



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:23 PM UTC

PDB ID : 9C7F / pdb_00009c7f
Title : Human monoclonal antibody MAD24-01 bound to the N-terminus of cleaved circumsporozoite protein
Authors : Moskovitz, R.; Wilson, I.A.
Deposited on : 2024-06-10
Resolution : 1.82 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

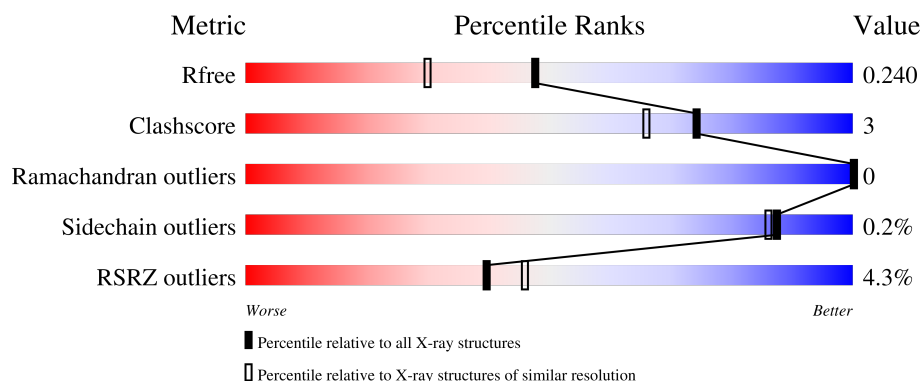
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	4% 94% 5%
1	C	225	7% 92% 8%
1	E	225	6% 93% 6%
1	H	225	4% 93% 6%
2	B	212	4% 91% 9%

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Mol	Chain	Length	Quality of chain
2	D	212	 % 95% 5%
2	F	212	 2% 96%
2	L	212	 3% 91% 9%
3	G	18	 6% 39% 6% 56%
3	I	18	 17% 44% 56%
3	J	18	 11% 44% 56%
3	Q	18	 11% 28% 17% 56%
4	K	3	 33% 33% 33%
4	M	3	 67% 33%
4	N	3	 67% 33%
4	O	3	 67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28545 atoms, of which 13397 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Monoclonal antibody MAD24-01 Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	223	Total	C	H	N	O	S	0	10	0
			3377	1071	1672	290	338	6			
1	A	223	Total	C	H	N	O	S	0	6	0
			3353	1065	1660	288	334	6			
1	C	225	Total	C	H	N	O	S	0	2	0
			3351	1065	1658	288	333	7			
1	E	223	Total	C	H	N	O	S	0	6	0
			3353	1065	1660	288	334	6			

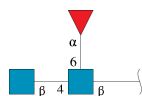
- Molecule 2 is a protein called Monoclonal antibody MAD24-01 Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	211	Total	C	H	N	O	S	0	6	0
			3268	1031	1618	281	332	6			
2	B	211	Total	C	H	N	O	S	0	8	0
			3297	1037	1634	288	333	5			
2	D	211	Total	C	H	N	O	S	0	0	0
			3223	1019	1594	278	327	5			
2	F	211	Total	C	H	N	O	S	0	3	0
			3239	1023	1603	279	329	5			

- Molecule 3 is a protein called Circumsporozoite protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	8	Total	C	H	N	O	0	0	0
			96	32	41	9	14			
3	G	8	Total	C	H	N	O	0	0	0
			96	32	41	9	14			
3	I	8	Total	C	H	N	O	0	0	0
			96	32	41	9	14			
3	J	8	Total	C	H	N	O	0	0	0
			96	32	41	9	14			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
4	M	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			
4	N	3	Total	C	H	N	O	0	0	0
			71	22	33	2	14			
4	O	3	Total	C	H	N	O	0	0	0
			71	22	33	2	14			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	206	Total	O	0	0
			206	206		
5	L	153	Total	O	0	0
			153	153		
5	A	184	Total	O	0	0
			184	184		
5	B	167	Total	O	0	0
			167	167		
5	C	191	Total	O	0	0
			191	191		
5	D	142	Total	O	0	0
			142	142		
5	E	191	Total	O	0	0
			191	191		
5	F	175	Total	O	0	0
			175	175		
5	Q	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		
5	I	2	Total	O	0	0
			2	2		
5	J	1	Total	O	0	0
			1	1		

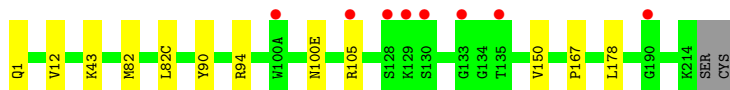
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

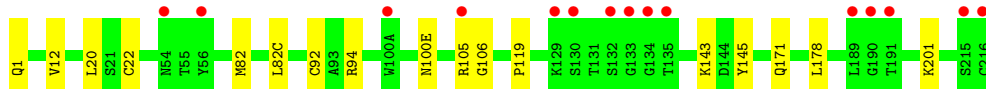
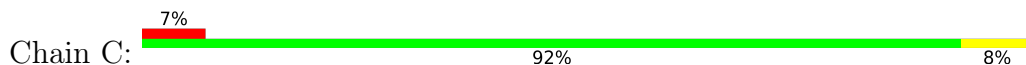
- Molecule 1: Monoclonal antibody MAD24-01 Fab Heavy Chain



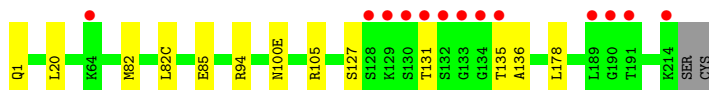
- Molecule 1: Monoclonal antibody MAD24-01 Fab Heavy Chain



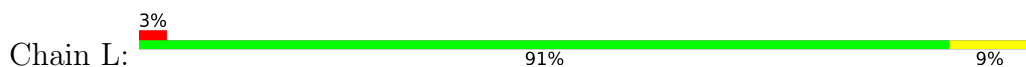
- Molecule 1: Monoclonal antibody MAD24-01 Fab Heavy Chain



