



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:56 PM UTC

PDB ID : 1RPQ / pdb_00001rpq
Title : High Affinity IgE Receptor (alpha chain) Complexed with Tight-Binding E131 'zeta' Peptide from Phage Display
Authors : Stamos, J.; Eigenbrot, C.; Nakamura, G.R.; Reynolds, M.E.; Yin, J.P.; Lowman, H.B.; Fairbrother, W.J.; Starovasnik, M.A.
Deposited on : 2003-12-03
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/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

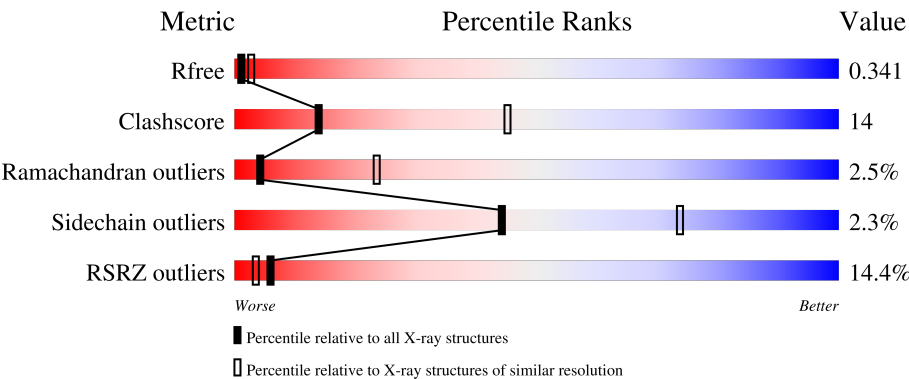
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



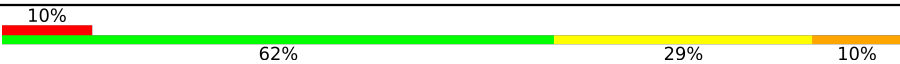
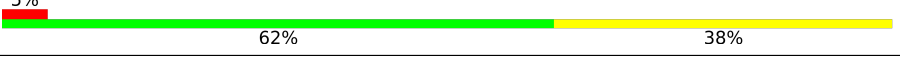
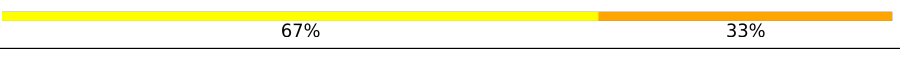
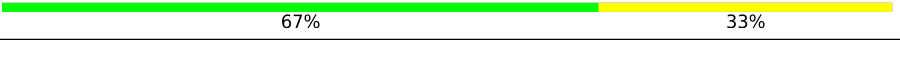
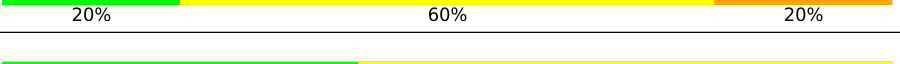
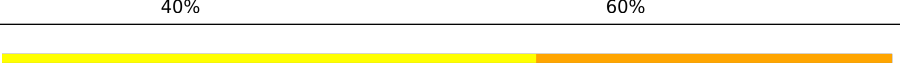
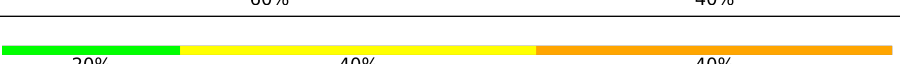
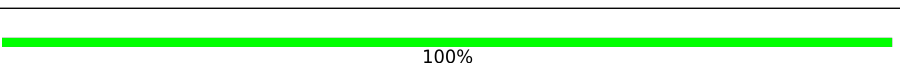
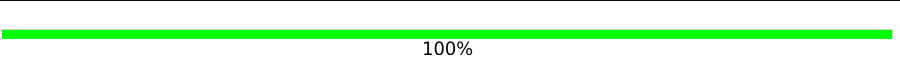
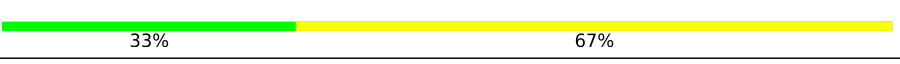
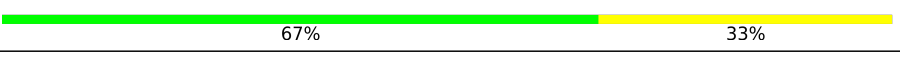
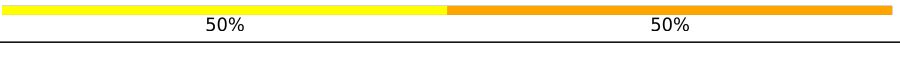
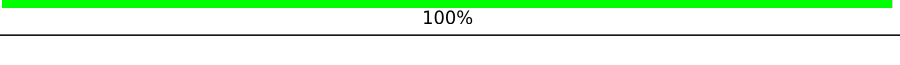
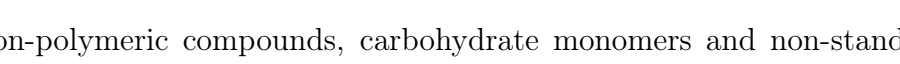
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	176	17% 66% 27% • 6%
1	B	176	13% 62% 31% • 7%
1	C	176	14% 60% 33% • 6%
1	D	176	13% 63% 30% • 5%
2	W	21	5% 90% 5% 5%

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Mol	Chain	Length	Quality of chain
2	X	21	
2	Y	21	
2	Z	21	
3	E	3	
3	H	3	
4	F	5	
4	I	5	
4	L	5	
4	O	5	
5	G	3	
5	J	3	
5	M	3	
5	P	3	
6	K	2	
6	N	2	

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	BMA	L	3	-	-	X	-
5	BMA	M	3	-	-	-	X
6	NAG	K	2	-	-	-	X
6	NAG	N	2	-	-	-	X
7	NAG	A	340	X	-	-	X
7	NAG	B	340	X	-	-	-
7	NAG	C	340	X	-	-	X
7	NAG	D	340	X	-	-	X
8	SO4	A	401	-	-	-	X
9	CIT	C	403	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6757 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.

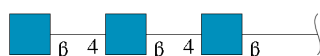
- Molecule 1 is a protein called High affinity immunoglobulin epsilon receptor alpha-subunit precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	44	0	0
			1350	861	222	262	5			
1	B	164	Total	C	N	O	S	47	0	0
			1342	857	220	260	5			
1	C	166	Total	C	N	O	S	61	0	0
			1361	870	223	263	5			
1	D	167	Total	C	N	O	S	6	0	0
			1372	879	224	264	5			

- Molecule 2 is a protein called Peptide E131.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	21	Total	C	N	O	S	4	0	0
			175	114	24	33	4			
2	X	21	Total	C	N	O	S	0	0	0
			175	114	24	33	4			
2	Y	21	Total	C	N	O	S	0	0	0
			175	114	24	33	4			
2	Z	21	Total	C	N	O	S	0	0	0
			175	114	24	33	4			

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



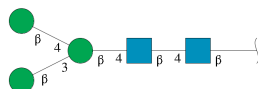
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			42	24	3	15			

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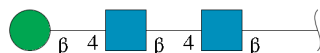
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]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
4	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	L	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



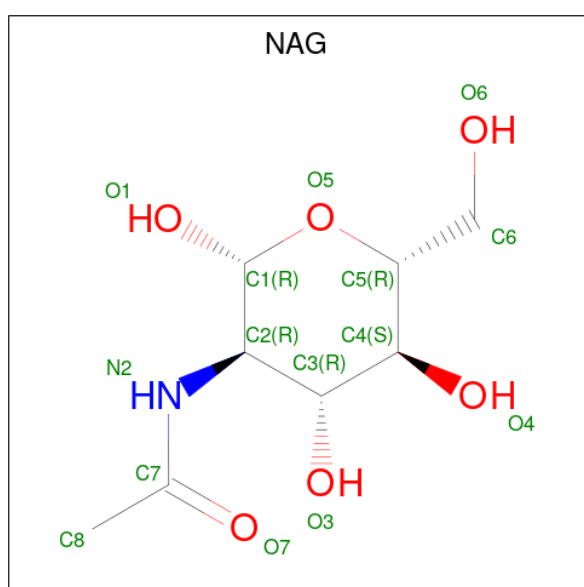
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

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



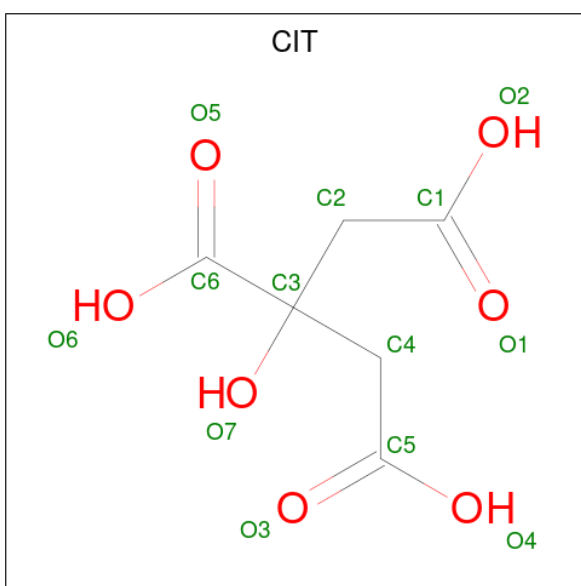
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	3	0
			5	4	1		
8	Z	1	Total	O	S	4	0
			5	4	1		

- Molecule 9 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).

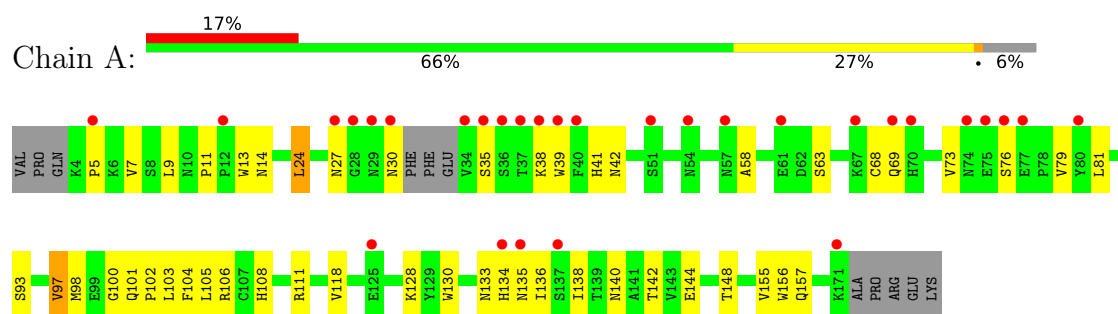


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			13	6	7		
9	D	1	Total	C	O	0	0
			13	6	7		

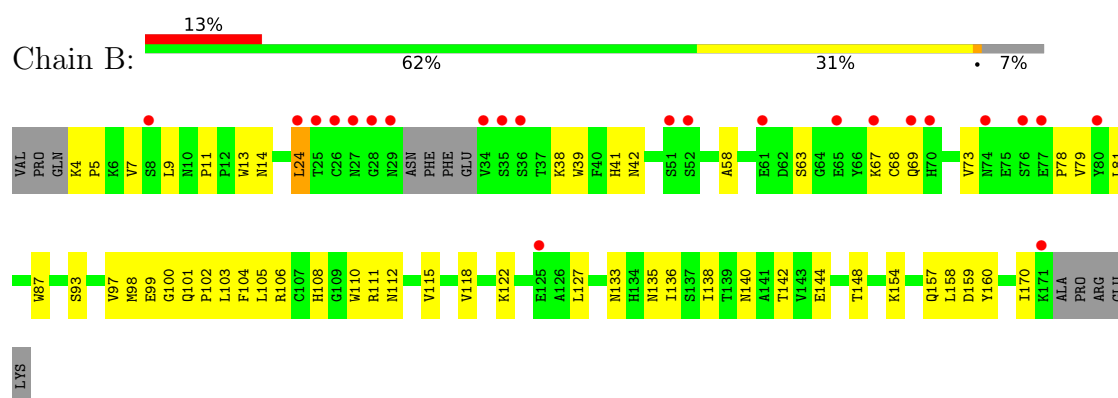
3 Residue-property plots

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 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.

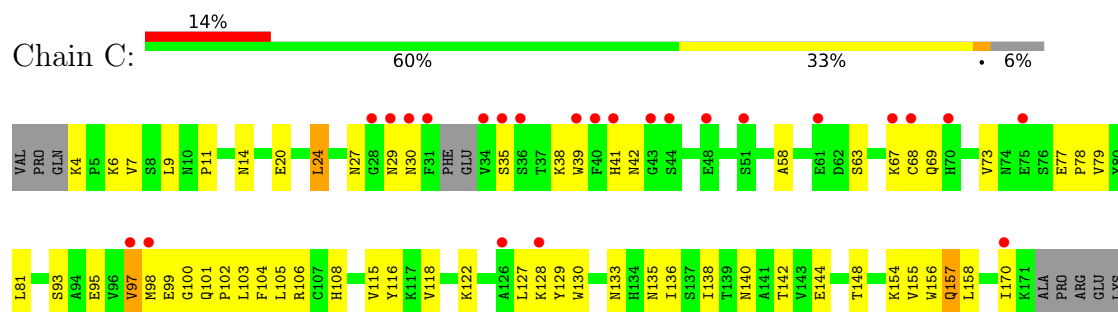
- Molecule 1: High affinity immunoglobulin epsilon receptor alpha-subunit precursor



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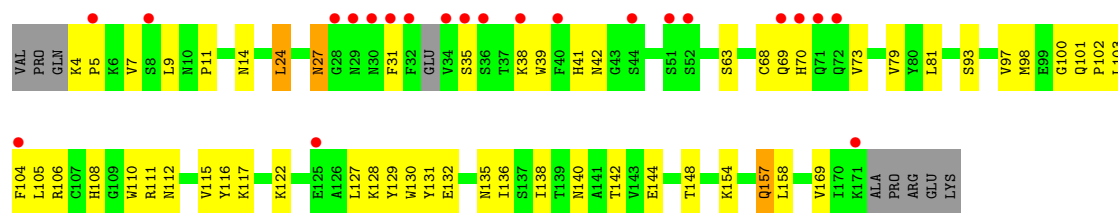


- Molecule 1: High affinity immunoglobulin epsilon receptor alpha-subunit precursor

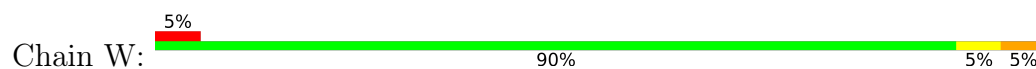


- Molecule 1: High affinity immunoglobulin epsilon receptor alpha-subunit precursor

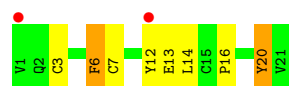




● Molecule 2: Peptide E131



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● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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



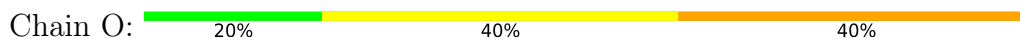
- Molecule 4: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	199.70Å 149.70Å 104.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-3.00) 97.1 (30.00-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.294 , 0.349 0.304 , 0.341	Depositor DCC
R_{free} test set	968 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, SO4, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/1387	0.88	4/1888 (0.2%)
1	B	0.49	0/1379	0.88	4/1877 (0.2%)
1	C	0.50	0/1399	0.88	4/1904 (0.2%)
1	D	0.59	1/1411 (0.1%)	1.00	4/1920 (0.2%)
2	W	0.50	0/181	1.00	1/248 (0.4%)
2	X	0.50	0/181	0.99	1/248 (0.4%)
2	Y	0.60	0/181	1.07	1/248 (0.4%)
2	Z	0.57	0/181	1.01	0/248
All	All	0.52	1/6300 (0.0%)	0.92	19/8581 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	PHE	CB-CG	-13.13	1.20	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	PHE	CA-CB-CG	21.91	135.71	113.80
1	A	11	PRO	CA-C-N	6.75	126.43	119.82
1	A	11	PRO	C-N-CA	6.75	126.43	119.82
1	C	11	PRO	CA-C-N	6.48	126.17	119.82
1	C	11	PRO	C-N-CA	6.48	126.17	119.82
1	D	11	PRO	CA-C-N	6.41	126.10	119.82
1	D	11	PRO	C-N-CA	6.41	126.10	119.82
1	B	11	PRO	CA-C-N	6.31	126.00	119.82
1	B	11	PRO	C-N-CA	6.31	126.00	119.82
2	Y	9	GLU	N-CA-C	-6.09	101.95	110.35
1	A	108	HIS	N-CA-C	5.87	118.76	109.96
1	D	108	HIS	N-CA-C	5.85	118.73	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	HIS	N-CA-C	5.82	118.69	109.96
1	B	108	HIS	N-CA-C	5.78	118.63	109.96
2	W	20	TYR	N-CA-C	5.75	119.43	110.17
1	C	97	VAL	N-CA-C	5.73	116.84	108.53
1	A	13	TRP	N-CA-C	5.70	117.36	109.15
1	B	13	TRP	N-CA-C	5.50	117.07	109.15
2	X	20	TYR	N-CA-C	5.19	119.88	113.50

There are no chirality outliers.

