



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:03 PM UTC

PDB ID : 7L06 / pdb_00007l06
EMDB ID : EMD-23095
Title : Cryo-EM structure of SARS-CoV-2 2P S ectodomain bound to two copies of domain-swapped antibody 2G12
Authors : Manne, K.; Henderson, R.; Acharya, P.
Deposited on : 2020-12-11
Resolution : 3.30 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:

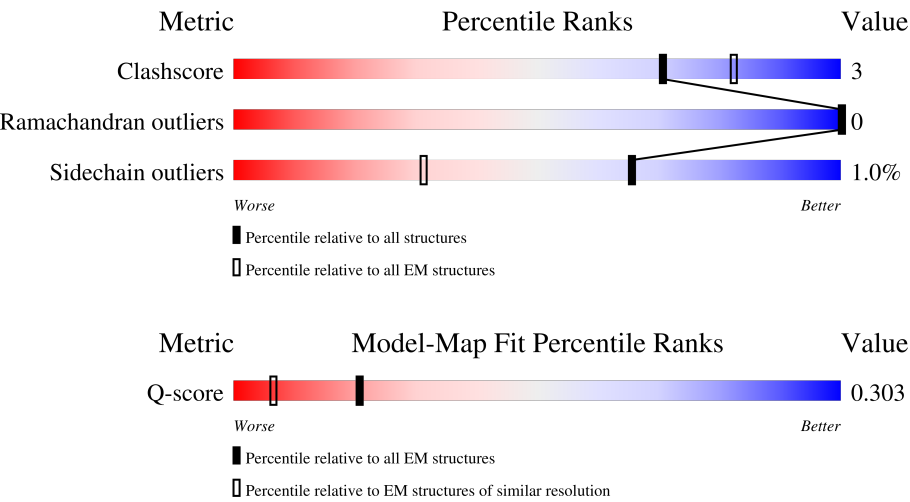
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

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



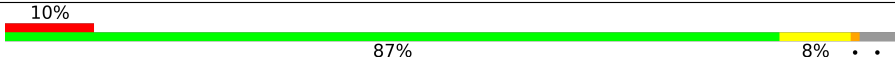
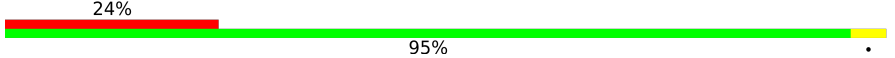
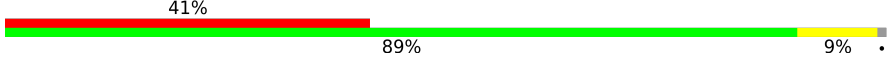
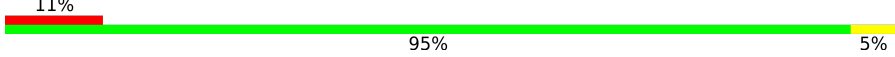
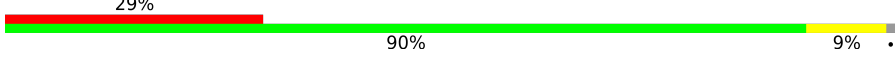
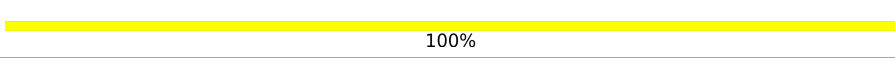
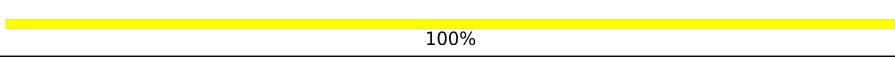
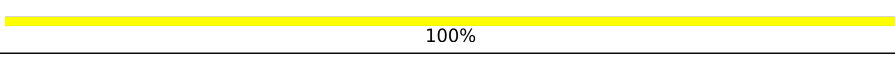
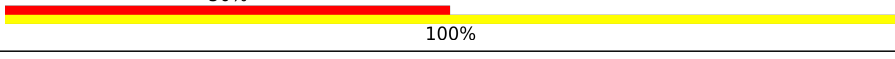
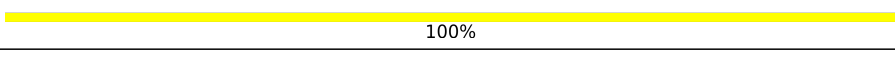
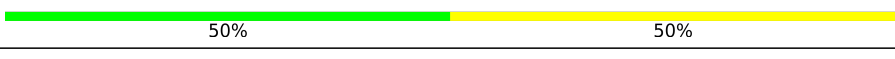
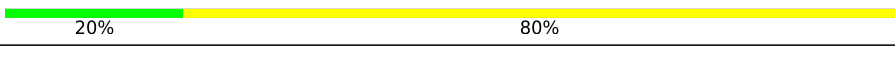
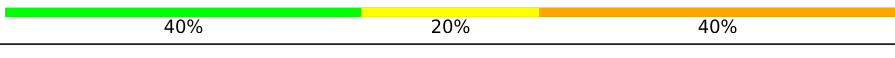
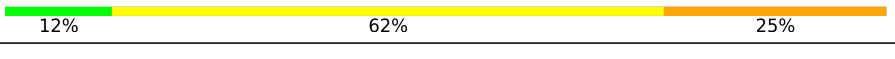
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1121	5% 82% 5% 13%
1	B	1121	6% 82% • 13%
1	C	1121	6% 81% 5% 13%
2	D	226	17% 87% 8% • •

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Mol	Chain	Length	Quality of chain
2	G	226	
2	H	226	
2	M	226	
3	E	213	
3	F	213	
3	K	213	
3	L	213	
4	I	2	
4	O	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	V	2	
4	Y	2	
5	J	5	
5	W	5	
6	N	8	
6	X	8	
7	P	5	
7	U	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	V	1	X	-	-	-
4	NAG	Y	1	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	W	4	-	-	X	-
5	MAN	W	5	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 72820 atoms, of which 35948 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	972	Total	C	H	N	O	S	0	0
			15038	4861	7434	1262	1448	33		
1	B	972	Total	C	H	N	O	S	0	0
			15038	4861	7434	1262	1448	33		
1	C	972	Total	C	H	N	O	S	0	0
			15018	4861	7414	1262	1448	33		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called 2G12 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		
2	G	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		
2	H	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		
2	M	218	Total	C	H	N	O	S	0	0
			3247	1032	1610	279	319	7		

- Molecule 3 is a protein called 2G12 light chain.

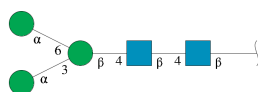
Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	213	Total	C	H	N	O	S	0	0
			3228	1027	1593	274	329	5		
3	F	211	Total	C	H	N	O	S	0	0
			3198	1018	1580	272	323	5		
3	K	213	Total	C	H	N	O	S	0	0
			3228	1027	1593	274	329	5		
3	L	211	Total	C	H	N	O	S	0	0
			3198	1018	1580	272	323	5		

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



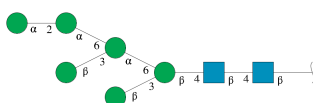
Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
4	O	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	Q	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	R	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	S	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	T	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
4	V	2	Total	C	H	N	O	0	0
			54	16	26	2	10		
4	Y	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



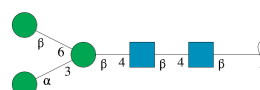
Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	5	Total	C	H	N	O	0	0
			118	34	57	2	25		
5	W	5	Total	C	H	N	O	0	0
			118	34	57	2	25		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	8	Total	C	H	N	O	0	0
			181	52	87	2	40		
6	X	8	Total	C	H	N	O	0	0
			181	52	87	2	40		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	5	Total	C	H	N	O	0	0
			74	34	13	2	25		
7	U	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

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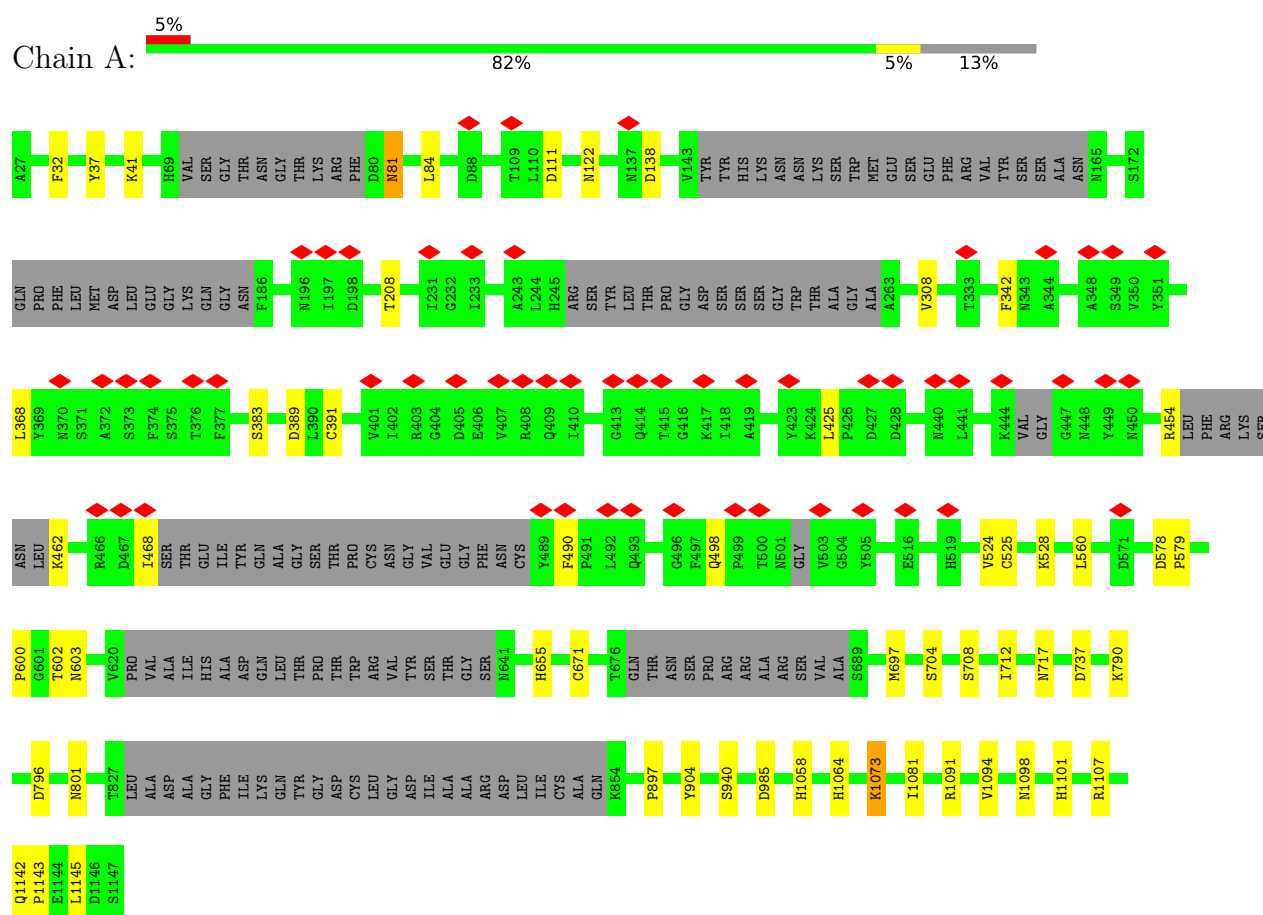
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Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
8	C	1	Total	C	H	N	O	0
			27	8	13	1	5	

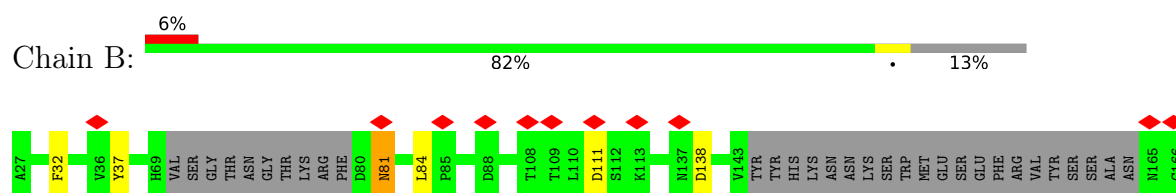
3 Residue-property plots

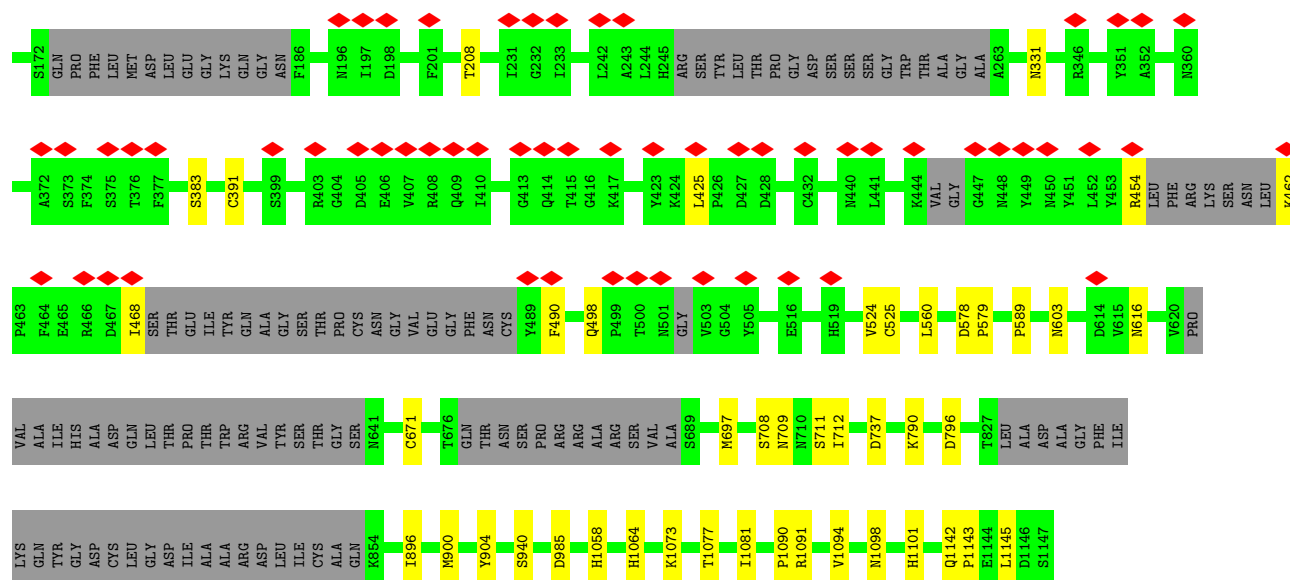
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

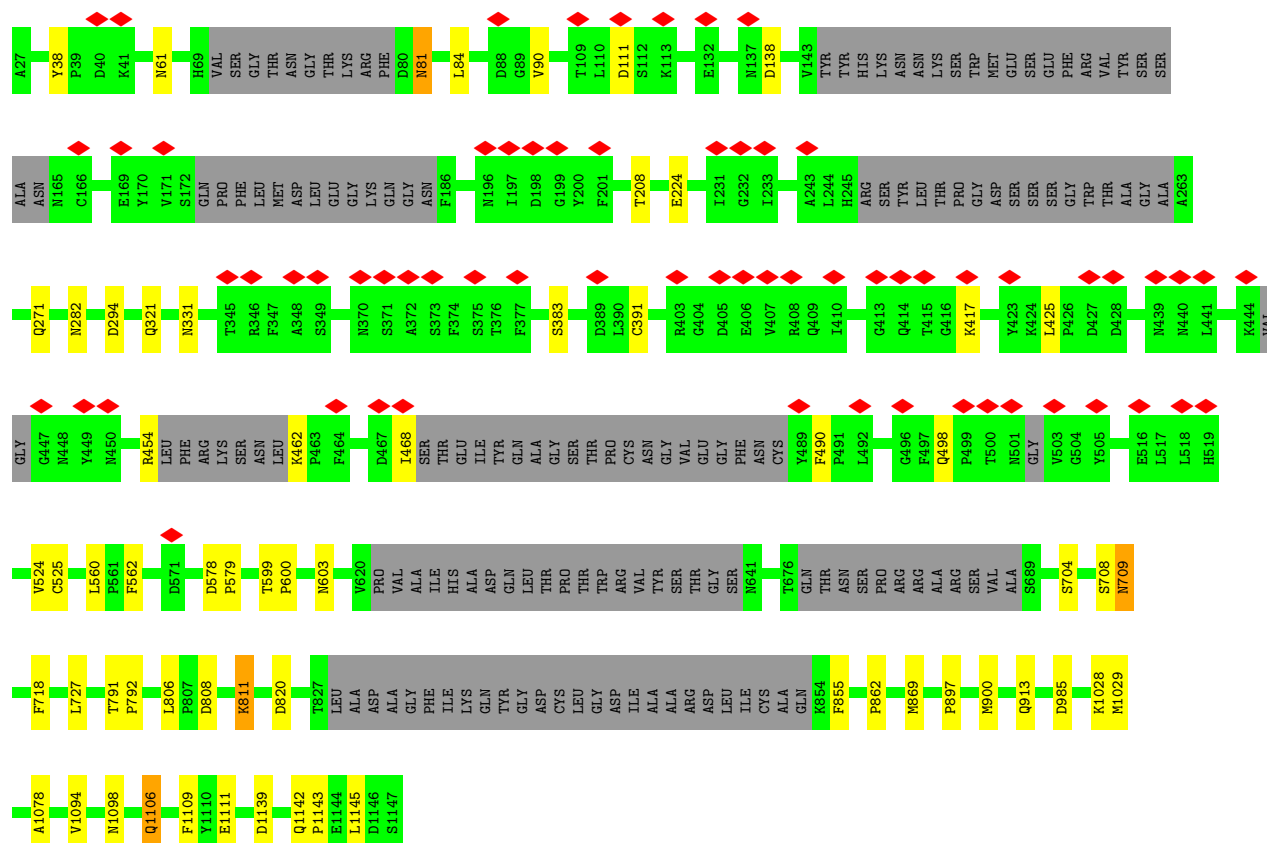
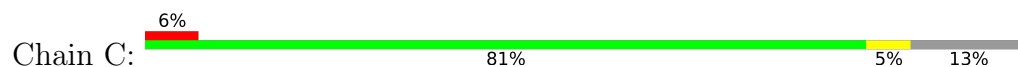


• Molecule 1: Spike glycoprotein

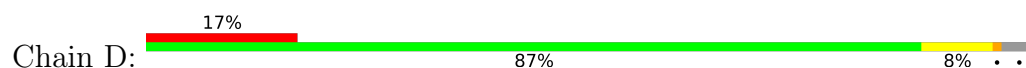


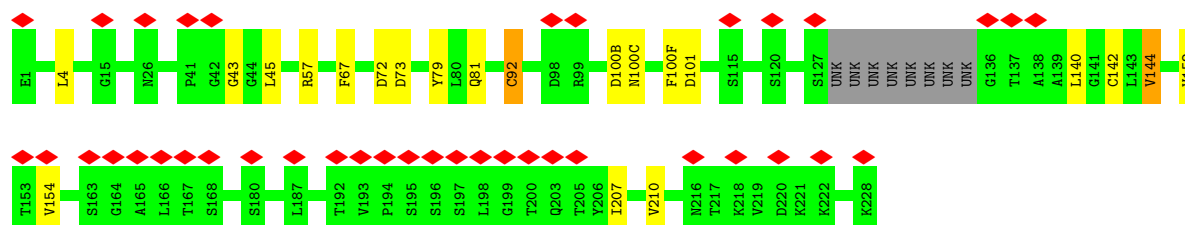


• Molecule 1: Spike glycoprotein

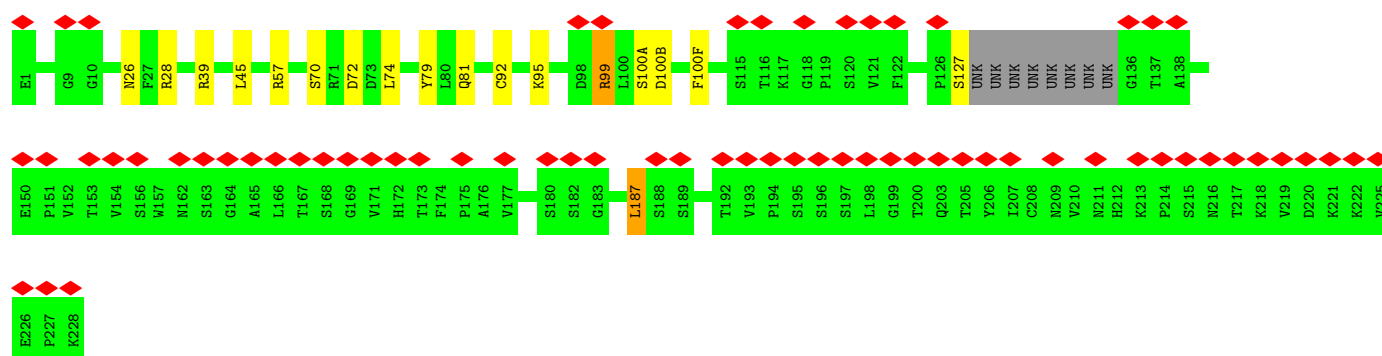
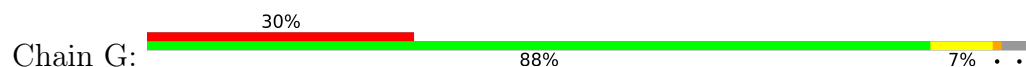