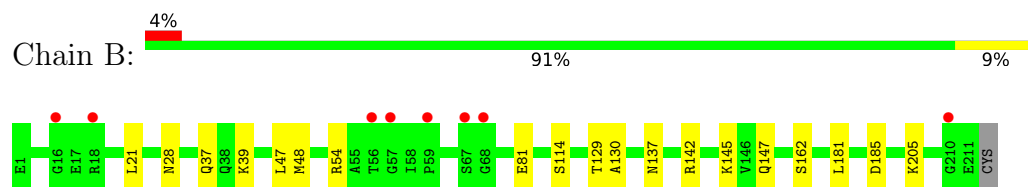
- Molecule 1: Monoclonal antibody MAD24-01 Fab Heavy Chain



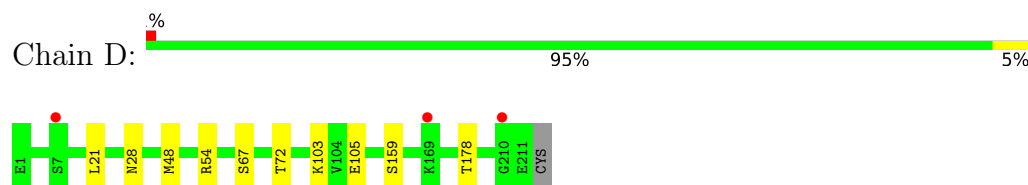
- Molecule 2: Monoclonal antibody MAD24-01 Fab Light Chain



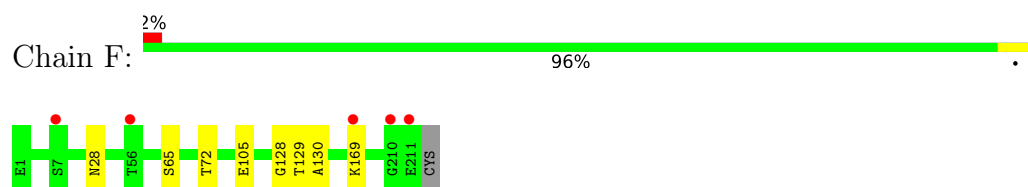
- Molecule 2: Monoclonal antibody MAD24-01 Fab Light Chain



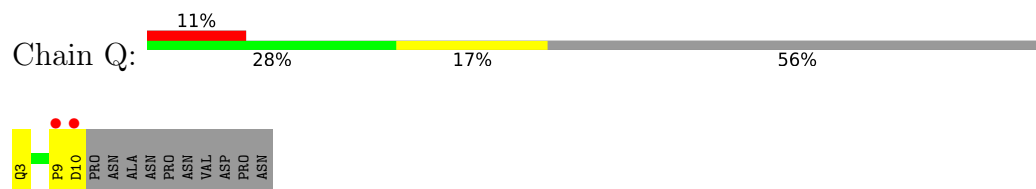
- Molecule 2: Monoclonal antibody MAD24-01 Fab Light Chain



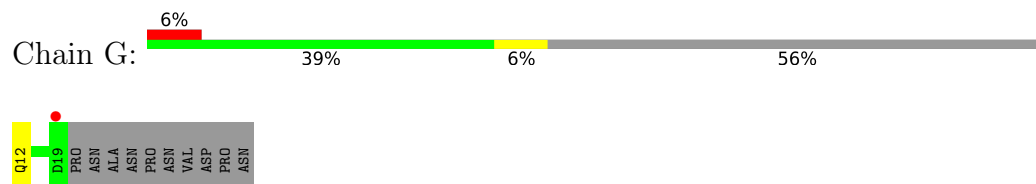
- Molecule 2: Monoclonal antibody MAD24-01 Fab Light Chain



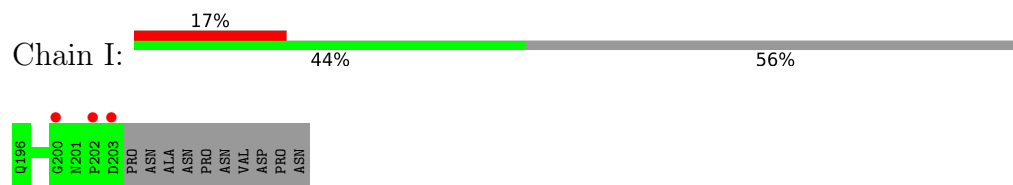
- Molecule 3: Circumsporozoite protein



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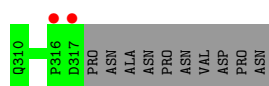


- Molecule 3: Circumsporozoite protein



- Molecule 3: Circumsporozoite protein





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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.54Å 88.32Å 168.95Å 90.00° 89.75° 90.00°	Depositor
Resolution (Å)	45.00 – 1.82 45.00 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.00-1.82) 98.3 (45.00-1.82)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, R_{free}	0.211 , 0.238 0.214 , 0.240	Depositor DCC
R_{free} test set	9581 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.060 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28545	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5899e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/1751	0.40	0/2383
1	C	0.16	0/1732	0.40	0/2357
1	E	0.17	0/1751	0.41	0/2383
1	H	0.17	0/1773	0.42	0/2412
2	B	0.16	0/1725	0.39	0/2341
2	D	0.17	0/1663	0.43	0/2258
2	F	0.17	0/1685	0.43	0/2289
2	L	0.16	0/1712	0.42	0/2325
3	G	0.14	0/49	0.38	0/69
3	I	0.17	0/49	0.38	0/69
3	J	0.17	0/49	0.48	0/69
3	Q	0.19	0/49	0.43	0/69
All	All	0.17	0/13988	0.41	0/19024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1693	1660	1638	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1693	1658	1652	12	0
1	E	1693	1660	1638	10	0
1	H	1705	1672	1641	12	0
2	B	1663	1634	1594	13	0
2	D	1629	1594	1594	7	0
2	F	1636	1603	1581	6	0
2	L	1650	1618	1586	13	0
3	G	55	41	41	0	0
3	I	55	41	41	0	0
3	J	55	41	41	0	0
3	Q	55	41	41	1	0
4	K	38	34	34	1	0
4	M	38	34	34	1	0
4	N	38	33	34	2	0
4	O	38	33	34	2	0
5	A	184	0	0	3	0
5	B	167	0	0	2	0
5	C	191	0	0	3	0
5	D	142	0	0	2	0
5	E	191	0	0	2	0
5	F	175	0	0	1	0
5	G	1	0	0	0	0
5	H	206	0	0	4	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
5	L	153	0	0	6	0
5	Q	1	0	0	0	0
All	All	15148	13397	13224	84	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.