There are no planarity outliers.

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	1350	0	1265	33	0
1	B	1342	0	1259	34	0
1	C	1361	0	1273	47	0
1	D	1372	0	1283	38	0
2	W	175	0	152	1	0
2	X	175	0	152	5	0
2	Y	175	0	152	4	0
2	Z	175	0	152	7	0
3	E	42	0	37	3	0
3	H	42	0	37	0	0
4	F	61	0	52	6	0
4	I	61	0	52	0	0
4	L	61	0	52	8	0
4	O	61	0	52	4	0
5	G	39	0	34	0	0
5	J	39	0	34	0	0
5	M	39	0	34	0	0
5	P	39	0	34	1	0
6	K	28	0	25	2	0
6	N	28	0	25	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	5	0	0	0	0
8	Z	5	0	0	0	0
9	C	13	0	5	5	0
9	D	13	0	5	3	0
All	All	6757	0	6218	182	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 14.

All (182) 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)
4:L:3:BMA:H61	4:L:5:BMA:O5	1.62	0.99
2:Z:6:PHE:HA	2:Z:9:GLU:HG2	1.42	0.99
3:E:2:NAG:H61	3:E:3:NAG:O5	1.67	0.95
4:O:3:BMA:H2	4:O:4:BMA:H2	1.50	0.91
4:O:3:BMA:C2	4:O:4:BMA:H2	2.10	0.82
1:D:105:LEU:HB2	1:D:136:ILE:CG2	2.16	0.76
1:C:157:GLN:HA	9:C:403:CIT:O4	1.86	0.75
1:A:30:ASN:C	5:P:1:NAG:H62	2.10	0.75
1:C:105:LEU:HB2	1:C:136:ILE:CG2	2.15	0.75
1:A:105:LEU:HB2	1:A:136:ILE:CG2	2.17	0.74
1:B:105:LEU:HB2	1:B:136:ILE:CG2	2.16	0.74
1:C:98:MET:O	1:C:101:GLN:HG2	1.92	0.68
1:B:14:ASN:O	1:B:81:LEU:HD12	1.94	0.65
1:D:110:TRP:CD1	1:D:111:ARG:HG3	2.32	0.65
1:A:98:MET:O	1:A:101:GLN:HG2	1.96	0.65
1:B:4:LYS:N	1:B:5:PRO:HD2	2.12	0.65
1:B:154:LYS:HA	1:B:158:LEU:O	1.96	0.64
1:C:118:VAL:HG21	1:C:133:ASN:HA	1.80	0.64
2:Z:4:PRO:HB2	2:Z:6:PHE:CD1	2.33	0.63
2:Z:15:CYS:HB3	2:Z:16:PRO:HD2	1.79	0.62
1:B:105:LEU:HB2	1:B:136:ILE:HG22	1.83	0.60
1:C:105:LEU:HB2	1:C:136:ILE:HG22	1.83	0.60
1:D:14:ASN:O	1:D:81:LEU:HD12	2.02	0.59
2:Y:16:PRO:HB2	2:Y:18:VAL:HG12	1.84	0.59
1:D:105:LEU:HB2	1:D:136:ILE:HG22	1.84	0.59
4:O:3:BMA:C2	4:O:4:BMA:C2	2.81	0.59
1:A:105:LEU:HB2	1:A:136:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLU:HA	6:K:1:NAG:H82	1.85	0.58
1:B:115:VAL:HB	1:B:133:ASN:HD22	1.69	0.57
1:B:9:LEU:HD22	1:B:24:LEU:HD22	1.87	0.57
1:C:116:TYR:CD1	9:C:403:CIT:H41	2.40	0.57
4:F:3:BMA:C6	4:F:5:BMA:C1	2.82	0.56
1:C:98:MET:H	1:C:101:GLN:NE2	2.03	0.56
1:D:158:LEU:HD12	2:Z:4:PRO:HD3	1.87	0.56
1:A:38:LYS:O	1:A:68:CYS:HA	2.06	0.56
1:C:9:LEU:HD22	1:C:24:LEU:HD22	1.86	0.56
1:C:116:TYR:HD1	9:C:403:CIT:O3	1.89	0.56
1:C:38:LYS:O	1:C:68:CYS:HA	2.05	0.56
1:D:142:THR:HG22	1:D:144:GLU:H	1.71	0.56
1:B:38:LYS:O	1:B:68:CYS:HA	2.05	0.56
1:C:14:ASN:O	1:C:81:LEU:HD12	2.06	0.56
1:C:142:THR:HG22	1:C:144:GLU:H	1.71	0.56
1:D:38:LYS:O	1:D:68:CYS:HA	2.05	0.56
1:A:9:LEU:HD22	1:A:24:LEU:HD22	1.87	0.56
1:B:118:VAL:HG21	1:B:133:ASN:HA	1.87	0.56
1:C:155:VAL:HG12	1:C:156:TRP:CD1	2.41	0.55
4:F:3:BMA:H61	4:F:5:BMA:O5	2.06	0.55
1:C:128:LYS:HD3	1:C:130:TRP:CH2	2.41	0.55
1:D:9:LEU:HD22	1:D:24:LEU:HD22	1.87	0.55
1:C:99:GLU:HB2	1:C:170:ILE:O	2.07	0.55
1:B:142:THR:HG22	1:B:144:GLU:H	1.72	0.54
4:L:2:NAG:O3	4:L:3:BMA:H2	2.08	0.53
1:D:129:TYR:CD2	1:D:129:TYR:C	2.87	0.53
1:A:142:THR:HG22	1:A:144:GLU:H	1.73	0.53
2:Z:10:LEU:HD12	2:Z:14:LEU:HD22	1.91	0.53
1:D:98:MET:O	1:D:101:GLN:HG2	2.09	0.52
1:A:157:GLN:HA	1:A:157:GLN:HE21	1.73	0.52
1:D:117:LYS:HE3	9:D:404:CIT:O6	2.09	0.52
1:A:103:LEU:HD23	1:A:138:ILE:HD12	1.92	0.52
4:L:3:BMA:H61	4:L:5:BMA:O6	2.10	0.52
1:A:106:ARG:HB2	1:A:135:ASN:ND2	2.25	0.51
1:D:131:TYR:HD2	1:D:132:GLU:HG2	1.75	0.51
1:C:158:LEU:HD12	2:Y:4:PRO:HD3	1.93	0.51
1:B:39:TRP:CZ3	1:B:68:CYS:HB3	2.46	0.51
1:D:106:ARG:HB2	1:D:135:ASN:ND2	2.26	0.51
1:D:39:TRP:CZ3	1:D:68:CYS:HB3	2.46	0.50
1:C:106:ARG:HB2	1:C:135:ASN:ND2	2.26	0.50
1:D:38:LYS:HB2	1:D:69:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:N	1:B:5:PRO:CD	2.75	0.50
1:B:98:MET:O	1:B:101:GLN:HG2	2.11	0.50
1:C:39:TRP:CZ3	1:C:68:CYS:HB3	2.47	0.50
1:D:103:LEU:HD23	1:D:138:ILE:HD12	1.93	0.50
1:A:39:TRP:CZ3	1:A:68:CYS:HB3	2.46	0.50
1:B:103:LEU:HD23	1:B:138:ILE:HD12	1.93	0.50
1:C:103:LEU:HD23	1:C:138:ILE:HD12	1.94	0.50
1:D:97:VAL:O	1:D:169:VAL:HA	2.11	0.50
1:B:38:LYS:HB2	1:B:69:GLN:HB3	1.94	0.49
1:C:157:GLN:CA	9:C:403:CIT:O4	2.57	0.49
1:B:87:TRP:CD1	1:B:160:TYR:CE2	3.00	0.49
1:C:128:LYS:HD3	1:C:130:TRP:HH2	1.77	0.49
1:C:38:LYS:HB2	1:C:69:GLN:HB3	1.94	0.49
2:Y:9:GLU:O	2:Y:10:LEU:HB3	2.12	0.49
2:W:13:GLU:HB3	2:W:20:TYR:CZ	2.47	0.49
1:A:38:LYS:HB2	1:A:69:GLN:HB3	1.94	0.49
1:C:6:LYS:H	1:C:27:ASN:CB	2.26	0.49
1:B:106:ARG:HB2	1:B:135:ASN:ND2	2.28	0.49
1:C:4:LYS:HE3	1:C:77:GLU:HG2	1.94	0.49
1:A:5:PRO:HG2	1:A:76:SER:HB3	1.95	0.48
1:D:101:GLN:HB2	1:D:102:PRO:HD2	1.95	0.48
4:L:3:BMA:C6	4:L:5:BMA:O5	2.48	0.48
1:C:105:LEU:HB2	1:C:136:ILE:HG23	1.96	0.48
1:B:157:GLN:HE21	1:B:157:GLN:HA	1.79	0.47
4:L:1:NAG:O3	4:L:2:NAG:O5	2.30	0.47
4:L:3:BMA:H61	4:L:5:BMA:C5	2.44	0.47
1:A:101:GLN:HB2	1:A:102:PRO:HD2	1.97	0.47
1:D:103:LEU:HB3	1:D:138:ILE:HB	1.97	0.47
4:L:3:BMA:C6	4:L:5:BMA:O6	2.63	0.47
1:A:42:ASN:HD22	4:F:1:NAG:C7	2.28	0.46
1:B:110:TRP:CG	2:X:16:PRO:HG3	2.51	0.46
1:D:7:VAL:HB	1:D:79:VAL:HG21	1.98	0.46
1:A:118:VAL:HG21	1:A:133:ASN:HA	1.97	0.46
1:A:155:VAL:HG12	1:A:156:TRP:CD1	2.50	0.46
1:A:156:TRP:O	1:A:157:GLN:HB2	2.15	0.46
1:B:101:GLN:HB2	1:B:102:PRO:HD2	1.97	0.46
1:B:110:TRP:CD1	1:B:111:ARG:HG3	2.50	0.46
1:C:101:GLN:HB2	1:C:102:PRO:HD2	1.96	0.46
4:F:3:BMA:C6	4:F:5:BMA:O5	2.63	0.46
1:B:103:LEU:HB3	1:B:138:ILE:HB	1.98	0.46
1:C:103:LEU:HB3	1:C:138:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:HIS:HE1	1:C:63:SER:O	1.99	0.46
2:X:13:GLU:HB3	2:X:20:TYR:CE1	2.51	0.46
1:A:7:VAL:HB	1:A:79:VAL:HG21	1.98	0.45
1:C:7:VAL:HB	1:C:79:VAL:HG21	1.98	0.45
1:B:7:VAL:HB	1:B:79:VAL:HG21	1.99	0.45
1:D:116:TYR:CD1	9:D:404:CIT:H41	2.51	0.45
4:F:3:BMA:H61	4:F:5:BMA:C1	2.47	0.45
1:C:100:GLY:HA2	1:C:140:ASN:OD1	2.17	0.45
1:C:97:VAL:HG21	1:C:103:LEU:HD13	1.98	0.45
1:D:128:LYS:HD3	1:D:130:TRP:CH2	2.52	0.45
1:B:105:LEU:HB2	1:B:136:ILE:HG23	1.97	0.45
1:D:131:TYR:CD2	1:D:132:GLU:HG2	2.52	0.45
1:B:97:VAL:HG21	1:B:103:LEU:HD13	1.99	0.45
1:C:14:ASN:ND2	1:C:95:GLU:OE1	2.50	0.45
2:X:6:PHE:CD2	2:X:6:PHE:C	2.94	0.45
1:A:98:MET:H	1:A:101:GLN:NE2	2.15	0.44
1:A:105:LEU:HB2	1:A:136:ILE:HG23	1.98	0.44
1:D:105:LEU:HB2	1:D:136:ILE:HG23	1.97	0.44
1:A:103:LEU:HB3	1:A:138:ILE:HB	1.98	0.44
1:D:97:VAL:HG21	1:D:103:LEU:HD13	1.99	0.44
1:D:4:LYS:HB3	1:D:5:PRO:HD3	2.00	0.44
2:Y:15:CYS:HB3	2:Y:16:PRO:CD	2.48	0.44
1:C:93:SER:HB3	1:C:104:PHE:HB2	2.00	0.44
1:B:41:HIS:HE1	1:B:63:SER:O	2.01	0.43
1:C:97:VAL:CG1	1:C:101:GLN:HG3	2.48	0.43
1:C:6:LYS:H	1:C:27:ASN:HB2	1.84	0.43
1:D:157:GLN:HA	9:D:404:CIT:O4	2.18	0.43
4:F:3:BMA:H61	4:F:5:BMA:C5	2.48	0.43
1:A:97:VAL:HG12	1:A:101:GLN:HG3	2.01	0.43
1:D:110:TRP:CD1	2:Z:16:PRO:HD3	2.54	0.43
1:A:128:LYS:HD3	1:A:130:TRP:CH2	2.54	0.43
1:B:93:SER:HB3	1:B:104:PHE:HB2	2.00	0.43
6:K:1:NAG:O3	6:K:2:NAG:C1	2.67	0.43
1:A:41:HIS:HE1	1:A:63:SER:O	2.02	0.42
1:A:156:TRP:HZ3	1:C:116:TYR:HE1	1.67	0.42
1:D:5:PRO:HA	1:D:27:ASN:CG	2.44	0.42
1:D:41:HIS:HE1	1:D:63:SER:O	2.02	0.42
1:D:110:TRP:NE1	1:D:111:ARG:HG3	2.34	0.42
1:B:99:GLU:HB2	1:B:170:ILE:O	2.19	0.42
1:A:41:HIS:O	1:A:42:ASN:HB2	2.19	0.42
1:B:41:HIS:O	1:B:42:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLY:HA2	1:B:140:ASN:OD1	2.19	0.42
1:D:115:VAL:HA	1:D:154:LYS:O	2.18	0.42
1:D:154:LYS:HB3	1:D:154:LYS:HE2	1.76	0.42
1:A:14:ASN:O	1:A:81:LEU:HD12	2.19	0.42
1:A:97:VAL:CG1	1:A:101:GLN:HG3	2.49	0.42
1:A:93:SER:HB3	1:A:104:PHE:HB2	2.02	0.42
1:B:97:VAL:HG13	1:B:101:GLN:HE21	1.84	0.42
1:C:122:LYS:HB2	1:C:127:LEU:HD11	2.01	0.42
1:C:154:LYS:HD3	9:C:403:CIT:O6	2.20	0.42
1:C:129:TYR:CD2	1:C:129:TYR:C	2.97	0.42
1:C:115:VAL:HA	1:C:154:LYS:O	2.20	0.41
3:E:2:NAG:H61	3:E:3:NAG:O6	2.19	0.41
1:D:122:LYS:HB2	1:D:127:LEU:HD11	2.02	0.41
1:C:41:HIS:O	1:C:42:ASN:HB2	2.20	0.41
1:C:97:VAL:HG13	1:C:101:GLN:HE21	1.85	0.41
1:D:93:SER:HB3	1:D:104:PHE:HB2	2.01	0.41
1:D:100:GLY:HA2	1:D:140:ASN:OD1	2.20	0.41
1:B:122:LYS:HB2	1:B:127:LEU:HD11	2.01	0.41
3:E:2:NAG:C6	3:E:3:NAG:O5	2.53	0.41
1:C:42:ASN:HD22	4:L:1:NAG:C7	2.31	0.41
1:A:9:LEU:CD2	1:A:24:LEU:HD22	2.51	0.41
1:D:41:HIS:O	1:D:42:ASN:HB2	2.20	0.41
1:C:97:VAL:HG12	1:C:101:GLN:HG3	2.03	0.40
1:A:100:GLY:HA2	1:A:140:ASN:OD1	2.21	0.40
1:A:130:TRP:CE2	1:A:134:HIS:HD2	2.40	0.40
1:B:9:LEU:CD2	1:B:24:LEU:HD22	2.51	0.40
1:B:67:LYS:HE2	1:B:78:PRO:HG3	2.04	0.40
1:C:98:MET:SD	1:C:99:GLU:O	2.79	0.40
1:D:42:ASN:HD22	4:O:1:NAG:C7	2.33	0.40
2:X:3:CYS:HB3	2:X:7:CYS:SG	2.61	0.40
1:C:67:LYS:HE2	1:C:78:PRO:HG3	2.04	0.40
2:X:12:TYR:CG	2:Z:10:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	161/176 (92%)	147 (91%)	9 (6%)	5 (3%)	3	19
1	B	160/176 (91%)	146 (91%)	12 (8%)	2 (1%)	9	38
1	C	162/176 (92%)	150 (93%)	7 (4%)	5 (3%)	3	19
1	D	163/176 (93%)	150 (92%)	10 (6%)	3 (2%)	6	31
2	W	19/21 (90%)	15 (79%)	4 (21%)	0	100	100
2	X	19/21 (90%)	16 (84%)	2 (10%)	1 (5%)	1	9
2	Y	19/21 (90%)	11 (58%)	7 (37%)	1 (5%)	1	9
2	Z	19/21 (90%)	18 (95%)	0	1 (5%)	1	9
All	All	722/788 (92%)	653 (90%)	51 (7%)	18 (2%)	4	23

