



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2023 – 03:15 pm GMT

PDB ID : 8A17
Title : Human PTPRM domains FN3-4, in spacegroup P3221
Authors : Shamin, M.; Graham, S.C.; Sharpe, H.J.; Deane, J.E.
Deposited on : 2022-05-31
Resolution : 3.09 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

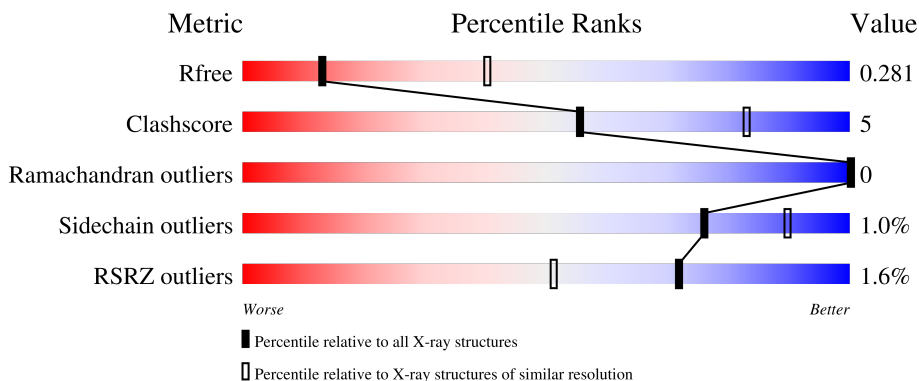
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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.



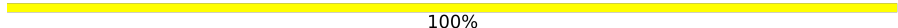
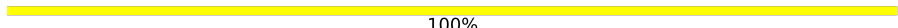
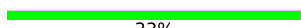
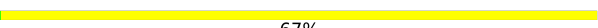
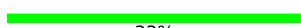
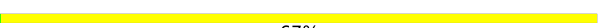
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	258	 82% 12% 5%
1	B	258	 82% 13% 5%
1	C	258	 81% 14% 5% 3%
1	D	258	 82% 12% 6% 2%
2	E	4	 25% 50% 25%

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Mol	Chain	Length	Quality of chain
2	G	4	 100%
2	I	4	 100%
3	F	5	 80%  20%
4	H	3	 33%  67%
4	J	3	 33%  67%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7989 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 Receptor-type tyrosine-protein phosphatase mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	1925	1236	316	369	4	0	0	0
1	B	244	1925	1236	316	369	4	0	0	0
1	C	244	1925	1236	316	369	4	0	0	0
1	D	243	1917	1229	315	369	4	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

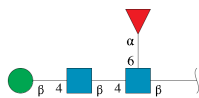
Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLU	-	cloning artifact	UNP P28827
A	476	THR	-	cloning artifact	UNP P28827
A	477	GLY	-	cloning artifact	UNP P28827
A	724	GLY	-	expression tag	UNP P28827
A	725	THR	-	expression tag	UNP P28827
A	726	LYS	-	expression tag	UNP P28827
A	727	HIS	-	expression tag	UNP P28827
A	728	HIS	-	expression tag	UNP P28827
A	729	HIS	-	expression tag	UNP P28827
A	730	HIS	-	expression tag	UNP P28827
A	731	HIS	-	expression tag	UNP P28827
A	732	HIS	-	expression tag	UNP P28827
B	475	GLU	-	cloning artifact	UNP P28827
B	476	THR	-	cloning artifact	UNP P28827
B	477	GLY	-	cloning artifact	UNP P28827
B	724	GLY	-	expression tag	UNP P28827
B	725	THR	-	expression tag	UNP P28827
B	726	LYS	-	expression tag	UNP P28827
B	727	HIS	-	expression tag	UNP P28827
B	728	HIS	-	expression tag	UNP P28827
B	729	HIS	-	expression tag	UNP P28827

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Chain	Residue	Modelled	Actual	Comment	Reference
B	730	HIS	-	expression tag	UNP P28827
B	731	HIS	-	expression tag	UNP P28827
B	732	HIS	-	expression tag	UNP P28827
C	475	GLU	-	cloning artifact	UNP P28827
C	476	THR	-	cloning artifact	UNP P28827
C	477	GLY	-	cloning artifact	UNP P28827
C	724	GLY	-	expression tag	UNP P28827
C	725	THR	-	expression tag	UNP P28827
C	726	LYS	-	expression tag	UNP P28827
C	727	HIS	-	expression tag	UNP P28827
C	728	HIS	-	expression tag	UNP P28827
C	729	HIS	-	expression tag	UNP P28827
C	730	HIS	-	expression tag	UNP P28827
C	731	HIS	-	expression tag	UNP P28827
C	732	HIS	-	expression tag	UNP P28827
D	475	GLU	-	cloning artifact	UNP P28827
D	476	THR	-	cloning artifact	UNP P28827
D	477	GLY	-	cloning artifact	UNP P28827
D	724	GLY	-	expression tag	UNP P28827
D	725	THR	-	expression tag	UNP P28827
D	726	LYS	-	expression tag	UNP P28827
D	727	HIS	-	expression tag	UNP P28827
D	728	HIS	-	expression tag	UNP P28827
D	729	HIS	-	expression tag	UNP P28827
D	730	HIS	-	expression tag	UNP P28827
D	731	HIS	-	expression tag	UNP P28827
D	732	HIS	-	expression tag	UNP P28827

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



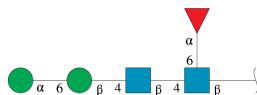
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	4	49	28	2	19	0	0	0
2	G	4	49	28	2	19	0	0	0

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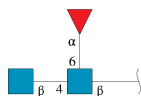
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	4	49	28	2	19	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



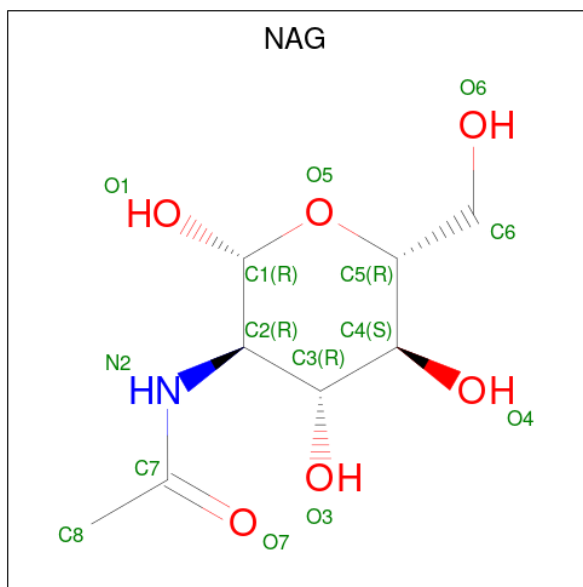
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	5	60	34	2	24	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	3	38	22	2	14	0	0	0
4	J	3	38	22	2	14	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

