



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 12:52 PM UTC

PDB ID : 5VL3 / pdb_00005vl3
Title : CD22 d1-d3 in complex with therapeutic Fab Epratuzumab
Authors : Sicard, T.; Ereno-Orbea, J.; Julien, J.P.
Deposited on : 2017-04-24
Resolution : 3.10 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

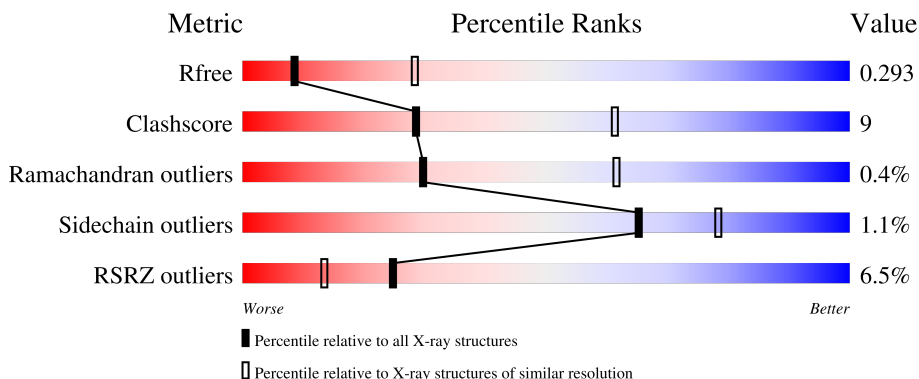
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	Q	323	2% 67% 26% 6%
1	R	323	4% 65% 25% 10%
1	S	323	9% 71% 20% 7%
1	T	323	10% 63% 26% 11%
2	A	222	3% 78% 18% .

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Mol	Chain	Length	Quality of chain
2	C	222	 6% 77% 18% 5%
2	E	222	 19% 70% 22% 7%
2	H	222	 2% 79% 17% 2%
3	B	222	 2% 85% 11% 2%
3	D	222	 3% 86% 11% 2%
3	F	222	 11% 83% 13% 2%
3	L	222	 85% 11% 2%
4	G	2	 100%
4	J	2	 100%
4	M	2	 100%
4	O	2	 100%
5	I	5	 60% 40%
6	K	4	 100%
6	P	4	 75% 25%
7	N	3	 33% 67%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22912 atoms, of which 0 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 B-cell receptor CD22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	303	Total	C	N	O	S	0	0	0
			2439	1544	415	467	13			
1	R	290	Total	C	N	O	S	0	0	0
			2332	1478	393	448	13			
1	S	299	Total	C	N	O	S	0	0	0
			2401	1518	409	461	13			
1	T	289	Total	C	N	O	S	0	0	0
			2324	1471	395	445	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	18	THR	-	expression tag	UNP P20273
Q	19	GLY	-	expression tag	UNP P20273
Q	20	ASP	-	expression tag	UNP P20273
Q	21	SER	-	expression tag	UNP P20273
Q	67	GLN	ASN	engineered mutation	UNP P20273
Q	112	GLN	ASN	engineered mutation	UNP P20273
Q	135	GLN	ASN	engineered mutation	UNP P20273
Q	164	GLN	ASN	engineered mutation	UNP P20273
Q	331	GLY	-	expression tag	UNP P20273
Q	332	GLY	-	expression tag	UNP P20273
Q	333	THR	-	expression tag	UNP P20273
Q	334	LYS	-	expression tag	UNP P20273
Q	335	HIS	-	expression tag	UNP P20273
Q	336	HIS	-	expression tag	UNP P20273
Q	337	HIS	-	expression tag	UNP P20273
Q	338	HIS	-	expression tag	UNP P20273
Q	339	HIS	-	expression tag	UNP P20273
Q	340	HIS	-	expression tag	UNP P20273
R	18	THR	-	expression tag	UNP P20273
R	19	GLY	-	expression tag	UNP P20273
R	20	ASP	-	expression tag	UNP P20273

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Chain	Residue	Modelled	Actual	Comment	Reference
R	21	SER	-	expression tag	UNP P20273
R	67	GLN	ASN	engineered mutation	UNP P20273
R	112	GLN	ASN	engineered mutation	UNP P20273
R	135	GLN	ASN	engineered mutation	UNP P20273
R	164	GLN	ASN	engineered mutation	UNP P20273
R	331	GLY	-	expression tag	UNP P20273
R	332	GLY	-	expression tag	UNP P20273
R	333	THR	-	expression tag	UNP P20273
R	334	LYS	-	expression tag	UNP P20273
R	335	HIS	-	expression tag	UNP P20273
R	336	HIS	-	expression tag	UNP P20273
R	337	HIS	-	expression tag	UNP P20273
R	338	HIS	-	expression tag	UNP P20273
R	339	HIS	-	expression tag	UNP P20273
R	340	HIS	-	expression tag	UNP P20273
S	18	THR	-	expression tag	UNP P20273
S	19	GLY	-	expression tag	UNP P20273
S	20	ASP	-	expression tag	UNP P20273
S	21	SER	-	expression tag	UNP P20273
S	67	GLN	ASN	engineered mutation	UNP P20273
S	112	GLN	ASN	engineered mutation	UNP P20273
S	135	GLN	ASN	engineered mutation	UNP P20273
S	164	GLN	ASN	engineered mutation	UNP P20273
S	331	GLY	-	expression tag	UNP P20273
S	332	GLY	-	expression tag	UNP P20273
S	333	THR	-	expression tag	UNP P20273
S	334	LYS	-	expression tag	UNP P20273
S	335	HIS	-	expression tag	UNP P20273
S	336	HIS	-	expression tag	UNP P20273
S	337	HIS	-	expression tag	UNP P20273
S	338	HIS	-	expression tag	UNP P20273
S	339	HIS	-	expression tag	UNP P20273
S	340	HIS	-	expression tag	UNP P20273
T	18	THR	-	expression tag	UNP P20273
T	19	GLY	-	expression tag	UNP P20273
T	20	ASP	-	expression tag	UNP P20273
T	21	SER	-	expression tag	UNP P20273
T	67	GLN	ASN	engineered mutation	UNP P20273
T	112	GLN	ASN	engineered mutation	UNP P20273
T	135	GLN	ASN	engineered mutation	UNP P20273
T	164	GLN	ASN	engineered mutation	UNP P20273
T	331	GLY	-	expression tag	UNP P20273

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Chain	Residue	Modelled	Actual	Comment	Reference
T	332	GLY	-	expression tag	UNP P20273
T	333	THR	-	expression tag	UNP P20273
T	334	LYS	-	expression tag	UNP P20273
T	335	HIS	-	expression tag	UNP P20273
T	336	HIS	-	expression tag	UNP P20273
T	337	HIS	-	expression tag	UNP P20273
T	338	HIS	-	expression tag	UNP P20273
T	339	HIS	-	expression tag	UNP P20273
T	340	HIS	-	expression tag	UNP P20273

- Molecule 2 is a protein called Epratuzumab Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	214	Total	C	N	O	S	0	0	0
			1640	1038	274	323	5			
2	C	212	Total	C	N	O	S	0	0	0
			1625	1029	271	320	5			
2	E	207	Total	C	N	O	S	0	0	0
			1595	1012	266	312	5			
2	H	214	Total	C	N	O	S	0	0	0
			1640	1038	274	323	5			

- Molecule 3 is a protein called Epratuzumab Fab Light Chain.

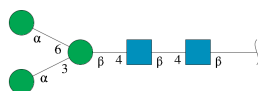
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	213	Total	C	N	O	S	0	0	0
			1642	1031	274	332	5			
3	D	216	Total	C	N	O	S	0	0	0
			1672	1050	281	336	5			
3	F	213	Total	C	N	O	S	0	0	0
			1642	1031	274	332	5			
3	L	213	Total	C	N	O	S	0	0	0
			1642	1031	274	332	5			

- 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				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	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.