The worst 5 of 84 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:H:214:LYS:NZ	5:H:301:HOH:O	1.74	1.20
2:B:142:ARG:NH2	5:B:303:HOH:O	1.97	0.98
1:C:22:CYS:SG	5:C:456:HOH:O	2.27	0.92
1:C:105:ARG:NE	5:C:301:HOH:O	2.01	0.89
2:B:185:ASP:OD2	5:B:301:HOH:O	1.92	0.87

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 X-ray entries followed by that with respect to entries of similar resolution.

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	227/225 (101%)	223 (98%)	4 (2%)	0	100	100
1	C	225/225 (100%)	221 (98%)	4 (2%)	0	100	100
1	E	227/225 (101%)	224 (99%)	3 (1%)	0	100	100
1	H	231/225 (103%)	227 (98%)	4 (2%)	0	100	100
2	B	217/212 (102%)	213 (98%)	4 (2%)	0	100	100
2	D	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
2	F	212/212 (100%)	207 (98%)	5 (2%)	0	100	100
2	L	215/212 (101%)	211 (98%)	4 (2%)	0	100	100
3	G	6/18 (33%)	6 (100%)	0	0	100	100
3	I	6/18 (33%)	6 (100%)	0	0	100	100
3	J	6/18 (33%)	6 (100%)	0	0	100	100
3	Q	6/18 (33%)	6 (100%)	0	0	100	100
All	All	1787/1820 (98%)	1754 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	191/187 (102%)	191 (100%)	0	100	100
1	C	189/187 (101%)	189 (100%)	0	100	100
1	E	191/187 (102%)	191 (100%)	0	100	100
1	H	194/187 (104%)	194 (100%)	0	100	100
2	B	189/183 (103%)	189 (100%)	0	100	100
2	D	182/183 (100%)	181 (100%)	1 (0%)	81	77
2	F	185/183 (101%)	184 (100%)	1 (0%)	81	77
2	L	188/183 (103%)	187 (100%)	1 (0%)	81	77
3	G	5/14 (36%)	5 (100%)	0	100	100
3	I	5/14 (36%)	5 (100%)	0	100	100
3	J	5/14 (36%)	5 (100%)	0	100	100
3	Q	5/14 (36%)	5 (100%)	0	100	100
All	All	1529/1536 (100%)	1526 (100%)	3 (0%)	87	86

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

Mol	Chain	Res	Type
2	L	105	GLU
2	D	105	GLU
2	F	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	189	HIS
2	F	152	ASN
1	E	39	GLN
1	A	100(E)	ASN
2	F	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
1	PCA	E	1	1	7,8,9	0.83	0	9,10,12	1.47	2 (22%)
1	PCA	H	1	1	7,8,9	0.85	0	9,10,12	1.44	2 (22%)
3	PCA	J	310	3	7,8,9	0.58	0	9,10,12	1.14	0
3	PCA	G	12	3	7,8,9	0.59	0	9,10,12	1.14	1 (11%)
1	PCA	A	1	1	7,8,9	0.87	0	9,10,12	1.40	2 (22%)
1	PCA	C	1	1	7,8,9	0.78	0	9,10,12	1.45	2 (22%)
3	PCA	Q	3	3	7,8,9	0.58	0	9,10,12	1.14	1 (11%)
3	PCA	I	196	3	7,8,9	0.57	0	9,10,12	1.15	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
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
3	PCA	J	310	3	-	0/0/11/13	0/1/1/1
3	PCA	G	12	3	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
3	PCA	Q	3	3	-	0/0/11/13	0/1/1/1
3	PCA	I	196	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	CB-CA-C	-2.46	109.29	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	PCA	CB-CA-C	-2.44	109.31	112.66
1	A	1	PCA	CB-CA-N	2.41	109.88	103.24
1	H	1	PCA	CB-CA-C	-2.28	109.52	112.66
1	H	1	PCA	CB-CA-N	2.13	109.11	103.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	K	1	4	14,14,15	1.28	2 (14%)	17,19,21	1.67	4 (23%)
4	NAG	K	2	4	14,14,15	0.72	0	17,19,21	1.02	1 (5%)
4	FUC	K	3	4	10,10,11	0.85	0	14,14,16	0.93	0
4	NAG	M	1	4	14,14,15	1.04	2 (14%)	17,19,21	1.58	4 (23%)
4	NAG	M	2	4	14,14,15	0.77	0	17,19,21	0.86	0
4	FUC	M	3	4	10,10,11	0.87	0	14,14,16	1.05	0
4	NAG	N	1	4	14,14,15	1.10	2 (14%)	17,19,21	1.96	6 (35%)
4	NAG	N	2	4	14,14,15	0.90	0	17,19,21	1.17	1 (5%)
4	FUC	N	3	4	10,10,11	0.64	0	14,14,16	1.22	2 (14%)
4	NAG	O	1	4	14,14,15	1.18	2 (14%)	17,19,21	2.11	7 (41%)
4	NAG	O	2	4	14,14,15	0.81	0	17,19,21	1.04	0
4	FUC	O	3	4	10,10,11	0.73	0	14,14,16	0.93	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	K	1	4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	FUC	K	3	4	-	-	0/1/1/1
4	NAG	M	1	4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	FUC	M	3	4	-	-	0/1/1/1
4	NAG	N	1	4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	FUC	N	3	4	-	-	0/1/1/1
4	NAG	O	1	4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	FUC	O	3	4	-	-	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	NAG	O5-C1	-3.03	1.38	1.43
4	O	1	NAG	C2-N2	-2.64	1.41	1.46
4	N	1	NAG	C2-N2	-2.57	1.42	1.46
4	M	1	NAG	O5-C1	-2.50	1.39	1.43
4	K	1	NAG	C1-C2	2.45	1.55	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1	NAG	C1-O5-C5	-4.85	105.69	112.19
4	N	1	NAG	O5-C1-C2	-4.36	104.55	111.29
4	O	1	NAG	O5-C1-C2	-3.94	105.19	111.29
4	N	1	NAG	O4-C4-C3	-3.77	101.50	110.38
4	K	1	NAG	C1-O5-C5	-3.40	107.63	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

