



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:14 AM BST

PDB ID : 6S0A
Title : Crystal Structure of Properdin (TSR domains N12 & 456)
Authors : van den Bos, R.M.; Pearce, N.M.; Gros, P.
Deposited on : 2019-06-14
Resolution : 2.52 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

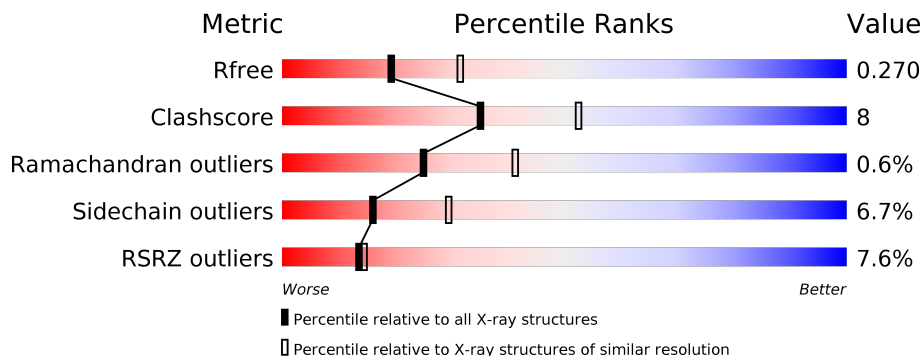
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	
2	B	166	
3	C	2	
3	E	2	
4	D	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	NAG	D	1	-	-	-	X
4	NAG	D	2	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2906 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 Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1557	962	289	284	22	0	0	0

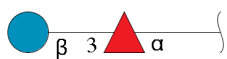
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP P27918
A	255	SER	-	expression tag	UNP P27918
A	470	ALA	-	expression tag	UNP P27918
A	471	ALA	-	expression tag	UNP P27918
A	472	ALA	-	expression tag	UNP P27918
A	473	HIS	-	expression tag	UNP P27918
A	474	HIS	-	expression tag	UNP P27918
A	475	HIS	-	expression tag	UNP P27918
A	476	HIS	-	expression tag	UNP P27918
A	477	HIS	-	expression tag	UNP P27918
A	478	HIS	-	expression tag	UNP P27918

- Molecule 2 is a protein called Properdin.

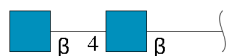
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	1148	697	210	221	20	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



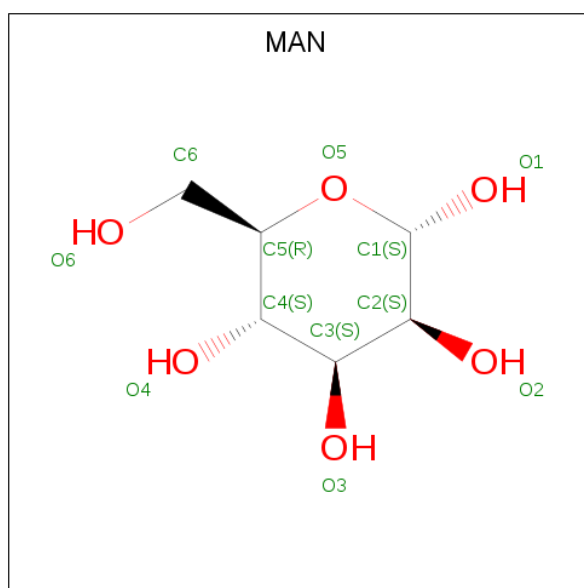
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			21	12	9			
3	E	2	Total	C	O	0	0	0
			21	12	9			

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



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

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



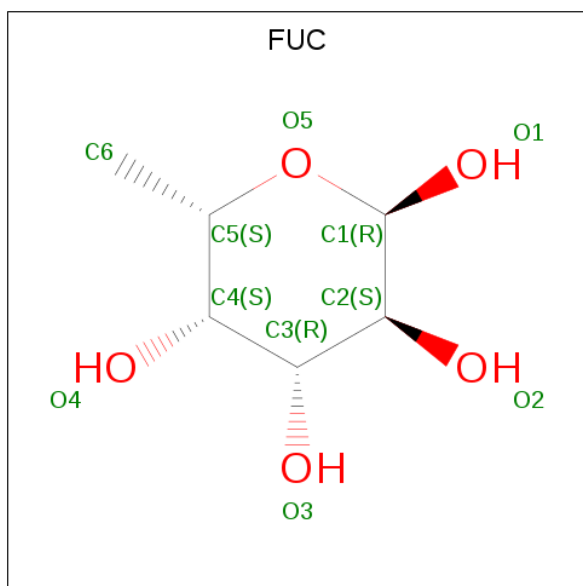
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