• Molecule 2: 2G12 heavy chain

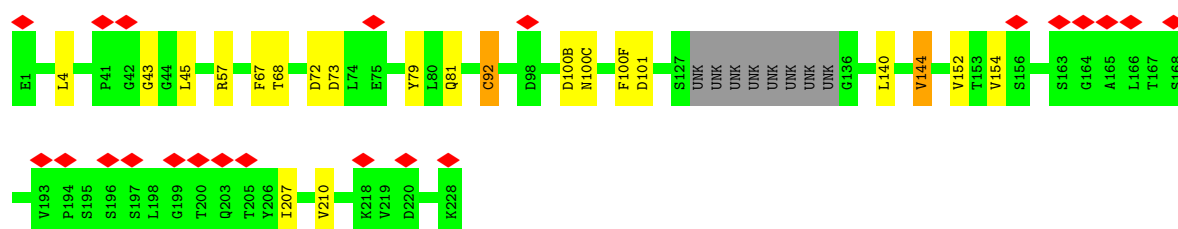
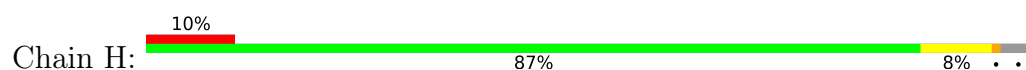




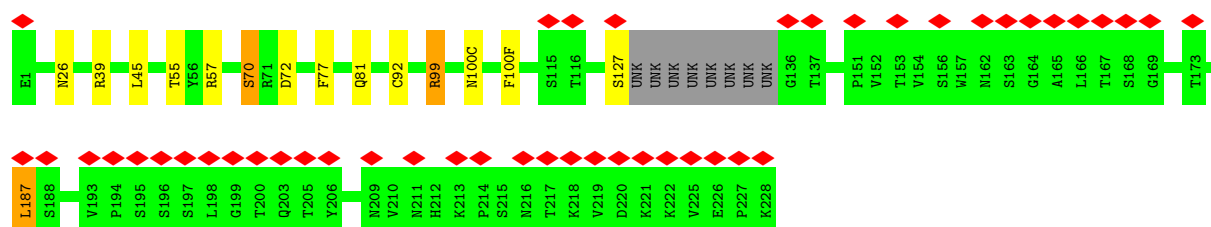
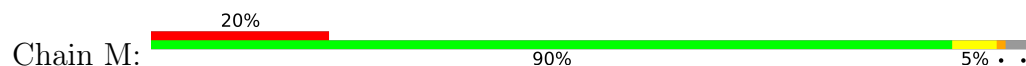
• Molecule 2: 2G12 heavy chain



• Molecule 2: 2G12 heavy chain

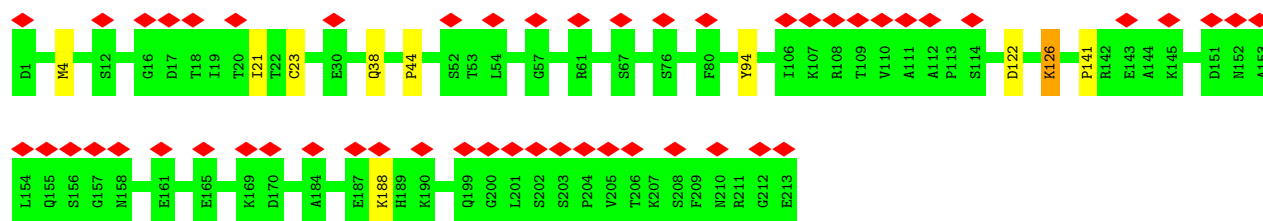


• Molecule 2: 2G12 heavy chain

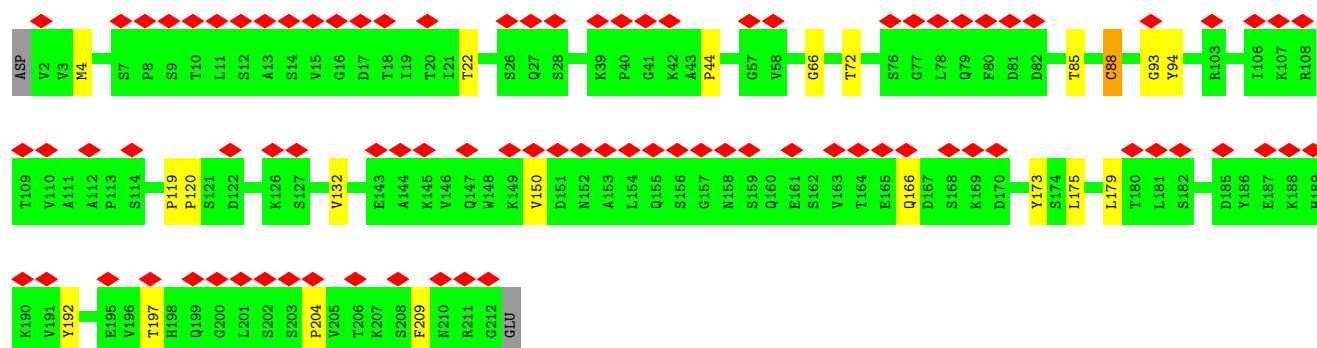
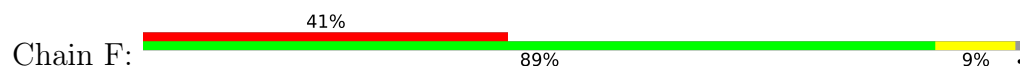


• Molecule 3: 2G12 light chain

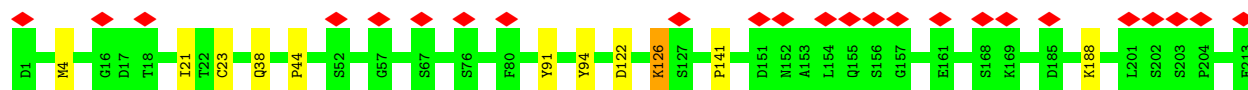




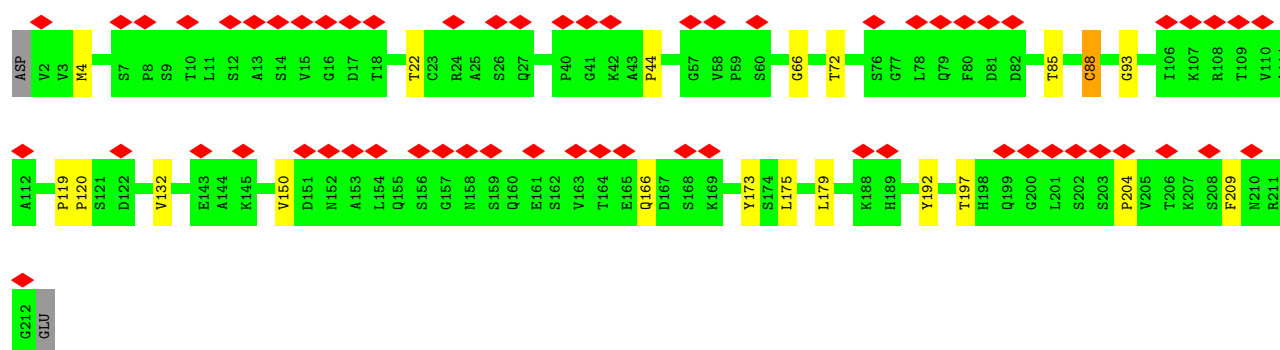
• Molecule 3: 2G12 light chain



• Molecule 3: 2G12 light chain



• Molecule 3: 2G12 light chain



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



MAG1
MAG2

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

Chain O:  50% 50%MAG1
MAG2

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

Chain Q:  100%MAG1
MAG2

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

Chain R:  100%MAG1
MAG2

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

Chain S:  50% 50%MAG1
MAG2

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

Chain T:  50% 100%MAG1
MAG2

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

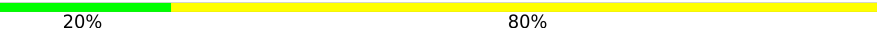
Chain V:  100%MAG1
MAG2

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

Chain Y: 

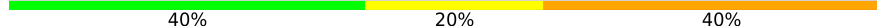


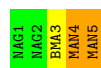
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 

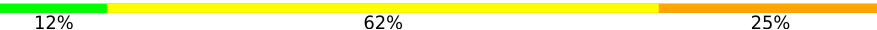


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



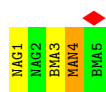
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



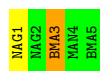
- Molecule 7: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 



- Molecule 7: α -D-mannopyranose-(1-3)-[β -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain U: 60% 20% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109774	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 ($e^-/\text{\AA}^2$)	66.43	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	1.636	Depositor
Minimum map value	-0.689	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.204	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, MAN, 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	0.81	4/7772 (0.1%)	1.23	33/10572 (0.3%)
1	B	0.80	4/7772 (0.1%)	1.24	34/10572 (0.3%)
1	C	0.81	2/7772 (0.0%)	1.03	59/10572 (0.6%)
2	D	0.81	1/1675 (0.1%)	1.30	8/2281 (0.4%)
2	G	0.70	0/1675	1.13	3/2281 (0.1%)
2	H	0.81	1/1675 (0.1%)	1.31	7/2281 (0.3%)
2	M	0.70	0/1675	1.13	3/2281 (0.1%)
3	E	0.71	0/1671	1.23	5/2269 (0.2%)
3	F	0.76	0/1654	1.02	2/2246 (0.1%)
3	K	0.71	0/1671	1.23	5/2269 (0.2%)
3	L	0.75	0/1654	1.02	2/2246 (0.1%)
All	All	0.79	12/36666 (0.0%)	1.17	161/49870 (0.3%)

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	1
1	B	0	1
3	E	0	1
3	K	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1081	ILE	C-O	-7.29	1.16	1.24
1	A	1081	ILE	C-O	-7.18	1.17	1.24
2	H	144	VAL	C-O	-5.76	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	ARG	NE-CZ	5.71	1.39	1.33
2	D	144	VAL	C-O	-5.69	1.17	1.24
1	B	454	ARG	NE-CZ	5.67	1.39	1.33
1	C	454	ARG	NE-CZ	5.52	1.39	1.33
1	A	737	ASP	CG-OD2	-5.34	1.15	1.25
1	B	737	ASP	CG-OD2	-5.34	1.15	1.25
1	B	468	ILE	CB-CG1	5.08	1.63	1.53
1	A	468	ILE	CB-CG1	5.03	1.63	1.53
1	C	468	ILE	CB-CG1	5.02	1.63	1.53

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	SER	CA-C-N	13.55	139.80	120.28
1	B	708	SER	C-N-CA	13.55	139.80	120.28
1	A	600	PRO	N-CA-C	-9.59	95.67	111.68
1	B	490	PHE	CA-C-N	7.35	127.52	119.87
1	B	490	PHE	C-N-CA	7.35	127.52	119.87
1	C	808	ASP	CA-C-N	7.34	127.04	119.56
1	C	808	ASP	C-N-CA	7.34	127.04	119.56
1	A	490	PHE	CA-C-N	7.31	127.47	119.87
1	A	490	PHE	C-N-CA	7.31	127.47	119.87
1	C	490	PHE	CA-C-N	7.30	127.47	119.87
1	C	490	PHE	C-N-CA	7.30	127.47	119.87
1	C	792	PRO	CA-C-N	7.18	126.89	119.56
1	C	792	PRO	C-N-CA	7.18	126.89	119.56
1	B	708	SER	CA-C-O	-7.10	113.04	120.99
1	A	708	SER	CA-C-O	-7.08	113.06	120.99
1	C	1139	ASP	CA-C-N	6.95	126.64	119.56
1	C	1139	ASP	C-N-CA	6.95	126.64	119.56
1	A	383	SER	CA-C-N	6.88	126.58	119.56
1	A	383	SER	C-N-CA	6.88	126.58	119.56
1	C	578	ASP	CA-C-N	6.87	126.50	119.56
1	C	578	ASP	C-N-CA	6.87	126.50	119.56
1	B	383	SER	CA-C-N	6.84	126.53	119.56
1	B	383	SER	C-N-CA	6.84	126.53	119.56
1	C	383	SER	CA-C-N	6.82	126.52	119.56
1	C	383	SER	C-N-CA	6.82	126.52	119.56
1	C	811	LYS	CA-C-N	6.82	126.52	119.56
1	C	811	LYS	C-N-CA	6.82	126.52	119.56
1	A	578	ASP	CA-C-N	6.79	126.42	119.56
1	A	578	ASP	C-N-CA	6.79	126.42	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	578	ASP	CA-C-N	6.75	126.38	119.56
1	B	578	ASP	C-N-CA	6.75	126.38	119.56
1	B	498	GLN	CA-C-N	6.71	126.41	119.56
1	B	498	GLN	C-N-CA	6.71	126.41	119.56
1	A	498	GLN	CA-C-N	6.71	126.40	119.56
1	A	498	GLN	C-N-CA	6.71	126.40	119.56
1	C	81	ASN	CA-C-N	6.69	126.63	120.21
1	C	81	ASN	C-N-CA	6.69	126.63	120.21
2	D	144	VAL	CA-C-O	-6.65	113.45	120.57
3	K	141	PRO	CA-C-N	6.61	129.80	120.28
3	K	141	PRO	C-N-CA	6.61	129.80	120.28
2	H	144	VAL	CA-C-O	-6.60	113.51	120.57
3	E	141	PRO	CA-C-N	6.58	129.76	120.28
3	E	141	PRO	C-N-CA	6.58	129.76	120.28
1	C	862	PRO	CA-C-N	6.58	126.49	119.85
1	C	862	PRO	C-N-CA	6.58	126.49	119.85
1	A	81	ASN	CA-C-N	6.53	126.48	120.21
1	A	81	ASN	C-N-CA	6.53	126.48	120.21
1	B	81	ASN	CA-C-N	6.49	126.44	120.21
1	B	81	ASN	C-N-CA	6.49	126.44	120.21
1	C	498	GLN	CA-C-N	6.48	126.17	119.56
1	C	498	GLN	C-N-CA	6.48	126.17	119.56
1	C	806	LEU	CA-C-N	6.45	126.40	119.76
1	C	806	LEU	C-N-CA	6.45	126.40	119.76
1	C	1078	ALA	CA-C-N	6.20	125.82	119.56
1	C	1078	ALA	C-N-CA	6.20	125.82	119.56
3	F	66	GLY	CA-C-O	-6.17	118.21	122.22
3	L	66	GLY	CA-C-O	-6.15	118.22	122.22
2	H	100(F)	PHE	CA-CB-CG	6.15	119.95	113.80
1	C	138	ASP	CA-C-N	6.10	126.42	119.83
1	C	138	ASP	C-N-CA	6.10	126.42	119.83
2	D	100(F)	PHE	CA-CB-CG	6.10	119.90	113.80
2	G	99	ARG	NE-CZ-NH2	6.03	124.63	119.20
2	M	99	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	B	138	ASP	CA-C-N	6.00	126.30	119.83
1	B	138	ASP	C-N-CA	6.00	126.30	119.83
1	A	138	ASP	CA-C-N	5.98	126.29	119.83
1	A	138	ASP	C-N-CA	5.98	126.29	119.83
1	C	224	GLU	CA-C-N	5.98	125.74	119.76
1	C	224	GLU	C-N-CA	5.98	125.74	119.76
1	C	38	TYR	CA-C-N	5.98	125.60	119.56
1	C	38	TYR	C-N-CA	5.98	125.60	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	GLN	CA-C-N	5.96	125.87	119.85
1	C	321	GLN	C-N-CA	5.96	125.87	119.85
1	C	524	VAL	CA-C-O	-5.92	114.02	120.71
3	K	21	ILE	CA-C-O	-5.90	115.47	121.67
3	E	21	ILE	CA-C-O	-5.87	115.50	121.67
1	C	727	LEU	CA-C-N	5.78	125.71	119.76
1	C	727	LEU	C-N-CA	5.78	125.71	119.76
1	B	796	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	796	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	1064	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	B	1064	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	C	985	ASP	CA-C-N	5.62	126.17	120.38
1	C	985	ASP	C-N-CA	5.62	126.17	120.38
1	B	985	ASP	CA-C-N	5.61	126.16	120.38
1	B	985	ASP	C-N-CA	5.61	126.16	120.38
2	H	207	ILE	CA-C-O	-5.56	115.39	121.28
2	D	207	ILE	CA-C-O	-5.55	115.39	121.28
1	A	985	ASP	CA-C-N	5.55	126.10	120.38
1	A	985	ASP	C-N-CA	5.55	126.10	120.38
1	C	90	VAL	N-CA-C	5.55	116.11	108.12
1	C	791	THR	CA-C-N	5.48	126.03	120.38
1	C	791	THR	C-N-CA	5.48	126.03	120.38
1	C	294	ASP	CA-C-N	5.46	125.81	119.47
1	C	294	ASP	C-N-CA	5.46	125.81	119.47
3	K	122	ASP	CA-C-N	5.43	127.55	120.28
3	K	122	ASP	C-N-CA	5.43	127.55	120.28
1	C	1111	GLU	CA-C-N	5.40	125.16	119.76
1	C	1111	GLU	C-N-CA	5.40	125.16	119.76
3	E	122	ASP	CA-C-N	5.35	127.45	120.28
3	E	122	ASP	C-N-CA	5.35	127.45	120.28
1	C	599	THR	CA-C-N	5.32	125.29	120.03
1	C	599	THR	C-N-CA	5.32	125.29	120.03
2	H	67	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	84	LEU	CA-C-N	5.30	125.24	119.78
1	A	84	LEU	C-N-CA	5.30	125.24	119.78
1	B	32	PHE	CA-C-N	5.27	130.82	122.60
1	B	32	PHE	C-N-CA	5.27	130.82	122.60
1	A	462	LYS	CA-C-N	5.26	125.51	119.83
1	A	462	LYS	C-N-CA	5.26	125.51	119.83
1	B	84	LEU	CA-C-N	5.26	125.20	119.78
1	B	84	LEU	C-N-CA	5.26	125.20	119.78
1	A	32	PHE	CA-C-N	5.25	130.80	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	PHE	C-N-CA	5.25	130.80	122.60
1	C	600	PRO	N-CA-C	-5.24	103.55	111.41
2	D	67	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	462	LYS	CA-C-N	5.23	125.47	119.83
1	C	462	LYS	C-N-CA	5.23	125.47	119.83
2	H	101	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	462	LYS	CA-C-N	5.22	125.47	119.83
1	B	462	LYS	C-N-CA	5.22	125.47	119.83
2	D	43	GLY	CA-C-N	5.22	125.87	120.60
2	D	43	GLY	C-N-CA	5.22	125.87	120.60
2	D	101	ASP	CA-CB-CG	5.22	117.82	112.60
2	H	43	GLY	CA-C-N	5.21	125.86	120.60
2	H	43	GLY	C-N-CA	5.21	125.86	120.60
1	C	560	LEU	CA-C-N	5.19	126.32	119.84
1	C	560	LEU	C-N-CA	5.19	126.32	119.84
1	C	84	LEU	CA-C-N	5.15	125.08	119.78
1	C	84	LEU	C-N-CA	5.15	125.08	119.78
1	A	560	LEU	CA-C-N	5.12	126.24	119.84
1	A	560	LEU	C-N-CA	5.12	126.24	119.84
1	B	1091	ARG	N-CA-C	-5.10	105.61	111.07
1	B	560	LEU	CA-C-N	5.10	126.22	119.84
1	B	560	LEU	C-N-CA	5.10	126.22	119.84
1	A	1091	ARG	N-CA-C	-5.10	105.61	111.07
2	M	100(F)	PHE	CA-CB-CG	5.10	118.90	113.80
1	C	208	THR	CA-C-N	5.09	124.85	119.76
1	C	208	THR	C-N-CA	5.09	124.85	119.76
1	A	1058	HIS	CB-CG-CD2	-5.09	124.59	131.20
1	B	208	THR	CA-C-N	5.08	124.84	119.76
1	B	208	THR	C-N-CA	5.08	124.84	119.76
1	B	1058	HIS	CB-CG-CD2	-5.07	124.61	131.20
3	F	88	CYS	CA-C-O	-5.07	116.04	121.56
1	A	425	LEU	CA-C-N	5.07	125.00	119.78
1	A	425	LEU	C-N-CA	5.07	125.00	119.78
2	G	100(F)	PHE	CA-CB-CG	5.05	118.85	113.80
2	G	26	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	1073	LYS	CA-C-O	-5.04	115.55	121.44
2	M	26	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	208	THR	CA-C-N	5.04	124.80	119.76
1	A	208	THR	C-N-CA	5.04	124.80	119.76
1	C	271	GLN	CA-C-N	5.04	126.14	119.84
1	C	271	GLN	C-N-CA	5.04	126.14	119.84
2	D	142	CYS	CA-C-O	-5.01	115.73	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	88	CYS	CA-C-O	-5.01	116.09	121.56
1	B	425	LEU	CA-C-N	5.01	124.94	119.78
1	B	425	LEU	C-N-CA	5.01	124.94	119.78
1	C	425	LEU	CA-C-N	5.01	124.94	119.78
1	C	425	LEU	C-N-CA	5.01	124.94	119.78
1	A	1073	LYS	CA-C-O	-5.01	115.58	121.44