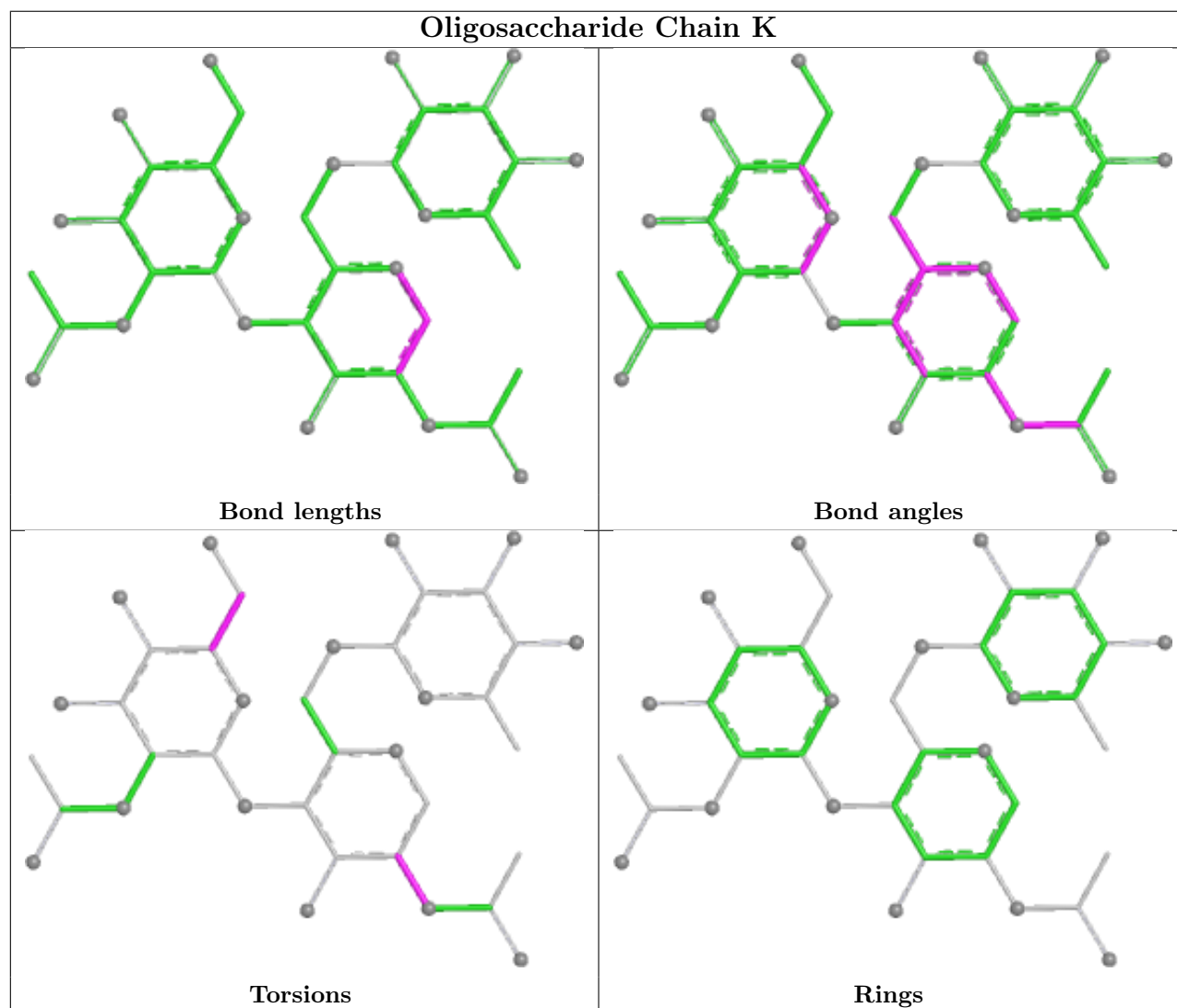
Mol	Chain	Res	Type	Atoms
4	K	1	NAG	C1-C2-N2-C7
4	K	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	K	2	NAG	C4-C5-C6-O6