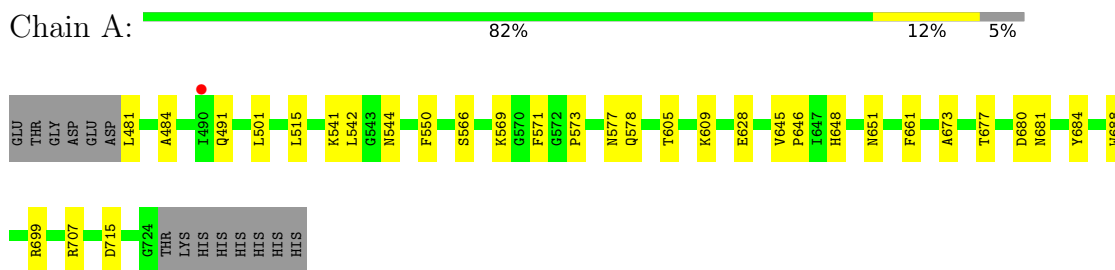


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

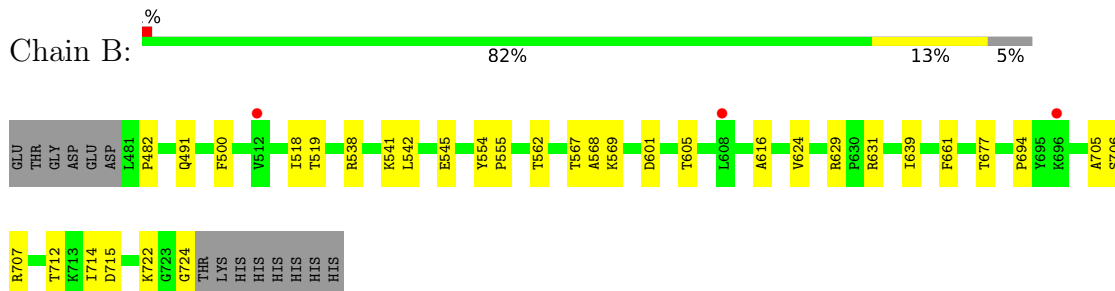
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

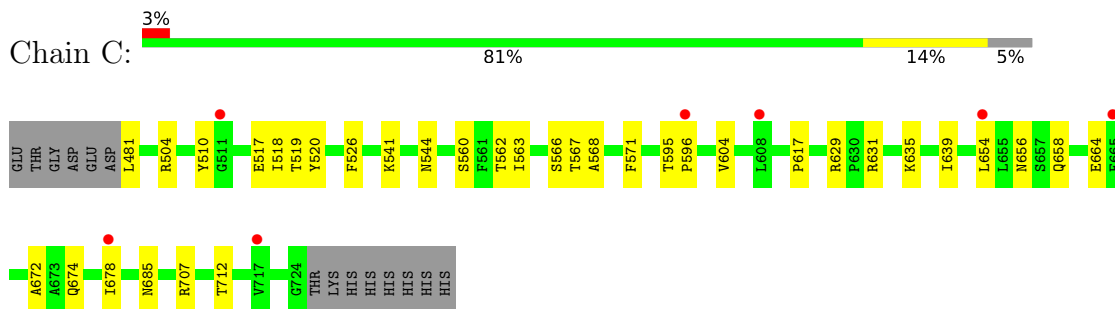
- Molecule 1: Receptor-type tyrosine-protein phosphatase mu



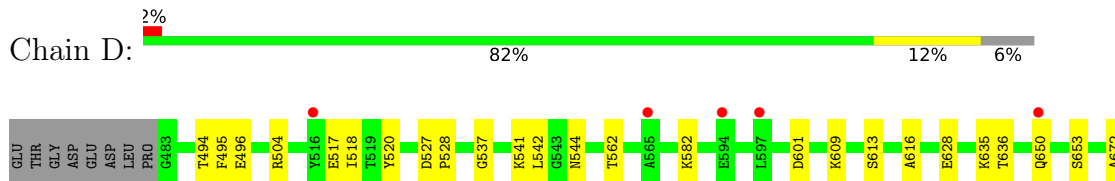
- Molecule 1: Receptor-type tyrosine-protein phosphatase mu



- Molecule 1: Receptor-type tyrosine-protein phosphatase mu



- Molecule 1: Receptor-type tyrosine-protein phosphatase mu





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

Chain E: 25% 50% 25%



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

Chain G: 100%



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

Chain I: 100%



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

Chain F: 80% 20%



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

Chain H: 33% 67%



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

Chain J: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.53Å 87.53Å 311.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.80 – 3.09 75.80 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.0 (75.80-3.09) 89.8 (75.80-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.16 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.243 , 0.290 0.236 , 0.281	Depositor DCC
R_{free} test set	1398 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	91.3	Xtrriage
Anisotropy	0.599	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 82.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7989	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, NAG, MAN, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/1979	0.77	0/2699
1	B	0.57	0/1979	0.79	1/2699 (0.0%)
1	C	0.51	0/1979	0.77	1/2699 (0.0%)
1	D	0.58	0/1970	0.79	1/2686 (0.0%)
All	All	0.56	0/7907	0.78	3/10783 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	542	LEU	CB-CG-CD1	-6.14	100.57	111.00
1	C	654	LEU	CA-CB-CG	5.88	128.81	115.30
1	D	542	LEU	CB-CG-CD1	-5.80	101.14	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1925	0	1877	23	0
1	B	1925	0	1876	26	0
1	C	1925	0	1876	22	0
1	D	1917	0	1865	21	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	49	0	43	1	0
2	G	49	0	43	2	0
2	I	49	0	43	2	0
3	F	60	0	52	0	1
4	H	38	0	34	0	0
4	J	38	0	34	0	0
5	B	14	0	13	0	0
All	All	7989	0	7756	80	1

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 5.