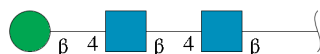
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



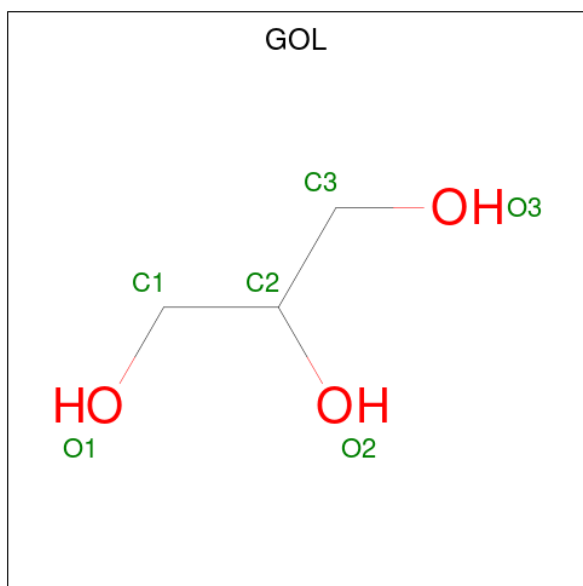
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
6	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



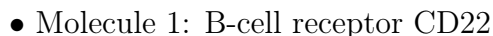
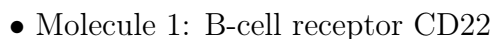
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

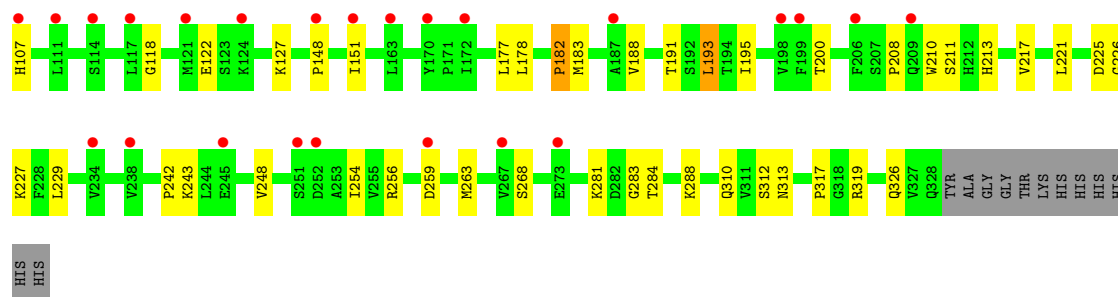
- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



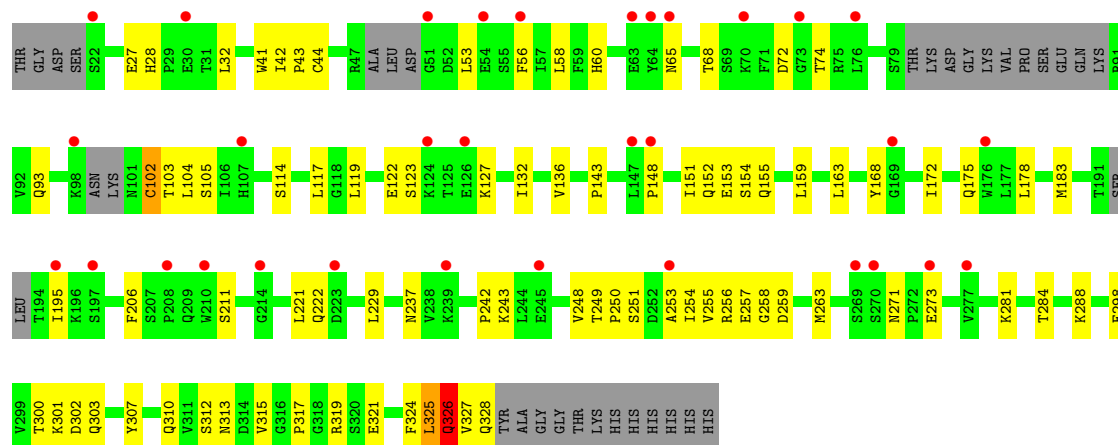
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	S	1	Total	C	O	0	0
			6	3	3		

- Molecule 1: B-cell receptor CD22

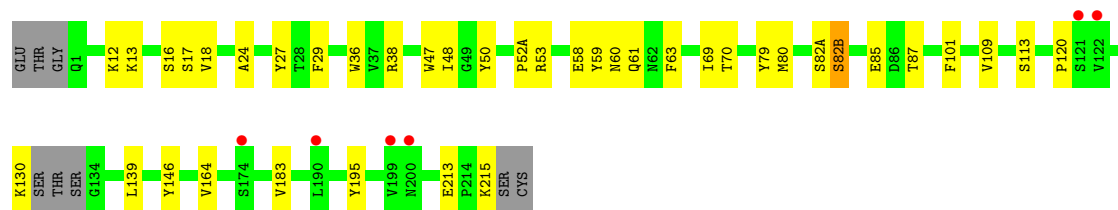
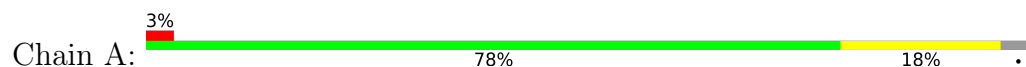




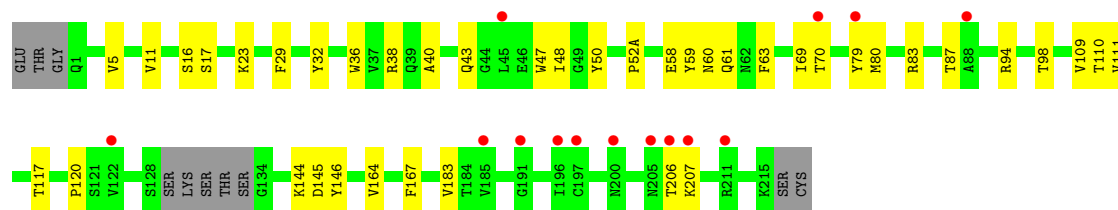
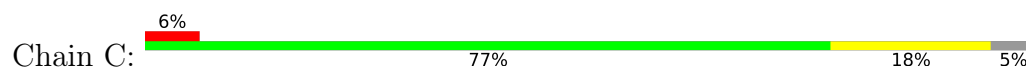
- Molecule 1: B-cell receptor CD22



- Molecule 2: Epratuzumab Fab Heavy Chain

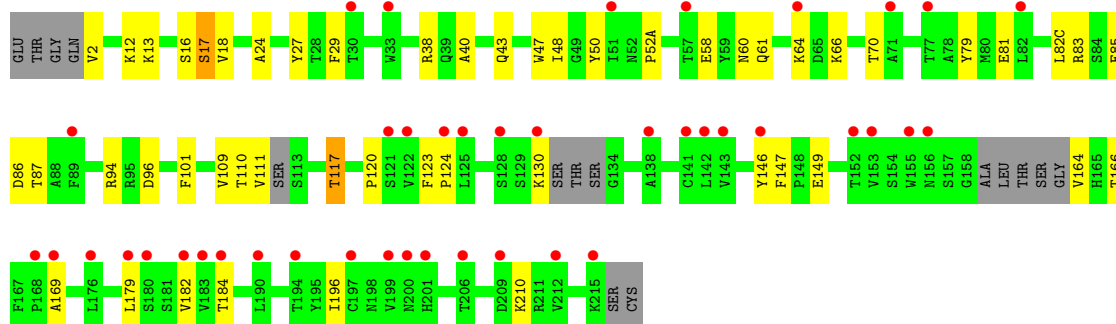


- Molecule 2: Epratuzumab Fab Heavy Chain



- Molecule 2: Epratuzumab Fab Heavy Chain

Chain E: 



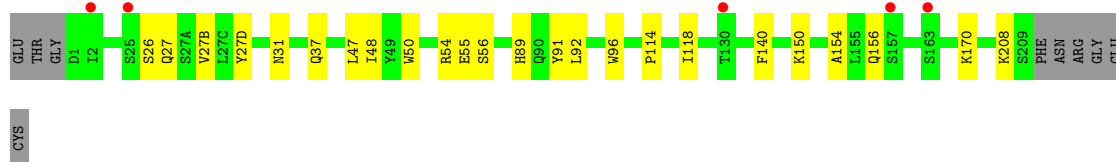
• Molecule 2: Epratuzumab Fab Heavy Chain

Chain H: 



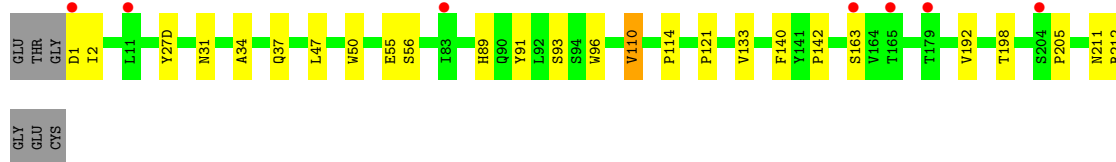
• Molecule 3: Epratuzumab Fab Light Chain

Chain B: 



• Molecule 3: Epratuzumab Fab Light Chain

Chain D: 



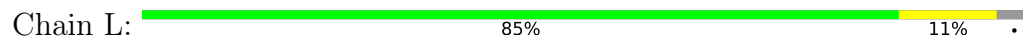
• Molecule 3: Epratuzumab Fab Light Chain

Chain F: 





• Molecule 3: Epratuzumab Fab Light Chain



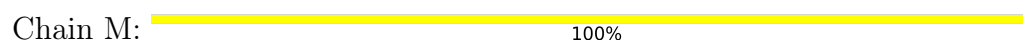
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