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	27	ASN
1	A	27	ASN
2	Y	2	GLN
1	C	29	ASN
1	A	35	SER
1	C	30	ASN
1	C	35	SER
1	D	35	SER
2	Z	17	ASP
1	A	73	VAL
1	A	111	ARG
2	X	6	PHE
1	A	58	ALA
1	B	58	ALA
1	C	58	ALA
1	B	73	VAL
1	D	73	VAL
1	C	73	VAL

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 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	151/161 (94%)	148 (98%)	3 (2%)	48	76
1	B	150/161 (93%)	146 (97%)	4 (3%)	39	71
1	C	152/161 (94%)	149 (98%)	3 (2%)	48	76
1	D	153/161 (95%)	148 (97%)	5 (3%)	33	67
2	W	21/21 (100%)	21 (100%)	0	100	100
2	X	21/21 (100%)	20 (95%)	1 (5%)	23	57
2	Y	21/21 (100%)	21 (100%)	0	100	100
2	Z	21/21 (100%)	21 (100%)	0	100	100
All	All	690/728 (95%)	674 (98%)	16 (2%)	44	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	97	VAL
1	A	148	THR
1	B	24	LEU
1	B	112	ASN
1	B	148	THR
1	B	159	ASP
1	C	24	LEU
1	C	148	THR
1	C	157	GLN
1	D	24	LEU
1	D	70	HIS
1	D	112	ASN
1	D	148	THR
1	D	157	GLN
2	X	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	41	HIS

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Mol	Chain	Res	Type
1	A	101	GLN
1	A	134	HIS
1	A	157	GLN
1	B	41	HIS
1	B	101	GLN
1	B	112	ASN
1	B	157	GLN
1	C	29	ASN
1	C	41	HIS
1	C	101	GLN
1	C	112	ASN
1	D	27	ASN
1	D	41	HIS
2	X	2	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

42 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	$\# Z > 2$
3	NAG	E	1	3,1	14,14,15	0.75	0	17,19,21	1.09	1 (5%)
3	NAG	E	2	3	14,14,15	0.78	1 (7%)	17,19,21	1.02	1 (5%)
3	NAG	E	3	3	14,14,15	0.59	0	17,19,21	0.79	0
4	NAG	F	1	4,1	14,14,15	0.46	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	2	4	14,14,15	0.67	0	17,19,21	1.64	2 (11%)
4	BMA	F	3	4	11,11,12	0.86	1 (9%)	15,15,17	1.49	3 (20%)
4	BMA	F	4	4	11,11,12	0.50	0	15,15,17	0.33	0
4	BMA	F	5	4	11,11,12	0.43	0	15,15,17	0.27	0
5	NAG	G	1	5,1	14,14,15	0.58	0	17,19,21	0.79	0
5	NAG	G	2	5	14,14,15	0.37	0	17,19,21	0.75	0
5	BMA	G	3	5	11,11,12	0.36	0	15,15,17	0.25	0
3	NAG	H	1	3,1	14,14,15	0.57	0	17,19,21	1.03	2 (11%)
3	NAG	H	2	3	14,14,15	0.60	0	17,19,21	0.76	0
3	NAG	H	3	3	14,14,15	0.55	0	17,19,21	0.70	0
4	NAG	I	1	4,1	14,14,15	0.65	0	17,19,21	0.94	1 (5%)
4	NAG	I	2	4	14,14,15	0.72	0	17,19,21	1.98	4 (23%)
4	BMA	I	3	4	11,11,12	0.51	0	15,15,17	1.04	1 (6%)
4	BMA	I	4	4	11,11,12	0.40	0	15,15,17	0.57	0
4	BMA	I	5	4	11,11,12	0.35	0	15,15,17	0.41	0
5	NAG	J	1	5,1	14,14,15	0.65	0	17,19,21	0.69	0
5	NAG	J	2	5	14,14,15	0.46	0	17,19,21	0.62	0
5	BMA	J	3	5	11,11,12	0.35	0	15,15,17	0.43	0
6	NAG	K	1	6,1	14,14,15	0.62	0	17,19,21	0.82	1 (5%)
6	NAG	K	2	6	14,14,15	0.39	0	17,19,21	0.66	0
4	NAG	L	1	4,1	14,14,15	0.57	0	17,19,21	0.72	0
4	NAG	L	2	4	14,14,15	0.71	0	17,19,21	2.01	3 (17%)
4	BMA	L	3	4	11,11,12	0.67	0	15,15,17	0.92	1 (6%)
4	BMA	L	4	4	11,11,12	0.57	0	15,15,17	0.64	1 (6%)
4	BMA	L	5	4	11,11,12	0.49	0	15,15,17	0.35	0
5	NAG	M	1	5,1	14,14,15	0.67	0	17,19,21	1.09	2 (11%)
5	NAG	M	2	5	14,14,15	0.67	1 (7%)	17,19,21	0.66	0
5	BMA	M	3	5	11,11,12	0.38	0	15,15,17	0.23	0
6	NAG	N	1	6,1	14,14,15	0.63	0	17,19,21	0.74	0
6	NAG	N	2	6	14,14,15	0.58	0	17,19,21	0.70	0
4	NAG	O	1	4,1	14,14,15	0.54	0	17,19,21	0.90	1 (5%)
4	NAG	O	2	4	14,14,15	0.83	0	17,19,21	2.01	3 (17%)
4	BMA	O	3	4	11,11,12	0.57	0	15,15,17	1.00	2 (13%)
4	BMA	O	4	4	11,11,12	0.39	0	15,15,17	0.44	0
4	BMA	O	5	4	11,11,12	0.34	0	15,15,17	0.31	0
5	NAG	P	1	5,1	14,14,15	0.74	0	17,19,21	0.73	0
5	NAG	P	2	5	14,14,15	0.50	0	17,19,21	0.66	0
5	BMA	P	3	5	11,11,12	0.37	0	15,15,17	0.26	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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	E	3	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	BMA	F	4	4	-	0/2/19/22	0/1/1/1
4	BMA	F	5	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	3	3	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	BMA	I	4	4	-	0/2/19/22	0/1/1/1
4	BMA	I	5	4	-	0/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	BMA	L	4	4	-	2/2/19/22	0/1/1/1
4	BMA	L	5	4	-	0/2/19/22	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
4	BMA	O	4	4	-	2/2/19/22	0/1/1/1
4	BMA	O	5	4	-	2/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C1-C2	2.25	1.57	1.52
5	M	2	NAG	C1-C2	2.03	1.55	1.52
3	E	2	NAG	C4-C5	2.00	1.57	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C4-C3-C2	-6.56	101.41	111.02
4	O	2	NAG	C4-C3-C2	-6.46	101.56	111.02
4	I	2	NAG	C4-C3-C2	-6.44	101.58	111.02
4	F	2	NAG	C4-C3-C2	-5.10	103.54	111.02
4	F	3	BMA	C1-C2-C3	4.24	115.82	109.64
5	M	1	NAG	C4-C3-C2	-3.08	106.51	111.02
4	I	3	BMA	C1-C2-C3	2.98	113.98	109.64
4	O	2	NAG	C2-N2-C7	-2.95	118.94	122.90
4	F	2	NAG	C2-N2-C7	-2.87	119.06	122.90
4	F	3	BMA	C1-O5-C5	2.87	116.03	112.19
4	O	3	BMA	C1-C2-C3	2.86	113.81	109.64
4	L	2	NAG	C2-N2-C7	-2.83	119.10	122.90
4	L	2	NAG	O4-C4-C3	2.82	117.03	110.38
4	I	1	NAG	C2-N2-C7	-2.70	119.28	122.90
4	L	3	BMA	C1-C2-C3	2.60	113.43	109.64
3	H	1	NAG	O5-C1-C2	-2.59	107.28	111.29
4	I	2	NAG	O4-C4-C5	2.50	115.48	109.32
6	K	1	NAG	C2-N2-C7	-2.45	119.62	122.90
4	I	2	NAG	C2-N2-C7	-2.42	119.66	122.90
3	H	1	NAG	C2-N2-C7	-2.35	119.75	122.90
3	E	2	NAG	O4-C4-C3	-2.32	104.91	110.38
5	M	1	NAG	C2-N2-C7	-2.27	119.86	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4	BMA	C1-O5-C5	2.19	115.12	112.19
3	E	1	NAG	C2-N2-C7	-2.19	119.97	122.90
4	I	2	NAG	O4-C4-C3	2.17	115.50	110.38
4	O	1	NAG	C2-N2-C7	-2.12	120.06	122.90
4	O	2	NAG	C1-O5-C5	2.03	114.91	112.19
4	F	3	BMA	C3-C4-C5	-2.02	106.58	110.23
4	O	3	BMA	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	3	NAG	C3-C2-N2-C7
4	O	3	BMA	C4-C5-C6-O6
4	L	4	BMA	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	F	5	BMA	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	O	4	BMA	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	L	4	BMA	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6
4	F	5	BMA	C4-C5-C6-O6
4	O	4	BMA	C4-C5-C6-O6
4	O	5	BMA	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
4	O	5	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	3	NAG	C4-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
5	J	3	BMA	C4-C5-C6-O6
5	J	3	BMA	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C3-C2-N2-C7
5	J	1	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
5	P	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7
5	P	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 24 short contacts:

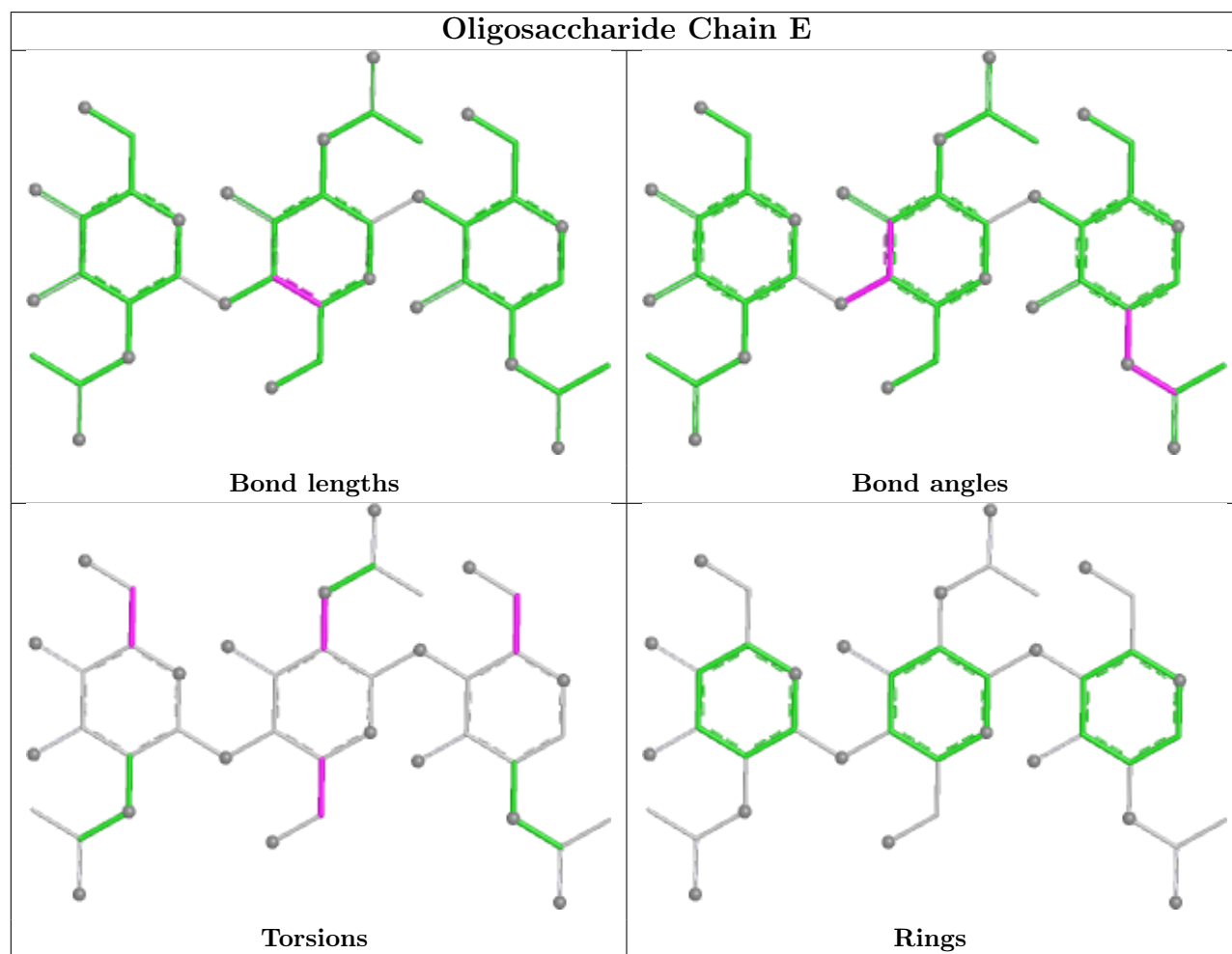
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	3	0
4	F	3	BMA	5	0
4	F	1	NAG	1	0
4	L	1	NAG	2	0
4	L	5	BMA	5	0
4	O	3	BMA	3	0
6	K	2	NAG	1	0
3	E	3	NAG	3	0
4	O	1	NAG	1	0
6	K	1	NAG	2	0
5	P	1	NAG	1	0
4	F	5	BMA	5	0

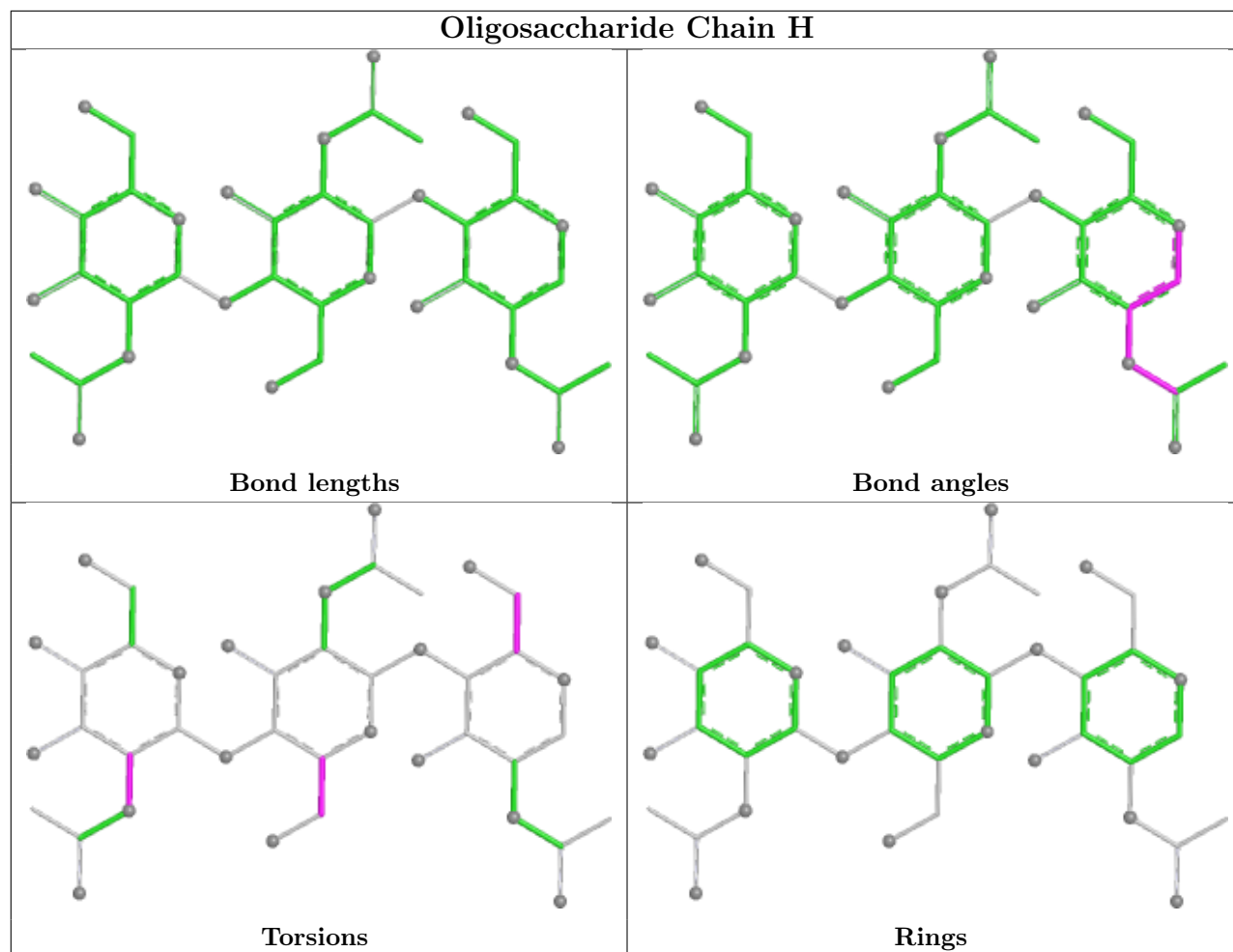
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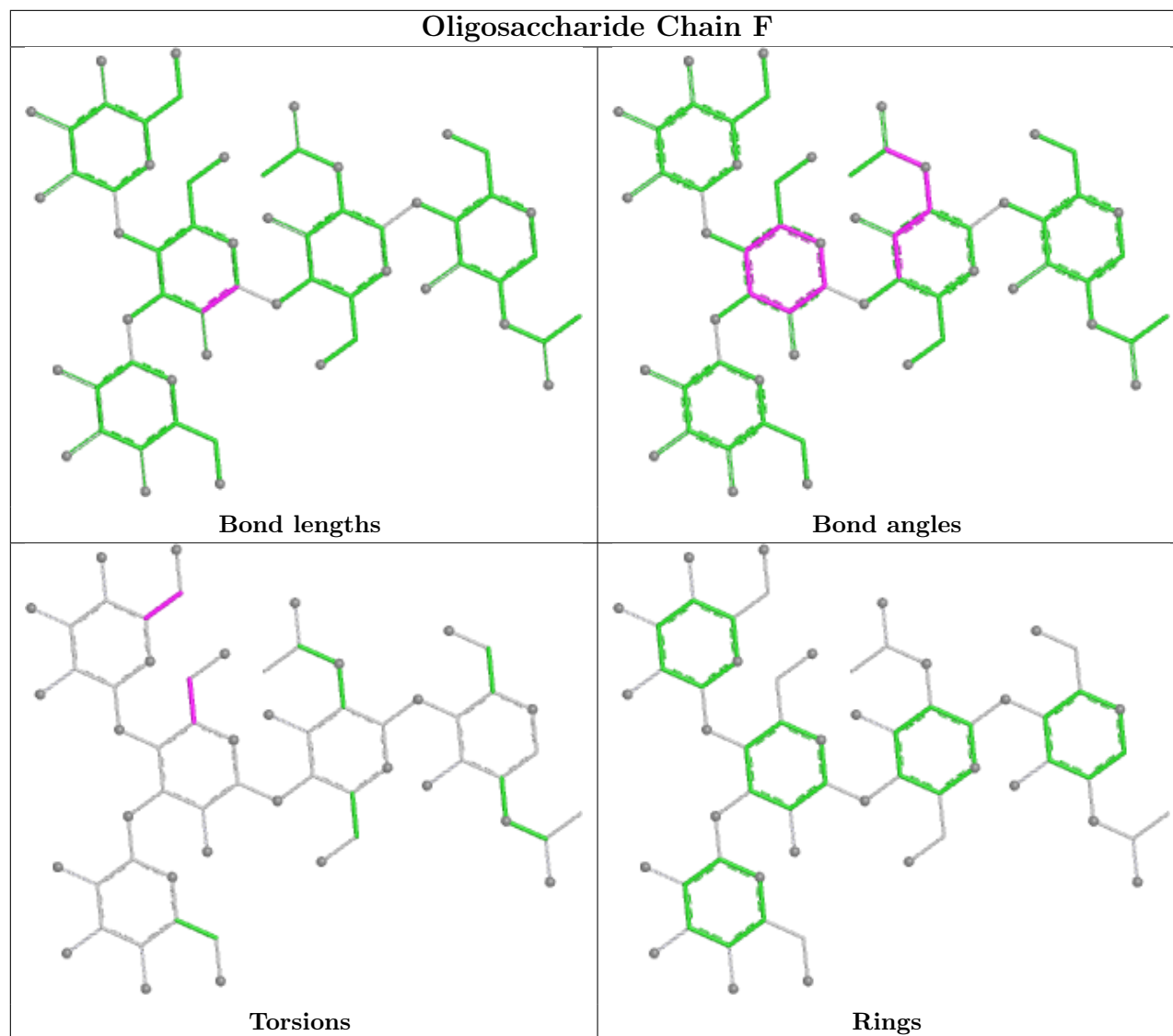
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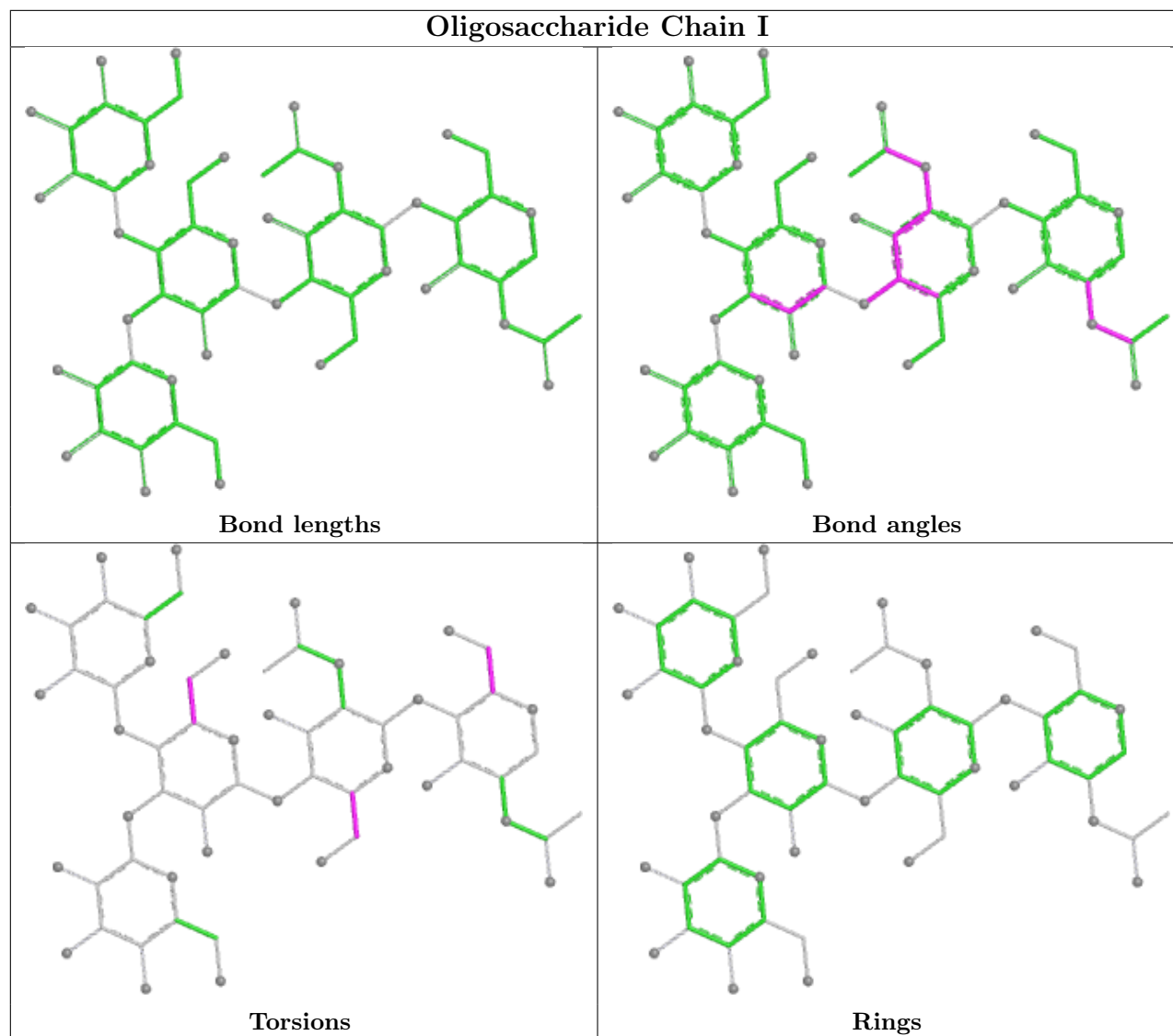
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	4	BMA	3	0
4	L	2	NAG	2	0
4	L	3	BMA	6	0