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	TYR	Sidechain
1	B	37	TYR	Sidechain
3	E	94	TYR	Sidechain
3	K	94	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	7604	7434	7420	58	0
1	B	7604	7434	7419	58	0
1	C	7604	7414	7419	43	0
2	D	1637	1610	1609	30	0
2	G	1637	1610	1608	56	0
2	H	1637	1610	1609	21	0
2	M	1637	1610	1609	26	0
3	E	1635	1593	1593	13	0
3	F	1618	1580	1580	18	0
3	K	1635	1593	1593	9	0
3	L	1618	1580	1580	15	0
4	I	28	26	25	0	0
4	O	28	25	25	5	0
4	Q	28	25	25	0	0
4	R	28	25	25	0	0
4	S	28	25	25	3	0
4	T	28	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	28	26	25	0	0
4	Y	28	25	25	7	0
5	J	61	57	52	4	0
5	W	61	57	52	12	0
6	N	94	87	79	5	0
6	X	94	87	79	6	0
7	P	61	13	52	4	0
7	U	61	52	52	4	0
8	A	112	104	104	11	0
8	B	126	117	117	13	0
8	C	112	104	104	10	0
All	All	36872	35948	35930	253	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 (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1098:ASN:HD21	4:S:1:NAG:C1	0.98	1.62
1:A:603:ASN:HD21	8:A:1304:NAG:C1	0.98	1.56
1:C:61:ASN:HD21	8:C:1203:NAG:C1	0.97	1.56
1:C:282:ASN:HD21	8:C:1204:NAG:C1	0.91	1.55
1:B:709:ASN:HD21	8:B:1309:NAG:C1	0.89	1.54
1:C:331:ASN:ND2	8:C:1205:NAG:C1	1.68	1.54
1:B:1098:ASN:ND2	4:Y:1:NAG:C1	1.69	1.52
1:B:616:ASN:HD21	8:B:1308:NAG:C1	0.90	1.52
1:A:1098:ASN:ND2	4:O:1:NAG:C1	1.68	1.52
1:A:717:ASN:ND2	6:N:1:NAG:C1	1.71	1.49
1:C:709:ASN:ND2	7:U:1:NAG:C1	1.71	1.49
1:A:801:ASN:ND2	5:J:1:NAG:C1	1.71	1.48
1:B:616:ASN:ND2	8:B:1308:NAG:C1	1.74	1.46
1:B:709:ASN:ND2	8:B:1309:NAG:C1	1.75	1.45
1:A:603:ASN:ND2	8:A:1304:NAG:C1	1.73	1.43
1:C:61:ASN:ND2	8:C:1203:NAG:C1	1.83	1.42
1:C:282:ASN:ND2	8:C:1204:NAG:C1	1.75	1.39
1:C:1098:ASN:ND2	4:S:1:NAG:C1	1.83	1.37
2:D:72:ASP:OD1	2:G:57:ARG:NH2	1.66	1.28
1:B:331:ASN:OD1	8:B:1302:NAG:C1	1.83	1.27
2:H:45:LEU:HD11	3:L:44:PRO:CG	1.70	1.19
1:A:704:SER:HB3	1:B:790:LYS:HE3	1.23	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:28:ARG:NH1	5:W:5:MAN:H5	1.68	1.08
2:H:45:LEU:HD11	3:L:44:PRO:HG2	1.06	1.06
2:H:57:ARG:NH1	2:M:72:ASP:OD2	1.89	1.04
2:H:45:LEU:CD1	3:L:44:PRO:HG2	1.88	1.02
2:H:72:ASP:OD2	2:M:57:ARG:NH1	1.93	1.00
2:D:45:LEU:HD11	3:F:44:PRO:HG2	1.43	0.99
2:D:57:ARG:NH1	2:G:72:ASP:OD2	1.96	0.99
3:E:38:GLN:HE22	2:G:39:ARG:HD2	1.27	0.96
1:B:1098:ASN:CG	4:Y:1:NAG:C1	2.38	0.96
2:D:79:TYR:OH	2:G:81:GLN:NE2	1.99	0.94
1:A:717:ASN:CG	6:N:1:NAG:C1	2.39	0.94
3:E:44:PRO:HG2	2:G:45:LEU:HD11	1.50	0.93
1:A:801:ASN:CG	5:J:1:NAG:C1	2.45	0.90
2:G:100(B):ASP:OD2	6:X:5:MAN:O6	1.91	0.89
1:A:1098:ASN:CG	4:O:1:NAG:C1	2.48	0.87
2:D:45:LEU:HD11	3:F:44:PRO:CG	2.08	0.83
2:G:28:ARG:HD3	5:W:5:MAN:H62	1.59	0.83
1:A:940:SER:CB	2:M:99:ARG:HD2	2.10	0.82
1:A:1094:VAL:CG2	1:B:904:TYR:OH	2.27	0.82
1:B:940:SER:CB	2:G:99:ARG:HD2	2.09	0.82
1:B:616:ASN:CG	8:B:1308:NAG:C1	2.54	0.80
2:D:79:TYR:HE1	2:G:81:GLN:HG3	1.45	0.80
2:H:72:ASP:OD1	2:M:57:ARG:NH2	2.14	0.80
1:A:603:ASN:CG	8:A:1304:NAG:C1	2.54	0.80
2:G:74:LEU:HD13	5:W:4:MAN:O4	1.82	0.79
2:G:28:ARG:NH1	5:W:5:MAN:C5	2.47	0.77
2:D:81:GLN:NE2	2:G:79:TYR:OH	2.14	0.77
2:D:72:ASP:CG	2:G:57:ARG:HH22	1.92	0.76
1:A:1098:ASN:ND2	4:O:1:NAG:C2	2.49	0.76
2:D:57:ARG:NH2	2:G:72:ASP:OD1	2.18	0.76
2:D:79:TYR:CE1	2:G:81:GLN:HG3	2.20	0.76
2:D:100(C):ASN:CG	3:F:93:GLY:HA2	2.13	0.73
2:H:72:ASP:CG	2:M:57:ARG:HH12	1.95	0.73
2:D:79:TYR:HE1	2:G:81:GLN:CG	2.00	0.73
1:A:704:SER:HB3	1:B:790:LYS:CE	2.12	0.72
3:E:38:GLN:CD	2:G:39:ARG:CZ	2.63	0.72
2:D:57:ARG:HH12	2:G:72:ASP:CG	1.98	0.72
2:M:187:LEU:C	2:M:187:LEU:HD12	2.15	0.72
2:D:72:ASP:OD1	2:G:57:ARG:CZ	2.33	0.72
2:H:57:ARG:NH2	2:M:72:ASP:OD1	2.19	0.71
2:G:187:LEU:HD12	2:G:187:LEU:C	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:95:LYS:HE3	6:X:6:MAN:O4	1.90	0.70
1:A:1094:VAL:HG22	1:B:904:TYR:OH	1.91	0.70
1:C:709:ASN:CG	7:U:1:NAG:C1	2.62	0.70
2:M:55:THR:HG21	6:N:3:BMA:H62	1.72	0.70
3:E:38:GLN:NE2	2:G:39:ARG:HD2	2.03	0.70
1:A:940:SER:OG	2:M:99:ARG:NH2	2.25	0.69
2:D:100(C):ASN:HB2	3:F:93:GLY:HA2	1.72	0.69
3:E:38:GLN:CD	2:G:39:ARG:NH1	2.50	0.69
3:F:94:TYR:HE1	7:P:4:MAN:HO6	1.41	0.69
1:B:940:SER:OG	2:G:99:ARG:NH2	2.26	0.69
2:D:72:ASP:CG	2:G:57:ARG:NH2	2.50	0.69
1:B:1101:HIS:ND1	4:Y:1:NAG:H5	2.08	0.69
2:G:74:LEU:HD13	5:W:4:MAN:H5	1.75	0.68
1:C:331:ASN:ND2	8:C:1205:NAG:C2	2.55	0.68
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.76	0.67
2:D:79:TYR:CZ	2:G:81:GLN:NE2	2.61	0.67
1:A:790:LYS:HE3	1:C:704:SER:HB3	1.76	0.67
2:D:100(C):ASN:CB	3:F:93:GLY:HA2	2.24	0.67
2:H:45:LEU:HD11	3:L:44:PRO:HG3	1.69	0.67
1:A:1094:VAL:HG21	1:B:904:TYR:OH	1.94	0.67
2:G:28:ARG:HH12	5:W:5:MAN:H5	1.59	0.66
1:A:1145:LEU:HD21	1:B:1145:LEU:HD12	1.78	0.65
1:C:391:CYS:CB	1:C:525:CYS:HA	2.27	0.65
3:E:44:PRO:CG	2:G:45:LEU:HD11	2.24	0.65
3:E:188:LYS:HE2	3:E:188:LYS:HA	1.79	0.64
1:B:391:CYS:HB2	1:B:524:VAL:O	1.97	0.64
3:K:188:LYS:HE2	3:K:188:LYS:HA	1.79	0.64
1:A:391:CYS:HB2	1:A:524:VAL:O	1.97	0.63
1:B:1098:ASN:OD1	4:Y:1:NAG:C1	2.47	0.63
1:A:391:CYS:CB	1:A:525:CYS:HA	2.29	0.63
1:A:940:SER:HB2	2:M:99:ARG:HD2	1.80	0.62
1:B:391:CYS:CB	1:B:525:CYS:HA	2.29	0.62
2:G:74:LEU:HD13	5:W:4:MAN:C5	2.29	0.62
1:C:282:ASN:CG	8:C:1204:NAG:C1	2.68	0.62
1:B:603:ASN:OD1	8:B:1304:NAG:C1	2.48	0.61
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.82	0.61
1:B:589:PRO:HD2	1:C:855:PHE:CD1	2.36	0.61
2:H:57:ARG:HH22	2:M:72:ASP:CG	2.07	0.61
1:B:1145:LEU:HD21	1:C:1145:LEU:HD12	1.83	0.61
1:A:41:LYS:HG2	1:C:562:PHE:HD1	1.66	0.61
1:A:579:PRO:O	8:A:1302:NAG:H82	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:TYR:CE1	2:G:81:GLN:CG	2.80	0.61
2:D:81:GLN:NE2	2:G:79:TYR:CZ	2.68	0.61
1:B:709:ASN:CG	8:B:1309:NAG:C1	2.69	0.60
1:A:717:ASN:OD1	6:N:1:NAG:C1	2.50	0.60
2:D:45:LEU:CD1	3:F:44:PRO:HG2	2.27	0.60
3:E:38:GLN:OE1	2:G:39:ARG:CZ	2.50	0.59
1:A:342:PHE:HB2	8:A:1303:NAG:H82	1.84	0.59
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.82	0.59
1:C:579:PRO:O	8:C:1205:NAG:H82	2.02	0.59
1:A:717:ASN:ND2	6:N:1:NAG:C2	2.61	0.59
1:C:61:ASN:CG	8:C:1203:NAG:C1	2.70	0.58
1:B:1098:ASN:ND2	4:Y:1:NAG:C2	2.63	0.58
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	2.39	0.58
1:A:655:HIS:ND1	8:A:1306:NAG:H62	2.20	0.57
1:B:331:ASN:CG	8:B:1302:NAG:C1	2.74	0.57
3:K:44:PRO:CG	2:M:45:LEU:HD11	2.34	0.57
2:H:100(B):ASP:OD1	7:U:3:BMA:O3	2.23	0.57
1:B:589:PRO:HG2	1:C:855:PHE:HB3	1.87	0.57
1:A:704:SER:CB	1:B:790:LYS:HE3	2.16	0.56
1:A:122:ASN:HD22	1:A:122:ASN:H	1.51	0.56
1:A:801:ASN:ND2	5:J:1:NAG:O5	2.34	0.56
2:G:28:ARG:NH1	5:W:5:MAN:O4	2.38	0.56
2:D:81:GLN:HG2	2:G:79:TYR:HE1	1.71	0.56
2:D:57:ARG:HH22	2:G:72:ASP:CG	2.14	0.56
1:B:603:ASN:CG	8:B:1304:NAG:C1	2.79	0.55
2:G:100(B):ASP:CG	6:X:5:MAN:O6	2.49	0.54
1:B:712:ILE:HD13	1:B:1094:VAL:HG11	1.90	0.54
3:K:44:PRO:HG2	2:M:45:LEU:HD11	1.90	0.54
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	1.90	0.53
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.41	0.53
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.43	0.53
1:B:1094:VAL:HG13	1:C:900:MET:HE1	1.90	0.53
3:L:4:MET:HE3	3:L:88:CYS:SG	2.49	0.53
2:G:74:LEU:CD1	5:W:4:MAN:O4	2.53	0.53
3:F:94:TYR:HE1	7:P:4:MAN:O6	1.92	0.53
1:C:1106:GLN:HG3	1:C:1109:PHE:O	2.09	0.53
3:F:166:GLN:HG3	3:F:173:TYR:CZ	2.43	0.52
3:E:38:GLN:HE22	2:G:39:ARG:CD	2.13	0.52
3:F:4:MET:HE3	3:F:88:CYS:SG	2.49	0.52
1:A:1145:LEU:HD21	1:B:1145:LEU:CD1	2.40	0.51
2:H:57:ARG:HH12	2:M:72:ASP:CG	2.03	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:HIS:ND1	4:O:1:NAG:H3	2.26	0.51
3:F:132:VAL:CG2	3:F:179:LEU:HB3	2.41	0.50
2:G:100(A):SER:O	6:X:6:MAN:H3	2.11	0.50
3:L:132:VAL:CG2	3:L:179:LEU:HB3	2.41	0.50
2:M:187:LEU:C	2:M:187:LEU:CD1	2.84	0.50
2:G:187:LEU:HD12	2:G:187:LEU:O	2.12	0.50
2:G:187:LEU:C	2:G:187:LEU:CD1	2.84	0.50
2:D:81:GLN:CG	2:G:79:TYR:HE1	2.25	0.50
2:G:74:LEU:HD22	5:W:4:MAN:H5	1.93	0.50
1:A:1107:ARG:HG2	1:B:904:TYR:CZ	2.46	0.50
2:D:81:GLN:HG3	2:G:79:TYR:OH	2.11	0.50
3:E:38:GLN:NE2	2:G:39:ARG:NH1	2.60	0.50
2:H:4:LEU:HD23	2:H:92:CYS:SG	2.52	0.49
2:H:68:THR:HG21	2:M:77:PHE:CE2	2.47	0.49
2:D:4:LEU:HD23	2:D:92:CYS:SG	2.52	0.49
1:A:391:CYS:HB3	1:A:525:CYS:HA	1.94	0.49
1:B:391:CYS:HB3	1:B:525:CYS:HA	1.94	0.49
1:A:1107:ARG:HG2	1:B:904:TYR:OH	2.13	0.48
1:C:61:ASN:ND2	8:C:1203:NAG:C2	2.72	0.48
2:M:187:LEU:HD12	2:M:187:LEU:O	2.12	0.48
1:A:904:TYR:OH	1:C:1094:VAL:HG11	2.13	0.48
1:B:940:SER:HB2	2:G:99:ARG:HD2	1.91	0.48
2:H:72:ASP:CG	2:M:57:ARG:HH22	2.13	0.48
2:D:154:VAL:HG22	2:D:210:VAL:HG22	1.96	0.47
2:H:154:VAL:HG22	2:H:210:VAL:HG22	1.96	0.47
3:F:4:MET:CE	3:F:88:CYS:SG	3.03	0.47
3:K:38:GLN:HE22	2:M:39:ARG:HD2	1.79	0.47
3:E:38:GLN:NE2	2:G:39:ARG:CD	2.75	0.47
3:L:4:MET:CE	3:L:88:CYS:SG	3.03	0.47
1:A:801:ASN:OD1	5:J:1:NAG:C1	2.62	0.47
1:B:1101:HIS:HD1	4:Y:1:NAG:H3	1.80	0.47
2:D:81:GLN:CG	2:G:79:TYR:CE1	2.98	0.46
3:E:4:MET:HB3	3:E:23:CYS:SG	2.55	0.46
3:K:4:MET:HB3	3:K:23:CYS:SG	2.55	0.46
1:A:1094:VAL:HG13	1:B:900:MET:HE1	1.97	0.46
2:H:72:ASP:OD2	2:M:70:SER:HA	2.15	0.46
1:C:1098:ASN:CG	4:S:1:NAG:C1	2.74	0.46
1:A:1098:ASN:OD1	4:O:1:NAG:C1	2.64	0.46
2:G:100(B):ASP:CG	6:X:5:MAN:HO6	2.08	0.46
1:A:389:ASP:OD1	1:A:528:LYS:NZ	2.39	0.46
2:H:144:VAL:HG11	2:H:152:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:GLN:NE2	2:M:77:PHE:CG	2.79	0.46
2:D:144:VAL:HG11	2:D:152:VAL:HG11	1.98	0.45
1:A:81:ASN:OD1	1:A:81:ASN:N	2.49	0.45
1:C:81:ASN:OD1	1:C:81:ASN:N	2.49	0.45
1:B:81:ASN:OD1	1:B:81:ASN:N	2.49	0.45
3:F:197:THR:HG22	3:F:204:PRO:HB3	1.99	0.45
1:A:897:PRO:CG	1:C:709:ASN:O	2.65	0.45
2:G:95:LYS:HE3	6:X:6:MAN:C4	2.47	0.45
3:K:44:PRO:HG3	2:M:45:LEU:HD11	1.99	0.45
3:K:91:TYR:CD2	2:M:100(C):ASN:ND2	2.85	0.45
3:F:22:THR:HG22	3:F:72:THR:HG22	1.99	0.45
1:B:589:PRO:HG2	1:C:855:PHE:CB	2.46	0.45
3:L:197:THR:HG22	3:L:204:PRO:HB3	1.99	0.44
1:B:1077:THR:OG1	1:C:900:MET:HE1	2.17	0.44
7:P:3:BMA:H3	7:P:4:MAN:H2	1.51	0.44
1:C:709:ASN:OD1	1:C:709:ASN:N	2.50	0.44
1:A:712:ILE:HD11	1:B:896:ILE:HD12	2.00	0.44
1:A:1107:ARG:CD	1:B:904:TYR:CE2	3.01	0.44
1:C:111:ASP:N	1:C:111:ASP:OD1	2.48	0.44
3:F:120:PRO:HD3	3:F:132:VAL:HG12	2.00	0.44
1:B:671:CYS:SG	1:B:697:MET:HB3	2.58	0.43
3:E:126:LYS:HA	3:E:126:LYS:CE	2.48	0.43
3:L:22:THR:HG22	3:L:72:THR:HG22	1.99	0.43
3:K:126:LYS:HA	3:K:126:LYS:CE	2.48	0.43
3:L:120:PRO:HD3	3:L:132:VAL:HG12	2.00	0.43
1:A:111:ASP:N	1:A:111:ASP:OD1	2.48	0.43
2:H:100(C):ASN:CG	3:L:93:GLY:HA2	2.44	0.43
2:M:92:CYS:O	2:M:92:CYS:SG	2.77	0.43
1:A:671:CYS:SG	1:A:697:MET:HB3	2.58	0.43
1:B:711:SER:O	1:C:897:PRO:HD3	2.18	0.43
1:C:718:PHE:CD1	1:C:718:PHE:C	2.97	0.43
2:G:74:LEU:HD13	5:W:4:MAN:C4	2.48	0.43
1:B:1145:LEU:HD21	1:C:1145:LEU:CD1	2.47	0.43
1:A:790:LYS:CE	1:C:704:SER:HB3	2.48	0.42
1:B:940:SER:OG	2:G:99:ARG:HD2	2.19	0.42
2:G:92:CYS:O	2:G:92:CYS:SG	2.77	0.42
1:B:697:MET:HG2	1:C:869:MET:HE1	2.01	0.42
2:D:100(B):ASP:OD1	7:P:3:BMA:O4	2.28	0.42
1:A:368:LEU:HD21	8:A:1303:NAG:H83	2.00	0.42
1:B:616:ASN:OD1	8:B:1308:NAG:C1	2.67	0.42
1:B:1090:PRO:O	1:C:913:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:ASN:ND2	7:U:1:NAG:C2	2.70	0.42
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.34	0.42
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.34	0.42
3:F:150:VAL:HG22	3:F:192:TYR:CD2	2.55	0.42
2:G:28:ARG:NH1	5:W:5:MAN:C4	2.82	0.42
1:A:603:ASN:ND2	8:A:1304:NAG:C2	2.73	0.42
8:B:1309:NAG:H3	8:B:1309:NAG:H82	2.01	0.42
1:A:368:LEU:CD2	8:A:1303:NAG:H83	2.50	0.42
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.35	0.42
3:L:119:PRO:HB3	3:L:209:PHE:CE1	2.55	0.42
3:L:175:LEU:C	3:L:175:LEU:HD23	2.46	0.41
3:F:119:PRO:HB3	3:F:209:PHE:CE1	2.55	0.41
3:L:150:VAL:HG22	3:L:192:TYR:CD2	2.55	0.41
3:K:38:GLN:NE2	2:M:39:ARG:HD2	2.35	0.41
1:A:1073:LYS:C	8:A:1305:NAG:H82	2.46	0.41
1:A:1073:LYS:HA	8:A:1305:NAG:H81	2.03	0.41
3:F:175:LEU:C	3:F:175:LEU:HD23	2.46	0.41
2:H:79:TYR:OH	2:M:81:GLN:NE2	2.39	0.41
1:B:579:PRO:O	8:B:1302:NAG:H82	2.21	0.41
1:A:308:VAL:HB	1:A:602:THR:HG23	2.03	0.40
1:B:1101:HIS:ND1	4:Y:1:NAG:H3	2.36	0.40
1:B:111:ASP:N	1:B:111:ASP:OD1	2.48	0.40
1:B:712:ILE:HG22	1:B:1077:THR:HB	2.03	0.40
1:C:1028:LYS:O	1:C:1029:MET:C	2.60	0.40
1:B:1094:VAL:HG13	1:C:900:MET:CE	2.51	0.40
1:C:391:CYS:HB3	1:C:525:CYS:HA	2.01	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	948/1121 (85%)	905 (96%)	43 (4%)	0	100	100
1	B	948/1121 (85%)	906 (96%)	42 (4%)	0	100	100
1	C	948/1121 (85%)	924 (98%)	24 (2%)	0	100	100
2	D	214/226 (95%)	204 (95%)	10 (5%)	0	100	100
2	G	214/226 (95%)	206 (96%)	8 (4%)	0	100	100
2	H	214/226 (95%)	203 (95%)	11 (5%)	0	100	100
2	M	214/226 (95%)	206 (96%)	8 (4%)	0	100	100
3	E	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
3	F	209/213 (98%)	203 (97%)	6 (3%)	0	100	100
3	K	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
3	L	209/213 (98%)	203 (97%)	6 (3%)	0	100	100
All	All	4540/5119 (89%)	4368 (96%)	172 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	C	711/972 (73%)	706 (99%)	5 (1%)	76	80
2	D	184/184 (100%)	181 (98%)	3 (2%)	55	72
2	G	184/184 (100%)	181 (98%)	3 (2%)	55	72
2	H	184/184 (100%)	181 (98%)	3 (2%)	55	72
2	M	184/184 (100%)	181 (98%)	3 (2%)	55	72
3	E	184/184 (100%)	183 (100%)	1 (0%)	81	83
3	F	182/184 (99%)	181 (100%)	1 (0%)	81	83
3	K	184/184 (100%)	183 (100%)	1 (0%)	81	83
3	L	182/184 (99%)	181 (100%)	1 (0%)	81	83
All	All	2179/2444 (89%)	2158 (99%)	21 (1%)	65	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	417	LYS
1	C	603	ASN
1	C	708	SER
1	C	709	ASN
1	C	1106	GLN
2	D	73	ASP
2	D	92	CYS
2	D	140	LEU
3	E	126	LYS
3	F	85	THR
2	G	70	SER
2	G	127	SER
2	G	187	LEU
2	H	73	ASP
2	H	92	CYS
2	H	140	LEU
3	K	126	LYS
3	L	85	THR
2	M	70	SER
2	M	127	SER
2	M	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	282	ASN
1	C	1071	GLN
1	C	1088	HIS
1	C	1098	ASN
2	D	81	GLN
3	E	38	GLN
3	E	137	ASN
3	E	138	ASN
3	E	147	GLN
3	F	210	ASN
2	G	81	GLN
2	G	203	GLN
2	H	32	HIS
3	K	38	GLN
3	K	137	ASN
3	K	138	ASN