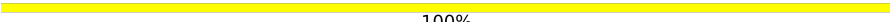
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• 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

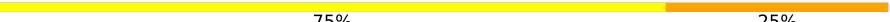


- Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

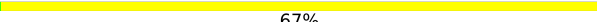
NAG1
NAG2
BMA3
MAN4

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

Chain P:  75%  25%

NAG1
NAG2
BMA3
MAN4

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

Chain N:  33%  67%

NAG1
NAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.11Å 90.22Å 136.63Å 70.83° 80.81° 80.99°	Depositor
Resolution (Å)	39.34 – 3.10 39.34 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (39.34-3.10) 94.1 (39.34-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.280 , 0.295 0.279 , 0.293	Depositor DCC
R_{free} test set	2000 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	22912	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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: BMA, GOL, 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	Q	0.22	0/2498	0.56	0/3388
1	R	0.19	0/2388	0.55	0/3241
1	S	0.21	0/2458	0.54	0/3335
1	T	0.23	0/2378	0.55	1/3223 (0.0%)
2	A	0.16	0/1682	0.42	0/2293
2	C	0.16	0/1667	0.44	0/2274
2	E	0.17	0/1635	0.48	0/2226
2	H	0.17	0/1682	0.44	0/2293
3	B	0.14	0/1680	0.43	0/2282
3	D	0.15	0/1711	0.41	0/2323
3	F	0.13	0/1680	0.40	0/2282
3	L	0.15	0/1680	0.41	0/2282
All	All	0.18	0/23139	0.48	1/31442 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	253	ALA	N-CA-C	5.33	115.43	108.07

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	Q	2439	0	2387	62	1
1	R	2332	0	2266	54	0
1	S	2401	0	2345	44	2
1	T	2324	0	2259	66	1
2	A	1640	0	1591	30	0
2	C	1625	0	1573	22	0
2	E	1595	0	1542	45	0
2	H	1640	0	1591	27	0
3	B	1642	0	1598	19	0
3	D	1672	0	1626	19	0
3	F	1642	0	1598	23	0
3	L	1642	0	1598	18	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	M	28	0	25	1	0
4	O	28	0	25	0	0
5	I	61	0	52	4	0
6	K	50	0	43	3	0
6	P	50	0	43	4	0
7	N	39	0	34	2	0
8	S	6	0	8	1	0
All	All	22912	0	22254	398	2

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 9.

The worst 5 of 398 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:Q:65:ASN:ND2	1:Q:72:ASP:OD2	1.95	1.00
1:R:65:ASN:ND2	1:R:72:ASP:OD2	1.99	0.95
1:R:147:LEU:HD11	1:R:234:VAL:HG11	1.52	0.89
2:E:50:TYR:HE2	2:E:58:GLU:HB2	1.47	0.78
2:H:130:LYS:HB3	3:L:208:LYS:NZ	1.99	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:127:LYS:NZ	1:S:122:GLU:OE2[1_556]	1.93	0.27
1:S:283:GLY:O	1:T:154:SER:OG[1_655]	2.17	0.03

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	Q	299/323 (93%)	287 (96%)	11 (4%)	1 (0%)	36	67
1	R	282/323 (87%)	271 (96%)	10 (4%)	1 (0%)	30	61
1	S	295/323 (91%)	280 (95%)	13 (4%)	2 (1%)	18	49
1	T	279/323 (86%)	266 (95%)	11 (4%)	2 (1%)	18	49
2	A	210/222 (95%)	201 (96%)	8 (4%)	1 (0%)	24	57
2	C	208/222 (94%)	198 (95%)	9 (4%)	1 (0%)	24	57
2	E	199/222 (90%)	191 (96%)	7 (4%)	1 (0%)	24	57
2	H	210/222 (95%)	203 (97%)	6 (3%)	1 (0%)	24	57
3	B	211/222 (95%)	202 (96%)	9 (4%)	0	100	100
3	D	214/222 (96%)	203 (95%)	11 (5%)	0	100	100
3	F	211/222 (95%)	203 (96%)	8 (4%)	0	100	100
3	L	211/222 (95%)	203 (96%)	8 (4%)	0	100	100
All	All	2829/3068 (92%)	2708 (96%)	111 (4%)	10 (0%)	30	61

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	226	GLY
2	C	117	THR
2	A	82(B)	SER
2	E	117	THR
1	T	326	GLN

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	Q	282/296 (95%)	276 (98%)	6 (2%)	47	71
1	R	270/296 (91%)	269 (100%)	1 (0%)	84	86
1	S	277/296 (94%)	269 (97%)	8 (3%)	37	66
1	T	268/296 (90%)	262 (98%)	6 (2%)	45	71
2	A	184/191 (96%)	184 (100%)	0	100	100
2	C	182/191 (95%)	181 (100%)	1 (0%)	81	85
2	E	179/191 (94%)	178 (99%)	1 (1%)	78	83
2	H	184/191 (96%)	183 (100%)	1 (0%)	81	85
3	B	188/195 (96%)	187 (100%)	1 (0%)	81	85
3	D	191/195 (98%)	190 (100%)	1 (0%)	81	85
3	F	188/195 (96%)	187 (100%)	1 (0%)	81	85
3	L	188/195 (96%)	187 (100%)	1 (0%)	81	85
All	All	2581/2728 (95%)	2553 (99%)	28 (1%)	65	78

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	326	GLN
3	L	130	THR
1	T	254	ILE
3	B	150	LYS
1	T	172	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	193	GLN
2	H	165	HIS
3	L	161	GLN
2	E	172	GLN
3	B	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 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	G	1	1,4	14,14,15	0.26	0	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	I	1	5,1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	I	2	5	14,14,15	0.63	0	17,19,21	0.50	0
5	BMA	I	3	5	11,11,12	1.17	2 (18%)	15,15,17	1.40	2 (13%)
5	MAN	I	4	5	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
5	MAN	I	5	5	11,11,12	0.69	0	15,15,17	0.96	2 (13%)
4	NAG	J	1	1,4	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	J	2	4	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	K	1	6,1	14,14,15	0.27	0	17,19,21	0.52	0
6	NAG	K	2	6	14,14,15	0.43	0	17,19,21	0.42	0
6	BMA	K	3	6	11,11,12	0.90	1 (9%)	15,15,17	1.11	2 (13%)
6	MAN	K	4	6	11,11,12	0.61	0	15,15,17	1.17	2 (13%)
4	NAG	M	1	1,4	14,14,15	0.57	0	17,19,21	0.49	0
4	NAG	M	2	4	14,14,15	0.22	0	17,19,21	0.54	0
7	NAG	N	1	7,1	14,14,15	0.24	0	17,19,21	0.62	0
7	NAG	N	2	7	14,14,15	0.27	0	17,19,21	0.55	0
7	BMA	N	3	7	11,11,12	0.66	0	15,15,17	0.75	0
4	NAG	O	1	1,4	14,14,15	0.28	0	17,19,21	0.75	0
4	NAG	O	2	4	14,14,15	0.28	0	17,19,21	0.44	0
6	NAG	P	1	6,1	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	P	2	6	14,14,15	0.34	0	17,19,21	0.43	0
6	BMA	P	3	6	11,11,12	0.83	0	15,15,17	1.01	1 (6%)
6	MAN	P	4	6	11,11,12	0.64	0	15,15,17	1.06	2 (13%)

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	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	0/1/1/1
5	MAN	I	5	5	-	0/2/19/22	1/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
6	MAN	K	4	6	-	2/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
7	NAG	N	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	3	BMA	O5-C1	-2.56	1.39	1.43
5	I	3	BMA	C4-C5	2.17	1.57	1.53
6	K	3	BMA	O5-C1	-2.05	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	4	MAN	C1-O5-C5	3.65	117.08	112.19
6	K	4	MAN	C1-O5-C5	3.55	116.95	112.19
5	I	3	BMA	C3-C4-C5	3.16	115.96	110.23
6	P	4	MAN	C1-O5-C5	3.00	116.21	112.19
5	I	3	BMA	C1-O5-C5	2.62	115.70	112.19

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
6	K	4	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
5	I	4	MAN	O5-C5-C6-O6