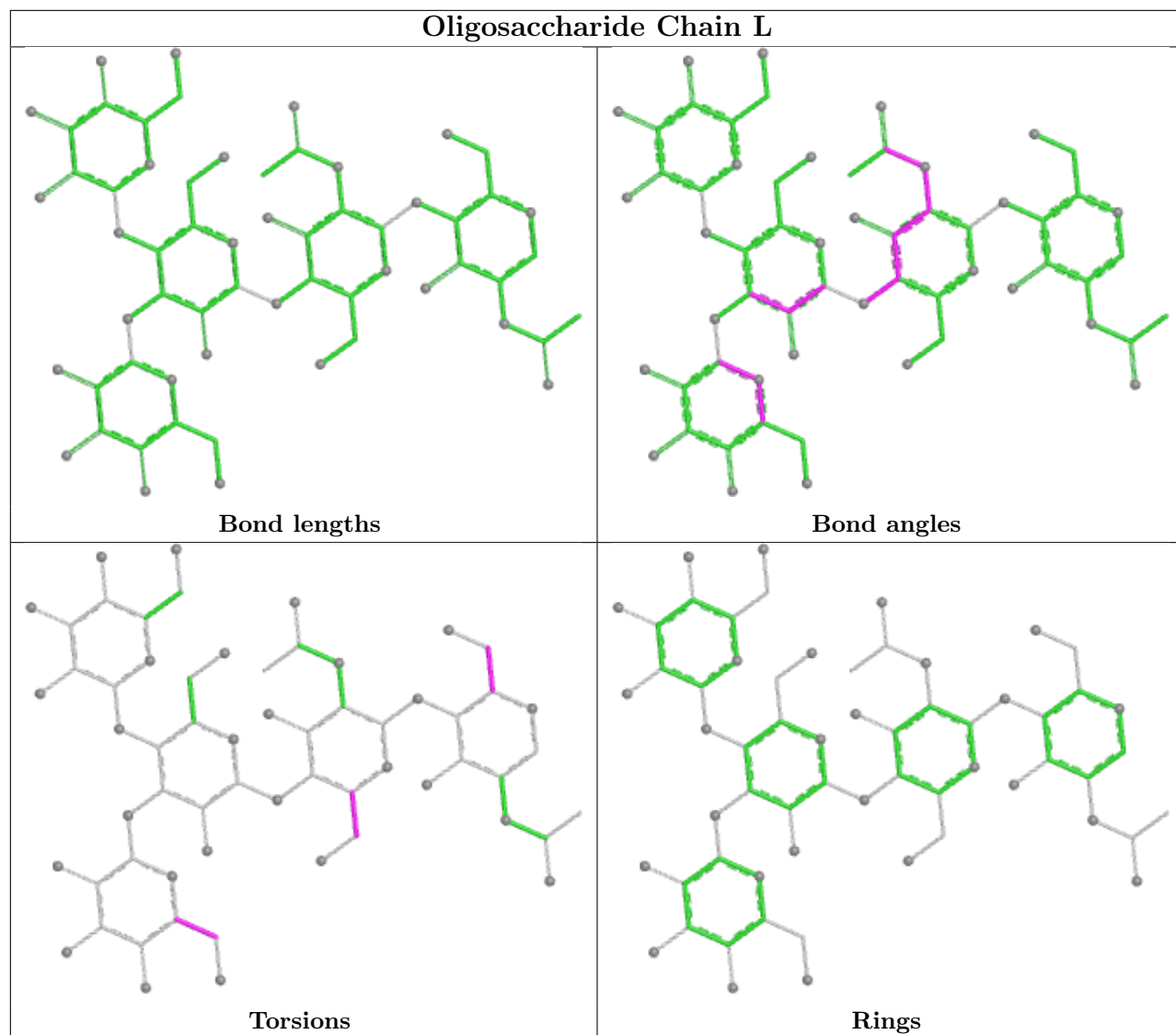
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

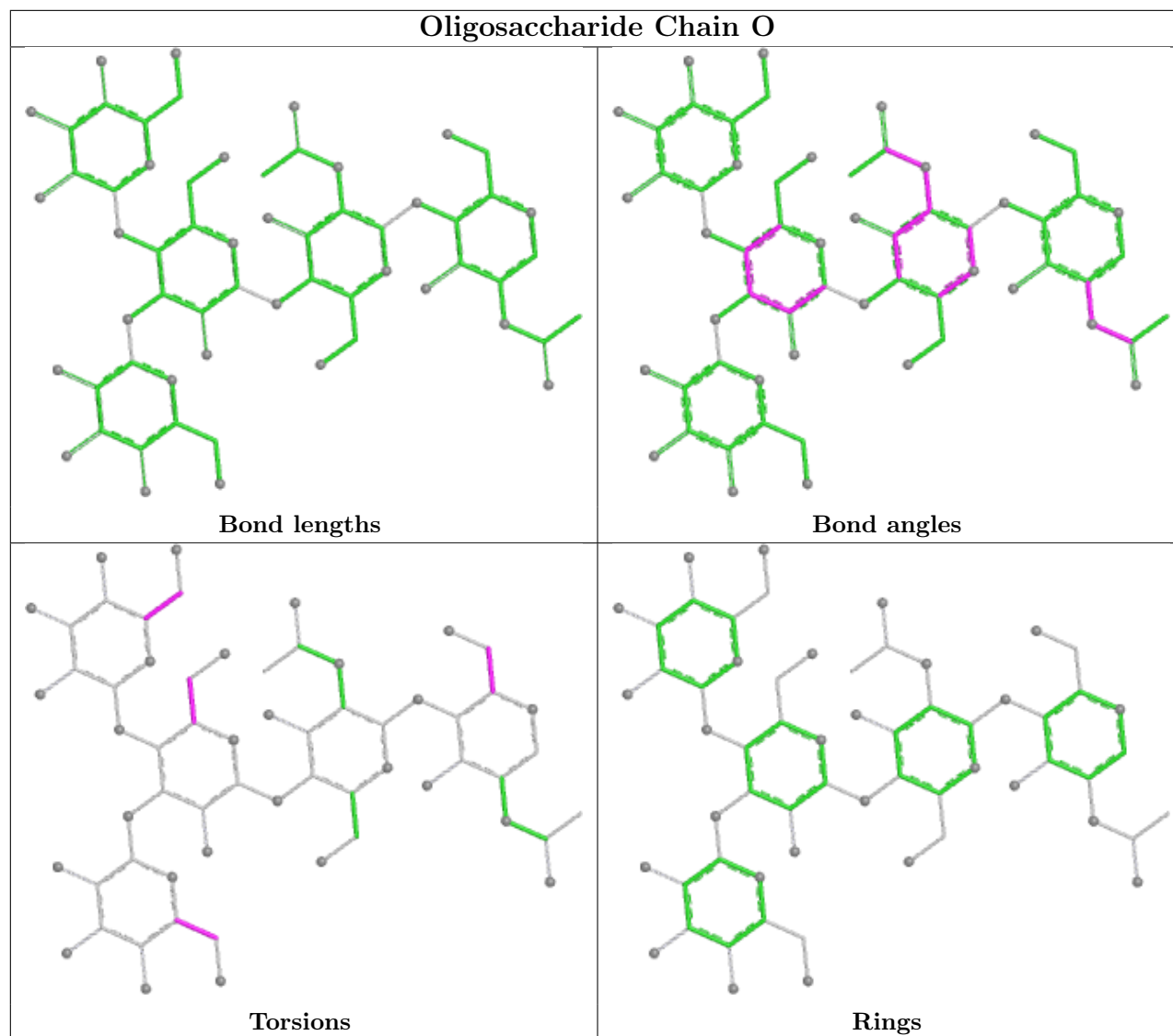


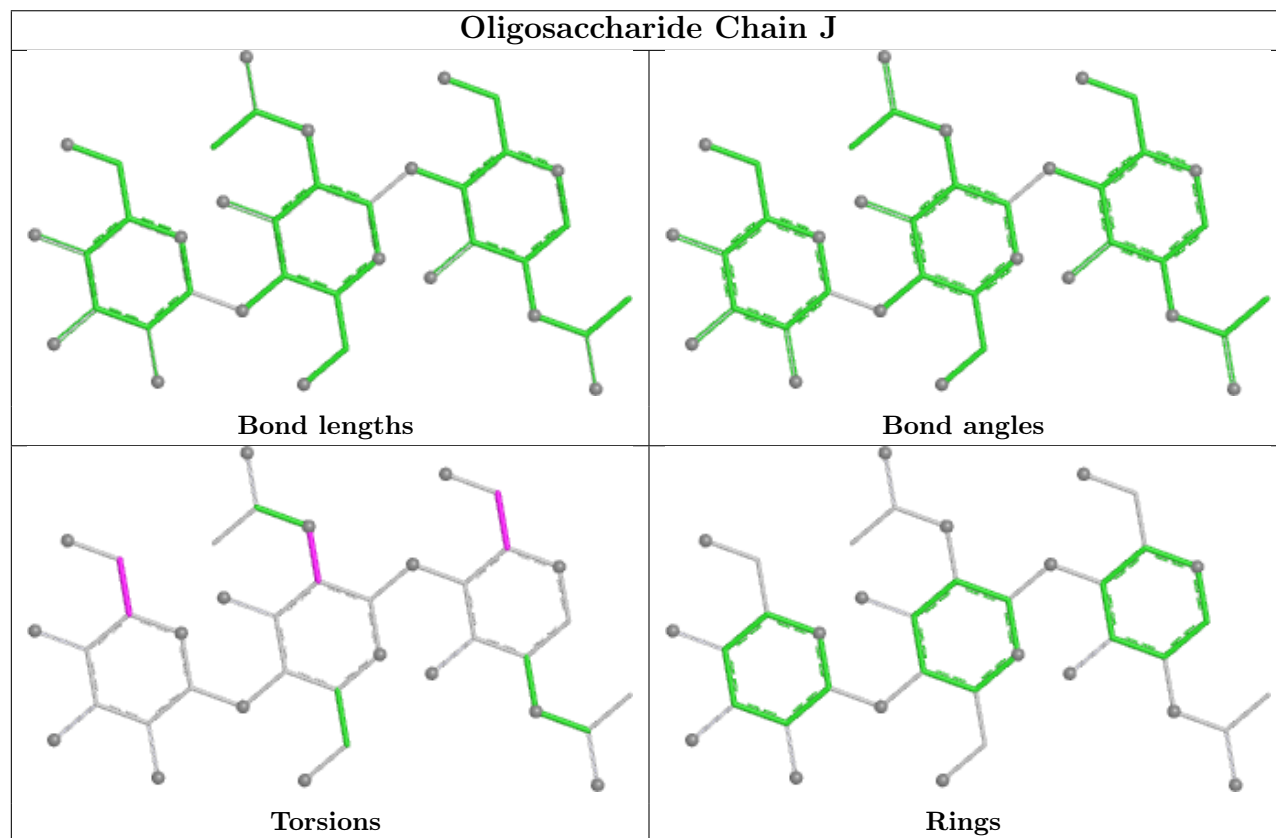
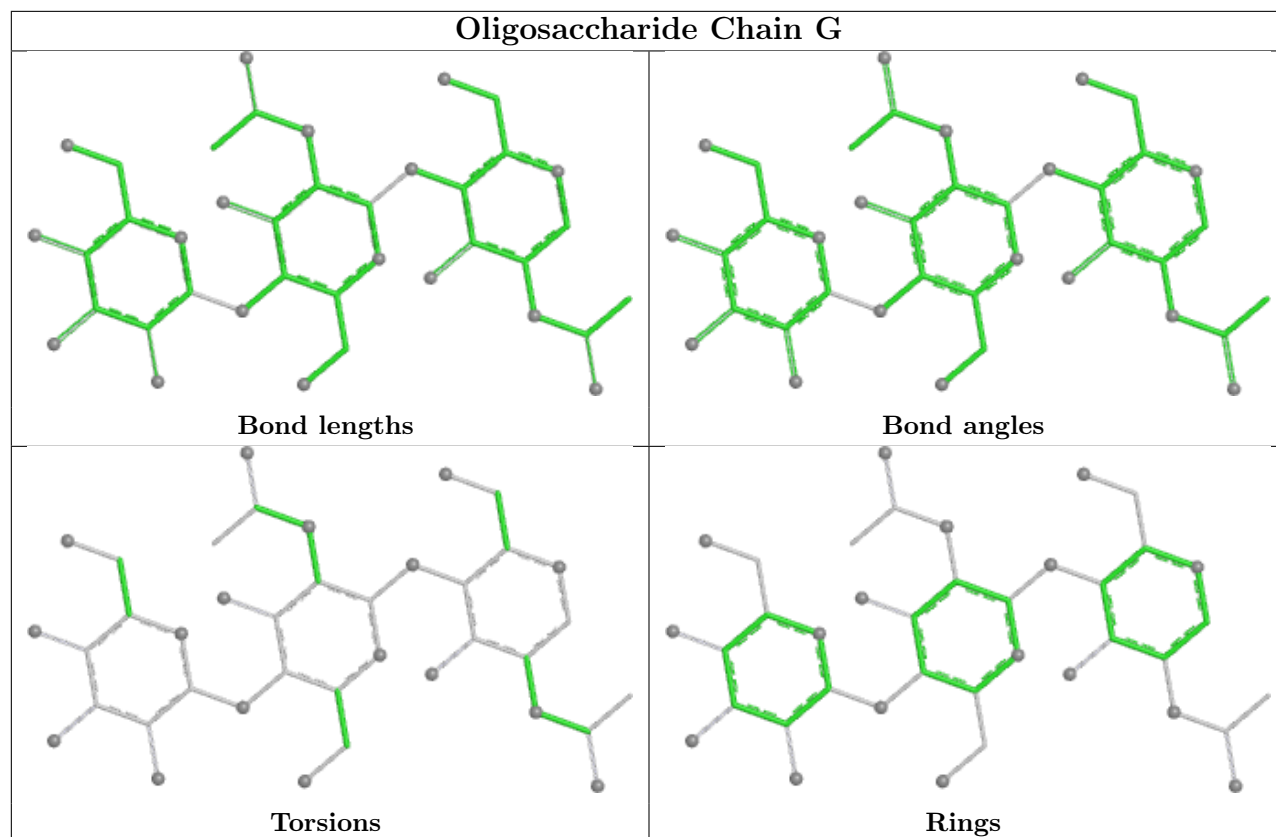