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Mol	Chain	Res	Type
3	K	147	GLN
3	K	160	GLN
3	L	210	ASN
2	M	203	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

52 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	I	1	4	14,14,15	1.53	2 (14%)	17,19,21	0.72	0
4	NAG	I	2	4	14,14,15	1.51	2 (14%)	17,19,21	0.63	0
5	NAG	J	1	5	14,14,15	0.98	0	17,19,21	0.68	0
5	NAG	J	2	5	14,14,15	0.96	0	17,19,21	0.77	0
5	BMA	J	3	5	11,11,12	1.03	1 (9%)	15,15,17	0.87	0
5	MAN	J	4	5	11,11,12	1.13	1 (9%)	15,15,17	1.47	2 (13%)
5	MAN	J	5	5	11,11,12	1.30	2 (18%)	15,15,17	0.69	0
6	NAG	N	1	6	14,14,15	1.07	1 (7%)	17,19,21	0.75	0
6	NAG	N	2	6	14,14,15	1.02	0	17,19,21	1.01	0
6	BMA	N	3	6	11,11,12	1.20	2 (18%)	15,15,17	1.23	1 (6%)
6	MAN	N	4	6	11,11,12	1.33	2 (18%)	15,15,17	1.22	2 (13%)
6	MAN	N	5	6	11,11,12	1.17	2 (18%)	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	N	6	6	11,11,12	1.23	2 (18%)	15,15,17	1.13	1 (6%)
6	BMA	N	7	6	11,11,12	1.03	1 (9%)	15,15,17	0.81	0
6	BMA	N	8	6	11,11,12	1.29	2 (18%)	15,15,17	1.00	1 (6%)
4	NAG	O	1	4	14,14,15	0.26	0	17,19,21	0.97	0
4	NAG	O	2	4	14,14,15	0.24	0	17,19,21	0.60	0
7	NAG	P	1	7	14,14,15	0.43	0	17,19,21	2.78	7 (41%)
7	NAG	P	2	7	14,14,15	0.46	0	17,19,21	0.98	0
7	BMA	P	3	7	11,11,12	0.40	0	15,15,17	0.84	0
7	MAN	P	4	7	11,11,12	0.23	0	15,15,17	0.84	1 (6%)
7	BMA	P	5	7	11,11,12	0.22	0	15,15,17	0.52	0
4	NAG	Q	1	1,4	14,14,15	1.46	2 (14%)	17,19,21	0.71	0
4	NAG	Q	2	4	14,14,15	1.47	2 (14%)	17,19,21	0.62	0
4	NAG	R	1	1,4	14,14,15	1.49	1 (7%)	17,19,21	0.73	0
4	NAG	R	2	4	14,14,15	1.49	2 (14%)	17,19,21	0.60	0
4	NAG	S	1	4	14,14,15	1.57	2 (14%)	17,19,21	0.79	0
4	NAG	S	2	4	14,14,15	1.36	2 (14%)	17,19,21	0.63	0
4	NAG	T	1	1,4	14,14,15	1.53	2 (14%)	17,19,21	0.71	0
4	NAG	T	2	4	14,14,15	1.52	2 (14%)	17,19,21	0.63	0
7	NAG	U	1	7	14,14,15	0.30	0	17,19,21	0.53	0
7	NAG	U	2	7	14,14,15	0.31	0	17,19,21	0.67	0
7	BMA	U	3	7	11,11,12	0.31	0	15,15,17	0.85	1 (6%)
7	MAN	U	4	7	11,11,12	0.22	0	15,15,17	0.82	0
7	BMA	U	5	7	11,11,12	0.23	0	15,15,17	0.77	0
4	NAG	V	1	1,4	14,14,15	1.53	2 (14%)	17,19,21	0.71	0
4	NAG	V	2	4	14,14,15	1.51	2 (14%)	17,19,21	0.64	0
5	NAG	W	1	5	14,14,15	0.98	0	17,19,21	0.69	0
5	NAG	W	2	5	14,14,15	0.96	0	17,19,21	0.77	0
5	BMA	W	3	5	11,11,12	1.03	1 (9%)	15,15,17	0.86	0
5	MAN	W	4	5	11,11,12	1.13	1 (9%)	15,15,17	1.48	2 (13%)
5	MAN	W	5	5	11,11,12	1.30	2 (18%)	15,15,17	0.70	0
6	NAG	X	1	1,6	14,14,15	1.06	1 (7%)	17,19,21	0.75	0
6	NAG	X	2	6	14,14,15	1.03	0	17,19,21	1.01	0
6	BMA	X	3	6	11,11,12	1.18	1 (9%)	15,15,17	1.24	1 (6%)
6	MAN	X	4	6	11,11,12	1.33	2 (18%)	15,15,17	1.22	2 (13%)
6	MAN	X	5	6	11,11,12	1.19	2 (18%)	15,15,17	0.90	1 (6%)
6	MAN	X	6	6	11,11,12	1.23	2 (18%)	15,15,17	1.12	1 (6%)
6	BMA	X	7	6	11,11,12	1.04	1 (9%)	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	X	8	6	11,11,12	1.28	2 (18%)	15,15,17	1.00	1 (6%)
4	NAG	Y	1	4	14,14,15	0.26	0	17,19,21	0.97	0
4	NAG	Y	2	4	14,14,15	0.26	0	17,19,21	0.60	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	I	1	4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	2/2/19/22	0/1/1/1
5	MAN	J	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6	-	1/6/23/26	0/1/1/1
6	NAG	N	2	6	-	1/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
6	MAN	N	6	6	-	0/2/19/22	0/1/1/1
6	BMA	N	7	6	-	0/2/19/22	0/1/1/1
6	BMA	N	8	6	-	0/2/19/22	0/1/1/1
4	NAG	O	1	4	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
7	NAG	P	1	7	-	4/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	2/2/19/22	0/1/1/1
7	MAN	P	4	7	-	1/2/19/22	0/1/1/1
7	BMA	P	5	7	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
7	NAG	U	1	7	-	4/6/23/26	0/1/1/1

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

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	C1-C2	4.16	1.58	1.52
4	R	1	NAG	C1-C2	4.11	1.57	1.52
4	T	1	NAG	C1-C2	4.10	1.57	1.52
4	I	1	NAG	C1-C2	4.10	1.57	1.52
4	V	1	NAG	C1-C2	4.07	1.57	1.52
4	T	2	NAG	C1-C2	4.06	1.57	1.52
4	Q	1	NAG	C1-C2	4.04	1.57	1.52
4	Q	2	NAG	C1-C2	4.00	1.57	1.52
4	I	2	NAG	C1-C2	3.96	1.57	1.52
4	R	2	NAG	C1-C2	3.93	1.57	1.52
4	V	2	NAG	C1-C2	3.93	1.57	1.52
4	S	2	NAG	C1-C2	3.14	1.56	1.52
6	N	8	BMA	O5-C5	2.97	1.49	1.43
6	X	8	BMA	O5-C5	2.94	1.49	1.43
6	X	6	MAN	O5-C5	2.87	1.49	1.43
6	N	6	MAN	O5-C5	2.86	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	5	MAN	O5-C5	2.78	1.48	1.43
5	W	5	MAN	O5-C5	2.70	1.48	1.43
4	S	1	NAG	O5-C5	2.61	1.48	1.43
5	W	4	MAN	O5-C5	2.57	1.48	1.43
5	J	4	MAN	O5-C5	2.56	1.48	1.43
4	V	2	NAG	O5-C5	2.55	1.48	1.43
6	X	4	MAN	O3-C3	2.52	1.49	1.43
4	I	2	NAG	O5-C5	2.52	1.48	1.43
4	S	2	NAG	O5-C5	2.52	1.48	1.43
6	N	4	MAN	O3-C3	2.51	1.49	1.43
4	R	2	NAG	O5-C5	2.50	1.48	1.43
4	T	2	NAG	O5-C5	2.46	1.48	1.43
6	N	6	MAN	O5-C1	2.45	1.47	1.43
6	X	6	MAN	O5-C1	2.43	1.47	1.43
6	X	7	BMA	O5-C5	2.40	1.48	1.43
6	N	3	BMA	O3-C3	2.39	1.48	1.43
6	X	3	BMA	O3-C3	2.39	1.48	1.43
6	N	7	BMA	O5-C5	2.39	1.48	1.43
4	Q	2	NAG	O5-C5	2.38	1.48	1.43
6	N	5	MAN	O5-C5	2.33	1.48	1.43
4	V	1	NAG	O5-C5	2.29	1.47	1.43
6	X	5	MAN	O5-C5	2.29	1.47	1.43
6	N	4	MAN	O5-C5	2.28	1.47	1.43
4	I	1	NAG	O5-C5	2.26	1.47	1.43
6	X	4	MAN	O5-C5	2.26	1.47	1.43
4	T	1	NAG	O5-C5	2.25	1.47	1.43
6	X	5	MAN	O5-C1	2.22	1.47	1.43
6	N	8	BMA	O5-C1	2.19	1.47	1.43
6	X	8	BMA	O5-C1	2.19	1.47	1.43
6	N	1	NAG	O5-C5	2.18	1.47	1.43
6	X	1	NAG	O5-C5	2.16	1.47	1.43
4	Q	1	NAG	O5-C5	2.14	1.47	1.43
5	W	5	MAN	O5-C1	2.13	1.47	1.43
6	N	5	MAN	O5-C1	2.13	1.47	1.43
5	J	5	MAN	O5-C1	2.05	1.47	1.43
6	N	3	BMA	O5-C5	2.05	1.47	1.43
5	J	3	BMA	O5-C5	2.02	1.47	1.43
5	W	3	BMA	O5-C5	2.02	1.47	1.43

All (25) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	1	NAG	C1-O5-C5	5.22	119.19	112.19
7	P	1	NAG	O3-C3-C2	4.78	119.33	109.40
5	W	4	MAN	C1-O5-C5	4.69	118.48	112.19
5	J	4	MAN	C1-O5-C5	4.66	118.43	112.19
6	X	3	BMA	C1-O5-C5	4.43	118.12	112.19
6	N	3	BMA	C1-O5-C5	4.35	118.01	112.19
7	P	1	NAG	O3-C3-C4	4.19	120.26	110.38
7	P	1	NAG	C4-C3-C2	3.93	116.78	111.02
7	P	1	NAG	C2-N2-C7	3.92	128.15	122.90
7	P	1	NAG	C8-C7-N2	3.40	121.76	116.12
6	N	6	MAN	C1-O5-C5	3.37	116.70	112.19
6	X	6	MAN	C1-O5-C5	3.34	116.66	112.19
6	N	8	BMA	C1-O5-C5	2.86	116.02	112.19
6	X	8	BMA	C1-O5-C5	2.86	116.02	112.19
7	P	1	NAG	O5-C5-C6	-2.85	102.11	107.66
6	X	4	MAN	C1-C2-C3	2.74	113.63	109.64
6	N	4	MAN	C1-C2-C3	2.73	113.61	109.64
5	W	4	MAN	O3-C3-C2	-2.68	104.59	110.05
6	N	5	MAN	C1-O5-C5	2.68	115.77	112.19
6	X	5	MAN	C1-O5-C5	2.65	115.74	112.19
5	J	4	MAN	O3-C3-C2	-2.65	104.64	110.05
7	P	4	MAN	C1-O5-C5	2.13	115.04	112.19
7	U	3	BMA	C2-C3-C4	-2.10	107.17	110.86
6	X	4	MAN	C1-O5-C5	2.07	114.95	112.19
6	N	4	MAN	C1-O5-C5	2.05	114.94	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	V	1	NAG	C1

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	O	2	NAG	C1-C2-N2-C7
4	O	2	NAG	C8-C7-N2-C2
4	O	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	Y	1	NAG	O7-C7-N2-C2
4	Y	2	NAG	C1-C2-N2-C7
4	Y	2	NAG	C8-C7-N2-C2
4	Y	2	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
7	U	1	NAG	O7-C7-N2-C2
7	U	2	NAG	C8-C7-N2-C2
7	U	2	NAG	O7-C7-N2-C2
7	U	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O5-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	U	3	BMA	O5-C5-C6-O6
7	U	3	BMA	C4-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	P	3	BMA	C4-C5-C6-O6
7	U	4	MAN	O5-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6
5	J	4	MAN	C4-C5-C6-O6
5	W	4	MAN	C4-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
5	J	4	MAN	O5-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
4	O	1	NAG	C3-C2-N2-C7
4	Y	1	NAG	C3-C2-N2-C7
6	N	1	NAG	C1-C2-N2-C7
6	N	2	NAG	C1-C2-N2-C7
6	X	1	NAG	C1-C2-N2-C7
6	X	2	NAG	C1-C2-N2-C7
7	U	2	NAG	C4-C5-C6-O6
7	P	4	MAN	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 50 short contacts:

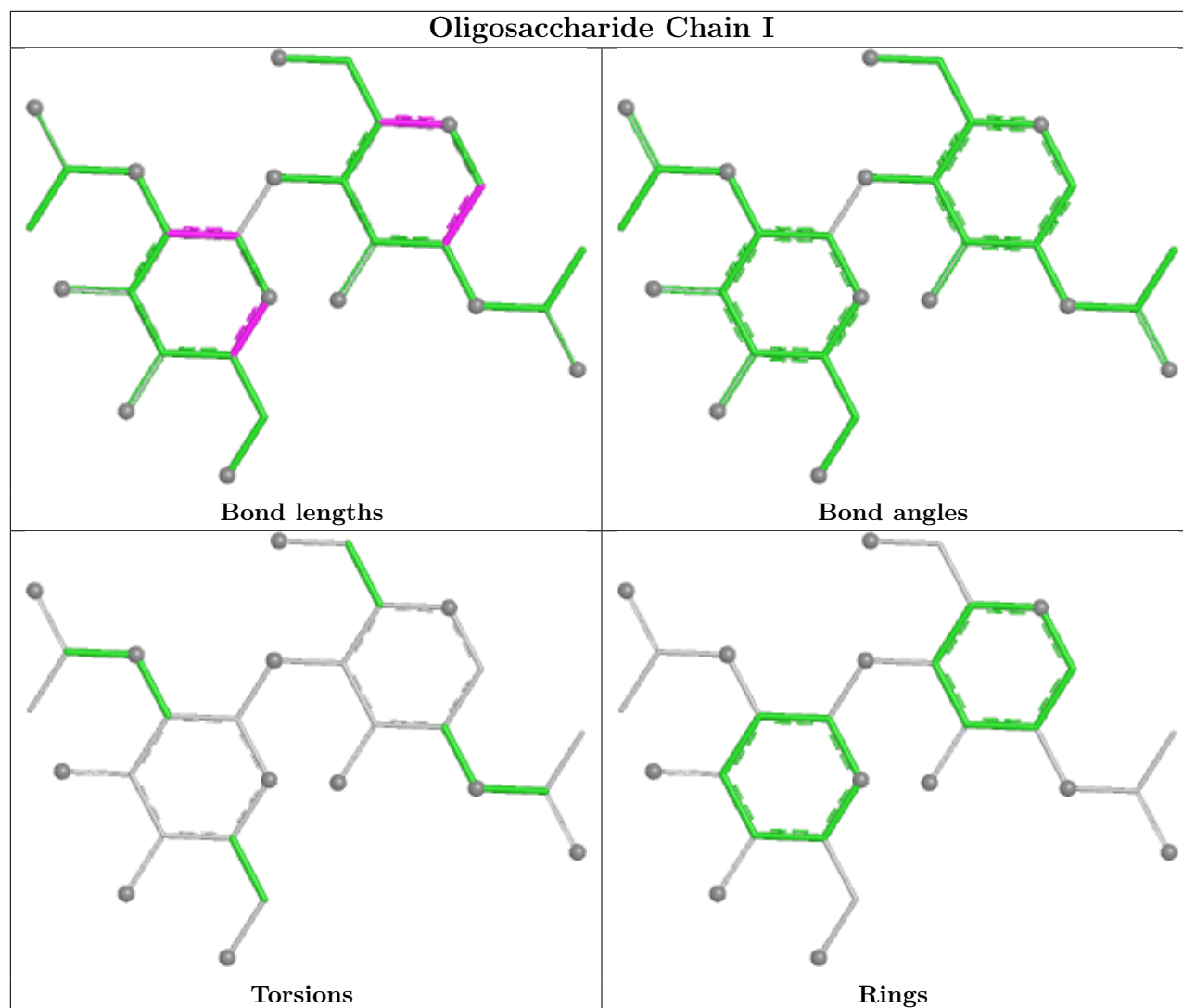
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	1	NAG	4	0
7	U	3	BMA	1	0
6	X	6	MAN	3	0

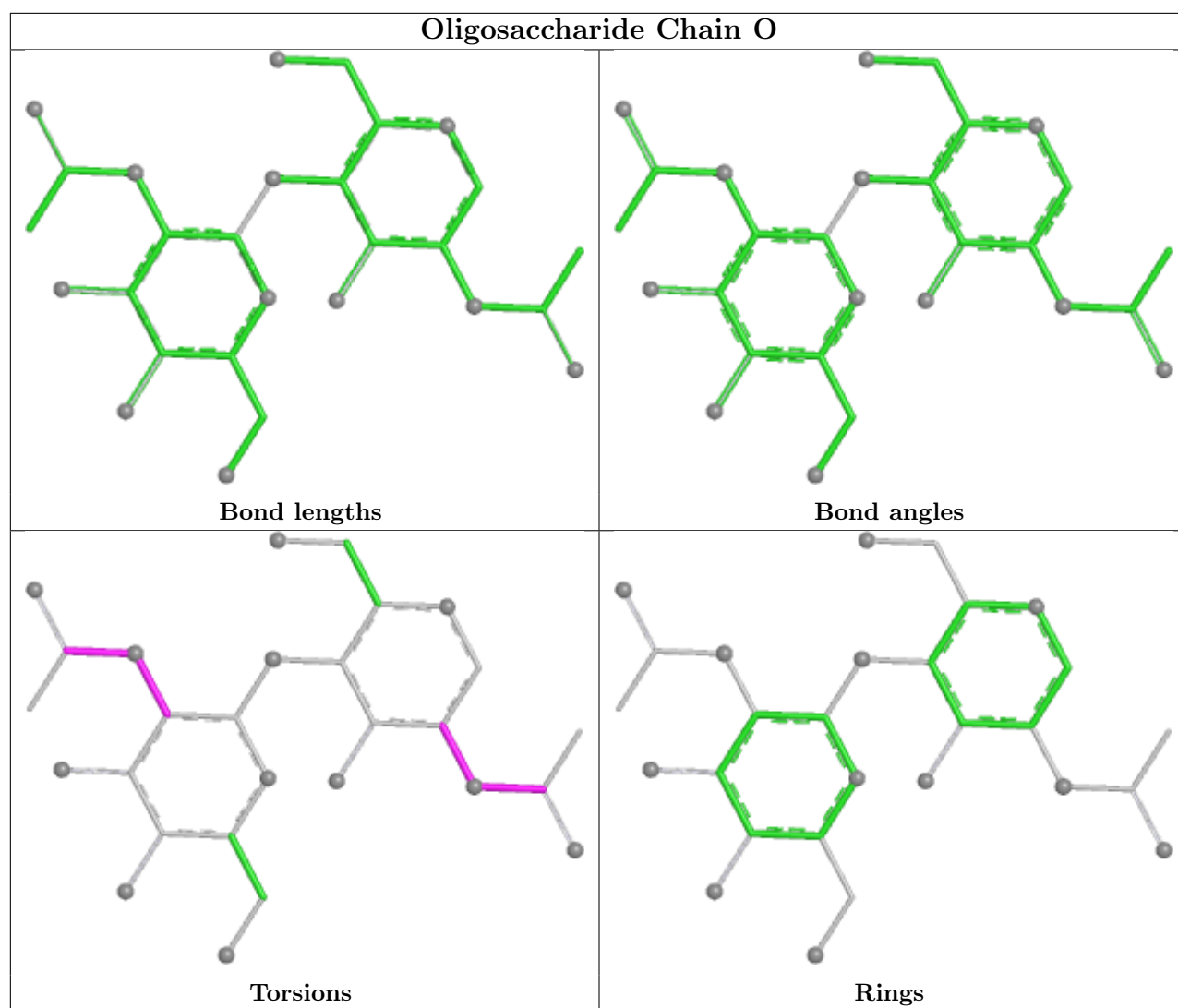
Continued on next page...