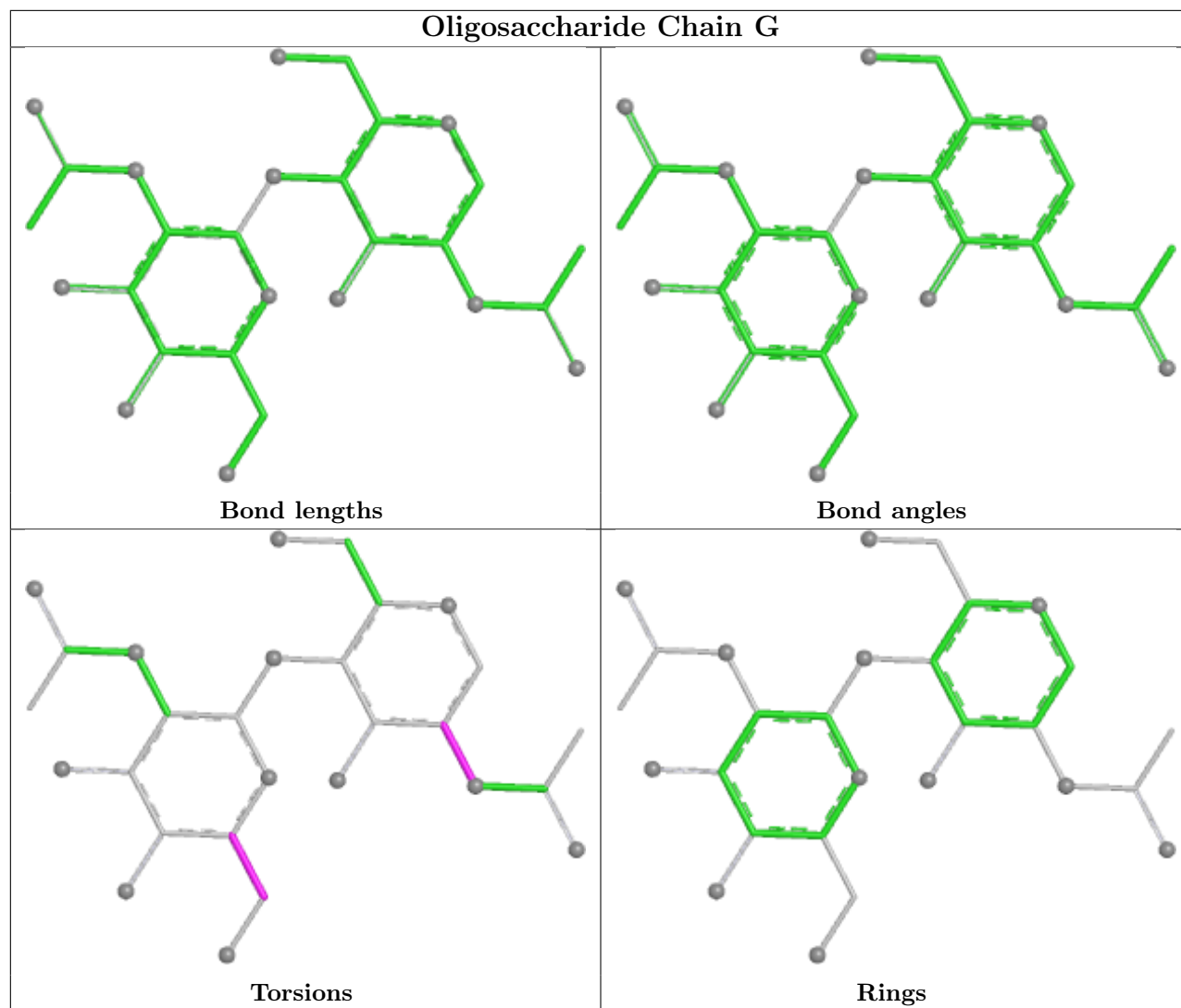
All (1) ring outliers are listed below:

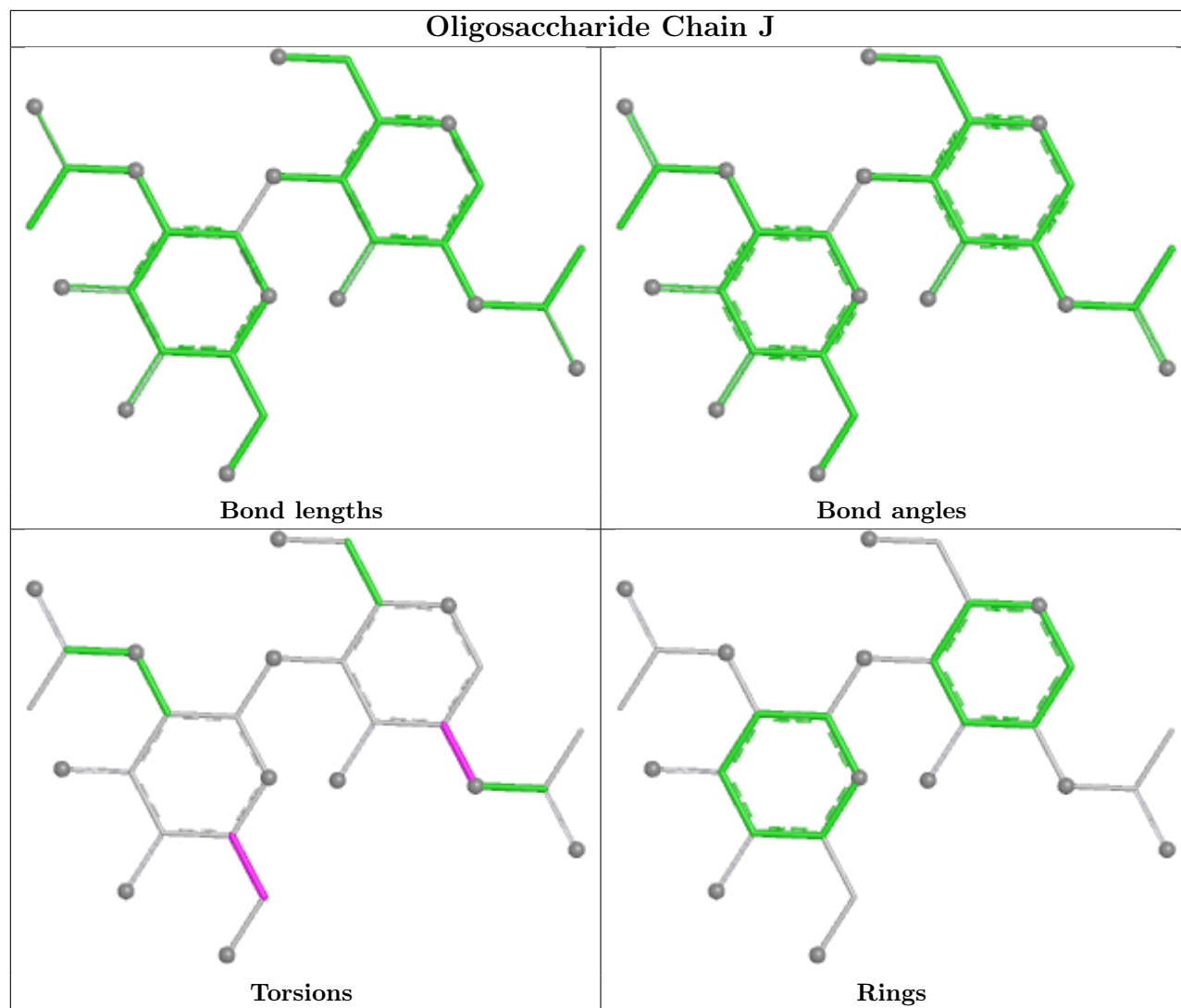
Mol	Chain	Res	Type	Atoms
5	I	5	MAN	C1-C2-C3-C4-C5-O5