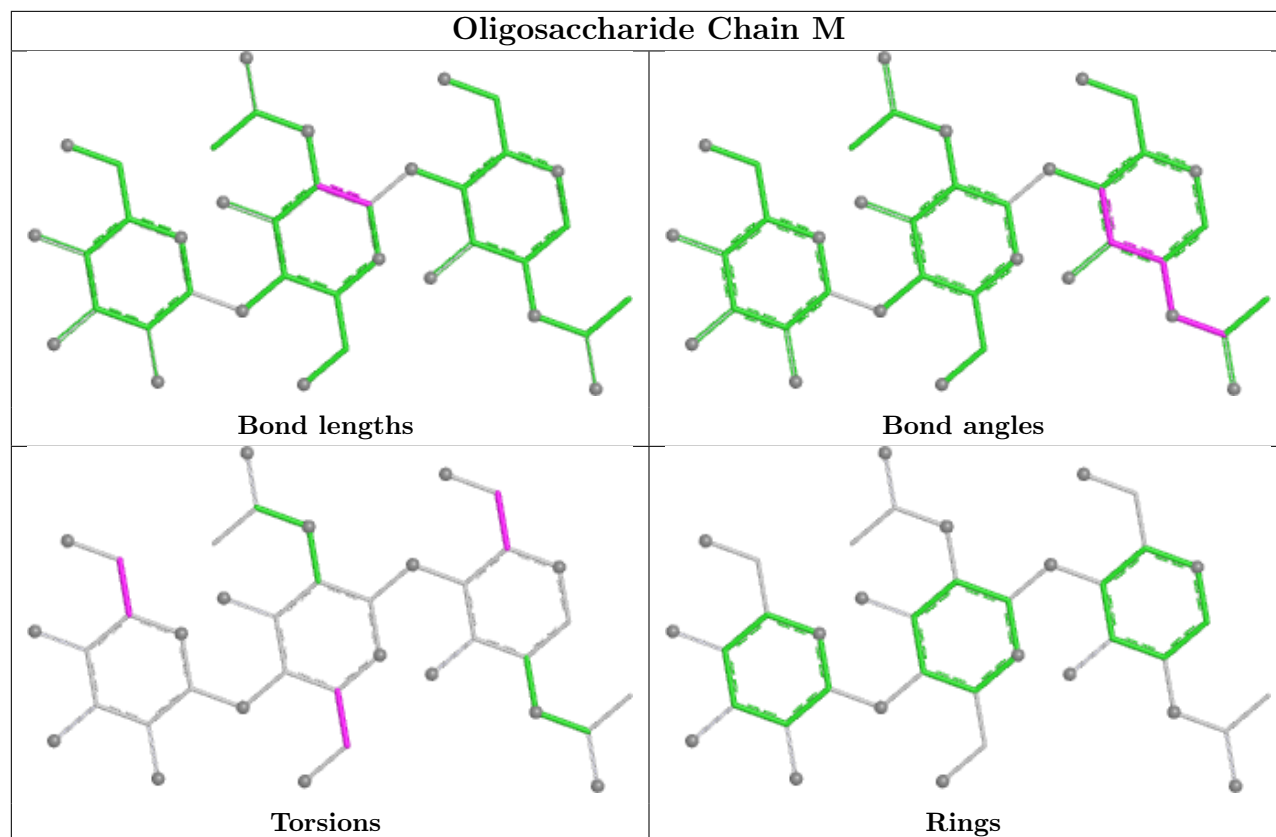




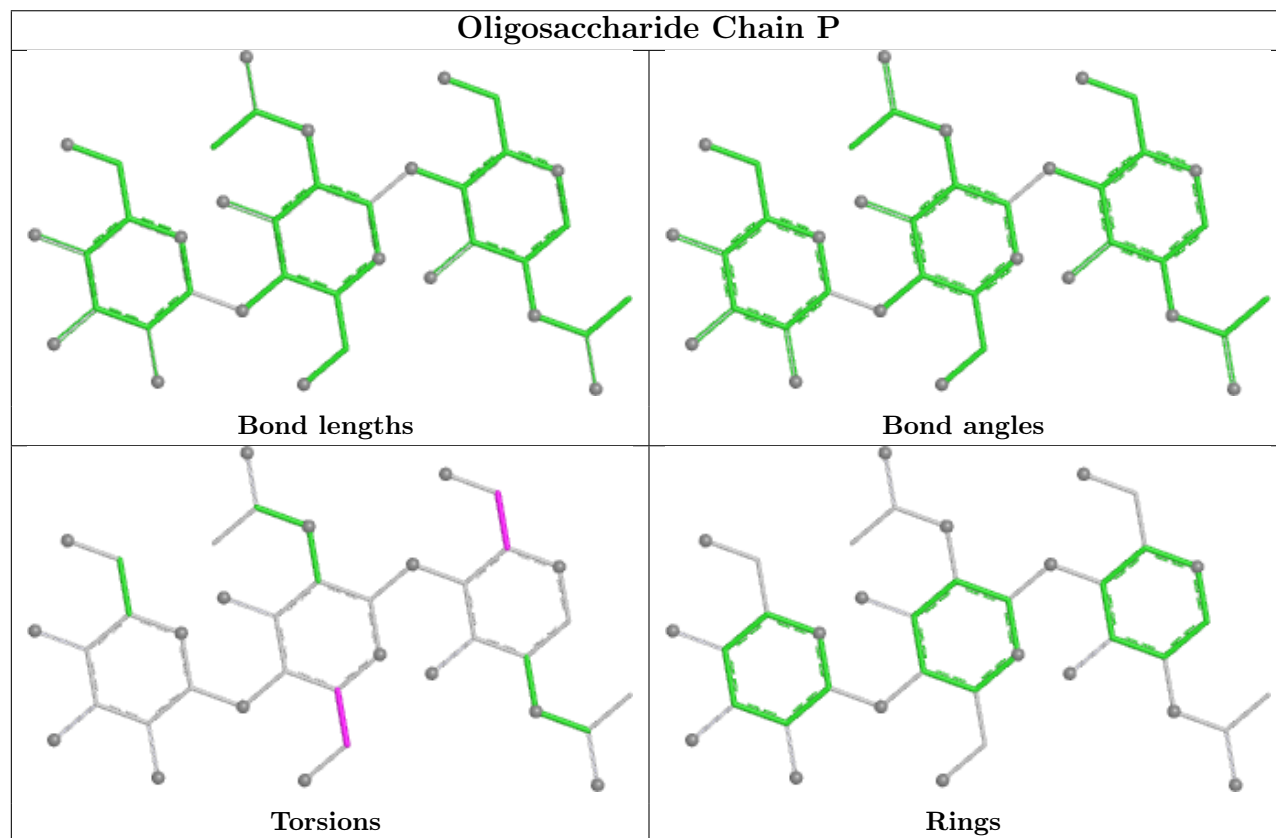


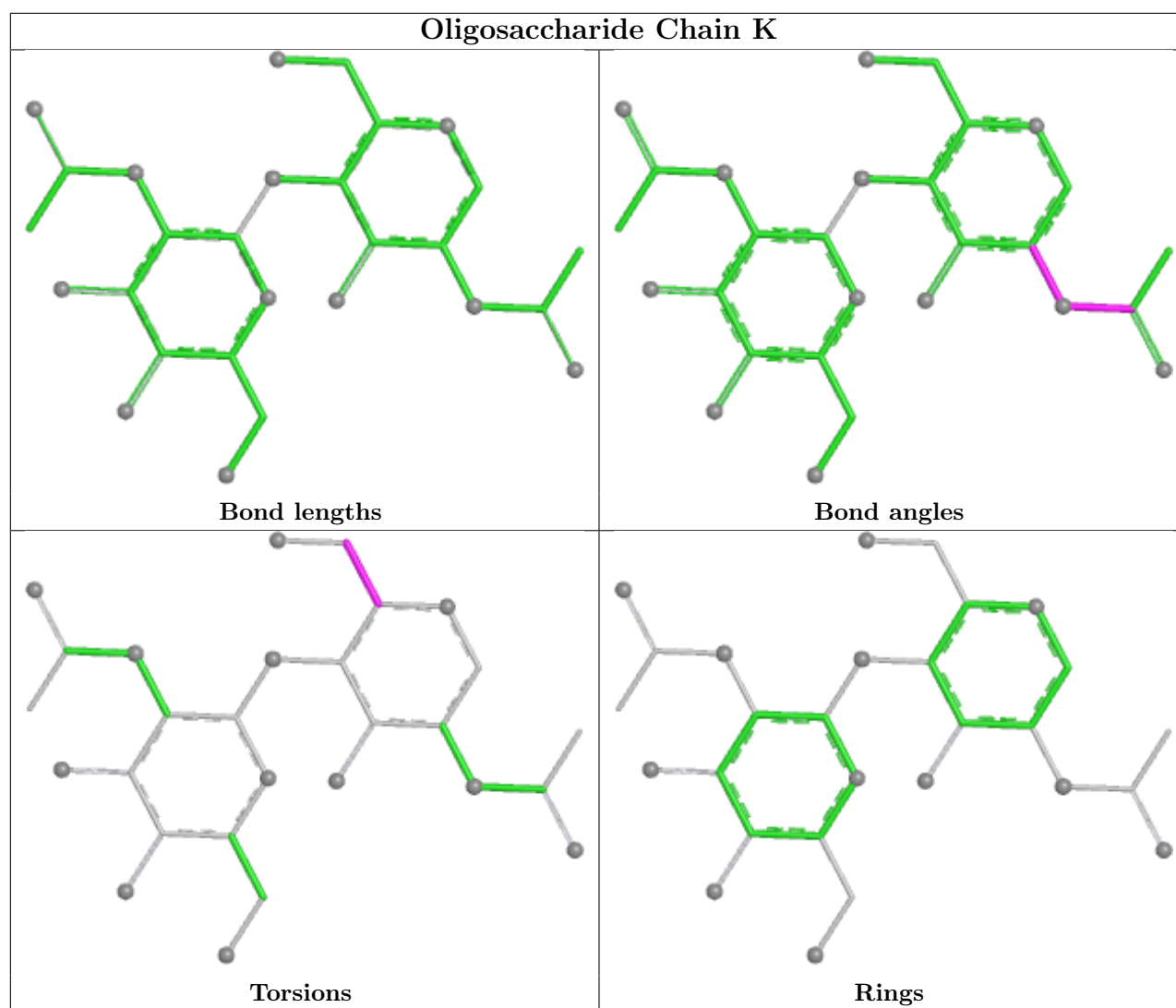


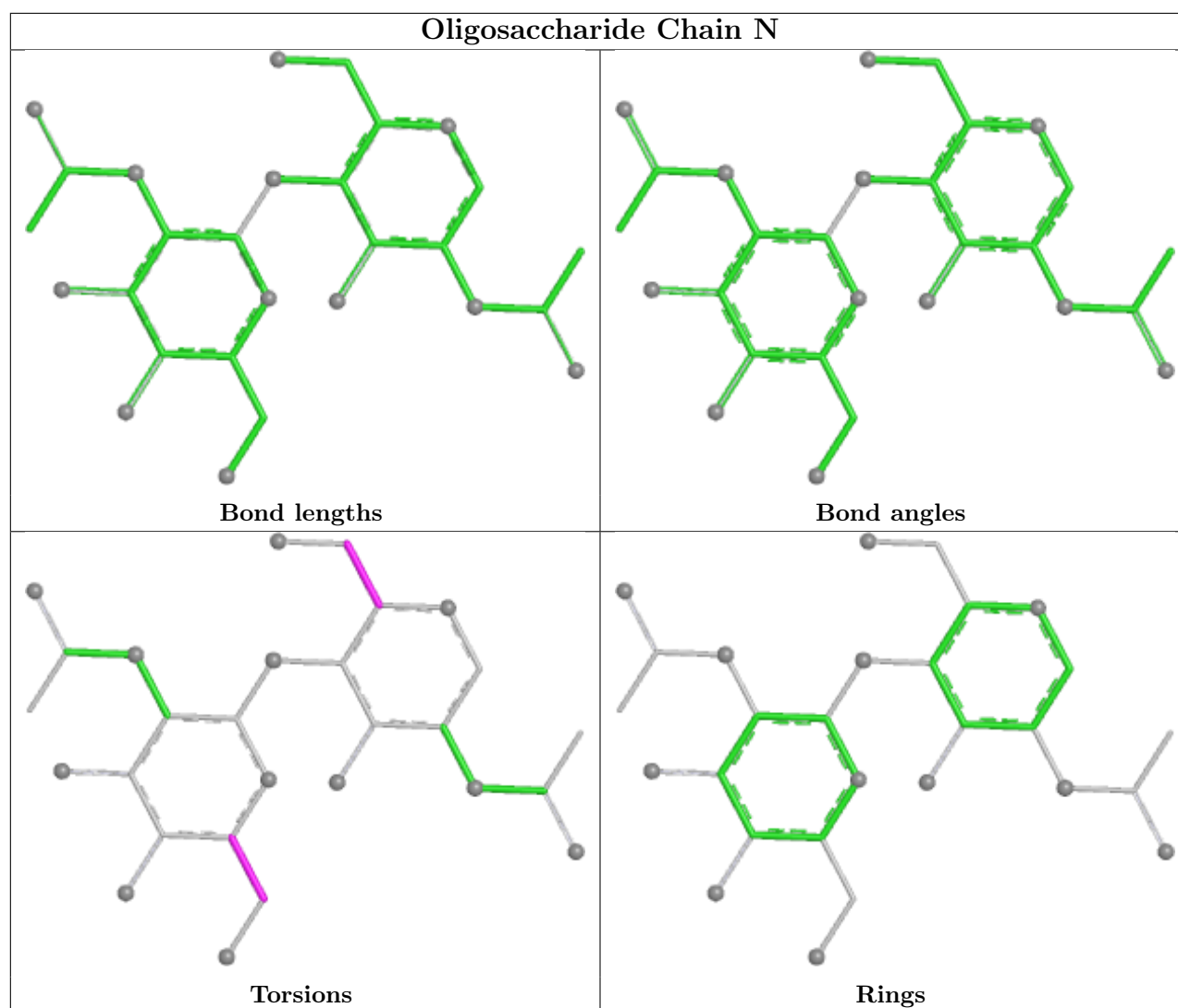
Oligosaccharide Chain M



Oligosaccharide Chain P







5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	340	1	14,14,15	0.71	1 (7%)	17,19,21	0.84	0
7	NAG	B	340	1	14,14,15	0.55	0	17,19,21	0.75	1 (5%)
9	CIT	D	404	-	12,12,12	2.41	5 (41%)	17,17,17	1.44	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	A	401	-	4,4,4	0.34	0	6,6,6	0.16	0
7	NAG	D	340	1	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
8	SO4	Z	402	-	4,4,4	0.28	0	6,6,6	0.19	0
7	NAG	C	340	1	14,14,15	0.41	0	17,19,21	0.70	0
9	CIT	C	403	-	12,12,12	2.68	5 (41%)	17,17,17	1.50	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	340	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	B	340	1	1/1/5/7	2/6/23/26	0/1/1/1
9	CIT	D	404	-	-	4/16/16/16	-
7	NAG	D	340	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	C	340	1	1/1/5/7	0/6/23/26	0/1/1/1
9	CIT	C	403	-	-	11/16/16/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	403	CIT	C3-C6	-5.30	1.48	1.53
9	C	403	CIT	O4-C5	-4.12	1.17	1.30
9	D	404	CIT	O1-C1	-3.56	1.10	1.22
9	D	404	CIT	O2-C1	-3.52	1.19	1.30
9	D	404	CIT	O4-C5	-3.44	1.19	1.30
9	C	403	CIT	O1-C1	-3.36	1.11	1.22
9	C	403	CIT	O3-C5	3.32	1.32	1.22
9	C	403	CIT	O2-C1	-3.29	1.19	1.30
9	D	404	CIT	O3-C5	3.26	1.32	1.22
9	D	404	CIT	C3-C6	-3.06	1.50	1.53
7	A	340	NAG	C1-C2	2.05	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	403	CIT	O6-C6-C3	3.50	119.86	113.14
9	D	404	CIT	O6-C6-C3	3.23	119.33	113.14
9	D	404	CIT	O4-C5-C4	2.51	122.29	114.35
7	B	340	NAG	C2-N2-C7	-2.42	119.66	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	403	CIT	O4-C5-C4	2.41	121.98	114.35
9	D	404	CIT	C3-C2-C1	2.32	120.27	113.92
9	D	404	CIT	O3-C5-C4	-2.28	116.49	122.95
7	D	340	NAG	C2-N2-C7	-2.22	119.92	122.90
9	C	403	CIT	O5-C6-C3	-2.18	117.86	122.09
9	C	403	CIT	C3-C2-C1	2.12	119.72	113.92

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	340	NAG	C1
7	B	340	NAG	C1
7	C	340	NAG	C1
7	D	340	NAG	C1