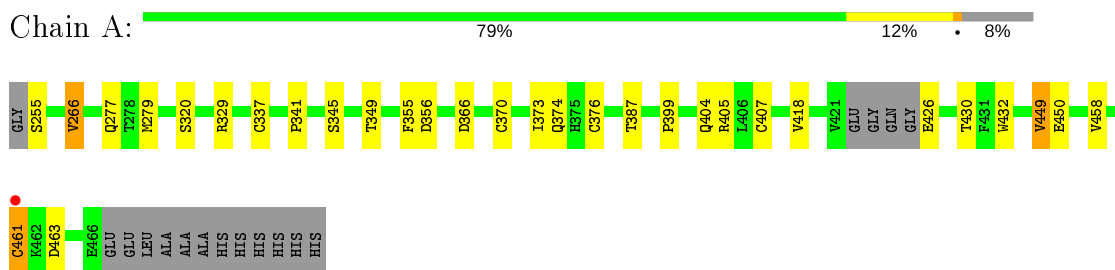
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	B	2	Total	O	0	0
			2	2		

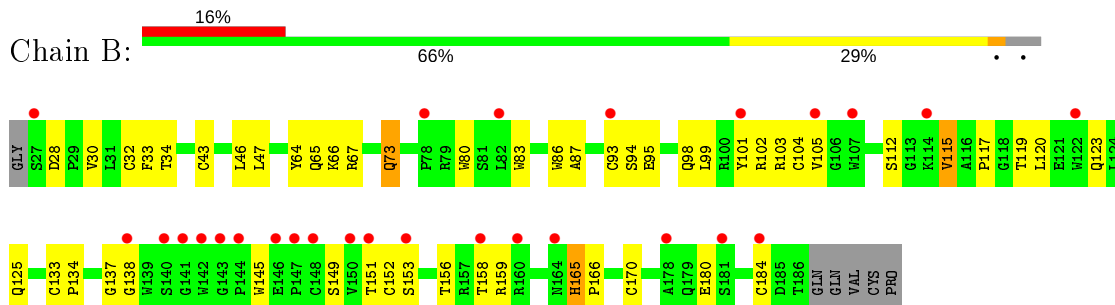
3 Residue-property plots [i](#)

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.

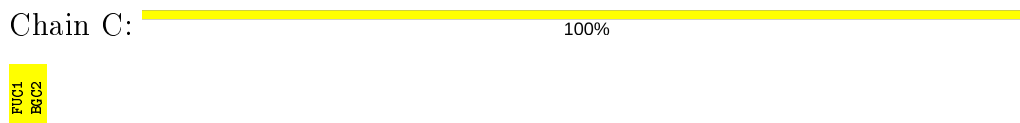
- Molecule 1: Properdin



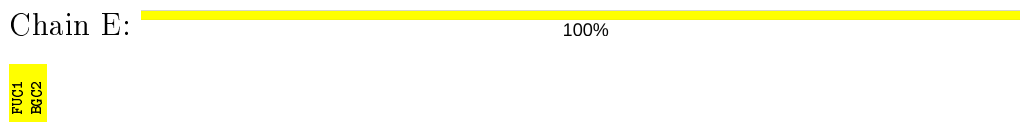
- Molecule 2: Properdin



- Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 3: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



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


Chain D:  100%

IMAGE
IMAGE2

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.75Å 114.75Å 232.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.88 – 2.52 102.88 – 2.52	Depositor EDS
% Data completeness (in resolution range)	60.5 (102.88-2.52) 60.5 (102.88-2.52)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.52Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.248 , 0.267 0.251 , 0.270	Depositor DCC
R_{free} test set	770 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2906	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: FUC, BGC, NAG, MAN

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	0.67	0/1610	0.86	0/2207
2	B	0.74	0/1179	0.87	0/1608
All	All	0.70	0/2789	0.87	0/3815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1557	0	1397	18	0
2	B	1148	0	999	30	0
3	C	21	0	19	0	0
3	E	21	0	19	0	0
4	D	28	0	25	0	0
5	A	77	0	70	1	0
5	B	33	0	30	0	0
6	B	10	0	10	0	0
7	A	9	0	0	0	0
7	B	2	0	0	0	0
All	All	2906	0	2569	45	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 8.