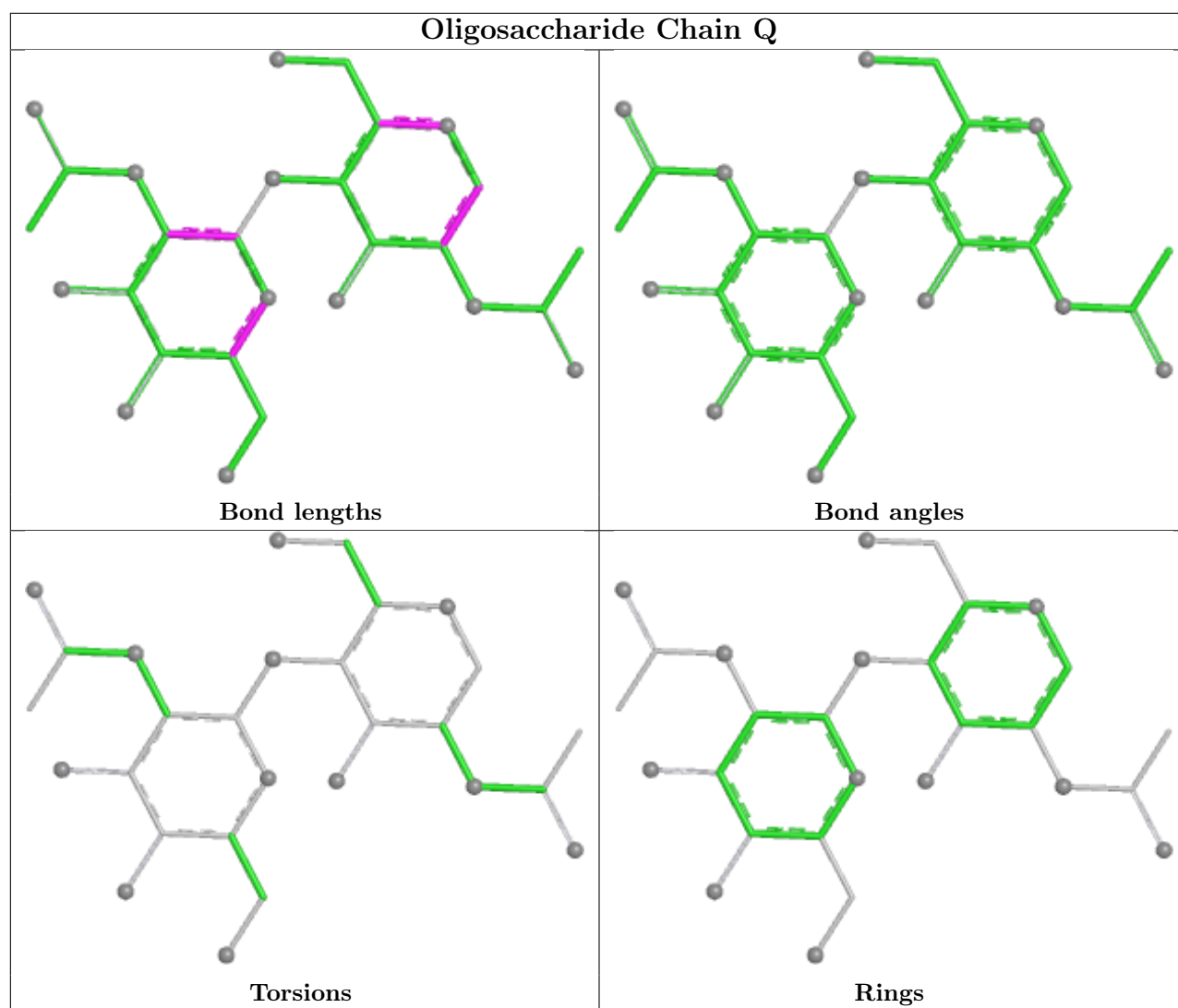
Continued from previous page...

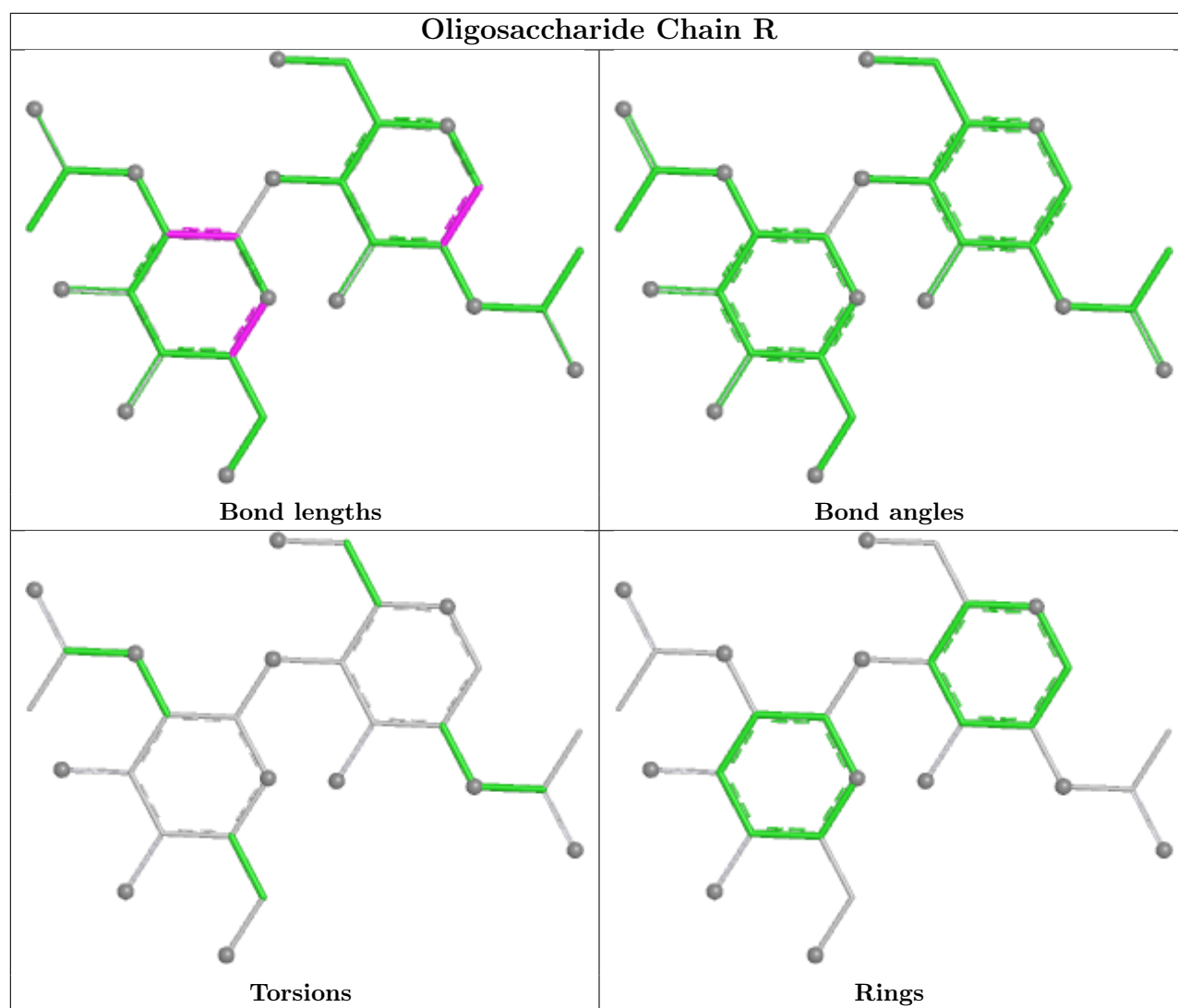
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	U	1	NAG	3	0
6	X	5	MAN	3	0
5	W	5	MAN	6	0
7	P	4	MAN	3	0
7	P	3	BMA	2	0
6	N	3	BMA	1	0
5	J	1	NAG	4	0
4	Y	1	NAG	7	0
4	S	1	NAG	3	0
5	W	4	MAN	6	0
4	O	1	NAG	5	0

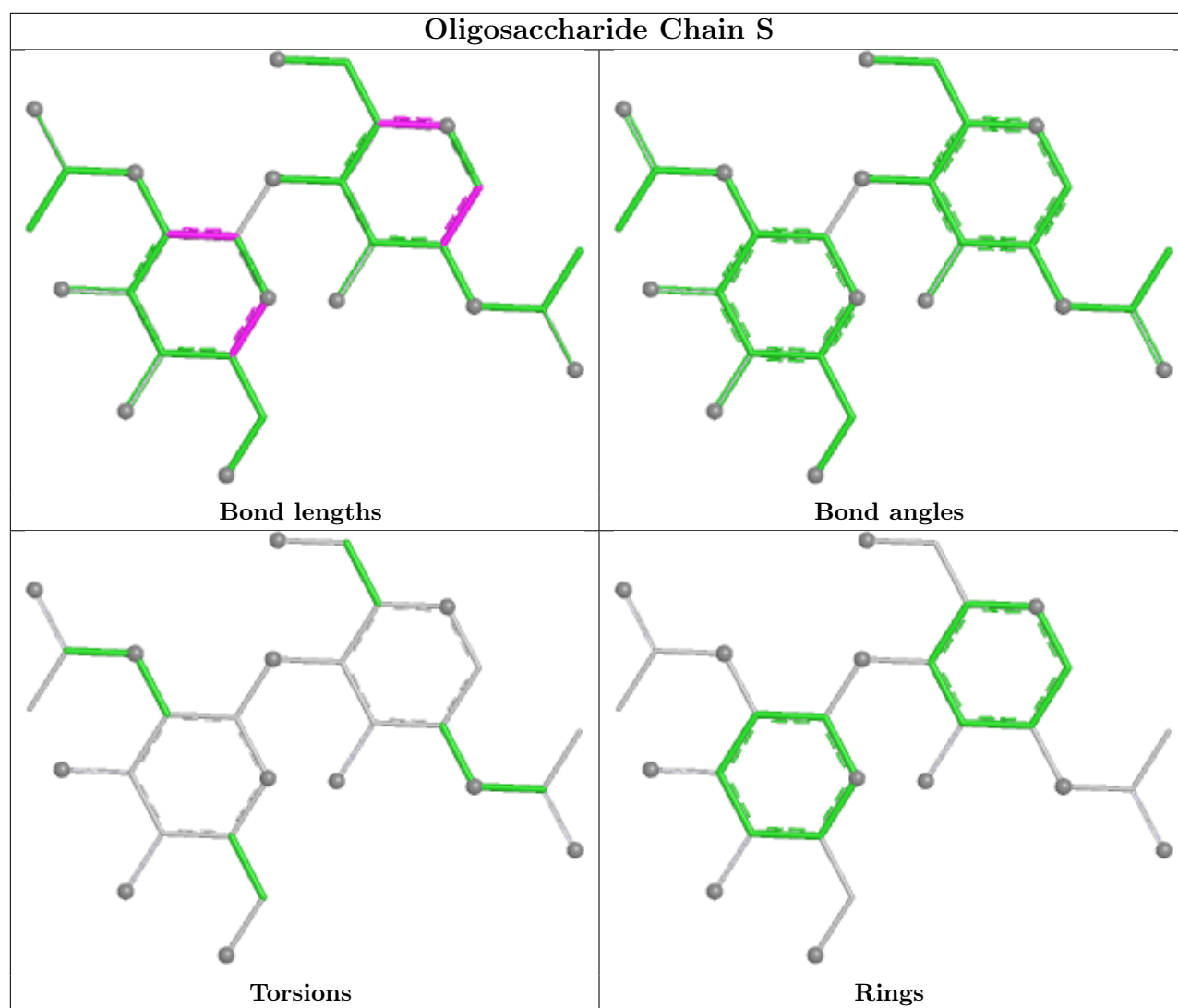
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