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	403	CIT	C1-C2-C3-O7
9	C	403	CIT	C1-C2-C3-C4
9	C	403	CIT	C1-C2-C3-C6
9	C	403	CIT	O7-C3-C6-O5
9	C	403	CIT	O7-C3-C6-O6
9	C	403	CIT	C4-C3-C6-O6
9	D	404	CIT	C2-C3-C6-O5
9	D	404	CIT	C2-C3-C6-O6
9	D	404	CIT	O7-C3-C6-O5
9	D	404	CIT	O7-C3-C6-O6
7	B	340	NAG	C4-C5-C6-O6
7	A	340	NAG	C4-C5-C6-O6
7	B	340	NAG	O5-C5-C6-O6
7	A	340	NAG	O5-C5-C6-O6
9	C	403	CIT	C4-C3-C6-O5
9	C	403	CIT	C2-C3-C6-O6
9	C	403	CIT	C2-C3-C6-O5
9	C	403	CIT	O1-C1-C2-C3
9	C	403	CIT	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	404	CIT	3	0
9	C	403	CIT	5	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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	161/176 (91%)	1.08	30 (18%) 3 2	29, 59, 108, 118	8 (4%)
1	B	160/176 (90%)	0.94	23 (14%) 6 3	31, 63, 109, 118	7 (4%)
1	C	162/176 (92%)	1.05	24 (14%) 5 3	11, 64, 109, 114	11 (6%)
1	D	167/176 (94%)	0.98	22 (13%) 7 4	15, 64, 111, 116	8 (4%)
2	W	21/21 (100%)	0.63	1 (4%) 35 19	43, 65, 92, 96	1 (4%)
2	X	21/21 (100%)	0.70	2 (9%) 14 7	50, 67, 93, 94	0
2	Y	21/21 (100%)	0.85	3 (14%) 6 3	48, 65, 93, 98	0
2	Z	21/21 (100%)	0.51	1 (4%) 35 19	49, 68, 92, 99	0
All	All	734/788 (93%)	0.98	106 (14%) 6 3	11, 63, 110, 118	35 (4%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	ASN	10.5
1	C	34	VAL	9.8
1	C	31	PHE	9.5
1	A	29	ASN	8.2
1	B	28	GLY	8.2
1	D	31	PHE	8.0
1	D	28	GLY	7.9
1	C	30	ASN	7.8
1	D	29	ASN	7.4
1	D	30	ASN	7.4
1	B	34	VAL	7.1
1	A	36	SER	6.7
1	A	28	GLY	6.6
1	D	32	PHE	6.6
1	C	28	GLY	6.4
1	A	40	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	35	SER	5.5
1	D	36	SER	5.5
1	B	36	SER	5.4
1	A	34	VAL	5.4
1	B	29	ASN	5.3
1	A	69	GLN	5.2
1	B	27	ASN	4.8
1	A	30	ASN	4.7
1	A	61	GLU	4.3
1	B	65	GLU	4.1
1	B	67	LYS	4.1
1	C	36	SER	3.9
1	D	44	SER	3.9
1	D	52	SER	3.8
1	D	34	VAL	3.8
1	D	70	HIS	3.8
1	D	71	GLN	3.7
2	Y	1	VAL	3.7
1	A	27	ASN	3.7
1	B	70	HIS	3.7
1	B	35	SER	3.6
1	A	51	SER	3.6
1	B	76	SER	3.6
1	C	68	CYS	3.5
2	Y	21	VAL	3.4
1	B	69	GLN	3.4
1	B	25	THR	3.2
1	A	70	HIS	3.2
1	A	38	LYS	3.2
1	A	134	HIS	3.2
1	A	75	GLU	3.1
1	C	98	MET	3.1
1	A	74	ASN	3.1
1	C	39	TRP	3.0
1	A	76	SER	3.0
1	A	80	TYR	3.0
1	C	51	SER	3.0
1	A	171	LYS	3.0
1	A	77	GLU	2.9
1	A	125	GLU	2.9
1	D	8	SER	2.9
1	C	70	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	35	SER	2.9
1	B	80	TYR	2.9
2	X	1	VAL	2.8
1	A	12	PRO	2.8
1	C	43	GLY	2.8
1	B	26	CYS	2.8
1	A	67	LYS	2.8
1	A	57	ASN	2.7
1	C	44	SER	2.7
1	A	37	THR	2.7
1	A	135	ASN	2.7
1	C	35	SER	2.7
1	D	125	GLU	2.7
1	A	137	SER	2.6
1	D	40	PHE	2.6
1	D	72	GLN	2.6
1	C	75	GLU	2.6
1	B	74	ASN	2.5
2	X	12	TYR	2.5
1	C	61	GLU	2.5
1	D	104	PHE	2.5
1	C	48	GLU	2.5
1	C	67	LYS	2.5
1	D	38	LYS	2.4
1	C	41	HIS	2.4
1	C	170	ILE	2.4
1	A	5	PRO	2.4
1	C	40	PHE	2.4
1	D	51	SER	2.3
1	B	8	SER	2.3
1	B	125	GLU	2.3
2	W	21	VAL	2.3
1	B	61	GLU	2.2
1	C	126	ALA	2.2
1	B	77	GLU	2.2
1	C	128	LYS	2.2
1	C	97	VAL	2.2
1	D	69	GLN	2.2
1	B	171	LYS	2.1
1	D	171	LYS	2.1
1	A	54	ASN	2.1
2	Y	2	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	Z	1	VAL	2.0
1	B	52	SER	2.0
1	A	39	TRP	2.0
1	D	5	PRO	2.0
1	B	24	LEU	2.0
1	B	51	SER	2.0

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 [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($\text{\AA}^2$)	Q<0.9
3	NAG	E	1	14/15	-	-	72,76,83,83	0
3	NAG	E	2	14/15	-	-	60,75,81,82	0
3	NAG	E	3	14/15	-	-	72,79,85,91	0
3	NAG	H	1	14/15	-	-	61,76,82,82	0
3	NAG	H	2	14/15	-	-	44,49,52,53	14
3	NAG	H	3	14/15	-	-	41,46,48,49	14
4	NAG	F	1	14/15	-	-	53,55,63,66	0
4	NAG	F	2	14/15	-	-	55,61,63,71	0
4	BMA	F	3	11/12	-	-	71,79,87,89	0
4	BMA	F	4	11/12	-	-	56,61,63,65	11
4	BMA	F	5	11/12	-	-	78,85,86,86	11
5	BMA	M	3	11/12	0.34	0.69	67,67,68,68	11
6	NAG	N	2	14/15	0.48	0.52	89,89,91,91	14
4	BMA	I	3	11/12	-	-	46,51,54,56	11
4	BMA	I	4	11/12	-	-	36,39,41,42	11
4	BMA	I	5	11/12	-	-	50,51,52,53	11
6	NAG	K	2	14/15	0.52	0.51	95,96,97,97	14
5	BMA	P	3	11/12	0.59	0.18	70,71,71,72	11
4	BMA	L	3	11/12	-	-	88,92,97,97	0
4	BMA	L	4	11/12	-	-	96,101,102,102	0
4	BMA	L	5	11/12	-	-	88,93,95,95	11
4	NAG	O	2	14/15	0.61	0.33	64,70,79,80	0

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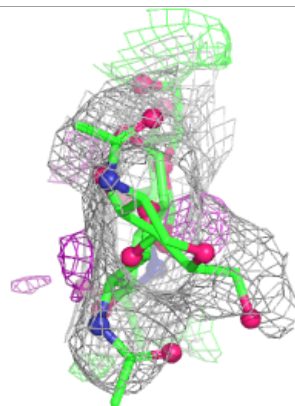
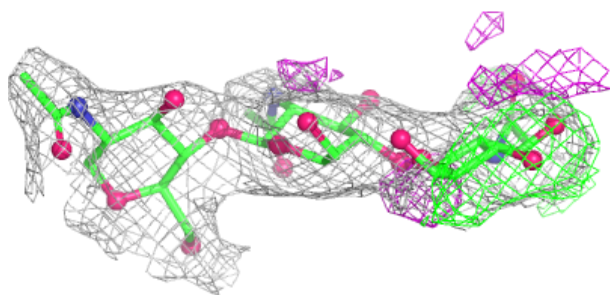
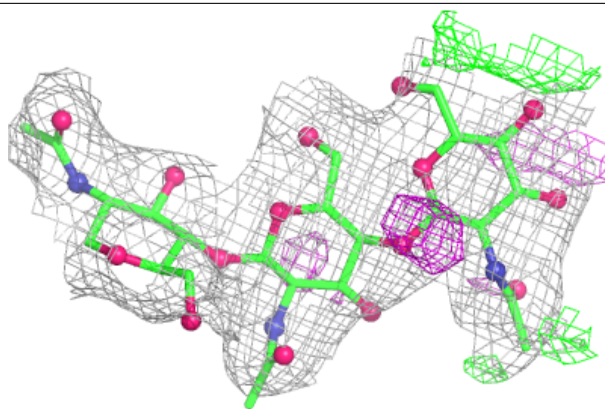
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	N	1	14/15	0.64	0.23	82,88,94,97	0
4	BMA	O	3	11/12	-	-	71,73,75,76	0
4	BMA	O	4	11/12	-	-	59,62,64,65	11
4	BMA	O	5	11/12	-	-	64,67,69,69	11
5	NAG	G	1	14/15	-	-	69,75,77,78	0
5	NAG	G	2	14/15	-	-	53,57,61,62	14
5	BMA	G	3	11/12	-	-	52,54,55,56	11
5	BMA	J	3	11/12	0.65	0.17	64,66,67,67	11
4	NAG	I	2	14/15	0.76	0.16	63,69,79,80	0
6	NAG	K	1	14/15	0.79	0.18	92,96,100,101	0
4	NAG	I	1	14/15	0.81	0.13	59,61,69,69	0
4	NAG	L	1	14/15	0.81	0.21	51,55,59,62	0
5	NAG	P	2	14/15	0.83	0.14	70,73,75,76	14
5	NAG	M	2	14/15	0.84	0.23	70,74,76,76	14
4	NAG	L	2	14/15	0.86	0.24	67,71,76,80	0
4	NAG	O	1	14/15	0.87	0.12	60,62,67,69	0
5	NAG	P	1	14/15	0.89	0.10	80,84,85,85	14
5	NAG	J	2	14/15	0.91	0.15	59,65,65,66	14
5	NAG	J	1	14/15	0.95	0.11	68,75,85,86	14
5	NAG	M	1	14/15	0.96	0.11	75,81,84,84	14

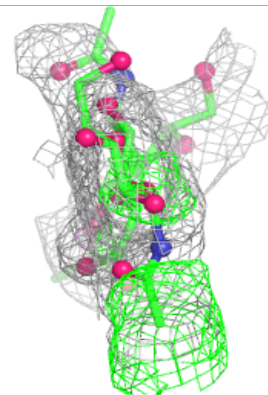
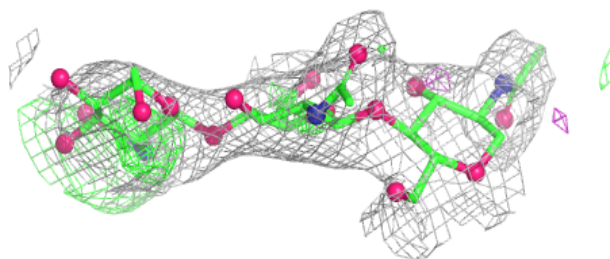
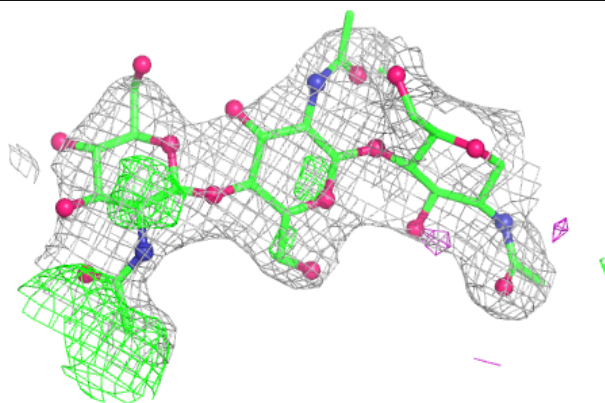
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

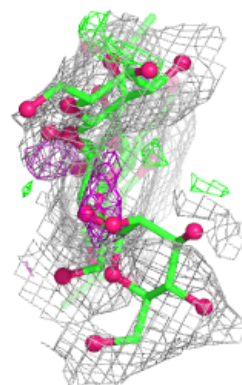
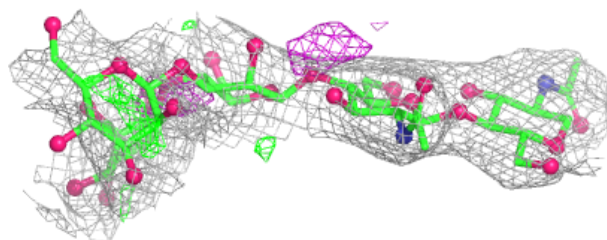
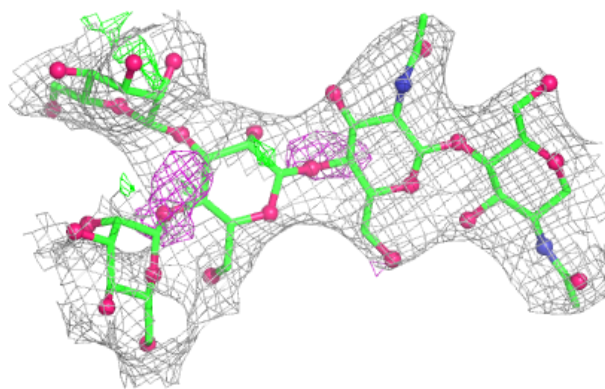
**Electron density around Chain H:**

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



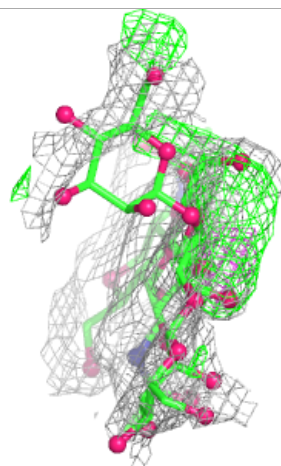
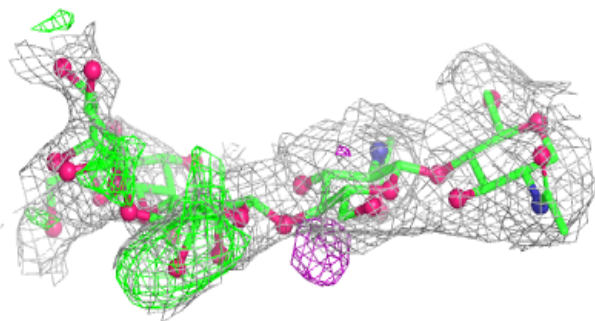
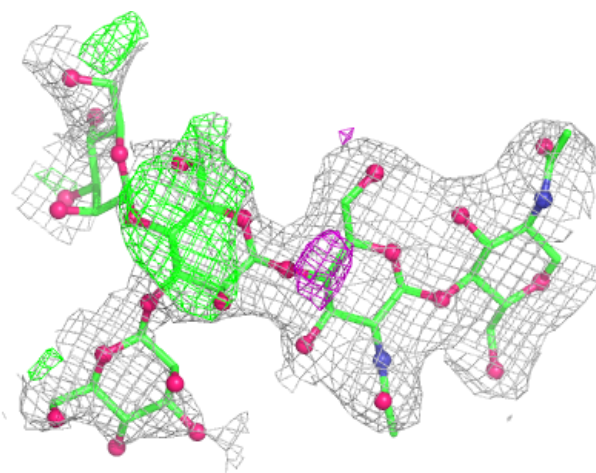
Electron density around Chain F:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