All (80) 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:A:484:ALA:HB2	1:A:573:PRO:HG2	1.55	0.86
1:A:707:ARG:NE	1:B:491:GLN:OE1	2.21	0.74
1:B:707:ARG:HE	1:B:712:THR:HG22	1.55	0.72
1:A:605:THR:OG1	1:A:677:THR:HG22	1.90	0.71
1:B:629:ARG:HH21	1:B:631:ARG:HH12	1.43	0.66
1:A:645:VAL:HG22	1:B:500:PHE:CZ	2.31	0.65
1:C:517:GLU:OE2	1:C:519:THR:HG23	1.97	0.65
1:B:605:THR:OG1	1:B:677:THR:HG22	1.98	0.63
1:A:491:GLN:HB2	1:B:707:ARG:HH22	1.65	0.60
1:B:601:ASP:O	1:B:722:LYS:HE2	2.03	0.58
1:D:544:ASN:ND2	2:I:1:NAG:O7	2.36	0.57
1:B:519:THR:HG22	1:B:538:ARG:HG2	1.87	0.57
1:D:628:GLU:OE2	1:D:699:ARG:NE	2.35	0.57
1:A:648:HIS:N	1:B:545:GLU:OE2	2.25	0.56
1:A:566:SER:HB2	1:A:571:PHE:CD1	2.40	0.55
1:C:664:GLU:O	1:C:685:ASN:ND2	2.33	0.54
1:D:520:TYR:CZ	1:D:537:GLY:HA3	2.44	0.52
1:D:601:ASP:HB3	1:D:694:PRO:HB3	1.91	0.52
1:A:491:GLN:HB2	1:B:707:ARG:NH2	2.25	0.51
1:C:639:ILE:H	1:C:639:ILE:HD12	1.73	0.51
1:A:688:TRP:O	1:A:688:TRP:CD1	2.64	0.51
1:D:495:PHE:O	1:D:582:LYS:N	2.43	0.51
1:B:518:ILE:HA	1:B:562:THR:O	2.10	0.50
1:C:566:SER:HB2	1:C:571:PHE:CD1	2.47	0.50
1:C:707:ARG:HG2	1:C:712:THR:HG22	1.94	0.50
1:D:707:ARG:HE	1:D:712:THR:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ASP:OD2	1:A:684:TYR:OH	2.26	0.50
1:D:494:THR:OG1	1:D:582:LYS:HE2	2.12	0.50
1:B:554:TYR:CG	1:B:555:PRO:HD2	2.47	0.49
1:D:650:GLN:HB3	2:G:1:NAG:H5	1.92	0.49
1:A:628:GLU:OE2	1:A:699:ARG:NE	2.40	0.49
1:B:519:THR:OG1	1:B:562:THR:HB	2.14	0.48
1:A:681:ASN:OD1	1:A:688:TRP:NE1	2.45	0.48
1:D:707:ARG:HG2	1:D:712:THR:HB	1.96	0.48
1:B:482:PRO:HG3	1:B:567:THR:H	1.79	0.47
1:A:577:ASN:OD1	1:A:578:GLN:N	2.44	0.47
1:A:544:ASN:HD22	2:E:1:NAG:C7	2.28	0.47
1:B:567:THR:HG22	1:B:569:LYS:H	1.80	0.46
1:D:613:SER:HB2	1:D:616:ALA:O	2.15	0.46
1:B:705:ALA:HB2	1:B:714:ILE:HG22	1.96	0.46
1:C:629:ARG:HH21	1:C:631:ARG:HH12	1.64	0.46
1:B:694:PRO:O	1:B:724:GLY:HA2	2.16	0.45
1:C:520:TYR:HA	1:C:560:SER:O	2.16	0.45
1:D:544:ASN:ND2	2:I:1:NAG:C7	2.80	0.45
1:A:481:LEU:HD11	1:A:569:LYS:O	2.17	0.45
1:B:629:ARG:NH2	1:B:631:ARG:HH12	2.12	0.45
1:C:504:ARG:NH2	1:D:685:ASN:HA	2.31	0.44
1:C:517:GLU:O	1:C:563:ILE:HA	2.17	0.44
1:C:629:ARG:NH1	1:C:658:GLN:OE1	2.51	0.44
1:B:707:ARG:HE	1:B:712:THR:CG2	2.27	0.44
1:A:651:ASN:ND2	1:B:545:GLU:HG2	2.32	0.44
1:C:604:VAL:O	1:C:678:ILE:N	2.50	0.43
1:B:624:VAL:HG22	1:B:661:PHE:CE1	2.53	0.43
1:C:566:SER:HB2	1:C:571:PHE:HD1	1.83	0.43
1:A:715:ASP:OD1	1:C:635:LYS:HE3	2.19	0.43
1:C:518:ILE:HA	1:C:562:THR:O	2.18	0.43
1:A:501:LEU:HA	1:A:501:LEU:HD12	1.79	0.43
1:A:542:LEU:HA	1:A:542:LEU:HD13	1.81	0.43
1:D:518:ILE:HA	1:D:562:THR:O	2.19	0.43
1:D:672:ALA:O	1:D:674:GLN:HG3	2.19	0.43
1:B:567:THR:HG22	1:B:568:ALA:N	2.34	0.43
1:B:629:ARG:HE	1:B:631:ARG:CZ	2.32	0.42
1:B:715:ASP:OD1	1:D:635:LYS:HE3	2.19	0.42
1:C:526:PHE:O	1:C:617:PRO:HD3	2.20	0.42
1:C:685:ASN:HA	1:D:504:ARG:NH2	2.35	0.42
1:C:685:ASN:OD1	1:D:504:ARG:NH1	2.52	0.42
1:B:639:ILE:HG23	1:D:636:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HB3	1:A:542:LEU:HD13	2.00	0.42
1:C:567:THR:HG22	1:C:568:ALA:N	2.35	0.42
1:A:646:PRO:HA	1:A:661:PHE:CZ	2.55	0.42
1:C:544:ASN:ND2	2:G:1:NAG:O7	2.51	0.41
1:D:707:ARG:HE	1:D:712:THR:CG2	2.33	0.41
1:D:496:GLU:HA	1:D:582:LYS:O	2.19	0.41
1:C:672:ALA:O	1:C:674:GLN:HG3	2.20	0.41
1:A:501:LEU:HB3	1:A:550:PHE:HE1	1.86	0.41
1:A:609:LYS:HG2	1:A:673:ALA:HB2	2.03	0.41
1:C:481:LEU:HD11	1:C:571:PHE:O	2.21	0.41
1:B:616:ALA:HB3	1:B:706:SER:HB3	2.02	0.41
1:D:527:ASP:OD1	1:D:528:PRO:HD2	2.22	0.40
1:C:595:THR:HG23	1:C:596:PRO:HD2	2.03	0.40

All (1) 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:D:653:SER:O	3:F:5:FUC:O4[6_454]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/258 (94%)	238 (98%)	4 (2%)	0	100	100
1	B	242/258 (94%)	239 (99%)	3 (1%)	0	100	100
1	C	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
1	D	241/258 (93%)	235 (98%)	6 (2%)	0	100	100
All	All	967/1032 (94%)	947 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/223 (94%)	209 (100%)	1 (0%)	88	94
1	B	210/223 (94%)	209 (100%)	1 (0%)	88	94
1	C	210/223 (94%)	207 (99%)	3 (1%)	67	86
1	D	209/223 (94%)	206 (99%)	3 (1%)	67	86
All	All	839/892 (94%)	831 (99%)	8 (1%)	76	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	541	LYS
1	B	541	LYS
1	C	510	TYR
1	C	541	LYS
1	C	656	ASN
1	D	517	GLU
1	D	541	LYS
1	D	609	LYS

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

Mol	Chain	Res	Type
1	A	651	ASN
1	A	718	GLN
1	B	718	GLN
1	C	718	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

23 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
2	NAG	E	1	2,1	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
2	NAG	E	2	2	14,14,15	0.41	0	17,19,21	0.81	0
2	BMA	E	3	2	11,11,12	1.34	2 (18%)	15,15,17	1.65	2 (13%)
2	FUC	E	4	2	10,10,11	1.59	2 (20%)	14,14,16	1.23	1 (7%)
3	NAG	F	1	1,3	14,14,15	0.47	0	17,19,21	0.95	2 (11%)
3	NAG	F	2	3	14,14,15	1.45	1 (7%)	17,19,21	1.35	2 (11%)
3	BMA	F	3	3	11,11,12	1.42	1 (9%)	15,15,17	1.13	2 (13%)
3	MAN	F	4	3	11,11,12	2.05	3 (27%)	15,15,17	1.88	4 (26%)
3	FUC	F	5	3	10,10,11	1.71	4 (40%)	14,14,16	1.22	2 (14%)
2	NAG	G	1	2,1	14,14,15	0.34	0	17,19,21	0.68	0
2	NAG	G	2	2	14,14,15	1.02	2 (14%)	17,19,21	0.99	1 (5%)
2	BMA	G	3	2	11,11,12	1.40	2 (18%)	15,15,17	1.42	1 (6%)
2	FUC	G	4	2	10,10,11	1.65	3 (30%)	14,14,16	1.18	1 (7%)
4	NAG	H	1	4,1	14,14,15	0.51	0	17,19,21	0.68	0
4	NAG	H	2	4	14,14,15	1.07	2 (14%)	17,19,21	0.71	0
4	FUC	H	3	4	10,10,11	1.40	1 (10%)	14,14,16	0.89	0
2	NAG	I	1	2,1	14,14,15	0.41	0	17,19,21	0.88	0
2	NAG	I	2	2	14,14,15	1.28	2 (14%)	17,19,21	0.88	1 (5%)
2	BMA	I	3	2	11,11,12	2.19	4 (36%)	15,15,17	1.14	1 (6%)
2	FUC	I	4	2	10,10,11	1.54	1 (10%)	14,14,16	1.11	0
4	NAG	J	1	4,1	14,14,15	0.45	0	17,19,21	0.41	0
4	NAG	J	2	4	14,14,15	0.65	1 (7%)	17,19,21	1.23	1 (5%)
4	FUC	J	3	4	10,10,11	1.50	2 (20%)	14,14,16	1.19	1 (7%)