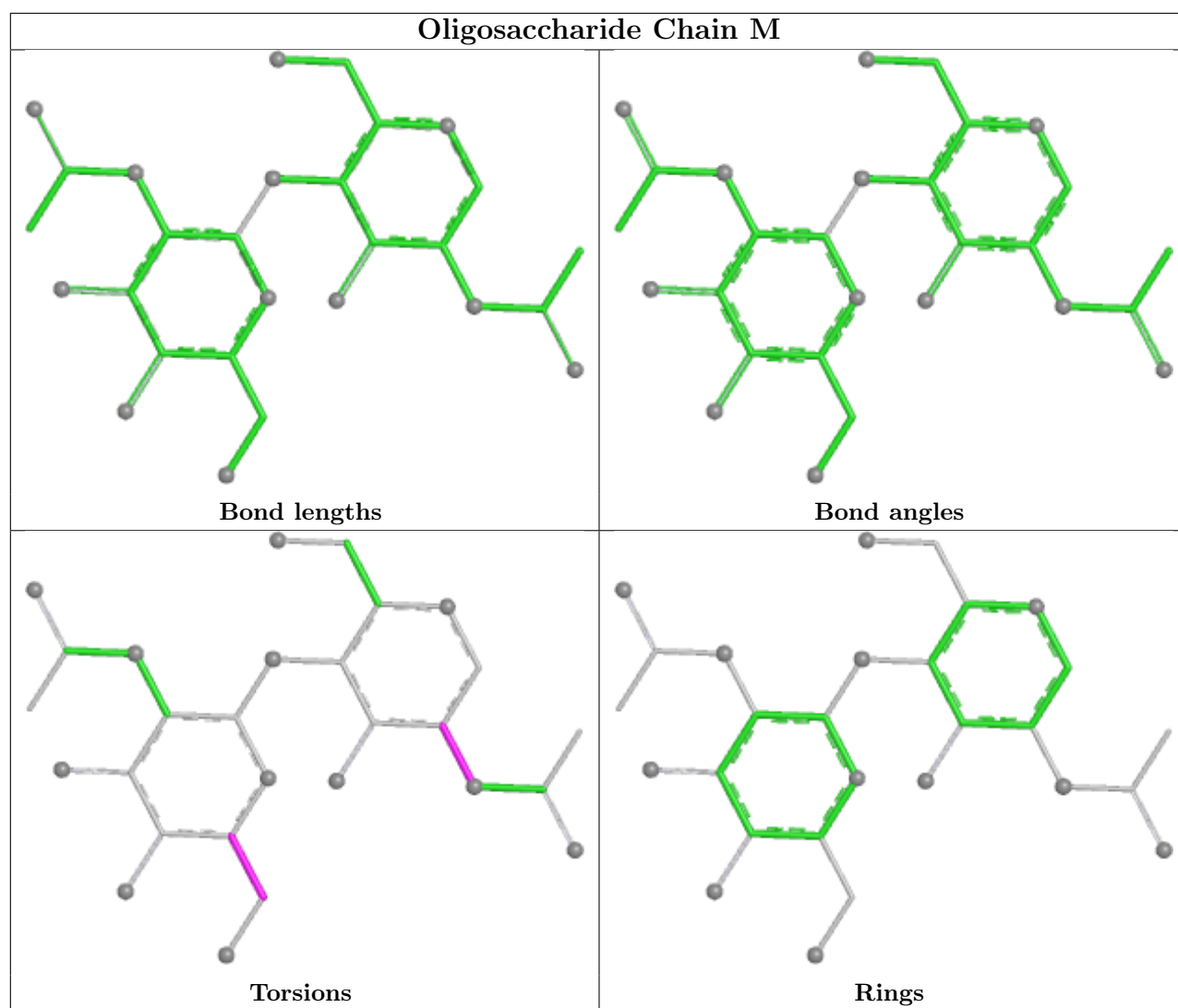
13 monomers are involved in 14 short contacts:

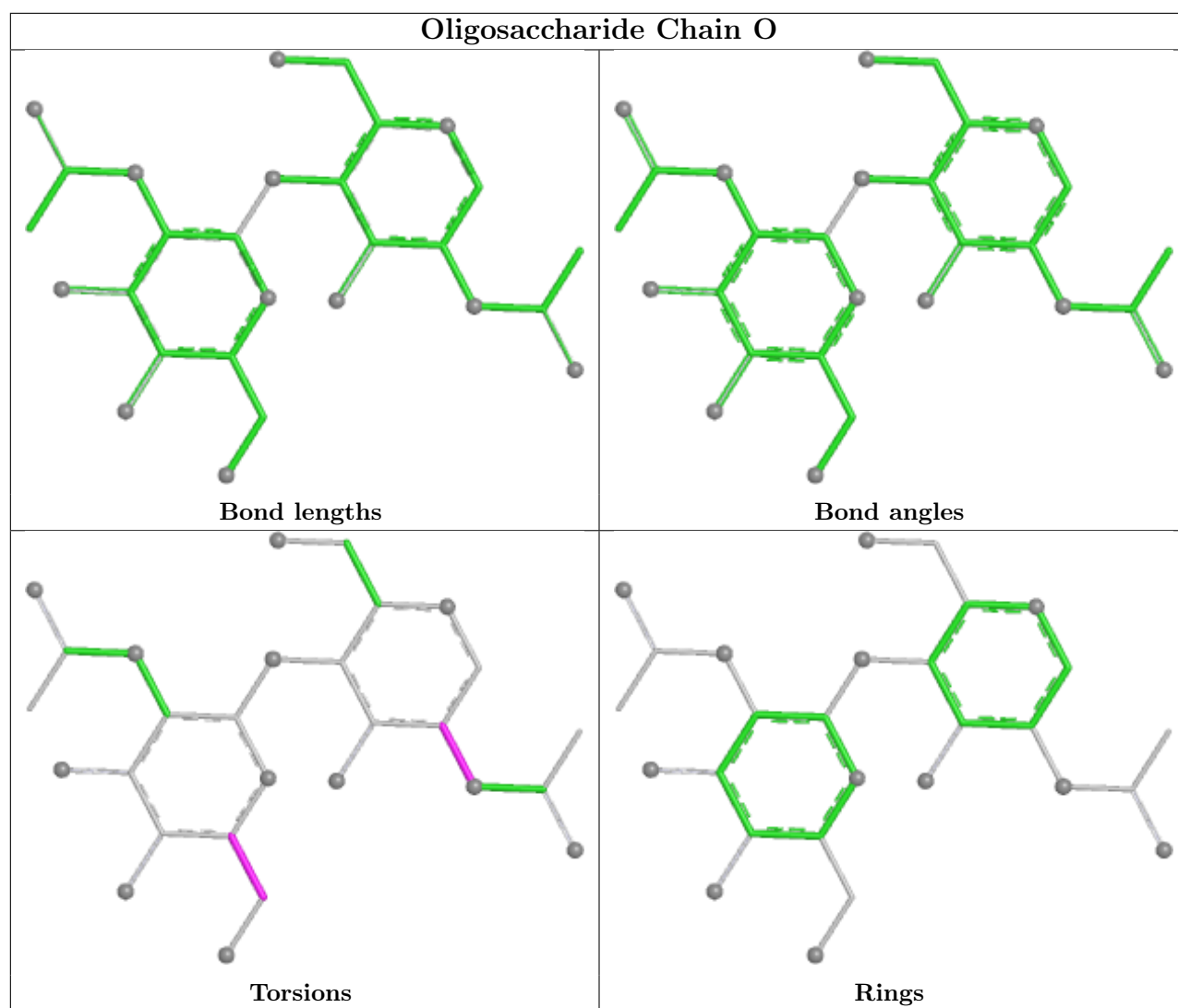
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	2	NAG	1	0
4	M	1	NAG	1	0
5	I	5	MAN	1	0
5	I	3	BMA	1	0
6	P	3	BMA	1	0
6	K	1	NAG	3	0
7	N	2	NAG	1	0
6	P	1	NAG	2	0
5	I	2	NAG	1	0
4	M	2	NAG	1	0
7	N	1	NAG	2	0
5	I	1	NAG	3	0
6	K	2	NAG	2	0

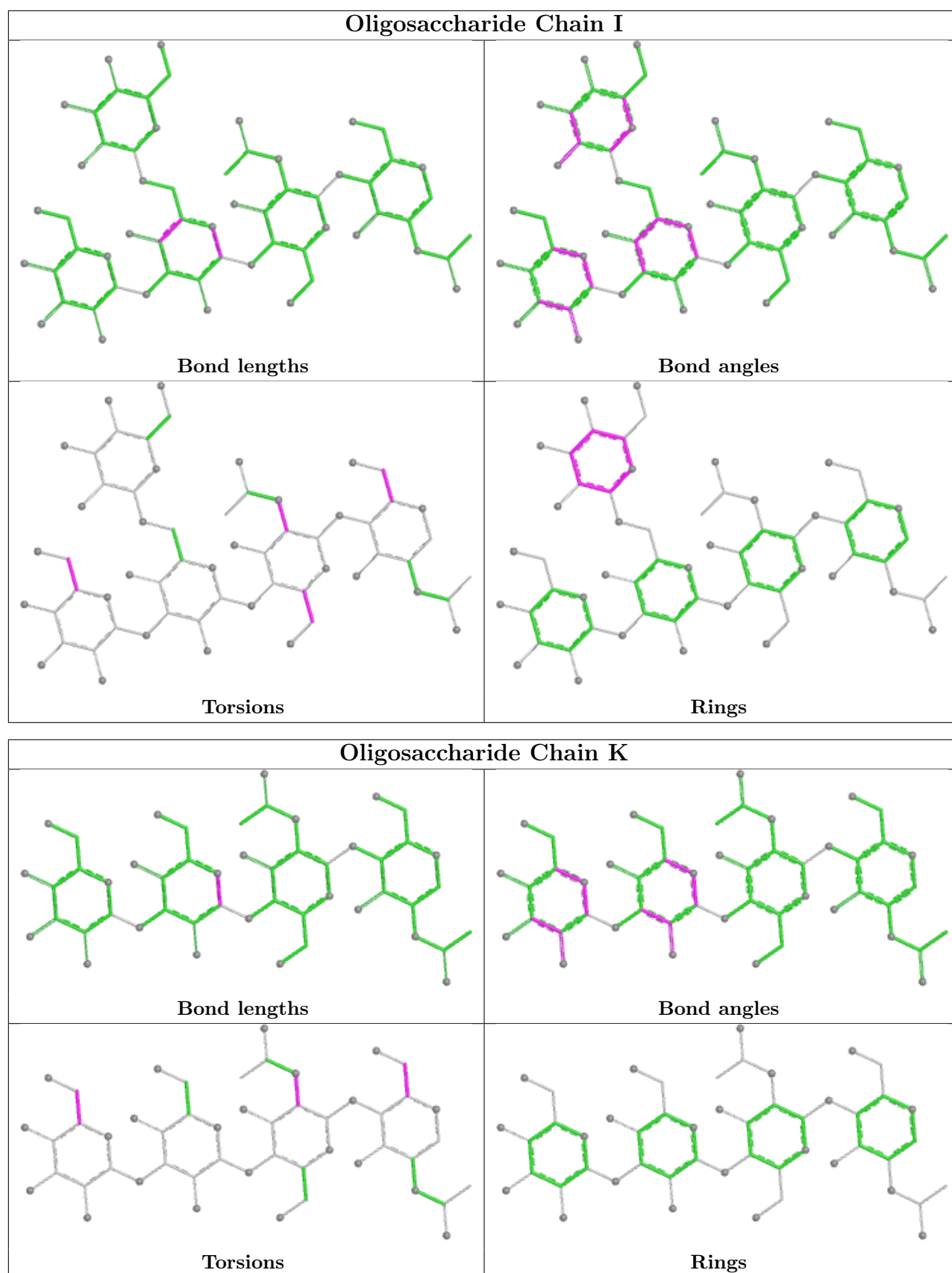
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