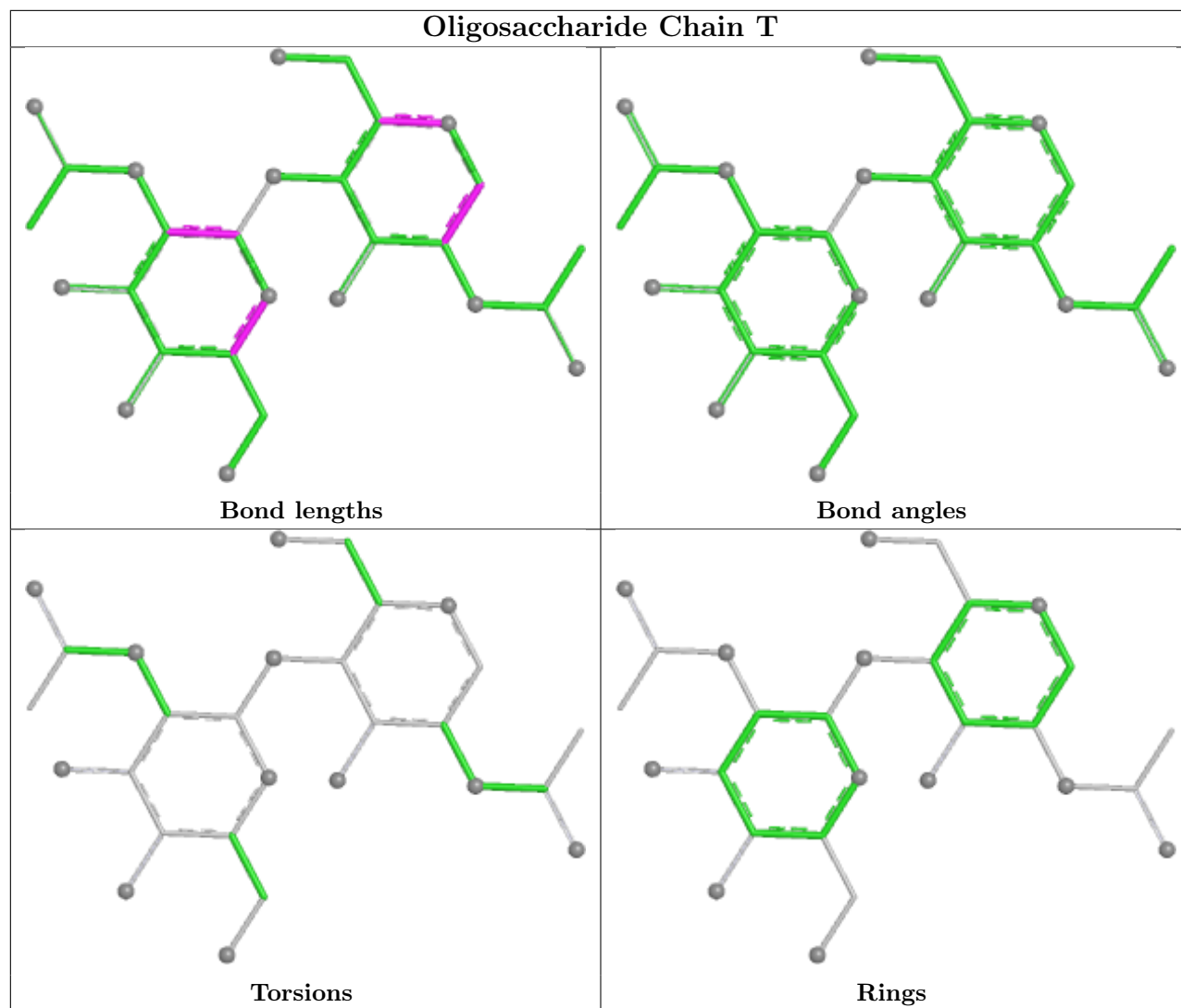


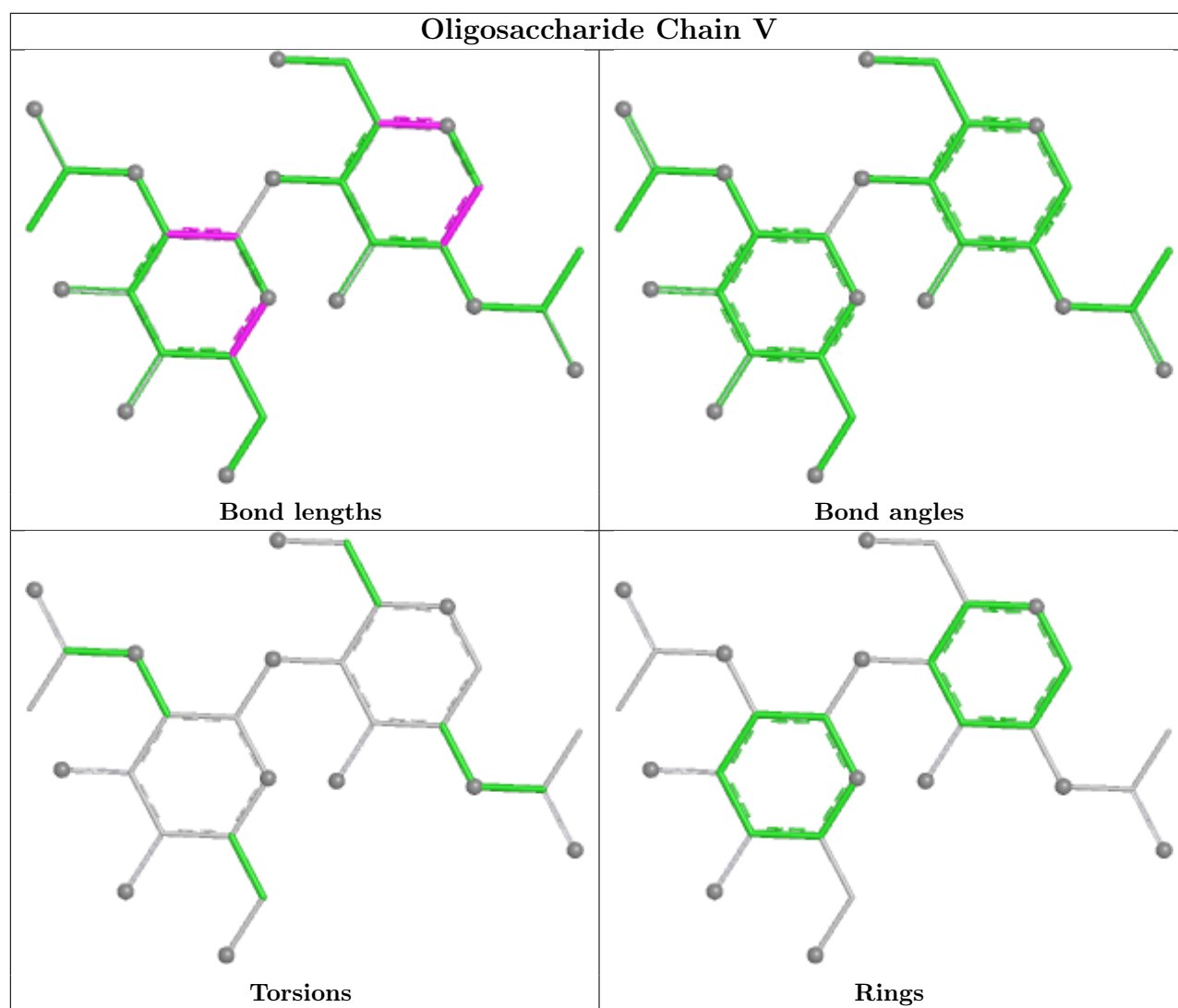


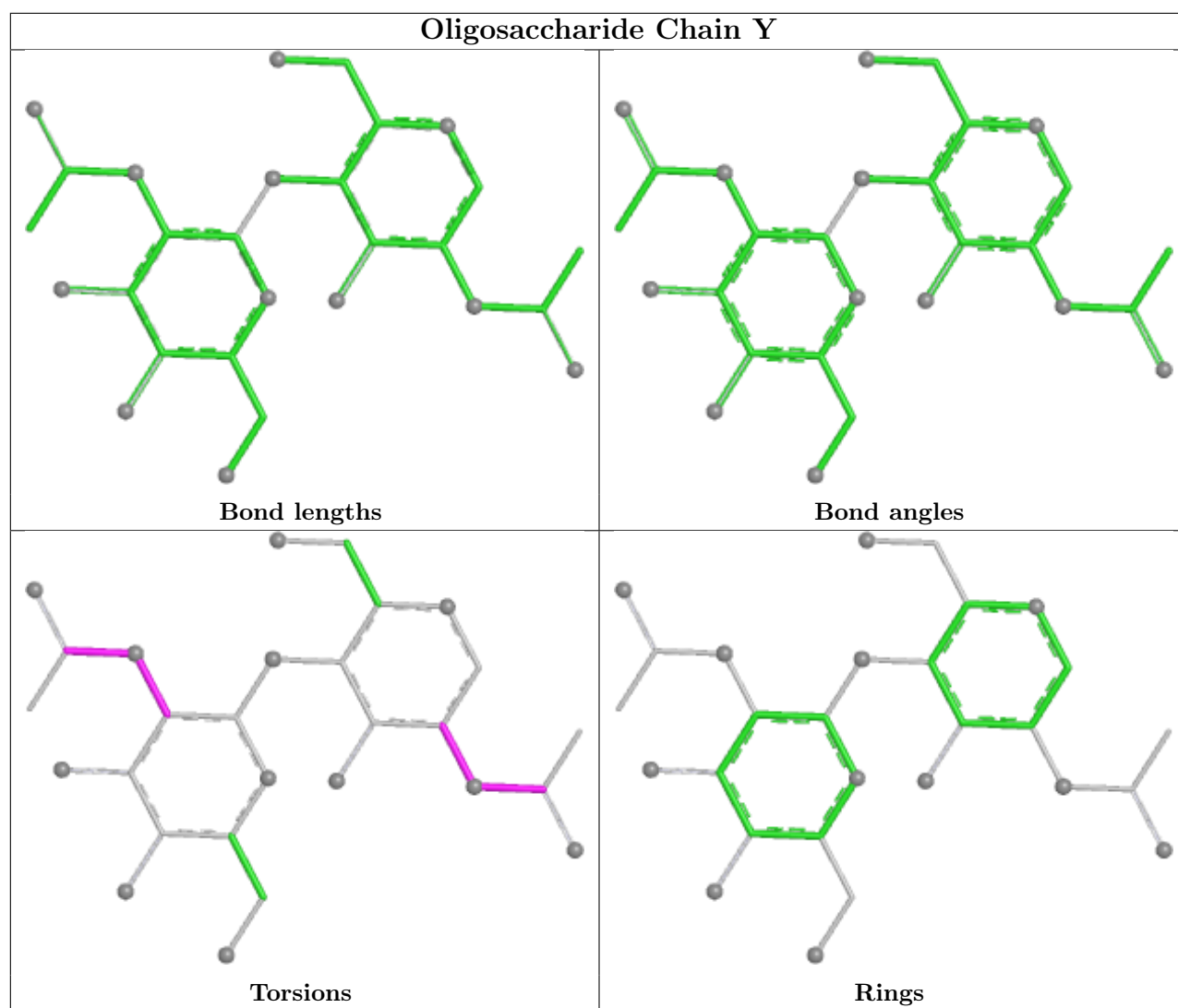


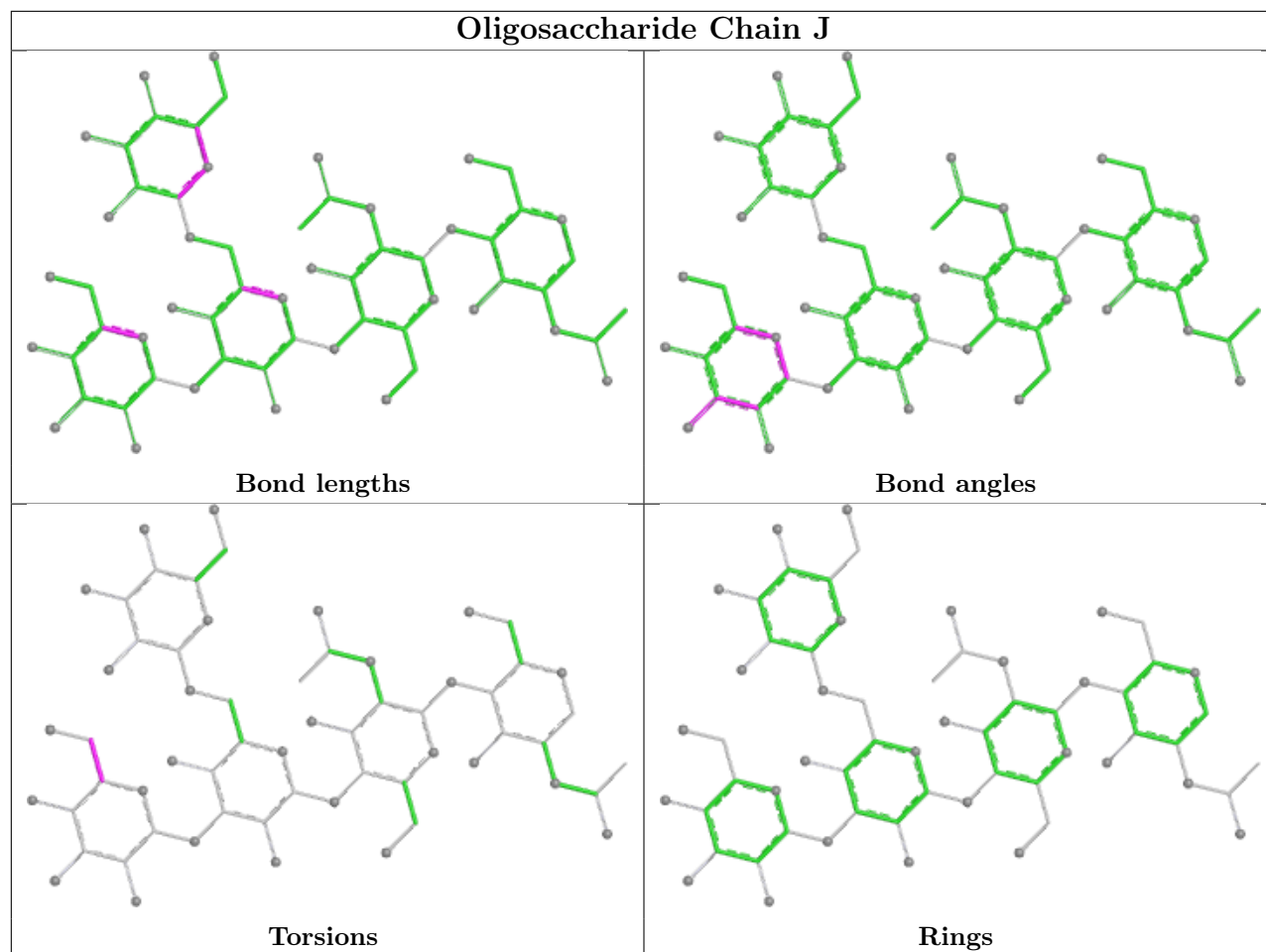


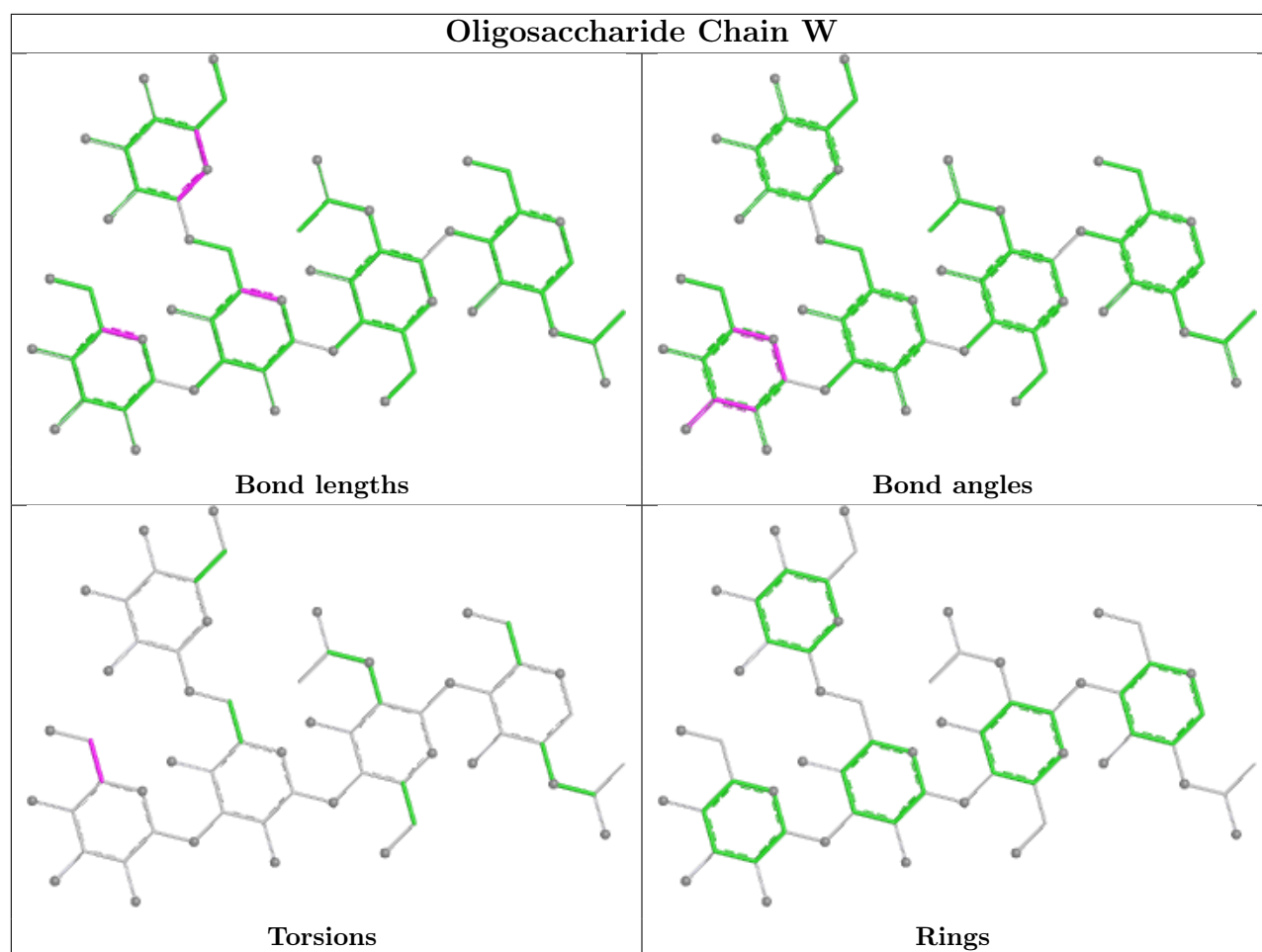


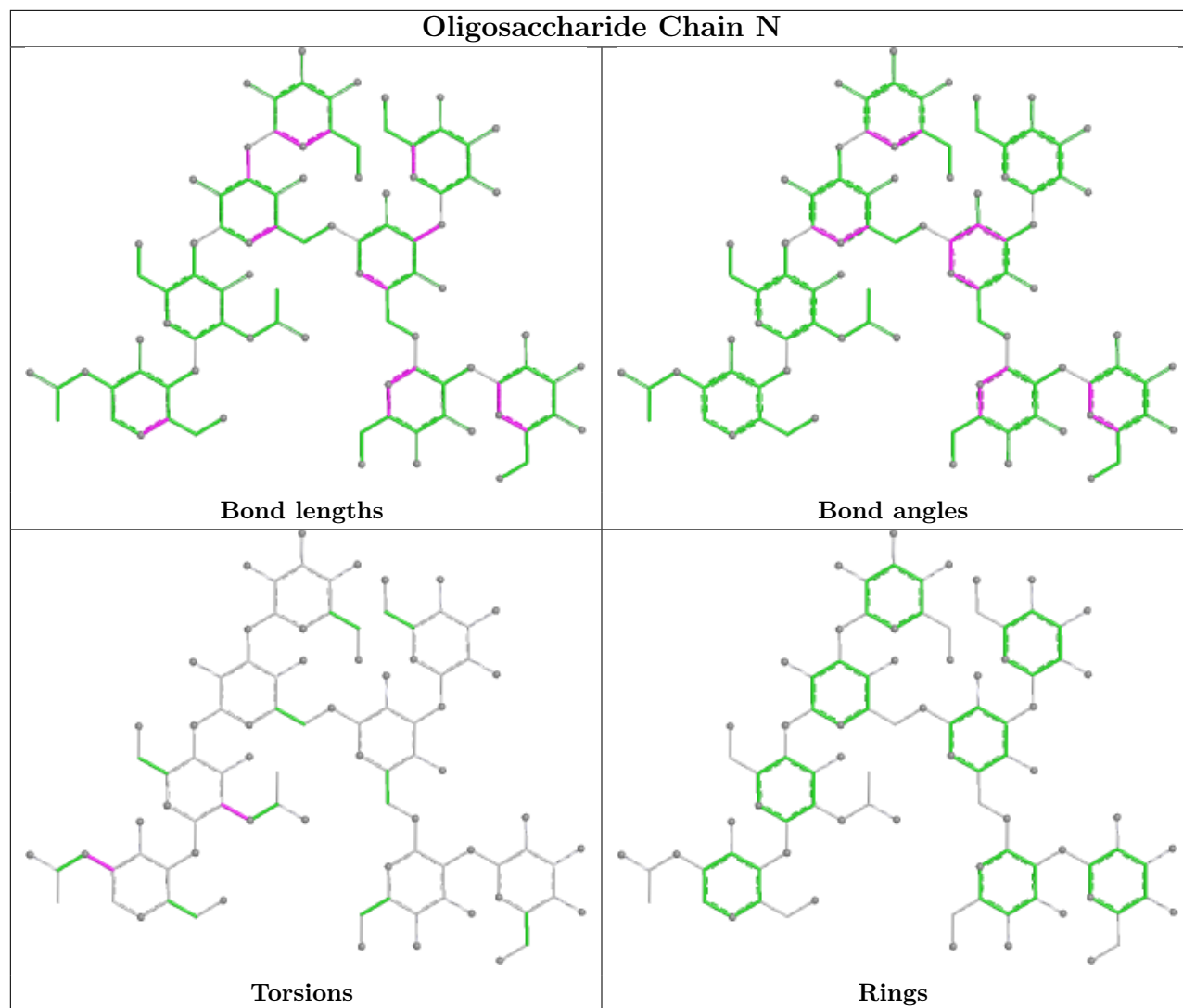


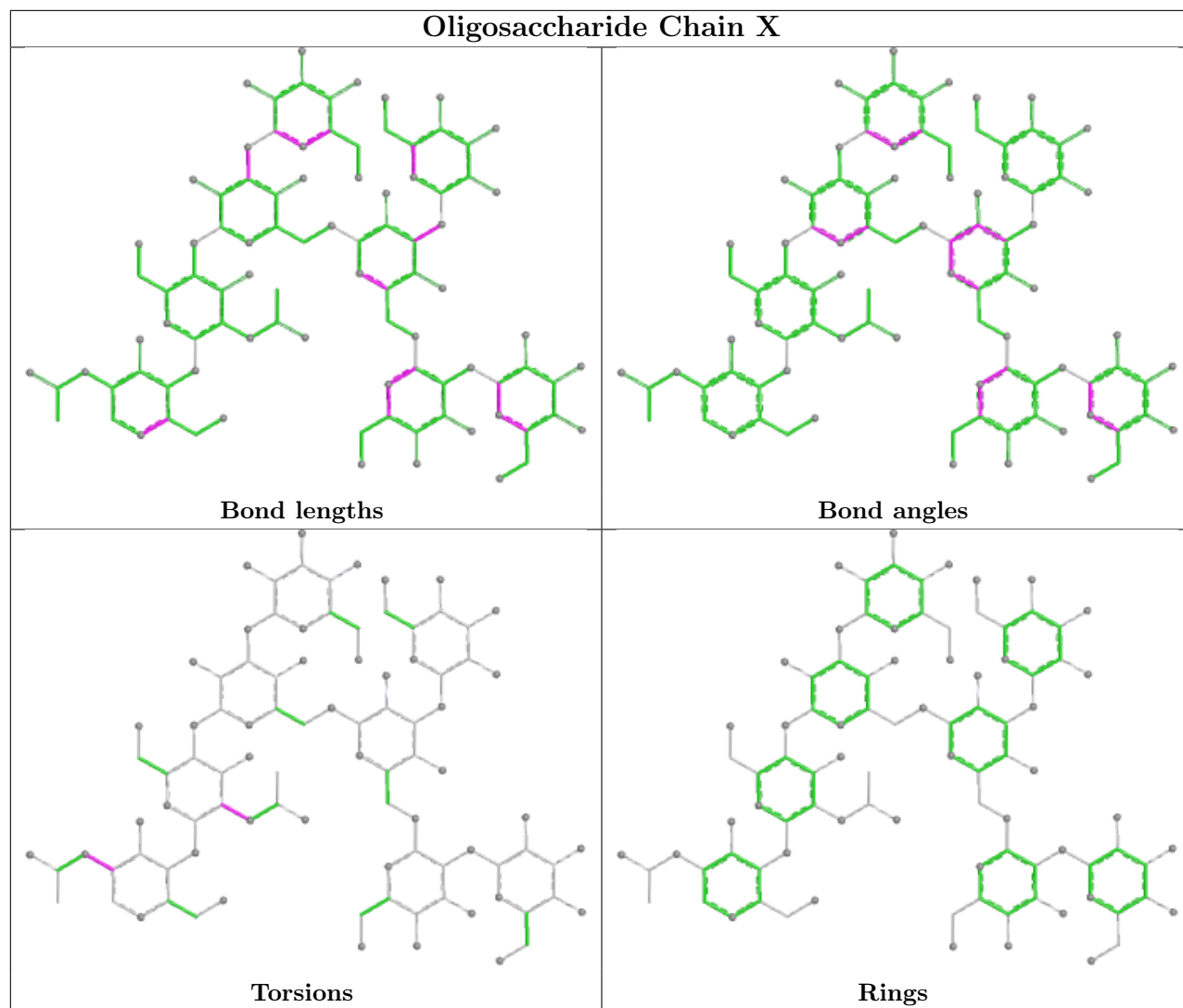


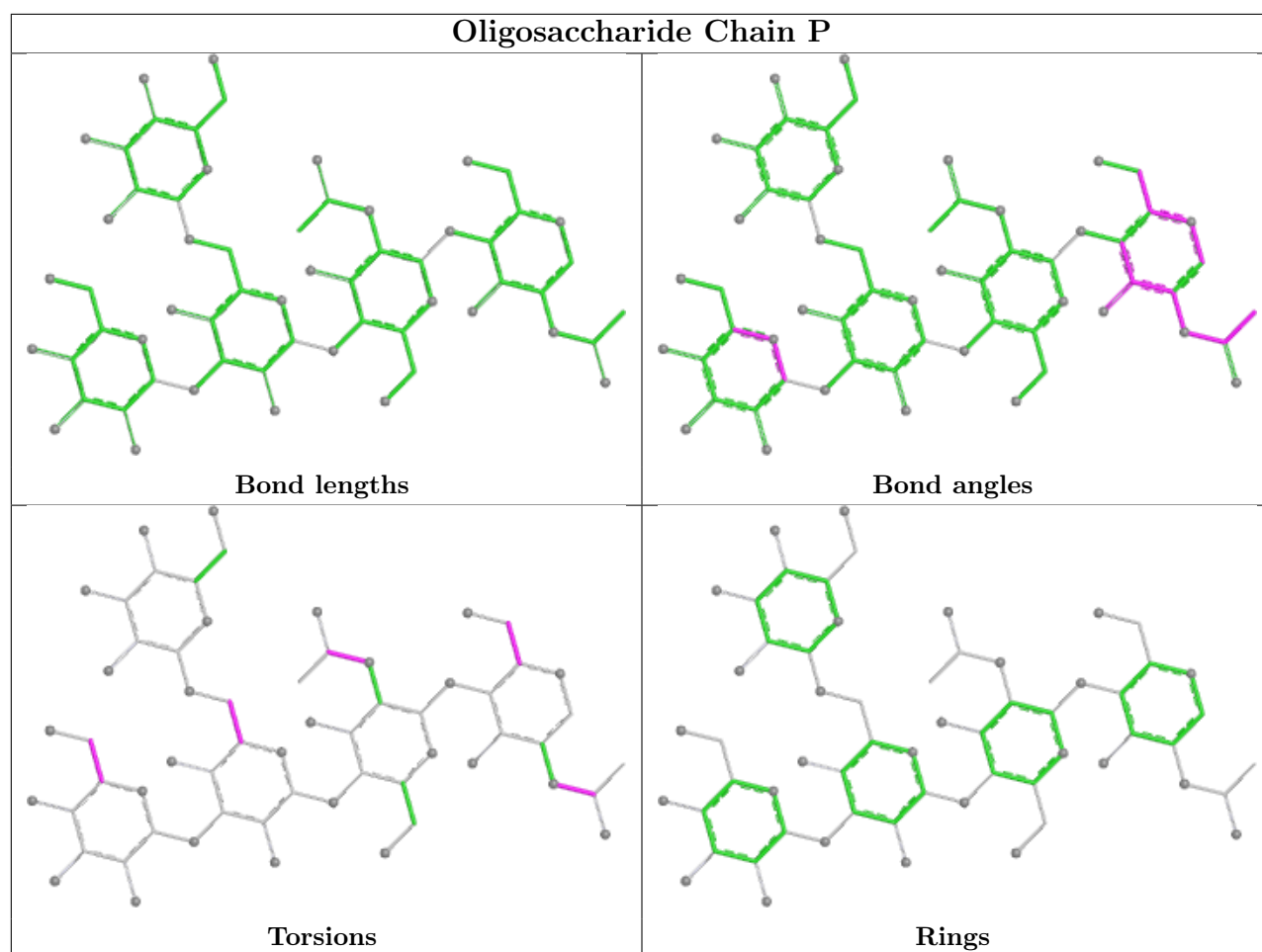


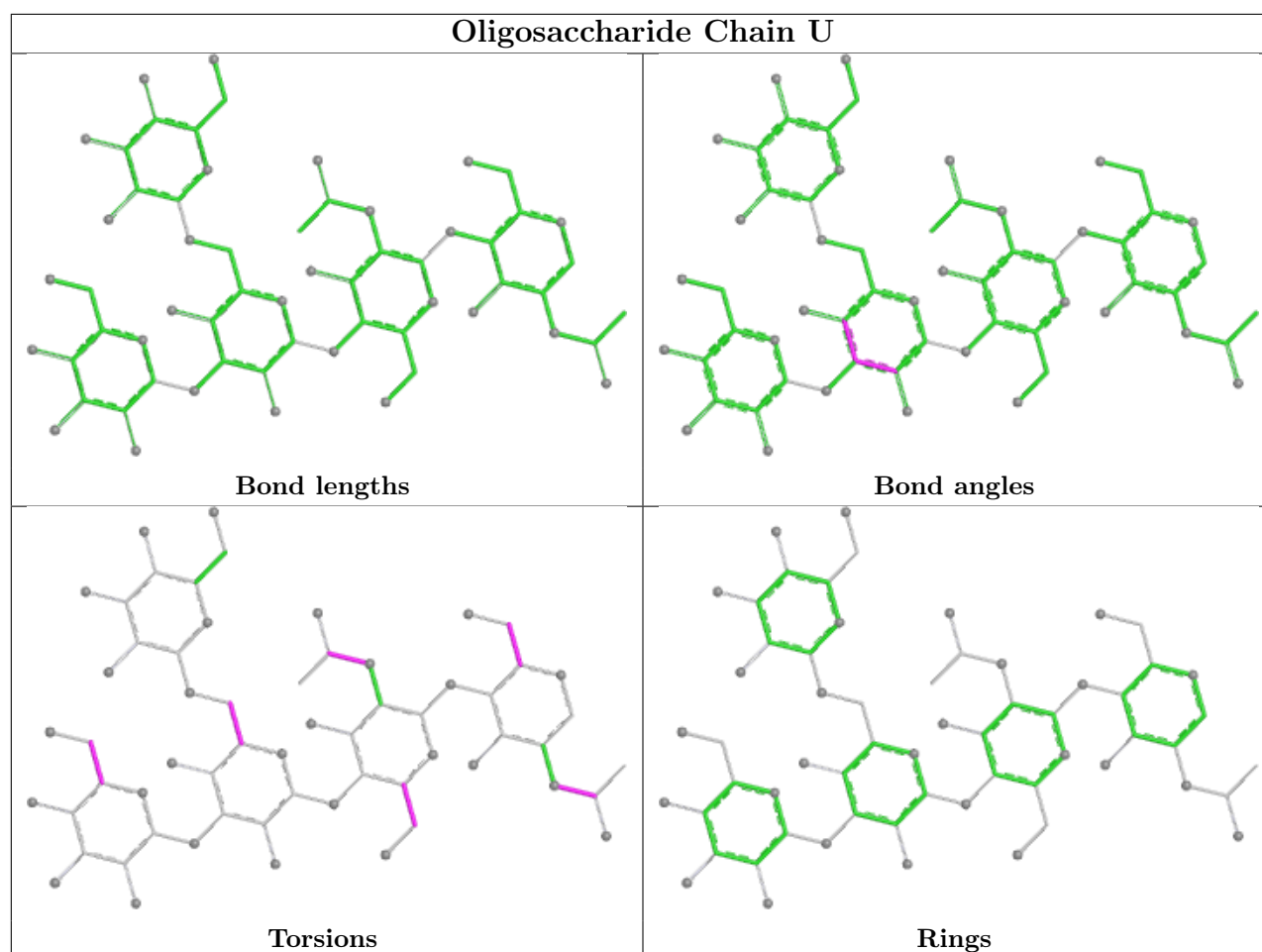












5.6 Ligand geometry [i](#)

25 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	$\# Z > 2$
8	NAG	B	1309	-	14,14,15	0.24	0	17,19,21	0.62	0
8	NAG	B	1307	1	14,14,15	0.24	0	17,19,21	0.72	0
8	NAG	B	1303	-	14,14,15	1.58	2 (14%)	17,19,21	0.74	0
8	NAG	C	1206	-	14,14,15	1.60	2 (14%)	17,19,21	0.74	0
8	NAG	B	1306	-	14,14,15	0.31	0	17,19,21	0.67	0
8	NAG	C	1203	-	14,14,15	1.62	2 (14%)	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	1307	1	14,14,15	0.24	0	17,19,21	0.71	0
8	NAG	A	1301	1	14,14,15	1.60	2 (14%)	17,19,21	0.64	0
8	NAG	C	1208	1	14,14,15	1.56	2 (14%)	17,19,21	0.73	0
8	NAG	C	1201	1	14,14,15	1.63	2 (14%)	17,19,21	0.78	0
8	NAG	C	1204	-	14,14,15	1.59	2 (14%)	17,19,21	0.74	0
8	NAG	A	1306	-	14,14,15	0.29	0	17,19,21	0.67	0
8	NAG	A	1305	-	14,14,15	1.50	2 (14%)	17,19,21	0.75	0
8	NAG	C	1205	-	14,14,15	1.66	2 (14%)	17,19,21	0.70	0
8	NAG	B	1308	-	14,14,15	0.28	0	17,19,21	0.66	0
8	NAG	A	1308	-	14,14,15	0.28	0	17,19,21	0.66	0
8	NAG	C	1207	1	14,14,15	1.62	2 (14%)	17,19,21	0.66	0
8	NAG	B	1302	-	14,14,15	1.66	2 (14%)	17,19,21	0.72	0
8	NAG	A	1304	-	14,14,15	1.63	2 (14%)	17,19,21	0.65	0
8	NAG	A	1303	-	14,14,15	1.59	2 (14%)	17,19,21	0.73	0
8	NAG	B	1304	-	14,14,15	1.61	2 (14%)	17,19,21	0.65	0
8	NAG	B	1301	1	14,14,15	1.60	2 (14%)	17,19,21	0.65	0
8	NAG	B	1305	1	14,14,15	1.50	2 (14%)	17,19,21	0.74	0
8	NAG	A	1302	-	14,14,15	1.65	2 (14%)	17,19,21	0.71	0
8	NAG	C	1202	1	14,14,15	1.52	2 (14%)	17,19,21	0.74	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
8	NAG	B	1309	-	-	4/6/23/26	0/1/1/1
8	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
8	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
8	NAG	C	1206	-	-	0/6/23/26	0/1/1/1
8	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
8	NAG	C	1203	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1208	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1201	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1204	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1306	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1305	-	-	1/6/23/26	0/1/1/1
8	NAG	C	1205	-	-	0/6/23/26	0/1/1/1
8	NAG	B	1308	-	-	3/6/23/26	0/1/1/1
8	NAG	A	1308	-	-	3/6/23/26	0/1/1/1
8	NAG	C	1207	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
8	NAG	A	1304	-	-	1/6/23/26	0/1/1/1
8	NAG	A	1303	-	-	0/6/23/26	0/1/1/1
8	NAG	B	1304	-	-	1/6/23/26	0/1/1/1
8	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1302	-	-	0/6/23/26	0/1/1/1
8	NAG	C	1202	1	-	1/6/23/26	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1302	NAG	C1-C2	4.74	1.58	1.52
8	C	1205	NAG	C1-C2	4.73	1.58	1.52
8	A	1302	NAG	C1-C2	4.69	1.58	1.52
8	C	1201	NAG	C1-C2	4.67	1.58	1.52
8	C	1203	NAG	C1-C2	4.58	1.58	1.52
8	A	1301	NAG	C1-C2	4.55	1.58	1.52
8	B	1301	NAG	C1-C2	4.50	1.58	1.52