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
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	FUC	E	4	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	FUC	F	5	3	-	-	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
2	FUC	G	4	2	-	-	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	FUC	I	4	2	-	-	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	-4.99	1.35	1.43
3	F	4	MAN	C1-C2	4.95	1.63	1.52
2	I	3	BMA	C2-C3	4.27	1.58	1.52
2	I	4	FUC	C2-C3	3.76	1.58	1.52
2	I	2	NAG	O5-C1	3.67	1.49	1.43
3	F	3	BMA	C1-C2	3.40	1.59	1.52
2	G	4	FUC	C1-C2	3.35	1.59	1.52
2	I	3	BMA	O5-C5	3.35	1.50	1.43
3	F	4	MAN	C2-C3	3.17	1.57	1.52
2	E	4	FUC	C2-C3	3.15	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NAG	C1-C2	3.05	1.56	1.52
2	I	3	BMA	C4-C3	3.03	1.60	1.52
4	J	3	FUC	C4-C5	2.95	1.59	1.52
2	I	3	BMA	O5-C1	2.90	1.48	1.43
2	I	2	NAG	C1-C2	2.77	1.56	1.52
3	F	5	FUC	C6-C5	2.64	1.57	1.51
2	G	4	FUC	C2-C3	2.54	1.56	1.52
2	G	2	NAG	C1-C2	2.52	1.56	1.52
2	G	2	NAG	O5-C1	2.47	1.47	1.43
3	F	4	MAN	O5-C1	2.36	1.47	1.43
4	H	2	NAG	O5-C1	2.32	1.47	1.43
4	H	3	FUC	C1-C2	2.31	1.57	1.52
3	F	5	FUC	O5-C1	2.31	1.47	1.43
3	F	5	FUC	C2-C3	2.30	1.55	1.52
2	G	3	BMA	C2-C3	2.25	1.55	1.52
2	E	3	BMA	C4-C3	2.21	1.58	1.52
4	J	3	FUC	C1-C2	2.20	1.57	1.52
2	E	4	FUC	C1-C2	2.13	1.57	1.52
2	E	3	BMA	C1-C2	2.12	1.57	1.52
3	F	5	FUC	C4-C3	2.09	1.57	1.52
4	J	2	NAG	O5-C1	2.06	1.47	1.43
2	G	4	FUC	O3-C3	2.01	1.47	1.43
2	G	3	BMA	C1-C2	2.00	1.56	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	4.51	118.31	112.19
3	F	4	MAN	C1-C2-C3	4.22	114.85	109.67
2	G	3	BMA	C1-O5-C5	4.21	117.90	112.19
4	J	2	NAG	C1-O5-C5	3.74	117.25	112.19
2	E	1	NAG	O4-C4-C3	-3.11	103.16	110.35
2	G	4	FUC	O2-C2-C1	3.00	115.29	109.15
3	F	2	NAG	C4-C3-C2	2.93	115.32	111.02
3	F	2	NAG	C1-O5-C5	-2.88	108.29	112.19
3	F	4	MAN	C1-O5-C5	2.82	116.02	112.19
2	E	3	BMA	C1-C2-C3	2.77	113.07	109.67
2	E	4	FUC	C1-C2-C3	2.76	113.06	109.67
2	I	3	BMA	O5-C5-C6	2.74	111.51	107.20
3	F	4	MAN	O5-C1-C2	2.68	114.90	110.77
3	F	5	FUC	C1-C2-C3	2.56	112.82	109.67
4	J	3	FUC	O5-C1-C2	2.41	114.49	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	O2-C2-C3	-2.41	105.32	110.14
2	I	2	NAG	C2-N2-C7	2.36	126.26	122.90
3	F	4	MAN	O2-C2-C1	2.35	113.95	109.15
3	F	3	BMA	O2-C2-C1	2.31	113.89	109.15
3	F	1	NAG	O4-C4-C3	-2.28	105.08	110.35
2	G	2	NAG	O4-C4-C5	-2.27	103.65	109.30
3	F	1	NAG	O3-C3-C2	2.08	113.78	109.47
3	F	5	FUC	C1-O5-C5	2.05	117.42	112.78

There are no chirality outliers.

All (18) torsion outliers are listed below:

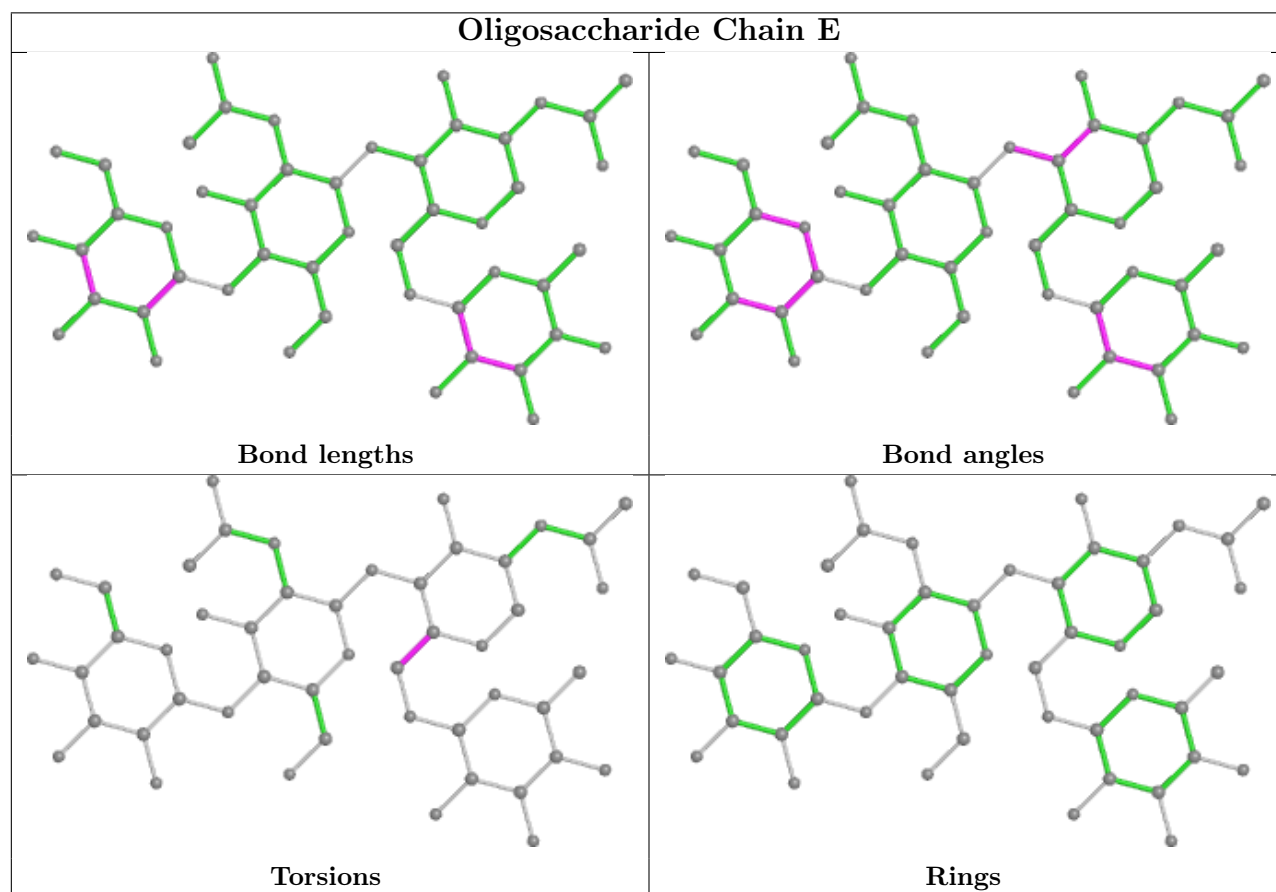
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
2	I	3	BMA	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
4	H	2	NAG	C3-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6