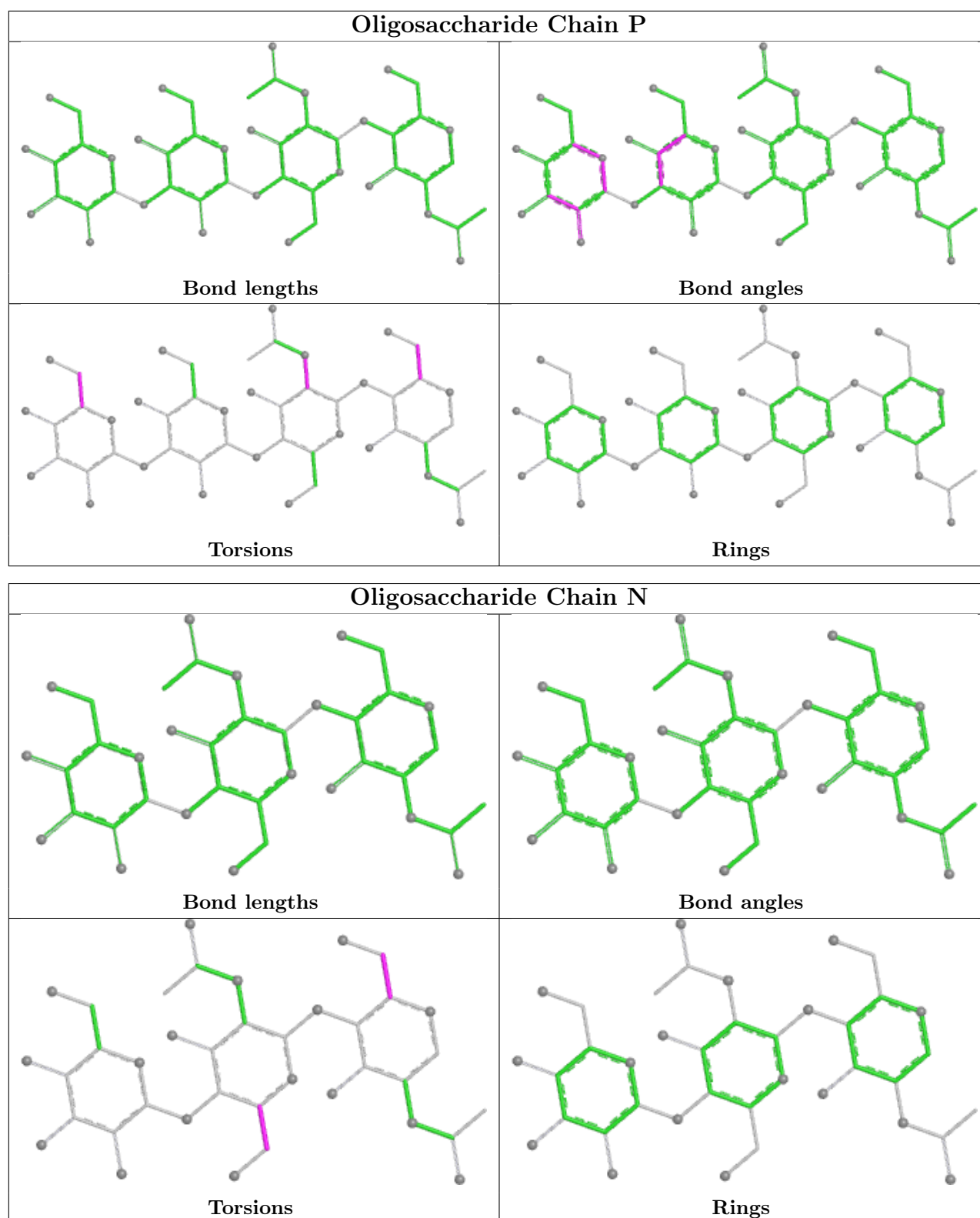












5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	S	1006	-	5,5,5	0.94	0	5,5,5	1.05	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	GOL	S	1006	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	1006	GOL	O1-C1-C2-C3
8	S	1006	GOL	C1-C2-C3-O3
8	S	1006	GOL	O2-C2-C3-O3
8	S	1006	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	S	1006	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	Q	303/323 (93%)	0.46	7 (2%) 61 39	34, 58, 81, 95	0
1	R	290/323 (89%)	0.58	14 (4%) 35 19	31, 63, 99, 112	0
1	S	299/323 (92%)	1.00	30 (10%) 12 6	65, 97, 114, 125	0
1	T	289/323 (89%)	1.08	32 (11%) 10 5	64, 97, 118, 144	0
2	A	214/222 (96%)	0.56	6 (2%) 55 34	30, 62, 101, 118	0
2	C	212/222 (95%)	0.96	14 (6%) 24 13	51, 75, 91, 107	0
2	E	207/222 (93%)	1.45	42 (20%) 3 1	68, 101, 119, 127	0
2	H	214/222 (96%)	0.44	5 (2%) 61 39	30, 53, 99, 116	0
3	B	213/222 (95%)	0.44	5 (2%) 61 39	26, 50, 91, 106	0
3	D	216/222 (97%)	0.79	7 (3%) 50 30	54, 66, 80, 98	0
3	F	213/222 (95%)	1.06	25 (11%) 9 5	57, 78, 111, 126	0
3	L	213/222 (95%)	0.35	1 (0%) 87 73	26, 49, 86, 98	0
All	All	2883/3068 (93%)	0.76	188 (6%) 25 13	26, 71, 109, 144	0

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	180	SER	4.6
2	E	155	TRP	4.3
2	E	141	CYS	4.1
3	F	135	CYS	4.0
1	S	238	VAL	3.9