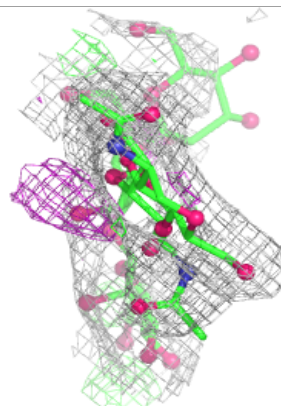
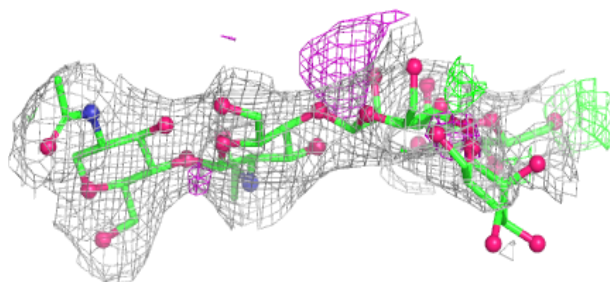
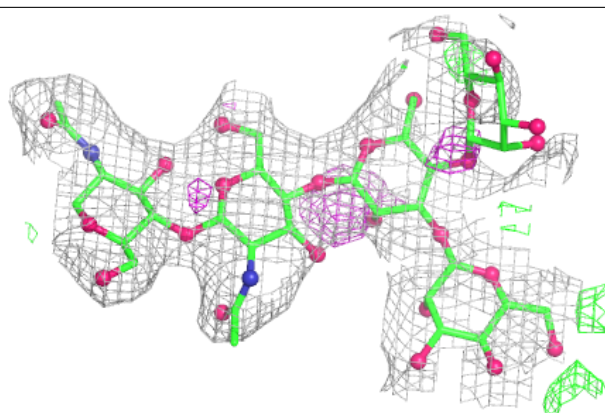
Electron density around Chain I:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

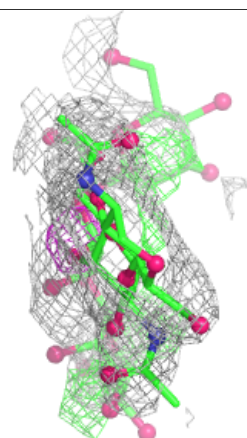
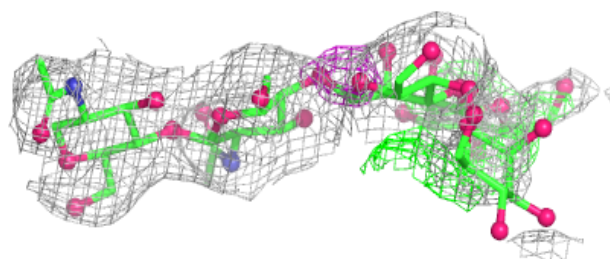
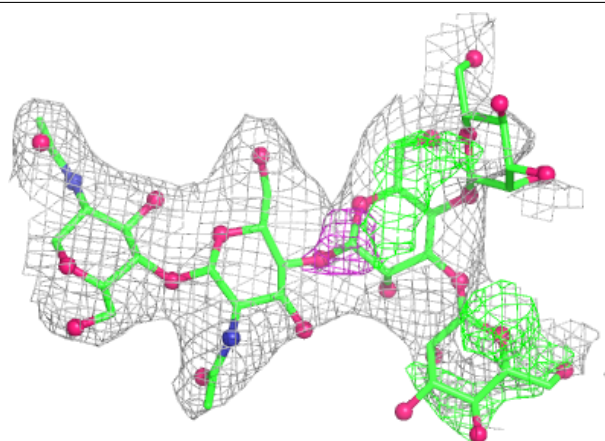


Electron density around Chain L:

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and green (positive)

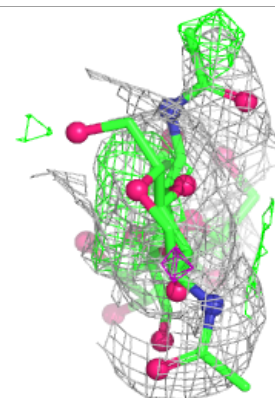
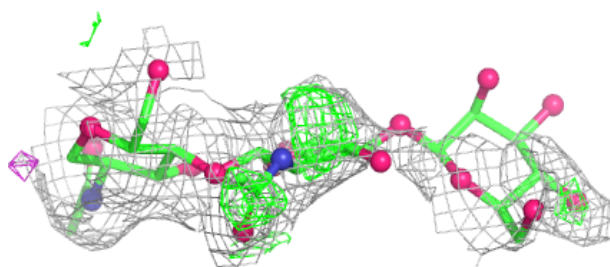
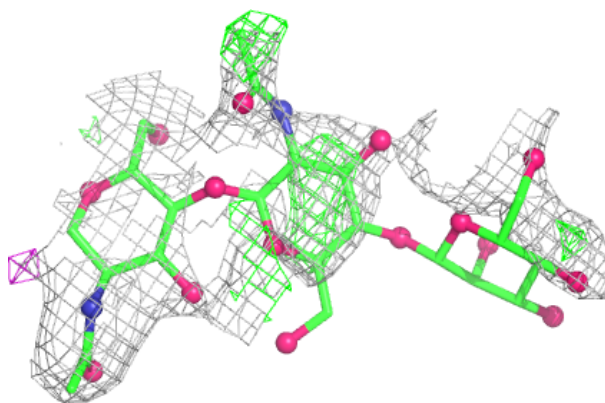
**Electron density around Chain O:**

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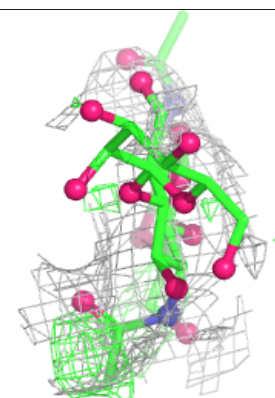
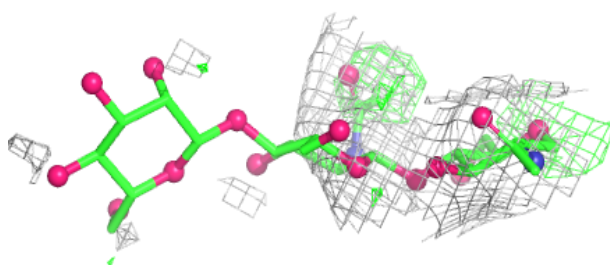
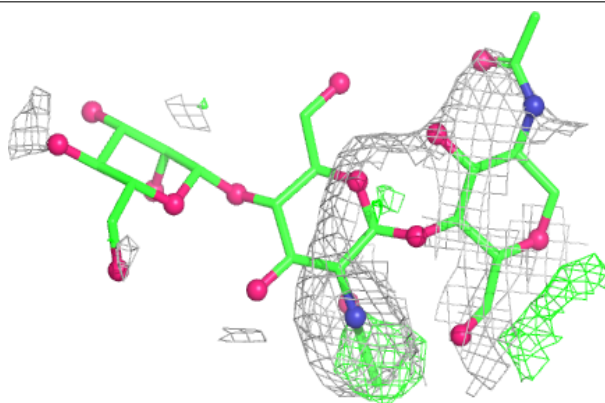


Electron density around Chain G:

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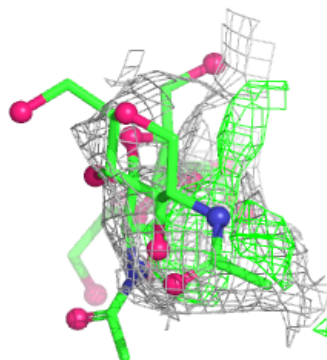
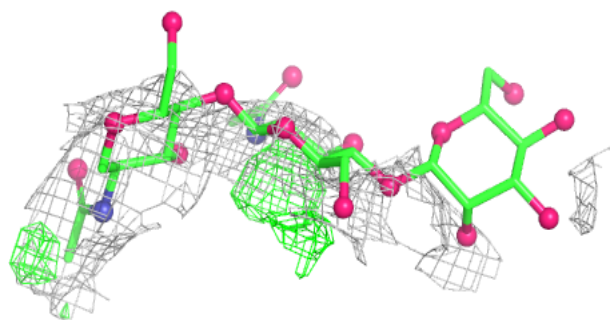
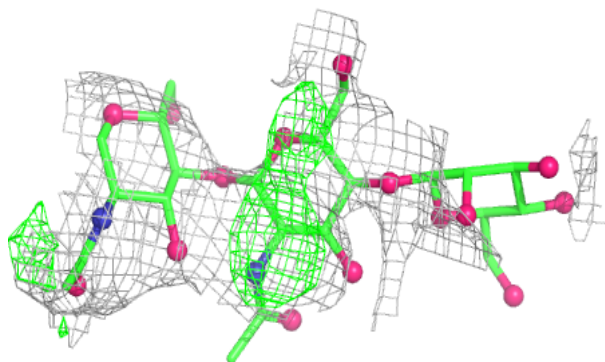
**Electron density around Chain J:**

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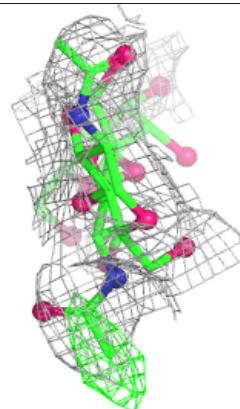
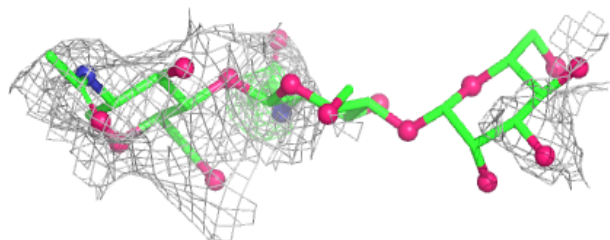
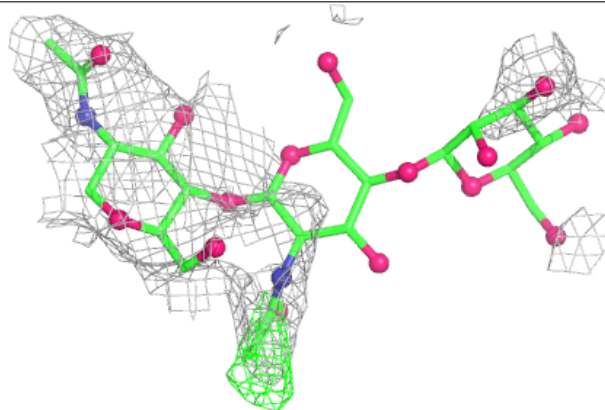


Electron density around Chain M:

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

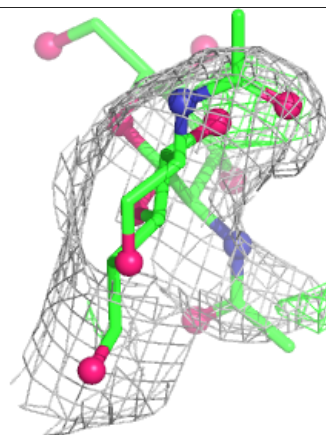
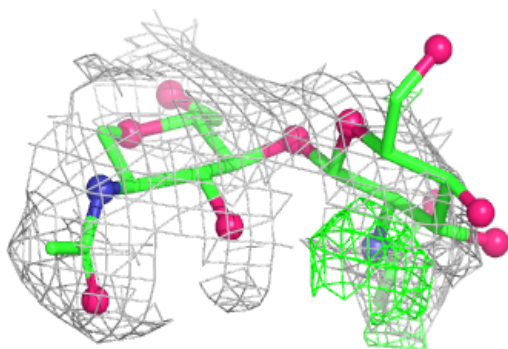
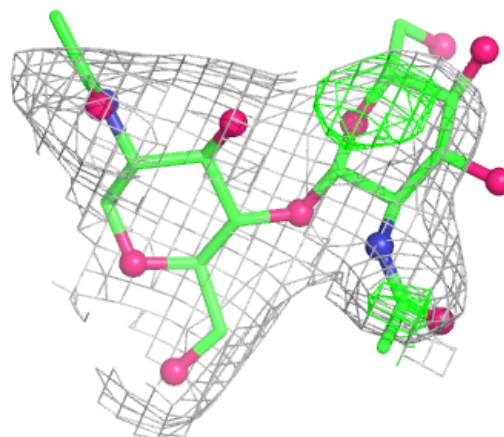
**Electron density around Chain P:**

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

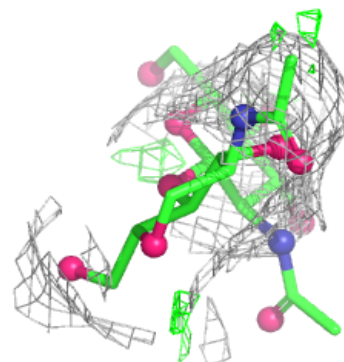
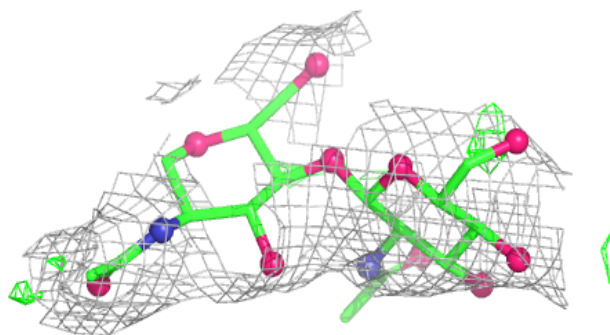
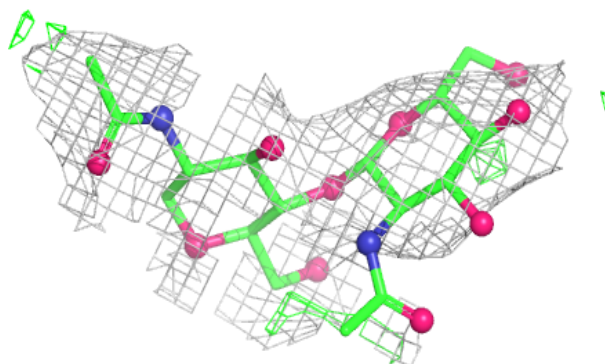


Electron density around Chain K:

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

**Electron density around Chain 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](#)

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
7	NAG	A	340	14/15	0.18	0.87	45,47,51,53	14
8	SO4	A	401	5/5	0.41	0.96	119,120,120,120	5
7	NAG	B	340	14/15	0.69	0.26	60,67,69,69	14
9	CIT	C	403	13/13	0.74	0.29	107,109,110,110	0
7	NAG	C	340	14/15	0.76	0.47	71,73,75,76	14
7	NAG	D	340	14/15	0.76	0.75	70,73,76,77	14
9	CIT	D	404	13/13	0.77	0.28	118,119,120,120	0
8	SO4	Z	402	5/5	0.92	0.37	25,25,26,26	5

6.5 Other polymers [i](#)

There are no such residues in this entry.