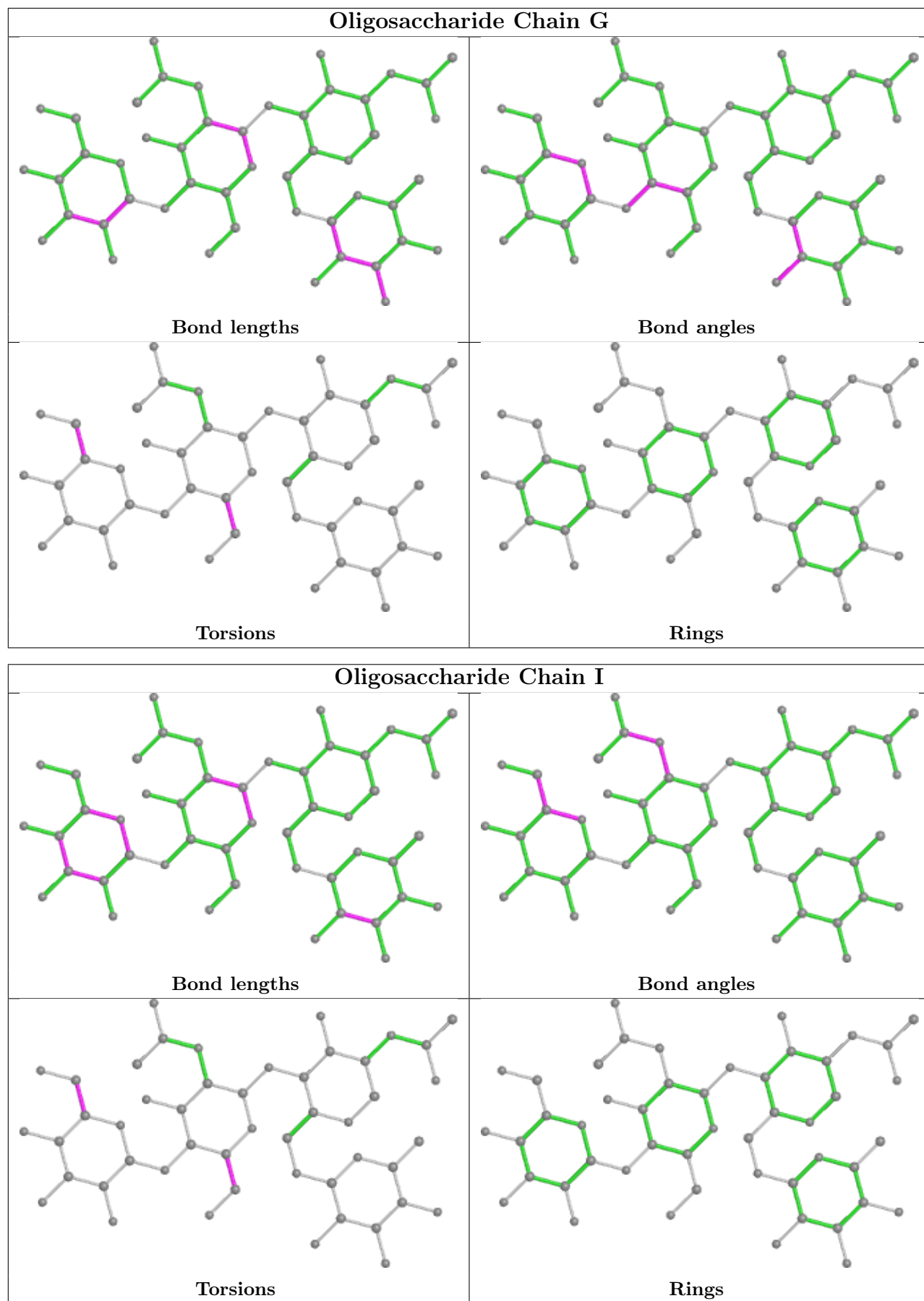
There are no ring outliers.

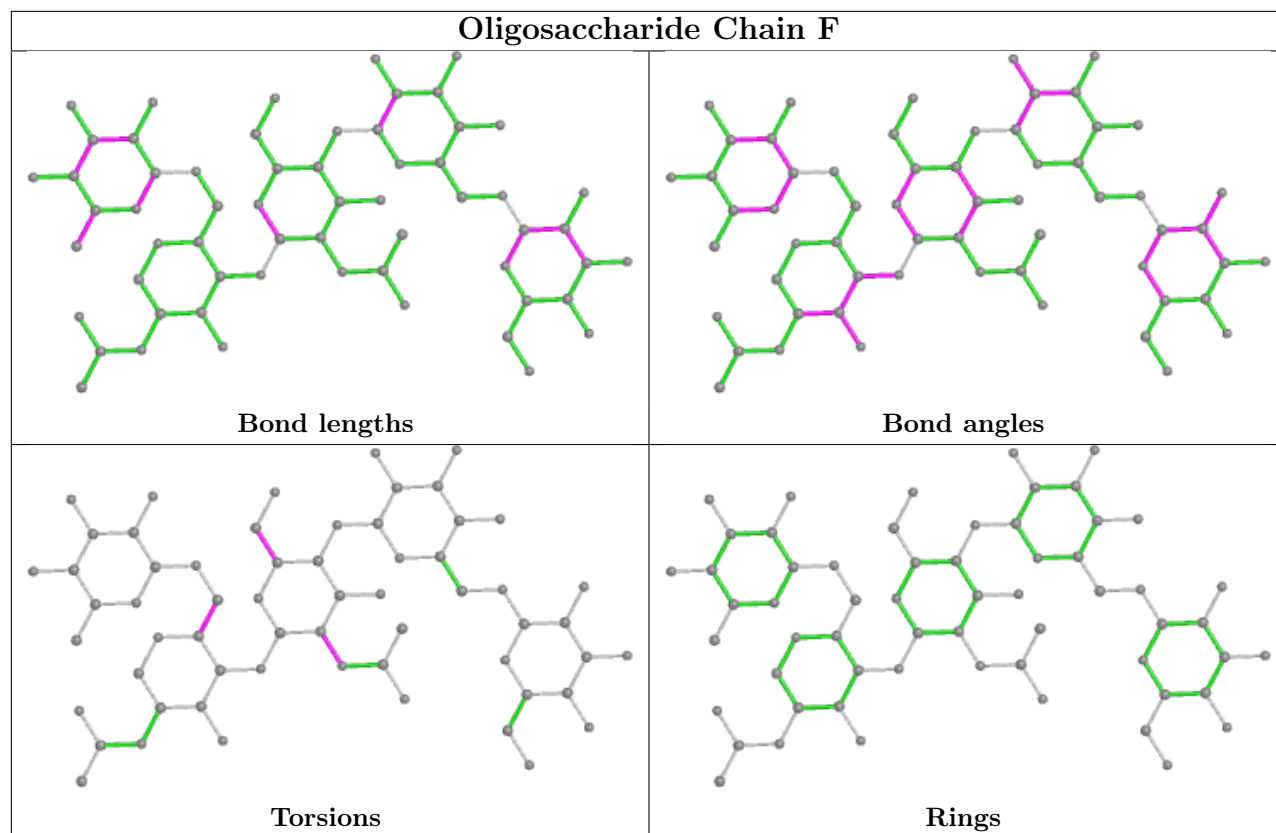
4 monomers are involved in 6 short contacts:

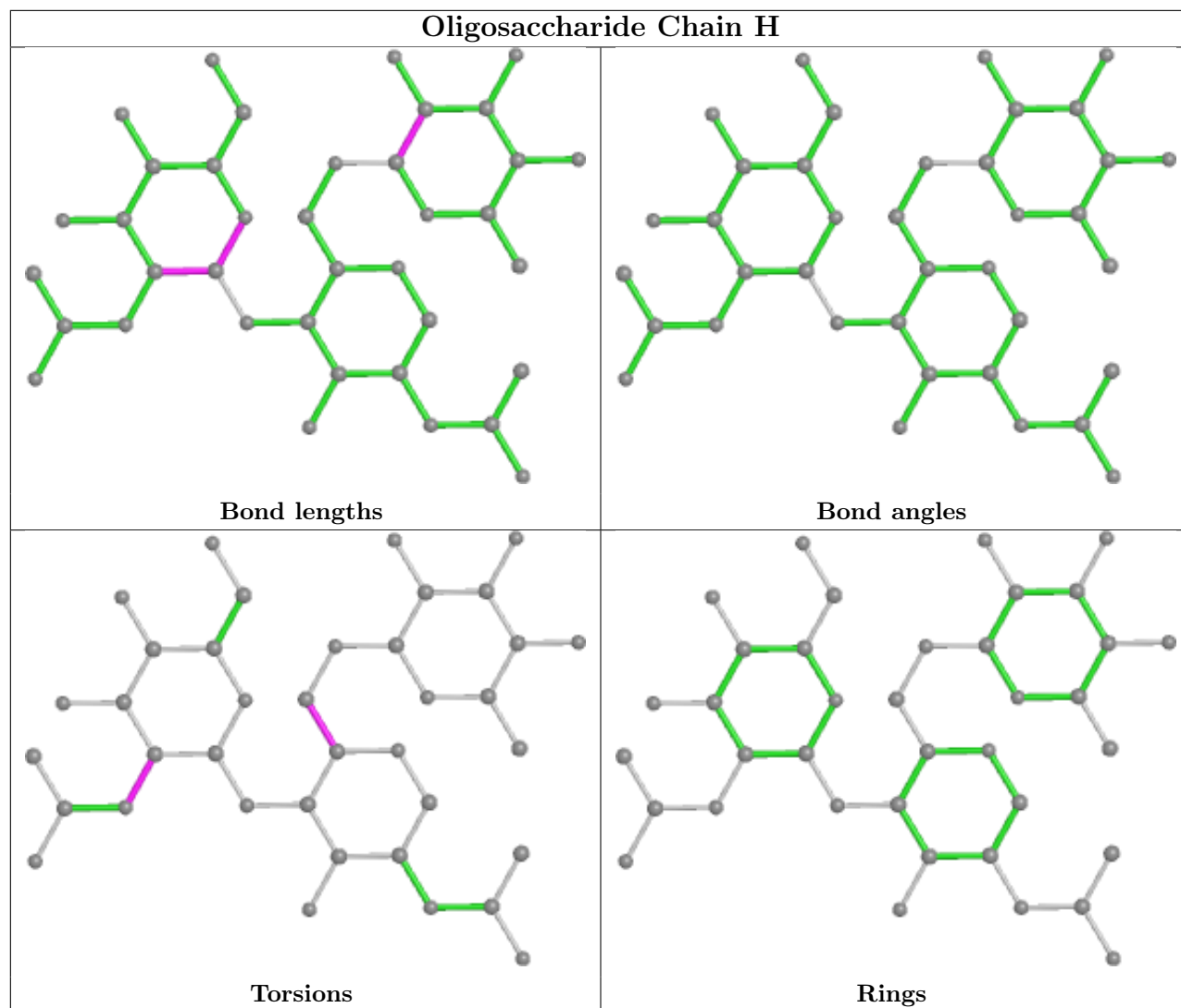
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	0
2	E	1	NAG	1	0
2	I	1	NAG	2	0
3	F	5	FUC	0	1

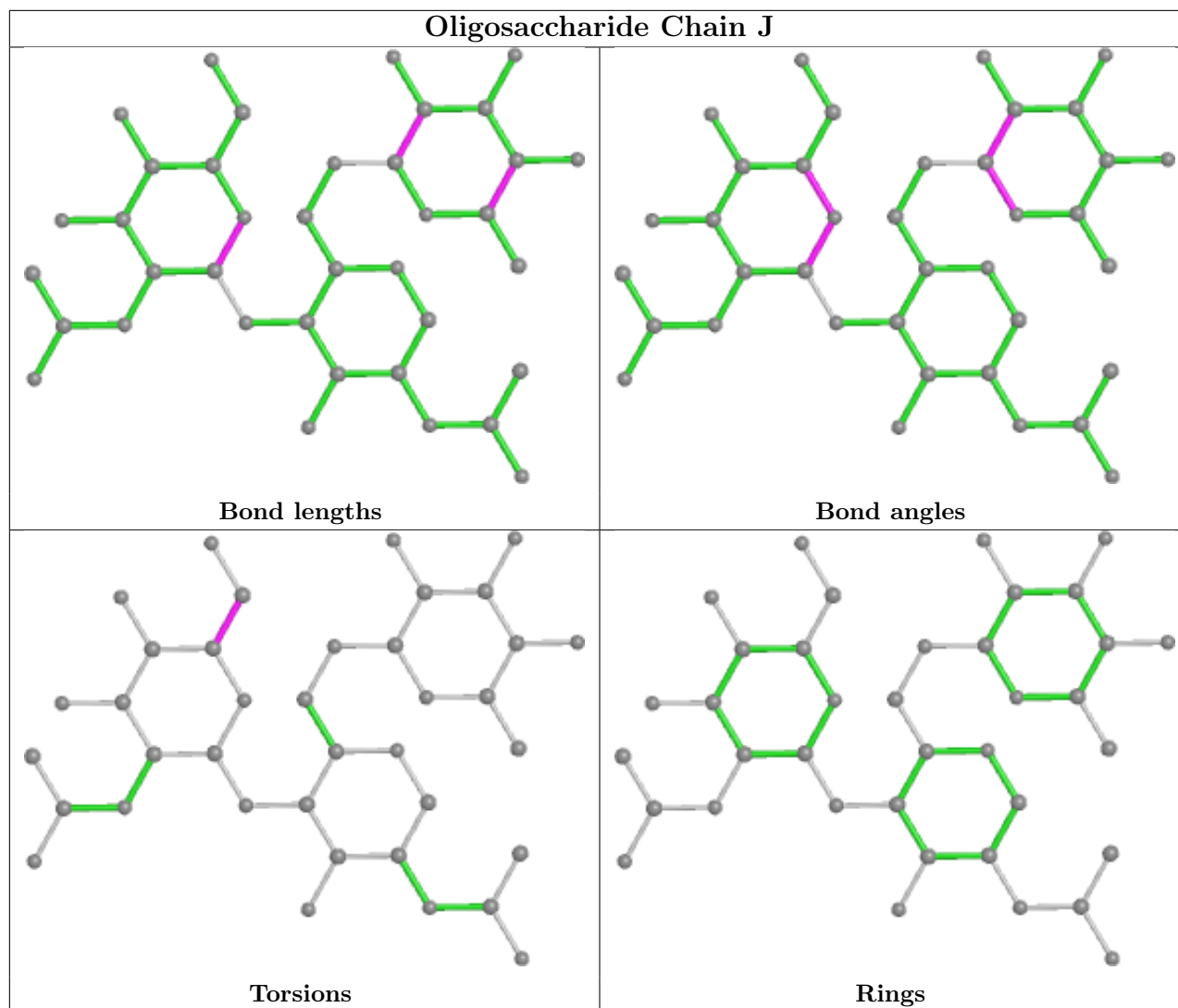
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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
5	NAG	B	801	1	14,14,15	1.78	1 (7%)	17,19,21	1.10	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	801	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	NAG	O5-C1	6.52	1.54	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	NAG	C1-O5-C5	4.05	117.67	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	NAG	C4-C5-C6-O6
5	B	801	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	244/258 (94%)	0.22	1 (0%) 92 84	73, 109, 143, 163	0
1	B	244/258 (94%)	0.26	3 (1%) 79 61	73, 107, 138, 190	0
1	C	244/258 (94%)	0.32	7 (2%) 51 28	76, 117, 155, 193	0
1	D	243/258 (94%)	0.39	5 (2%) 63 43	77, 109, 143, 183	0
All	All	975/1032 (94%)	0.30	16 (1%) 72 51	73, 110, 148, 193	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	597	LEU	3.6
1	D	594	GLU	3.1
1	C	654	LEU	2.9
1	C	665	PHE	2.5
1	D	516	TYR	2.4
1	C	511	GLY	2.3
1	C	678	ILE	2.3
1	C	717	VAL	2.2
1	B	608	LEU	2.2
1	A	490	ILE	2.2
1	C	596	PRO	2.1
1	B	696	LYS	2.1
1	C	608	LEU	2.1
1	B	512	VAL	2.1
1	D	650	GLN	2.0
1	D	565	ALA	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