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

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

6.3 Carbohydrates ⓘ

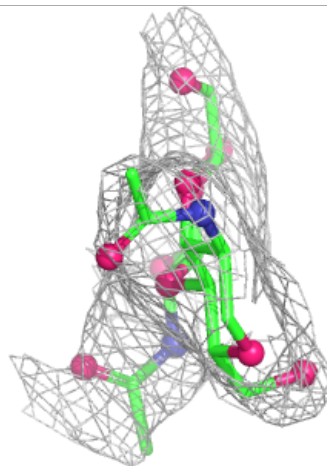
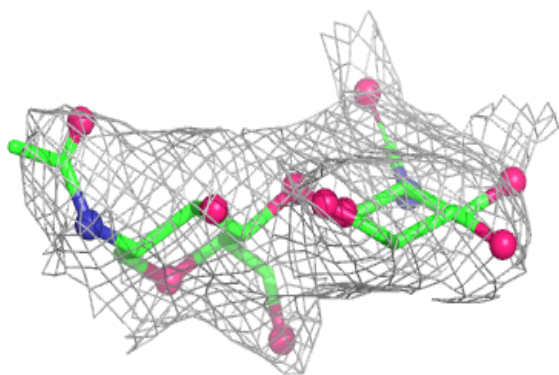
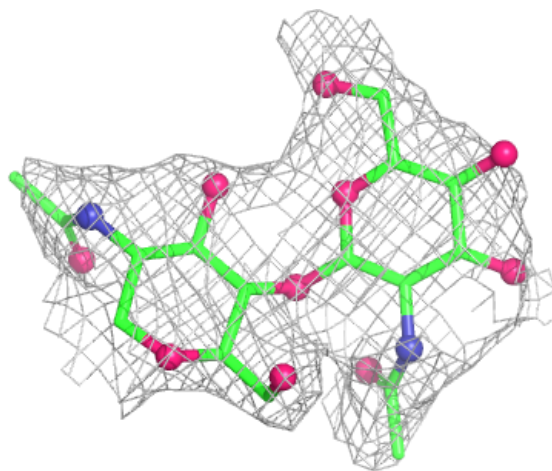
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G	1	14/15	-	-	57,71,78,79	0
4	NAG	G	2	14/15	-	-	48,71,81,90	0
4	NAG	J	1	14/15	-	-	54,68,73,76	0
4	NAG	J	2	14/15	-	-	49,70,78,90	0
6	BMA	P	3	11/12	0.70	0.12	110,119,125,128	0
4	NAG	O	2	14/15	0.71	0.13	101,123,133,142	0
6	MAN	P	4	11/12	0.74	0.14	103,122,130,141	0
7	NAG	N	2	14/15	0.76	0.15	88,113,121,128	0
5	NAG	I	1	14/15	-	-	57,68,73,76	0
5	NAG	I	2	14/15	-	-	58,83,91,99	0
5	BMA	I	3	11/12	-	-	86,96,101,105	0
5	MAN	I	4	11/12	-	-	83,98,106,119	0
5	MAN	I	5	11/12	-	-	89,106,114,116	0
6	NAG	K	1	14/15	-	-	66,75,79,81	0
6	NAG	K	2	14/15	-	-	59,86,94,99	0
6	BMA	K	3	11/12	-	-	86,95,101,105	0
6	MAN	K	4	11/12	-	-	86,104,112,124	0
4	NAG	M	2	14/15	0.78	0.11	94,116,125,135	0
6	NAG	P	2	14/15	0.80	0.13	89,113,120,129	0
7	BMA	N	3	11/12	0.81	0.11	108,117,122,125	0
4	NAG	O	1	14/15	0.85	0.12	100,115,121,123	0
7	NAG	N	1	14/15	0.85	0.11	90,101,106,108	0
6	NAG	P	1	14/15	0.87	0.10	91,102,107,108	0
4	NAG	M	1	14/15	0.90	0.10	99,113,119,121	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.

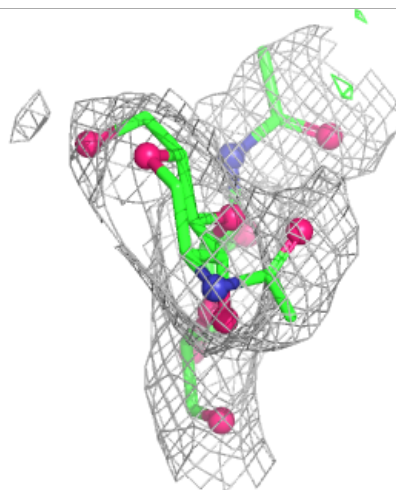
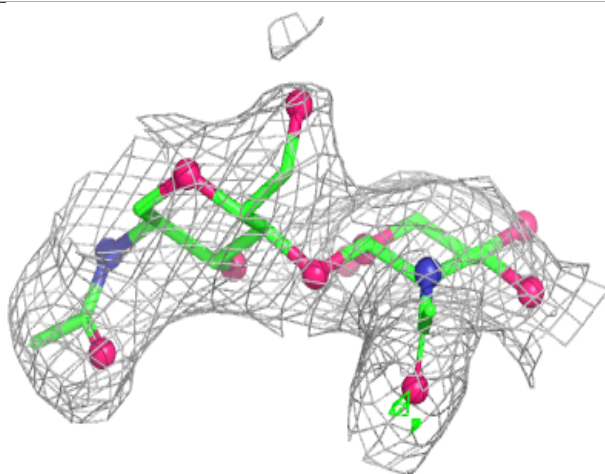
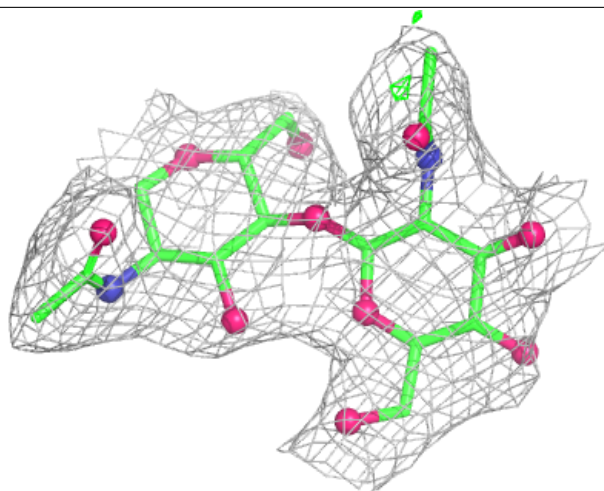
Electron density around Chain G:

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



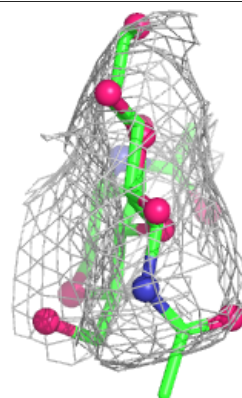
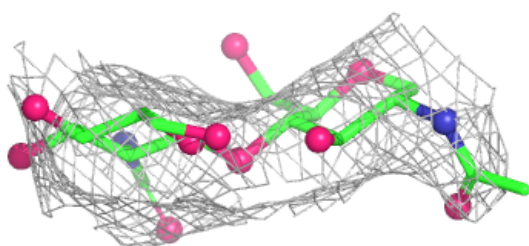
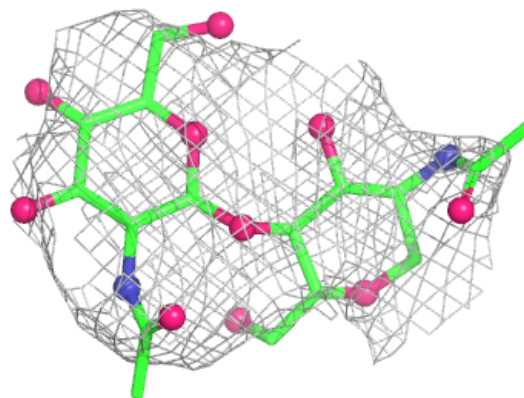
Electron density around Chain J:

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

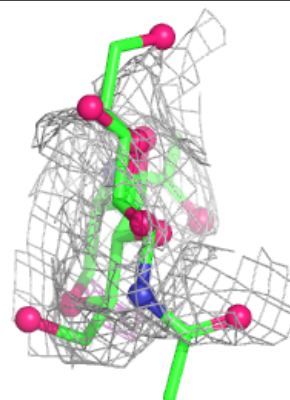
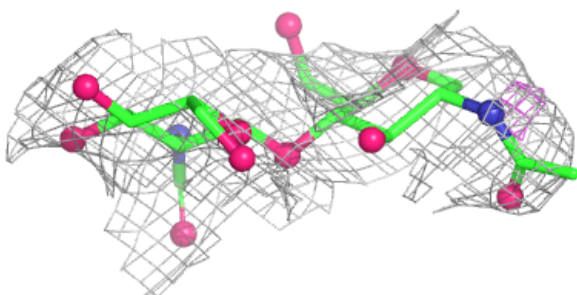
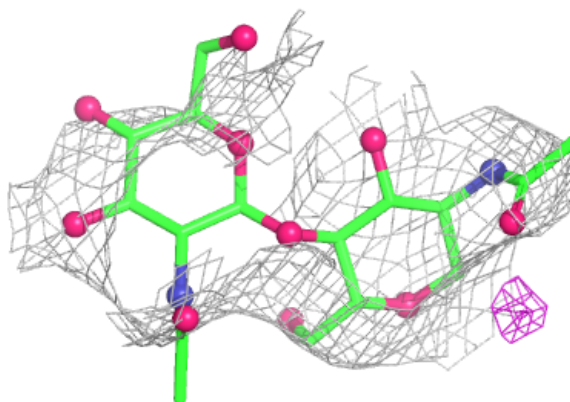


Electron density around Chain M:

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

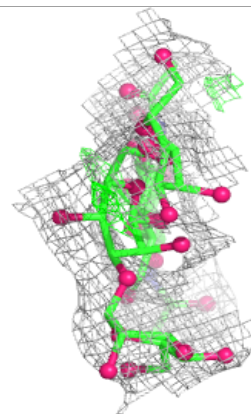
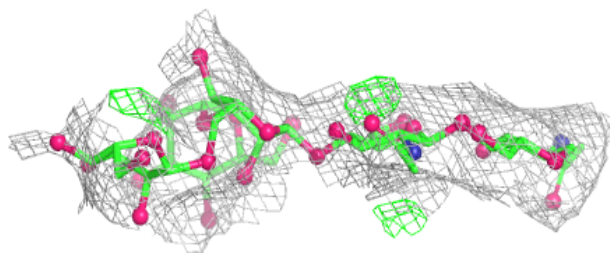
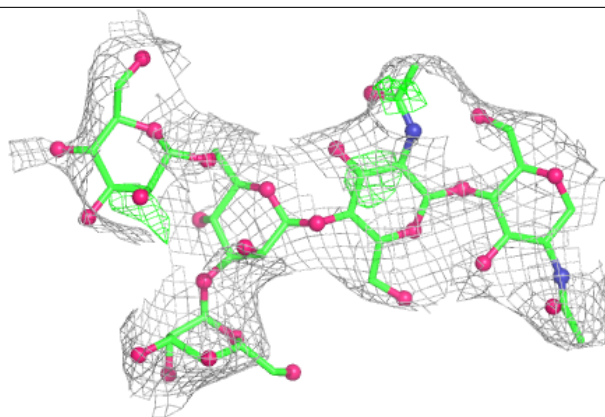
**Electron density around Chain O:**

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

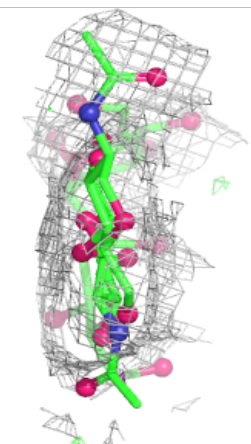
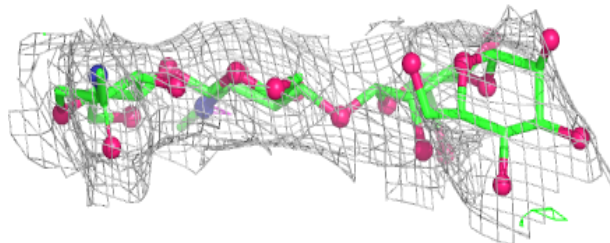
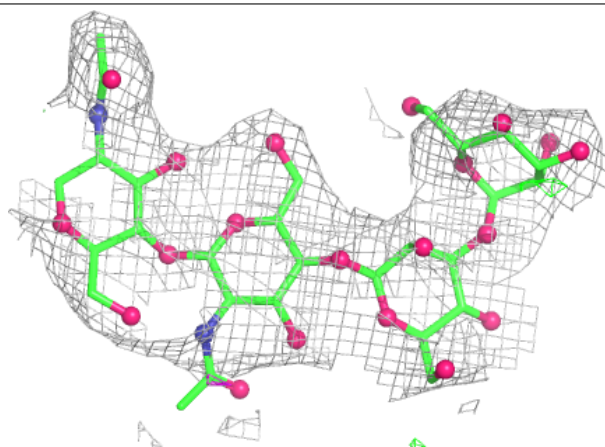


Electron density around Chain I:

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

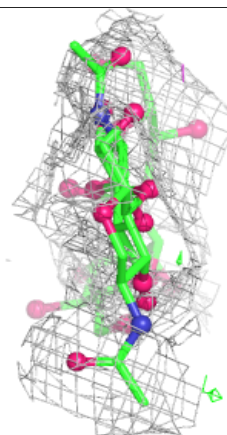
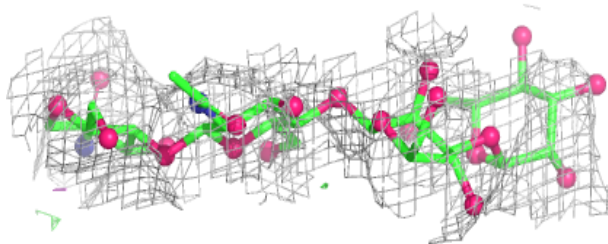
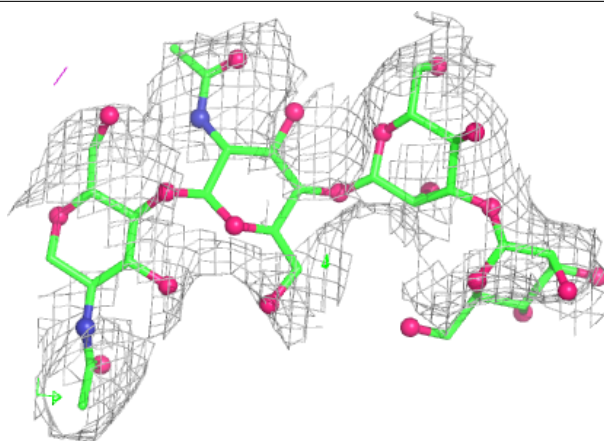
**Electron density around Chain K:**

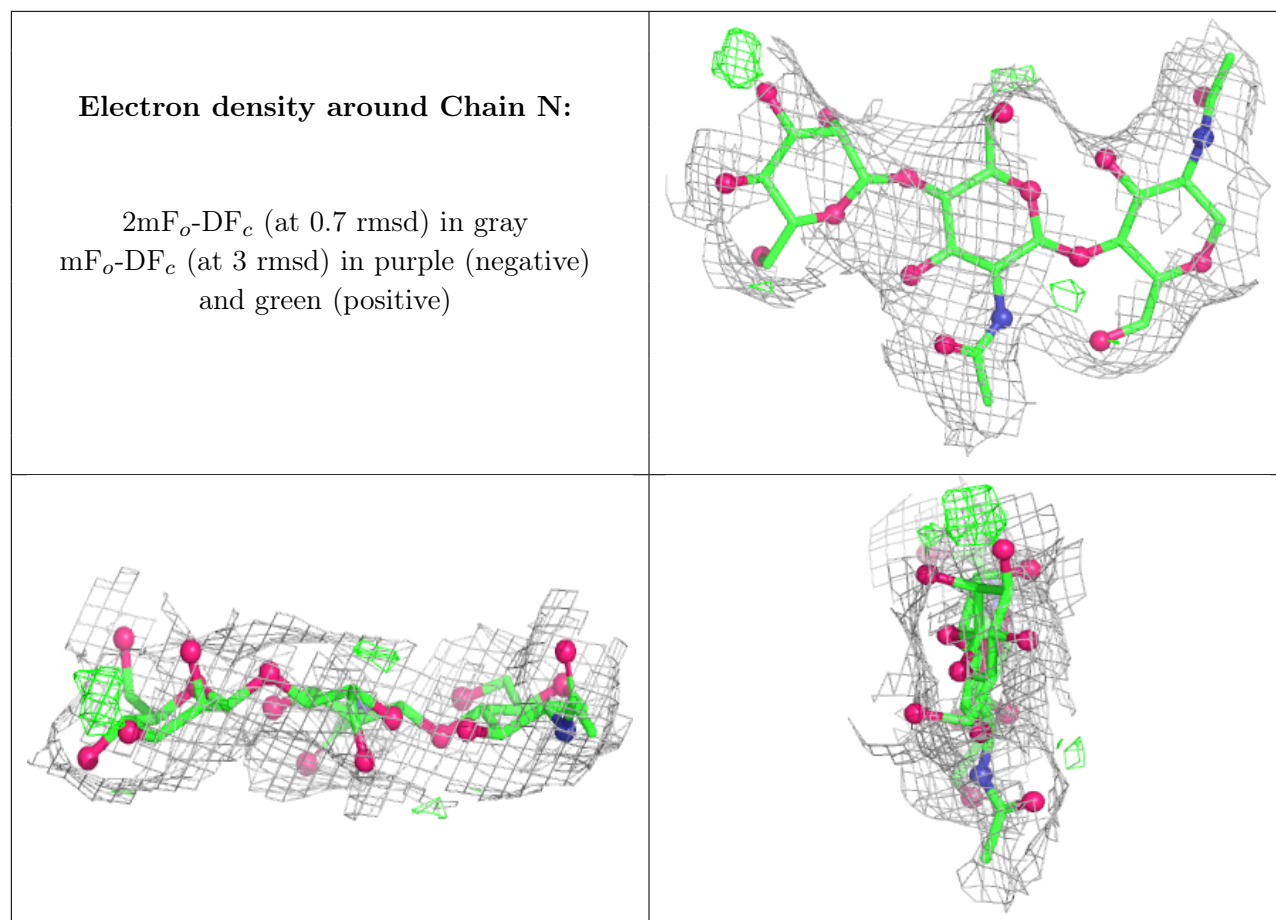
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

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





6.4 Ligands [i](#)

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
8	GOL	S	1006	6/6	0.73	0.23	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.