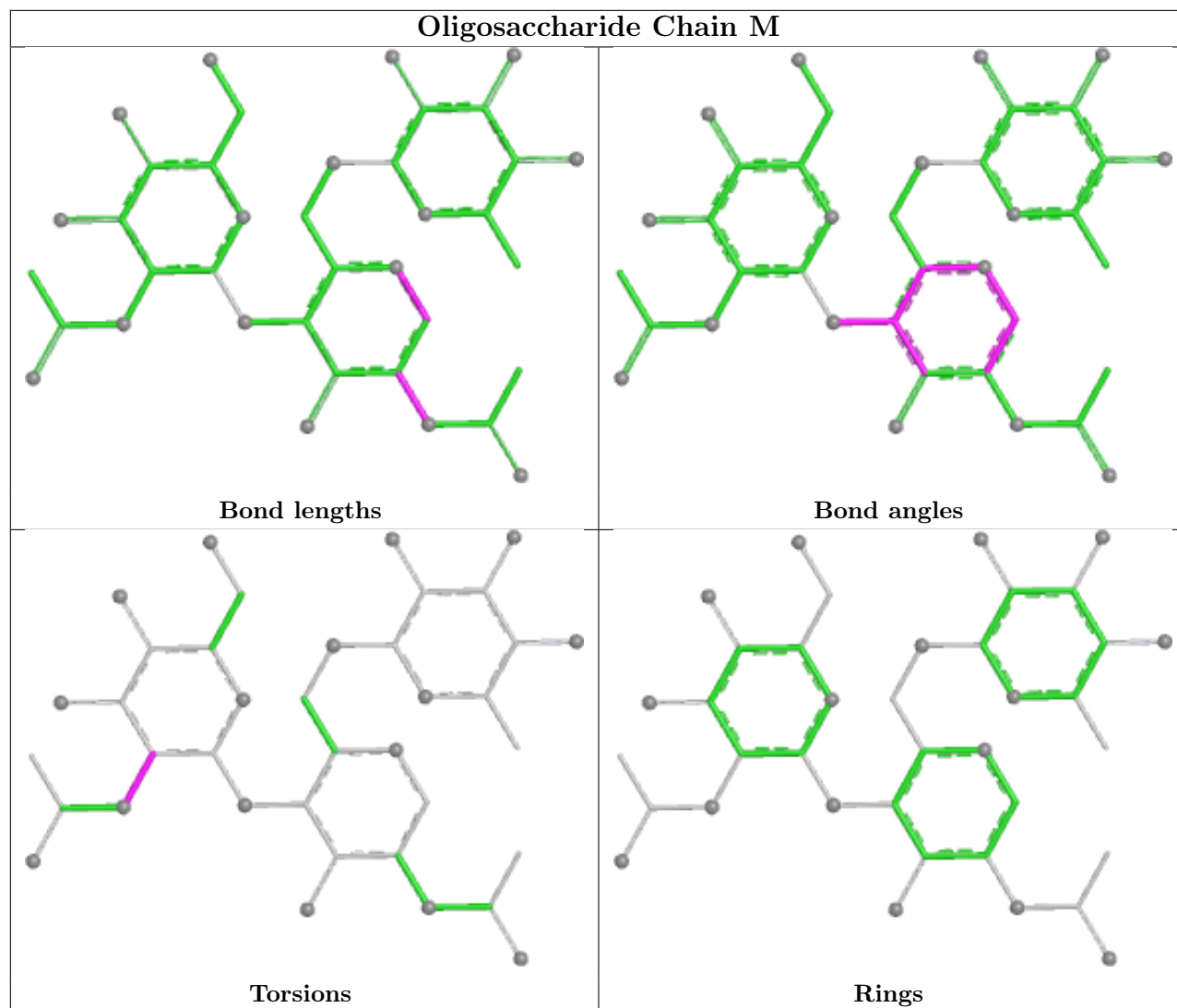
There are no ring outliers.

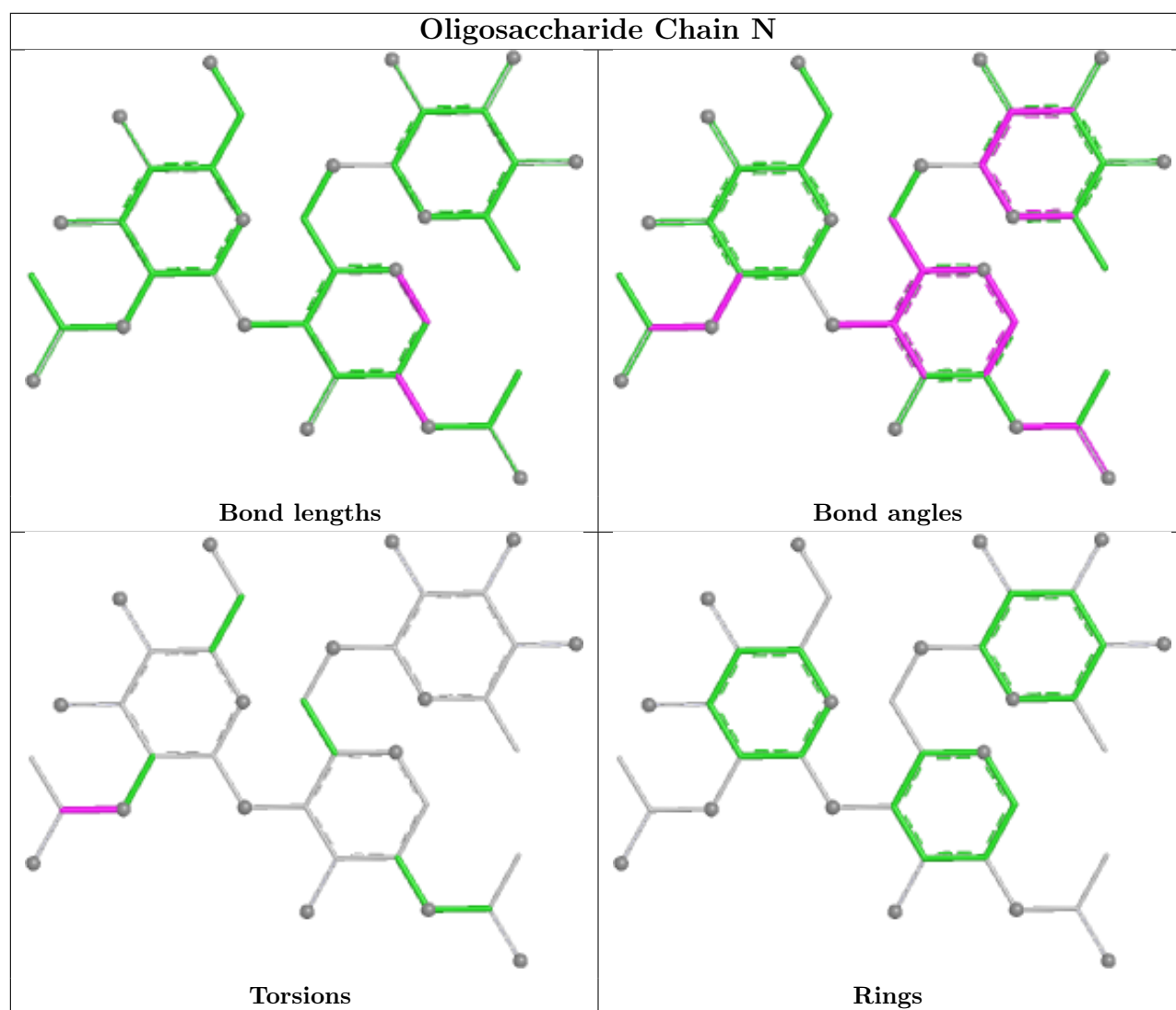
4 monomers are involved in 6 short contacts:

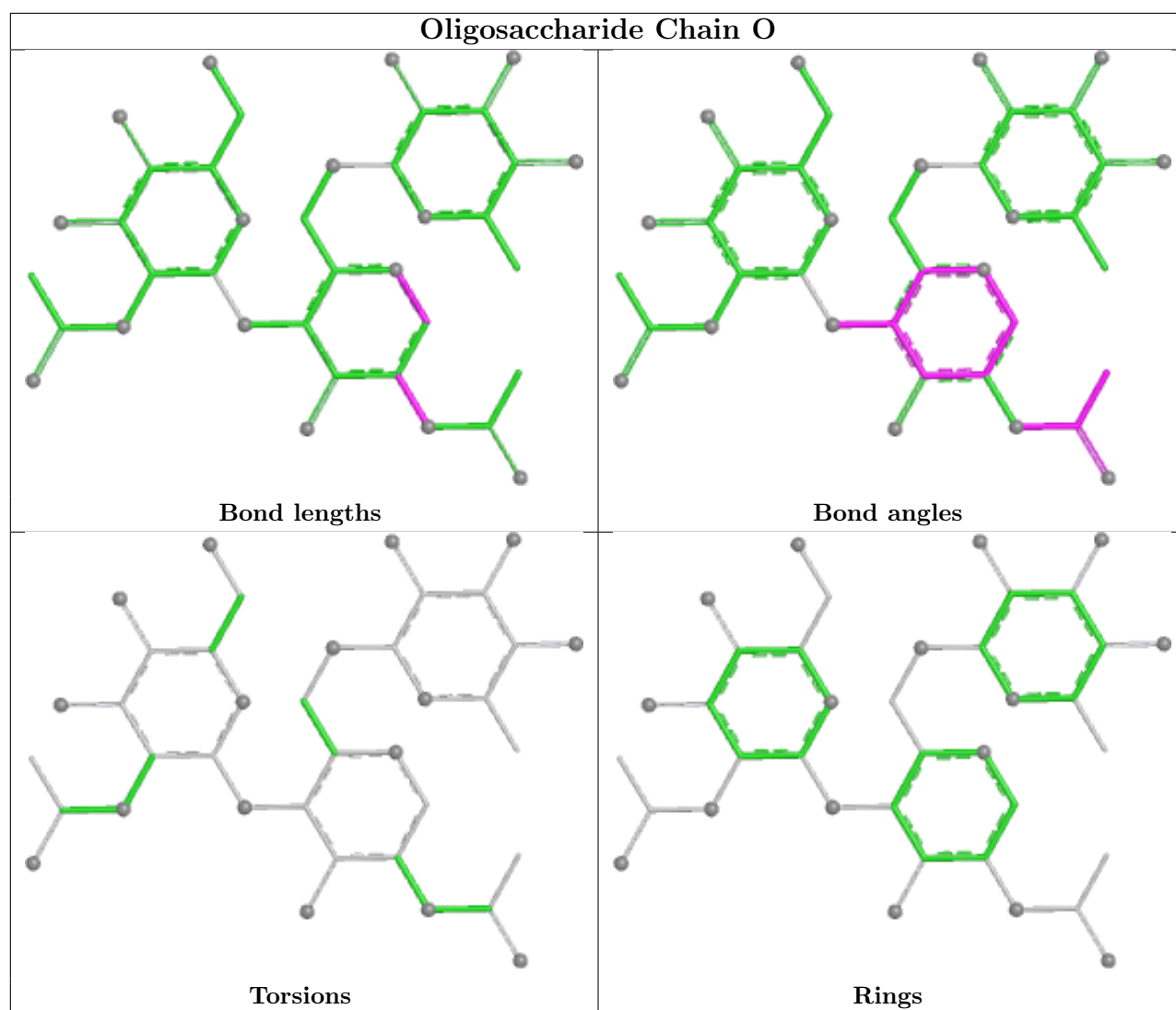
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	1	NAG	2	0
4	N	1	NAG	2	0
4	M	1	NAG	1	0
4	K	1	NAG	1	0

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](#)

There are no ligands in this entry.

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/225 (98%)	0.05	8 (3%) 46 53	9, 24, 40, 63	3 (1%)
1	C	224/225 (99%)	0.21	15 (6%) 24 27	9, 27, 42, 57	1 (0%)
1	E	222/225 (98%)	-0.04	13 (5%) 28 32	9, 23, 43, 52	3 (1%)
1	H	222/225 (98%)	-0.03	9 (4%) 41 47	8, 23, 38, 72	5 (2%)
2	B	211/212 (99%)	0.27	8 (3%) 44 50	10, 27, 42, 53	4 (1%)
2	D	211/212 (99%)	0.07	3 (1%) 73 79	17, 26, 39, 56	0
2	F	211/212 (99%)	-0.09	5 (2%) 59 66	12, 24, 36, 55	1 (0%)
2	L	211/212 (99%)	0.09	6 (2%) 55 60	10, 26, 39, 47	3 (1%)
3	G	7/18 (38%)	1.01	1 (14%) 6 6	32, 34, 47, 53	0
3	I	7/18 (38%)	1.67	3 (42%) 0 0	35, 39, 56, 62	0
3	J	7/18 (38%)	1.29	2 (28%) 1 1	33, 37, 52, 60	0
3	Q	7/18 (38%)	1.03	2 (28%) 1 1	31, 35, 52, 68	0
All	All	1762/1820 (96%)	0.09	75 (4%) 40 46	8, 25, 41, 72	20 (1%)