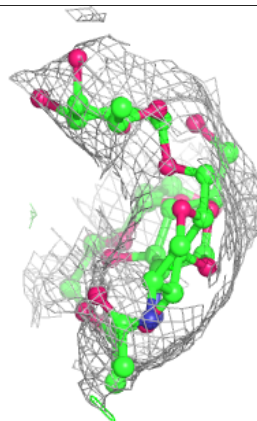
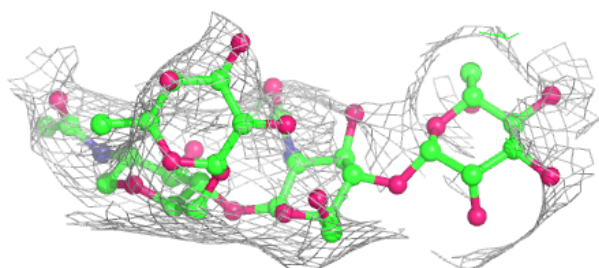
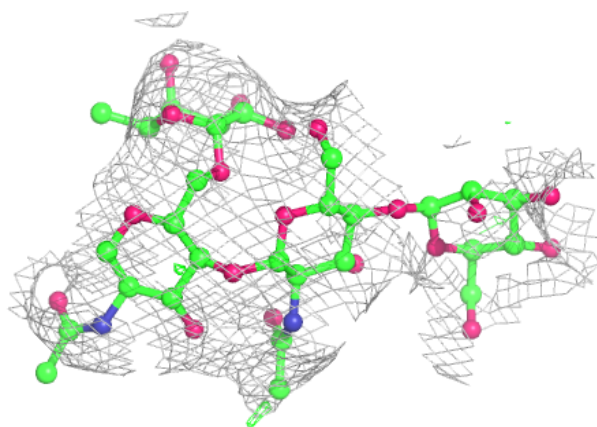
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	J	2	14/15	0.61	0.30	142,152,156,158	0
2	BMA	E	3	11/12	0.65	0.23	149,161,166,169	0
2	BMA	I	3	11/12	0.69	0.26	144,151,163,165	0
2	NAG	I	2	14/15	0.69	0.28	129,141,145,152	0
4	NAG	H	2	14/15	0.70	0.34	155,164,166,168	0
4	FUC	H	3	10/11	0.76	0.27	154,157,163,165	0
4	FUC	J	3	10/11	0.76	0.26	130,142,147,149	0
3	MAN	F	4	11/12	0.79	0.17	136,148,154,157	0
2	BMA	G	3	11/12	0.80	0.20	144,153,158,161	0
3	BMA	F	3	11/12	0.85	0.12	143,147,152,160	0
2	NAG	G	2	14/15	0.85	0.17	129,136,141,148	0
4	NAG	H	1	14/15	0.86	0.17	146,153,158,160	0
2	NAG	E	2	14/15	0.87	0.14	124,137,149,155	0
2	FUC	G	4	10/11	0.88	0.31	110,123,132,134	0
3	NAG	F	2	14/15	0.88	0.19	110,123,129,134	0
2	FUC	E	4	10/11	0.88	0.28	128,133,140,141	0
3	FUC	F	5	10/11	0.89	0.40	101,110,114,121	0
2	FUC	I	4	10/11	0.89	0.24	113,118,124,133	0
4	NAG	J	1	14/15	0.91	0.24	131,136,142,145	0
3	NAG	F	1	14/15	0.93	0.25	79,93,107,108	0
2	NAG	I	1	14/15	0.94	0.19	96,101,120,121	0
2	NAG	G	1	14/15	0.94	0.21	105,116,124,125	0
2	NAG	E	1	14/15	0.94	0.24	110,118,126,128	0

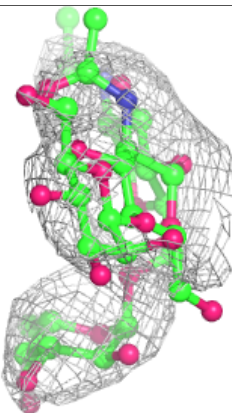
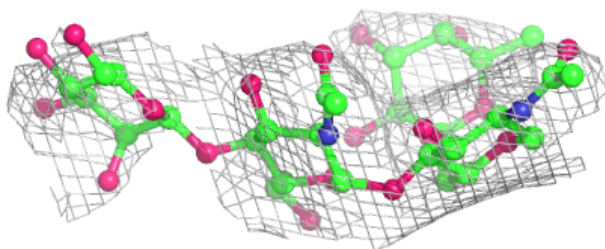
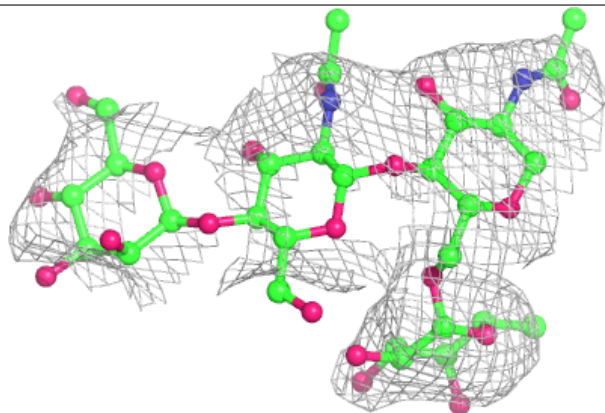
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

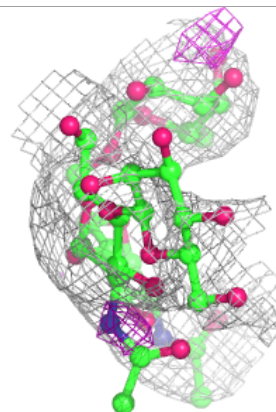
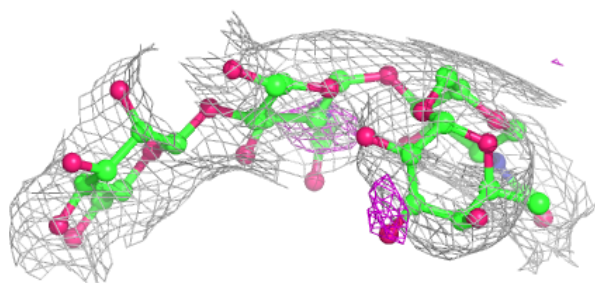
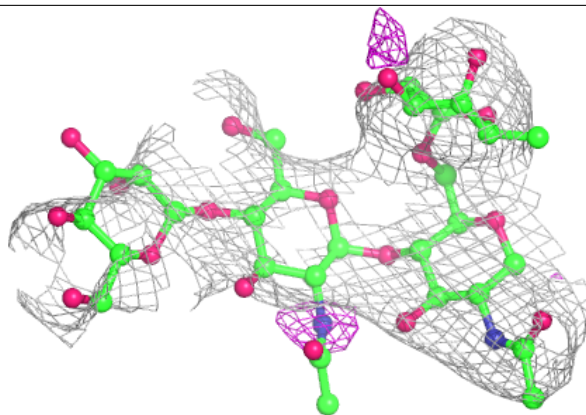
**Electron density around Chain G:**