8	A	1304	NAG	C1-C2	4.49	1.58	1.52
8	C	1207	NAG	C1-C2	4.48	1.58	1.52
8	B	1304	NAG	C1-C2	4.46	1.58	1.52
8	A	1303	NAG	C1-C2	4.42	1.58	1.52
8	C	1204	NAG	C1-C2	4.42	1.58	1.52
8	C	1208	NAG	C1-C2	4.42	1.58	1.52
8	C	1206	NAG	C1-C2	4.41	1.58	1.52
8	B	1303	NAG	C1-C2	4.38	1.58	1.52
8	C	1202	NAG	C1-C2	4.34	1.58	1.52
8	B	1305	NAG	C1-C2	4.29	1.58	1.52
8	A	1305	NAG	C1-C2	4.25	1.58	1.52
8	A	1302	NAG	O5-C5	2.58	1.48	1.43
8	B	1302	NAG	O5-C5	2.54	1.48	1.43
8	C	1205	NAG	O5-C5	2.51	1.48	1.43
8	A	1304	NAG	O5-C5	2.49	1.48	1.43
8	B	1304	NAG	O5-C5	2.47	1.48	1.43
8	C	1204	NAG	O5-C5	2.47	1.48	1.43
8	C	1207	NAG	O5-C5	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1206	NAG	O5-C5	2.38	1.48	1.43
8	C	1208	NAG	O5-C5	2.37	1.48	1.43
8	A	1303	NAG	O5-C5	2.33	1.48	1.43
8	B	1303	NAG	O5-C5	2.33	1.48	1.43
8	B	1301	NAG	O5-C5	2.29	1.47	1.43
8	C	1201	NAG	O5-C5	2.28	1.47	1.43
8	C	1203	NAG	O5-C5	2.28	1.47	1.43
8	A	1301	NAG	O5-C5	2.27	1.47	1.43
8	C	1202	NAG	O5-C5	2.12	1.47	1.43
8	A	1305	NAG	O5-C5	2.07	1.47	1.43
8	B	1305	NAG	O5-C5	2.06	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1307	NAG	C1-C2-N2-C7
8	A	1307	NAG	C8-C7-N2-C2
8	A	1307	NAG	O7-C7-N2-C2
8	A	1308	NAG	C1-C2-N2-C7
8	A	1308	NAG	C8-C7-N2-C2
8	A	1308	NAG	O7-C7-N2-C2
8	B	1307	NAG	C1-C2-N2-C7
8	B	1307	NAG	C8-C7-N2-C2
8	B	1307	NAG	O7-C7-N2-C2
8	B	1308	NAG	C1-C2-N2-C7
8	B	1308	NAG	C8-C7-N2-C2
8	B	1308	NAG	O7-C7-N2-C2
8	B	1309	NAG	C1-C2-N2-C7
8	B	1309	NAG	C8-C7-N2-C2
8	B	1309	NAG	O7-C7-N2-C2
8	A	1306	NAG	C8-C7-N2-C2
8	B	1306	NAG	C8-C7-N2-C2
8	A	1306	NAG	O7-C7-N2-C2
8	B	1306	NAG	O7-C7-N2-C2
8	A	1305	NAG	O5-C5-C6-O6
8	B	1305	NAG	O5-C5-C6-O6
8	C	1202	NAG	O5-C5-C6-O6
8	B	1309	NAG	O5-C5-C6-O6
8	A	1304	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	B	1304	NAG	C4-C5-C6-O6
8	C	1207	NAG	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1309	NAG	4	0
8	C	1203	NAG	4	0
8	C	1204	NAG	3	0
8	A	1306	NAG	1	0
8	A	1305	NAG	2	0
8	C	1205	NAG	3	0
8	B	1308	NAG	4	0
8	B	1302	NAG	3	0
8	A	1304	NAG	4	0
8	A	1303	NAG	3	0
8	B	1304	NAG	2	0
8	A	1302	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.

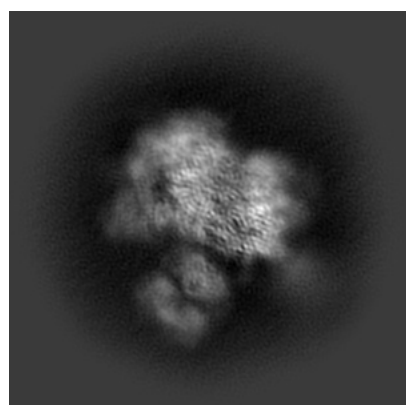
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23095. These allow visual inspection of the internal detail of the map and identification of artifacts.

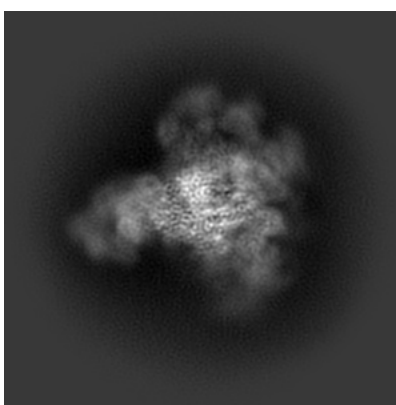
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

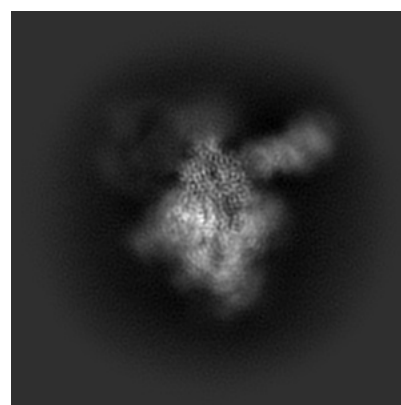
6.1.1 Primary map



X



Y

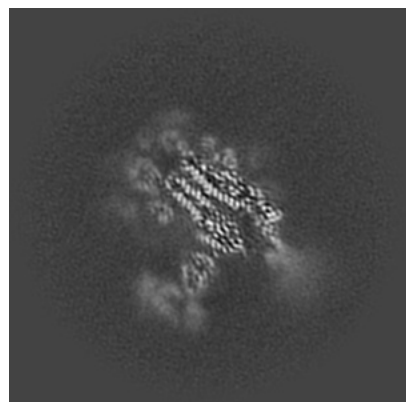


Z

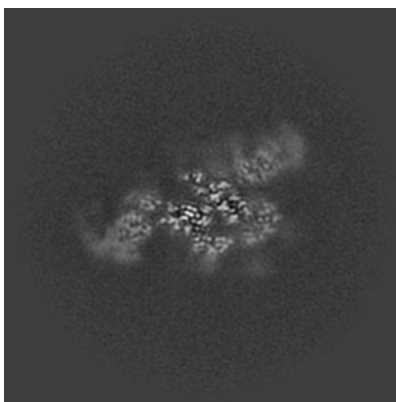
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

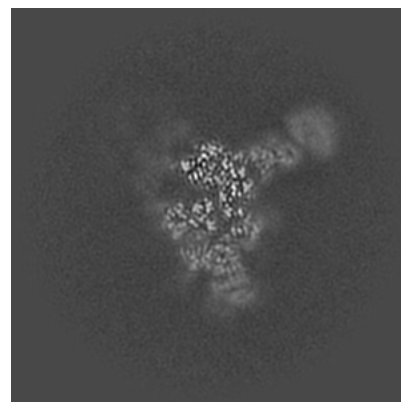
6.2.1 Primary map



X Index: 160



Y Index: 160

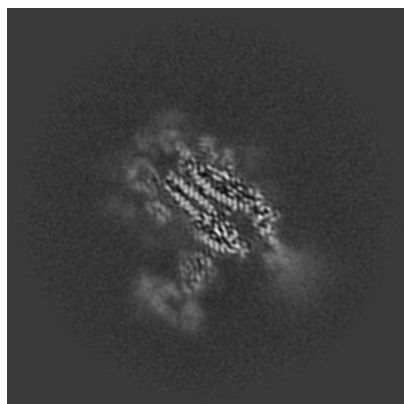


Z Index: 160

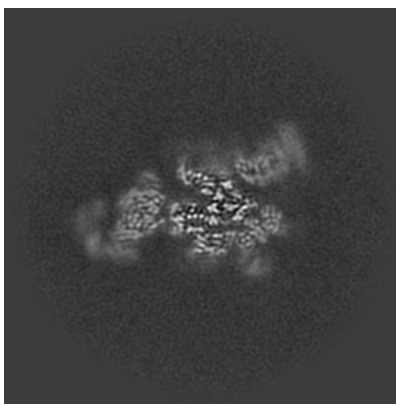
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

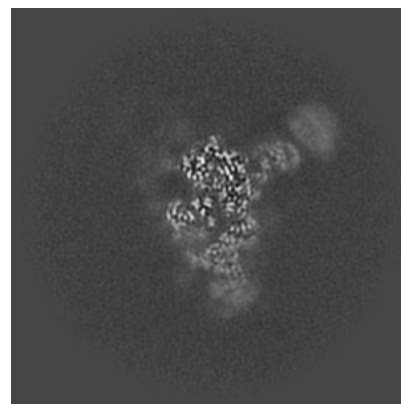
6.3.1 Primary map



X Index: 159



Y Index: 155

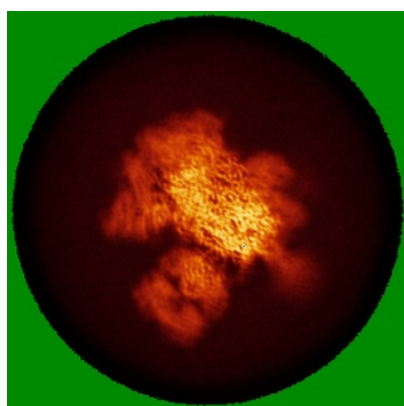


Z Index: 157

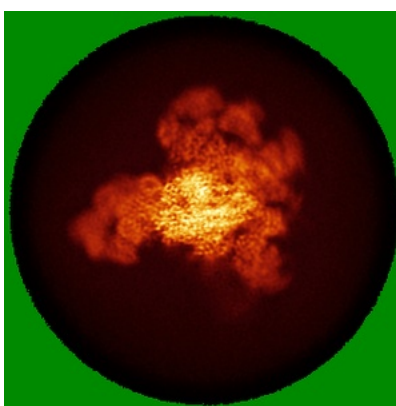
The images above show the largest variance slices of the map in three orthogonal directions.