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	130	SER	5.4
1	E	130	SER	5.2
1	C	190	GLY	5.0
2	L	48[A]	MET	4.8
2	D	210	GLY	4.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	A	1	8/9	0.72	0.22	35,51,59,67	0
1	PCA	C	1	8/9	0.90	0.10	26,33,40,40	0
1	PCA	E	1	8/9	0.91	0.10	26,31,40,40	0
3	PCA	G	12	8/9	0.92	0.09	23,28,34,34	0
1	PCA	H	1	8/9	0.93	0.08	22,27,34,34	0
3	PCA	I	196	8/9	0.94	0.07	25,29,36,36	0
3	PCA	J	310	8/9	0.94	0.08	25,28,35,35	0
3	PCA	Q	3	8/9	0.96	0.07	20,27,31,34	0

6.3 Carbohydrates [i](#)

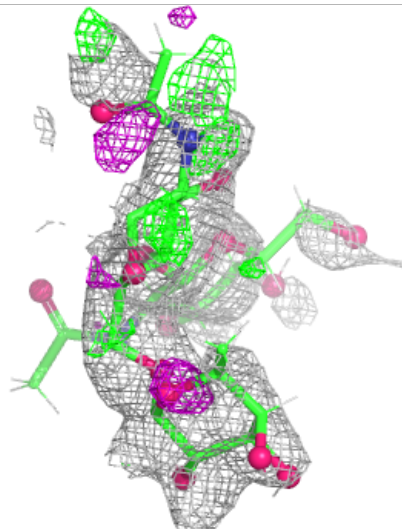
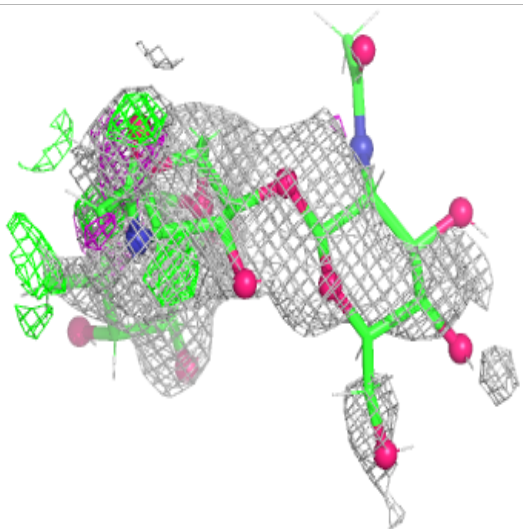
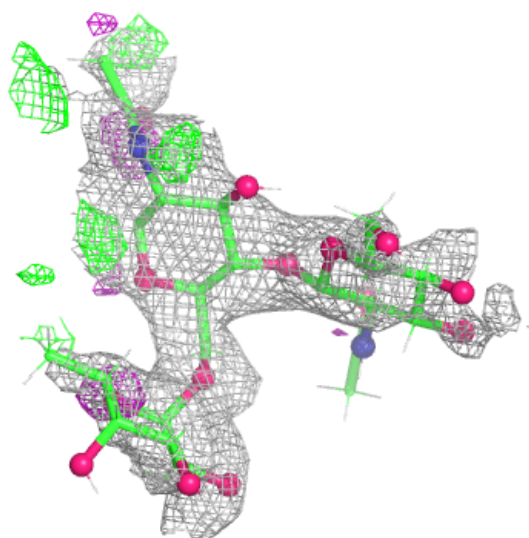
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	K	1	14/15	-	-	54,64,75,79	0
4	NAG	K	2	14/15	-	-	66,78,92,96	0
4	FUC	K	3	10/11	-	-	61,71,83,84	0
4	FUC	N	3	10/11	0.22	0.25	46,57,67,69	0
4	NAG	O	2	14/15	0.36	0.24	41,51,62,70	0
4	NAG	M	2	14/15	0.47	0.19	62,67,80,82	0
4	FUC	M	3	10/11	0.47	0.21	56,67,80,84	0
4	NAG	N	2	14/15	0.67	0.16	49,66,81,86	0
4	NAG	M	1	14/15	0.68	0.22	43,52,66,67	0
4	NAG	N	1	14/15	0.72	0.17	33,41,56,59	0
4	FUC	O	3	10/11	0.77	0.14	40,46,55,56	0
4	NAG	O	1	14/15	0.81	0.14	31,37,43,46	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

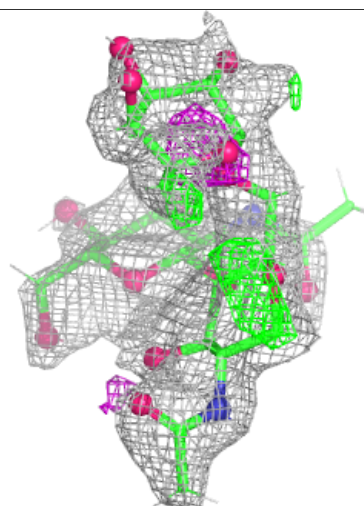
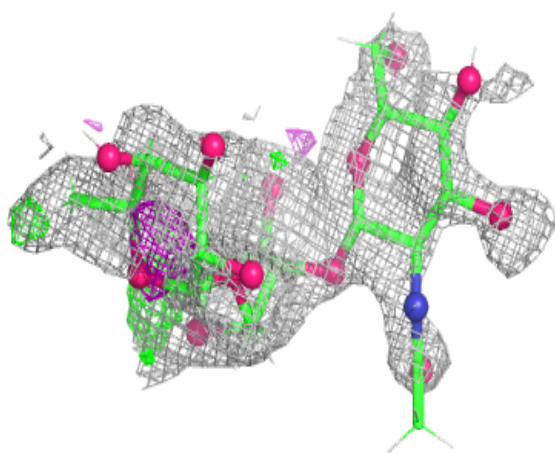
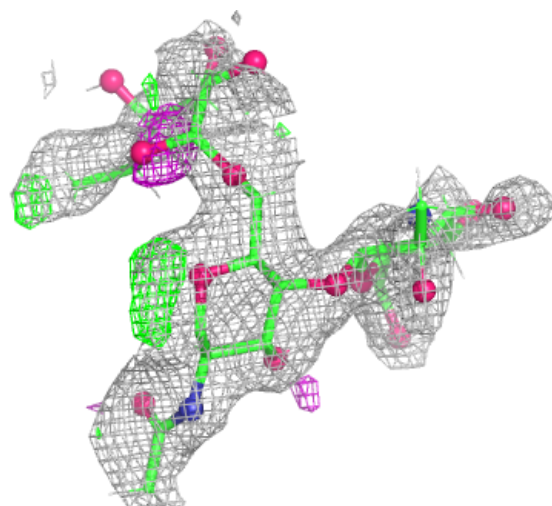
Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