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

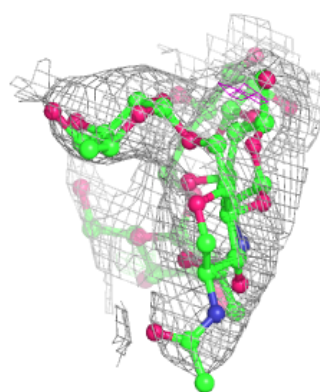
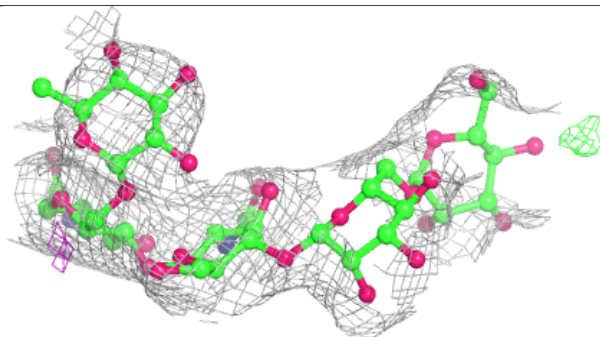
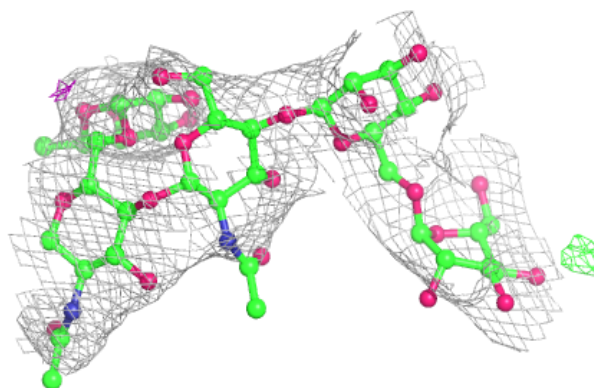


Electron density around Chain I:

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

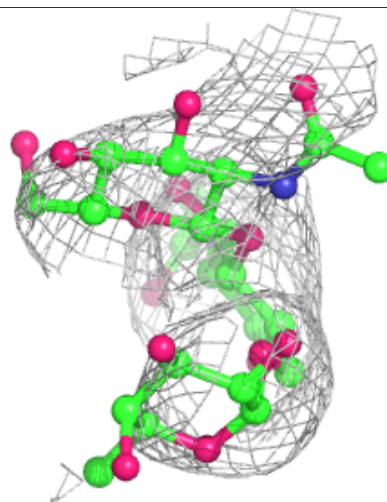
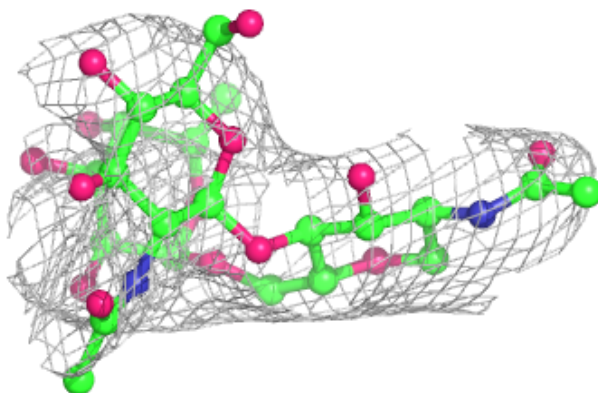
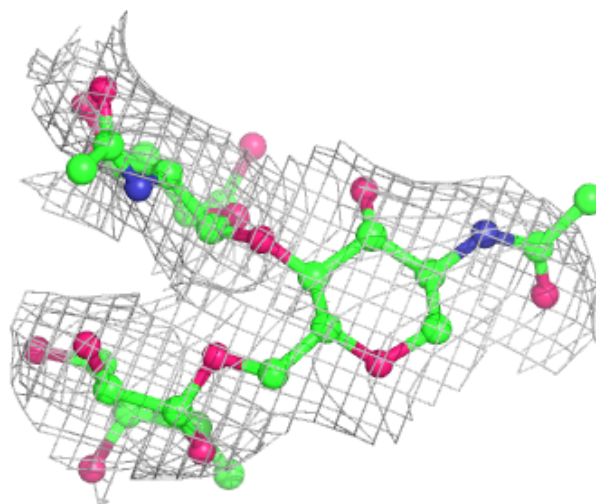
**Electron density around Chain F:**

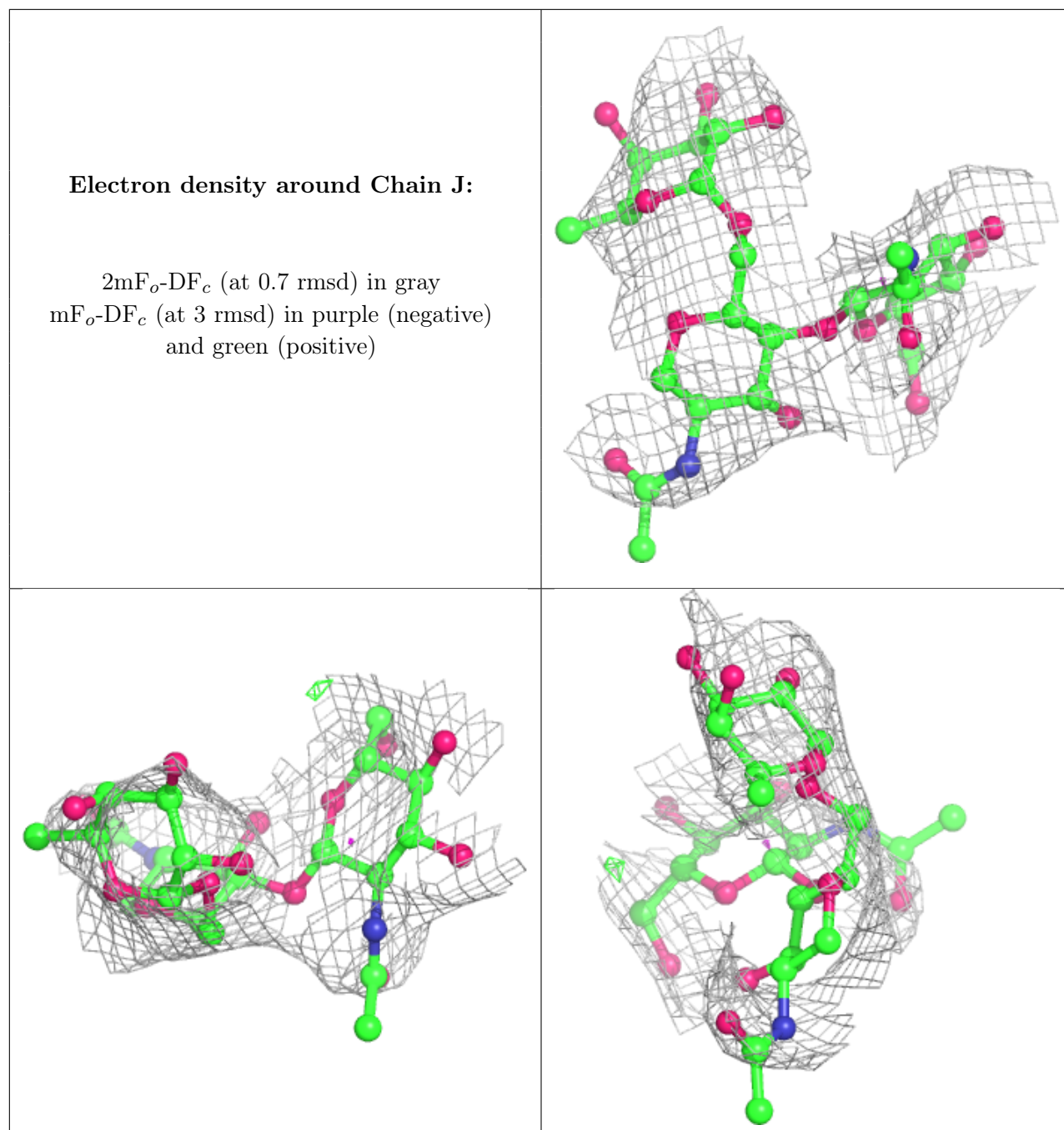
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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(\AA^2)	Q<0.9
5	NAG	B	801	14/15	0.78	0.21	120,130,134,135	0

6.5 Other polymers [i](#)

There are no such residues in this entry.