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

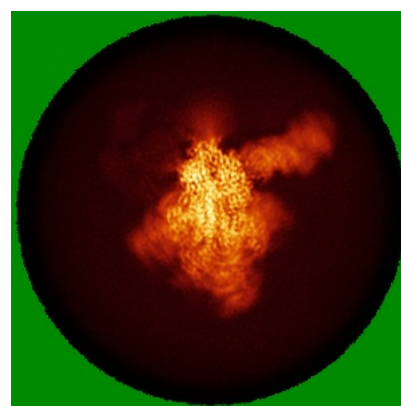
6.4.1 Primary map



X



Y

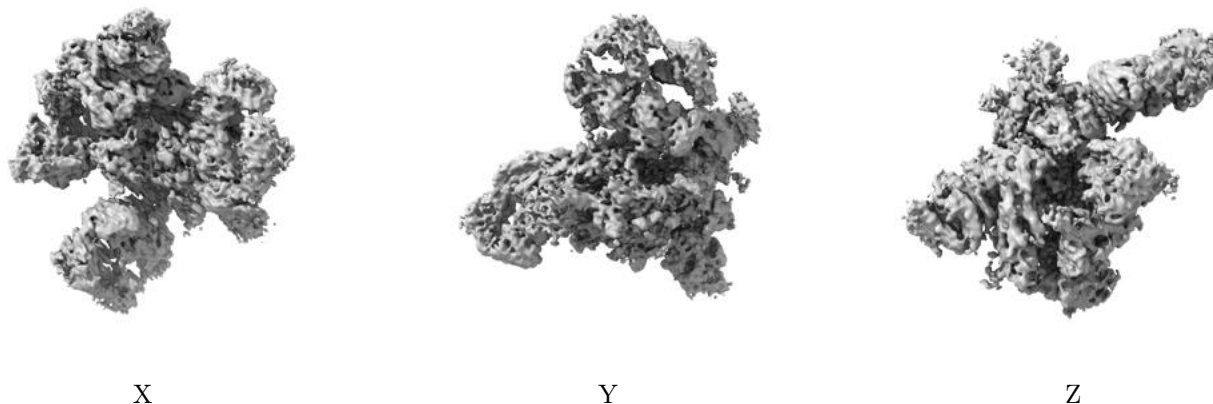


Z

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

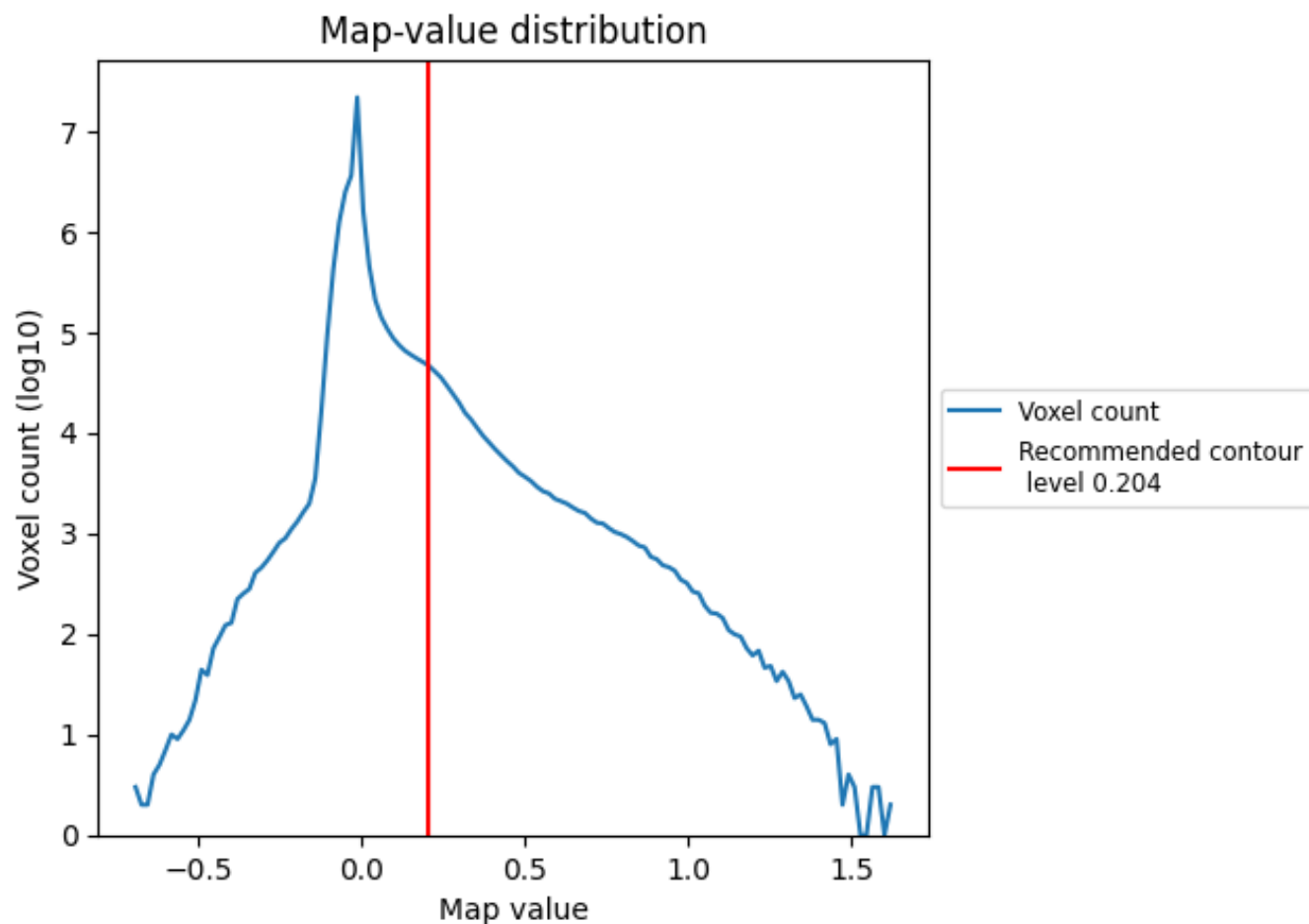
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

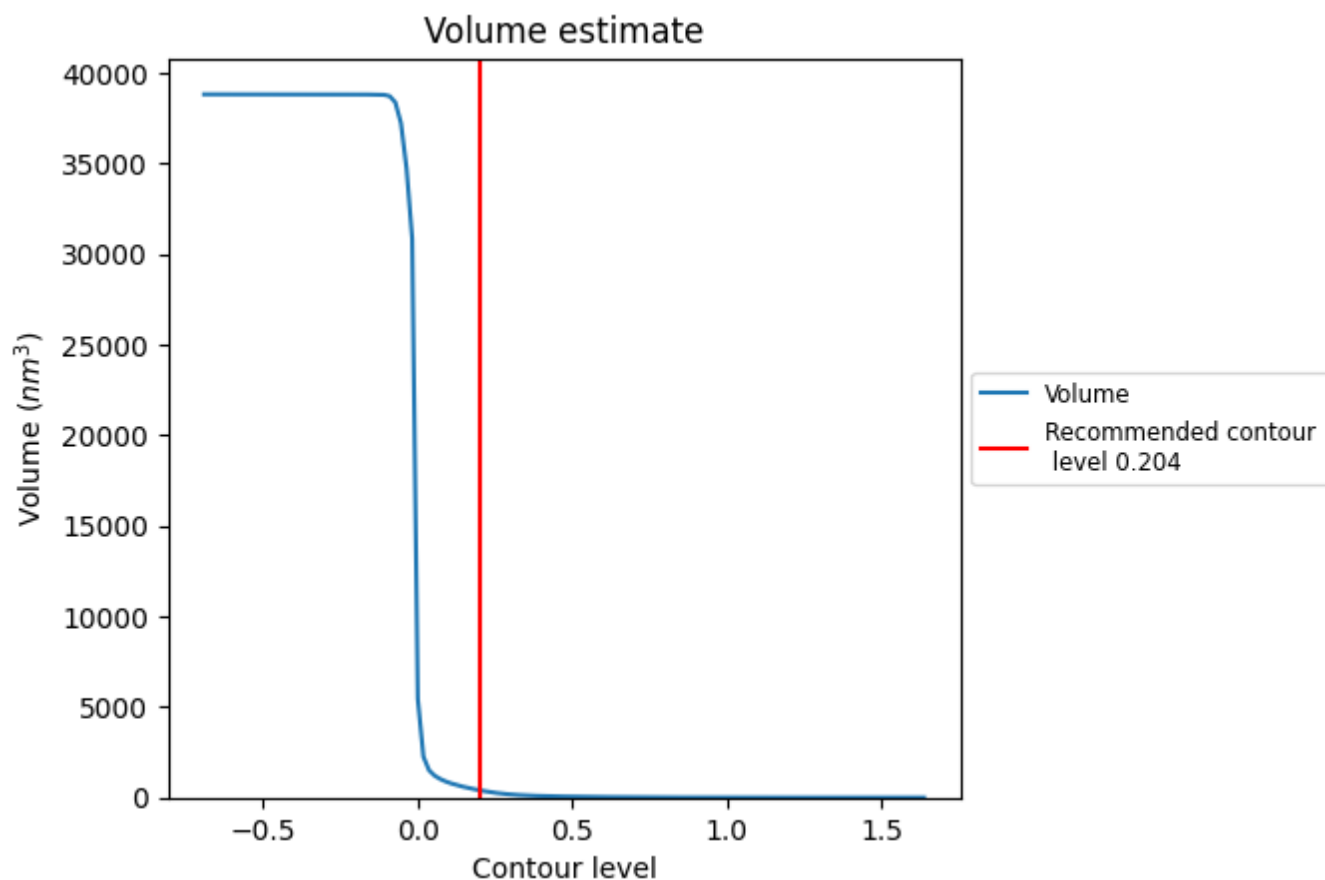
This section contains the results of statistical analysis of the map.

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.

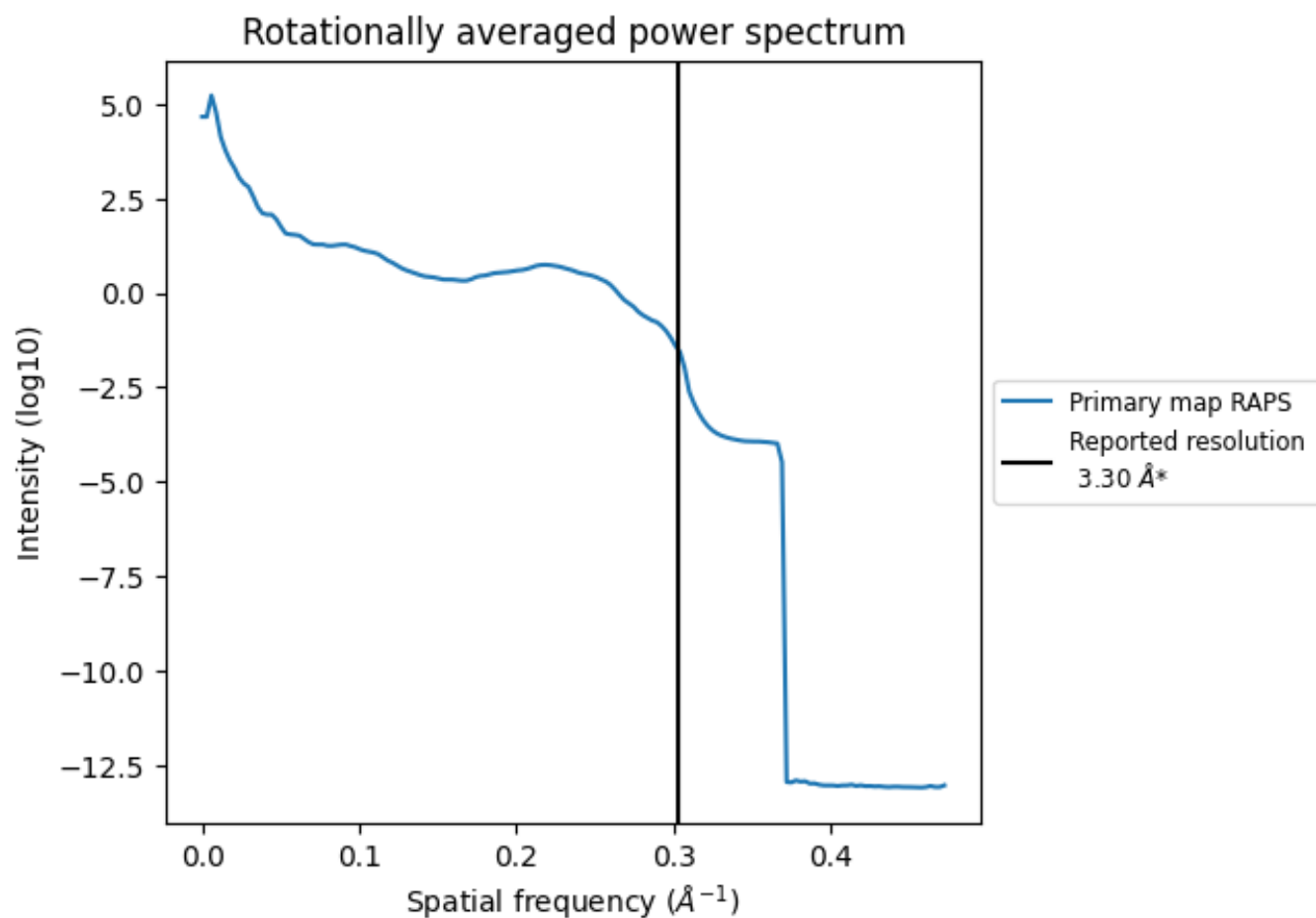
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 394 nm³; this corresponds to an approximate mass of 356 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 0.303 Å⁻¹

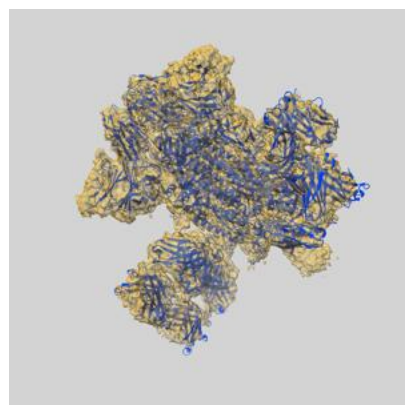
8 Fourier-Shell correlation ⓘ

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

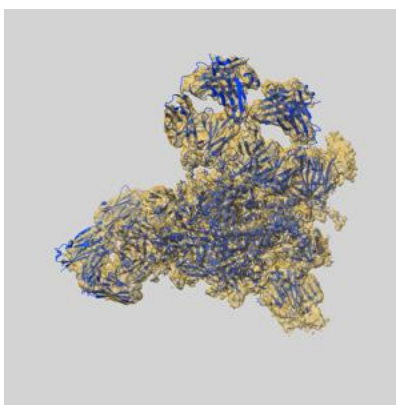
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23095 and PDB model 7L06. Per-residue inclusion information can be found in section 3 on page 10.

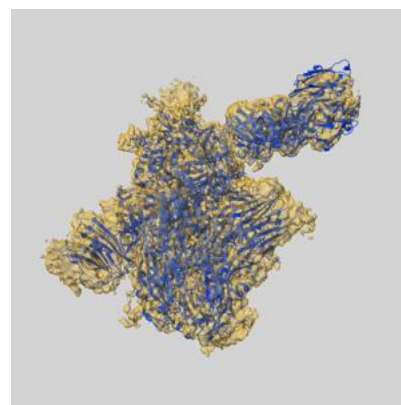
9.1 Map-model overlay [i](#)



X



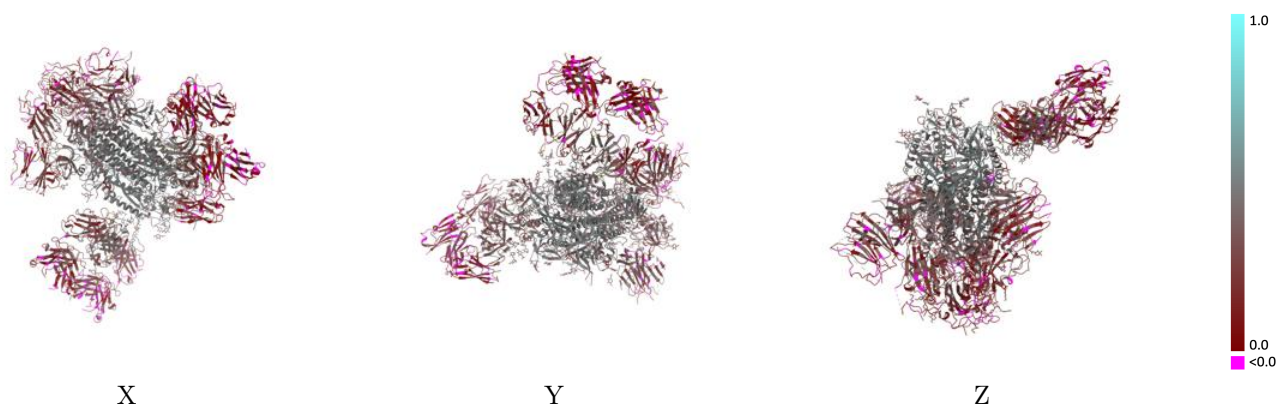
Y



Z

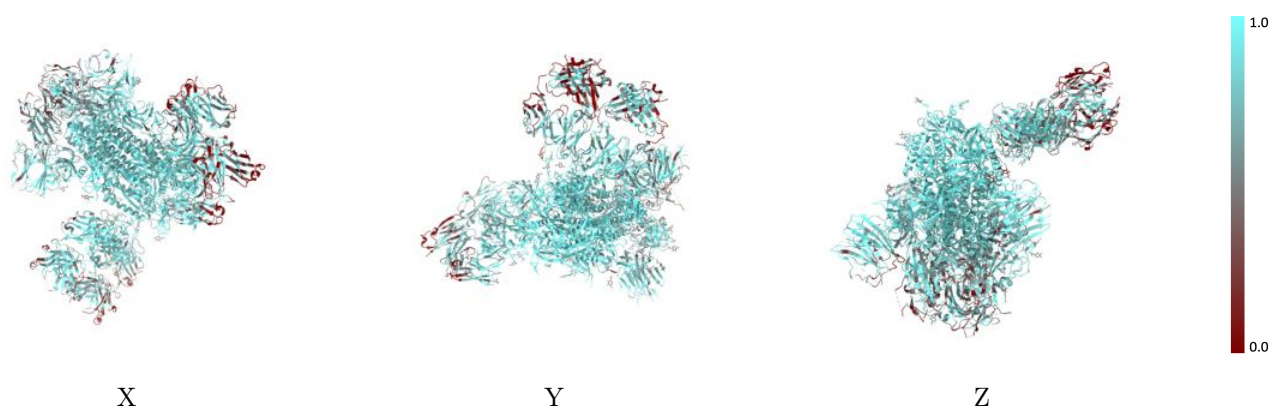
The images above show the 3D surface view of the map at the recommended contour level 0.204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



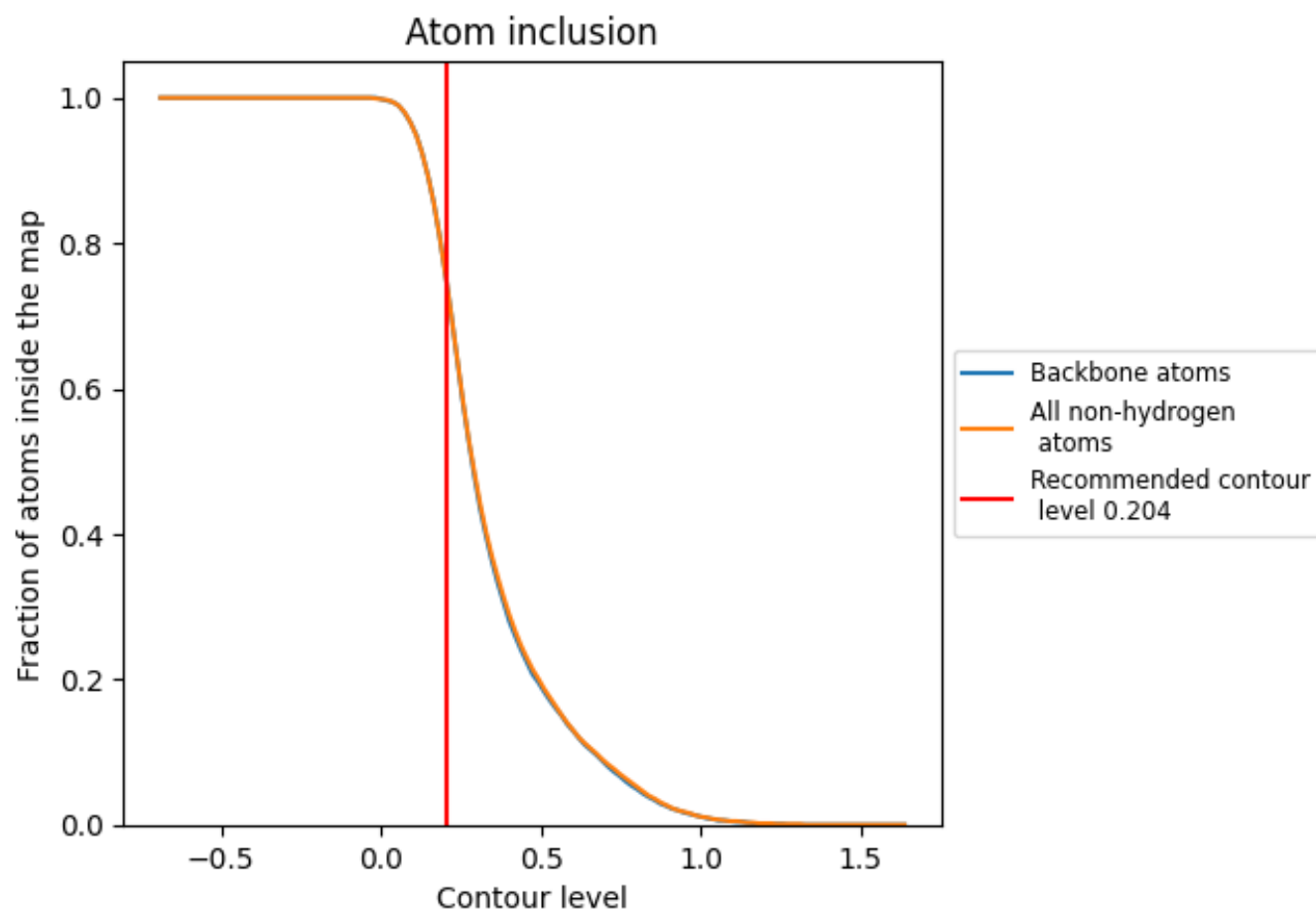
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.204).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.3030
A	 0.8200	 0.3570
B	 0.8040	 0.3540
C	 0.8130	 0.3450
D	 0.6710	 0.2270
E	 0.6160	 0.1540
F	 0.5110	 0.1520
G	 0.6070	 0.2480
H	 0.7830	 0.2620
I	 0.7140	 0.3660
J	 0.9340	 0.4440
K	 0.7410	 0.2320
L	 0.6040	 0.1260
M	 0.6980	 0.2800
N	 0.8620	 0.4490
O	 0.9290	 0.4210
P	 0.6890	 0.3770
Q	 0.7860	 0.4320
R	 0.7140	 0.2620
S	 0.8570	 0.3640
T	 0.6790	 0.2900
U	 0.7870	 0.3520
V	 0.7500	 0.3110
W	 0.9020	 0.4530
X	 0.8720	 0.4370
Y	 0.8210	 0.3480