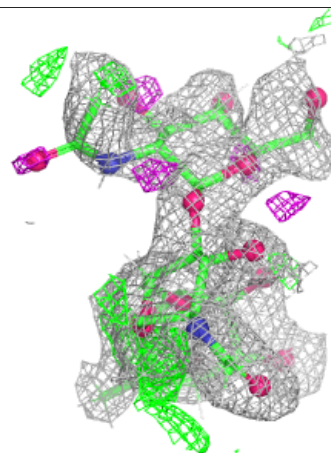
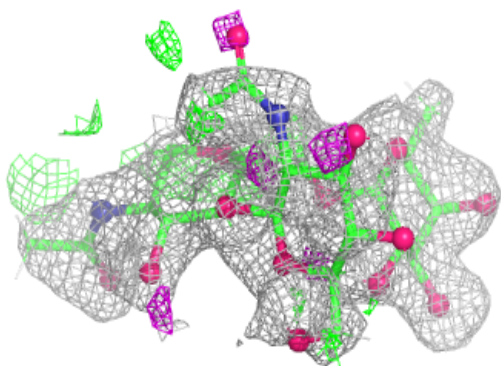
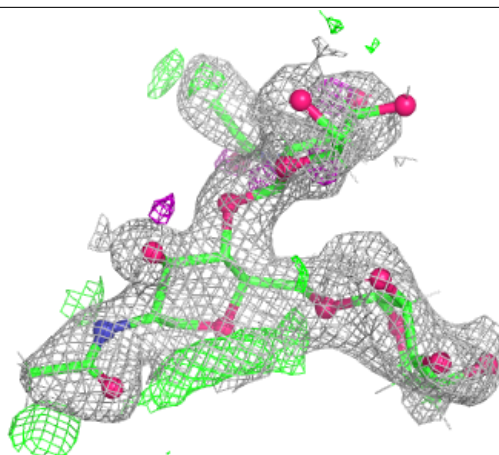
Electron density around Chain M:

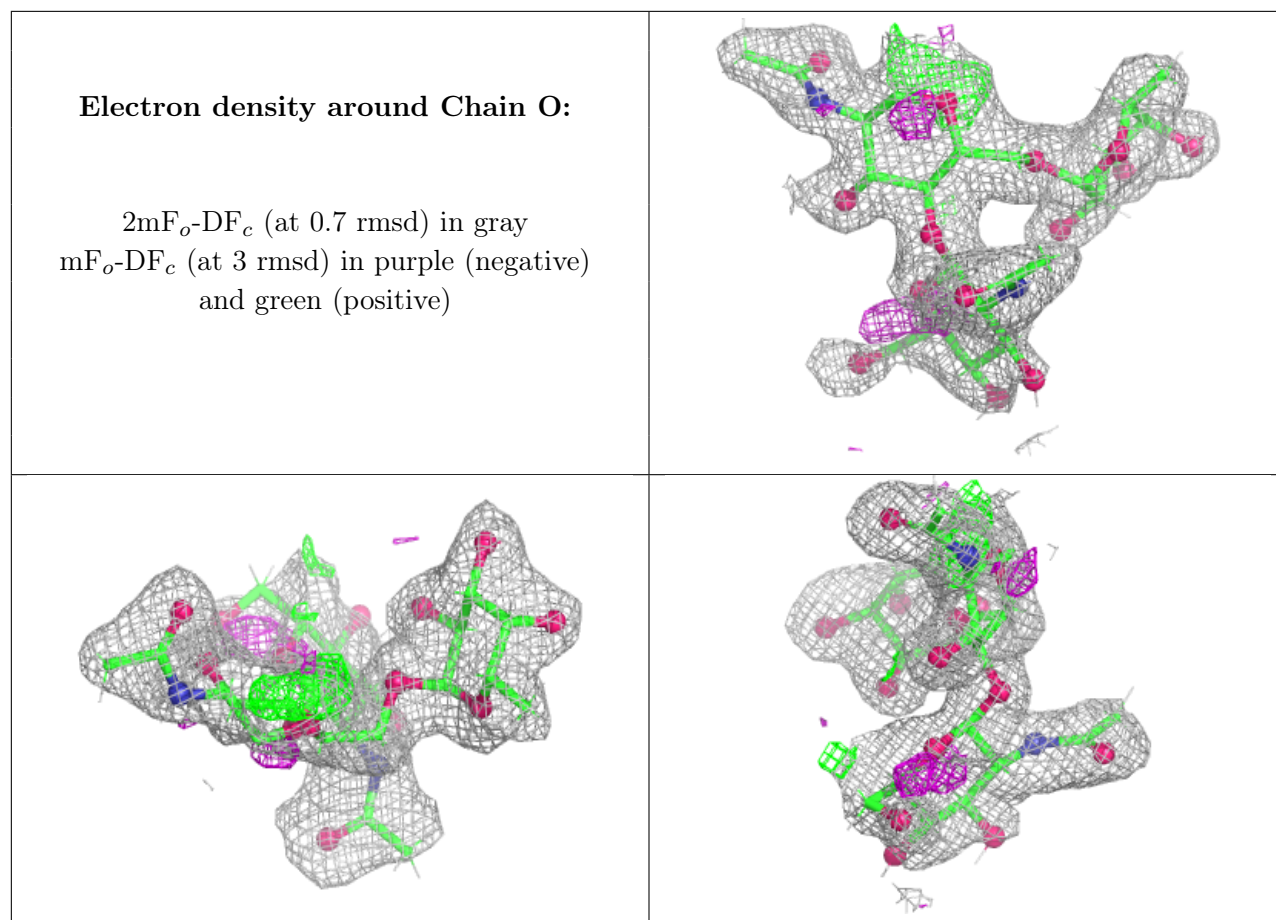
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.