All (45) 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)
2:B:165:HIS:CB	2:B:166:PRO:HD3	1.95	0.95
2:B:165:HIS:CB	2:B:166:PRO:CD	2.45	0.95
2:B:115:VAL:HG22	2:B:119:THR:HG21	1.68	0.75
2:B:30:VAL:HG22	2:B:65:GLN:O	1.93	0.68
2:B:104:CYS:HB3	2:B:117:PRO:HA	1.78	0.66
1:A:329:ARG:NH1	1:A:341:PRO:O	2.31	0.64
2:B:73:GLN:HE21	2:B:105:VAL:HA	1.67	0.59
2:B:138:GLY:HA3	2:B:166:PRO:HD2	1.88	0.56
1:A:266:VAL:HG13	1:A:279:MET:O	2.07	0.54
2:B:138:GLY:CA	2:B:166:PRO:HD2	2.40	0.51
2:B:145:TRP:CE3	2:B:159:ARG:HB2	2.45	0.51
2:B:32:CYS:O	2:B:46:LEU:HD12	2.11	0.51
1:A:418:VAL:O	1:A:426:GLU:HA	2.12	0.50
1:A:374:GLN:HG3	1:A:432:TRP:CZ3	2.47	0.49
2:B:133:CYS:SG	2:B:134:PRO:HD2	2.52	0.49
1:A:405:ARG:HB2	1:A:449:VAL:HG22	1.93	0.49
2:B:30:VAL:HG23	2:B:66:LYS:HA	1.94	0.48
2:B:33:PHE:CD2	2:B:43:CYS:HB3	2.49	0.47
1:A:337:CYS:N	1:A:376:CYS:SG	2.88	0.47
1:A:399:PRO:HG2	1:A:458:VAL:HG11	1.96	0.47
2:B:137:GLY:HA2	2:B:166:PRO:O	2.15	0.46
2:B:101:TYR:HB2	2:B:120:LEU:HD22	1.98	0.46
2:B:94:SER:OG	2:B:95:GLU:N	2.49	0.46
2:B:30:VAL:HG21	2:B:64:TYR:CD2	2.51	0.46
2:B:33:PHE:CG	2:B:43:CYS:HB3	2.51	0.45
1:A:374:GLN:HG3	1:A:432:TRP:HZ3	1.82	0.45
1:A:463:ASP:OD1	2:B:103:ARG:NH1	2.45	0.44
2:B:158:THR:HA	2:B:180:GLU:O	2.17	0.44
1:A:370:CYS:HA	1:A:430:THR:O	2.18	0.44
2:B:86:TRP:CH2	2:B:125:GLN:HB2	2.52	0.44
1:A:387:THR:HA	5:A:509:MAN:O2	2.18	0.43
2:B:104:CYS:CB	2:B:117:PRO:HA	2.47	0.43
2:B:80:TRP:HE1	2:B:112:SER:HB2	1.83	0.43
2:B:98:GLN:OE1	2:B:125:GLN:NE2	2.52	0.42
1:A:373:ILE:HA	1:A:376:CYS:SG	2.60	0.42
1:A:461:CYS:HB3	2:B:99:LEU:HD13	2.01	0.41
2:B:145:TRP:CZ3	2:B:159:ARG:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:TRP:CE3	2:B:102:ARG:HG3	2.55	0.41
1:A:404:GLN:NE2	1:A:450:GLU:OE2	2.52	0.41
1:A:374:GLN:CG	1:A:432:TRP:CZ3	3.03	0.41
1:A:345:SER:HA	1:A:366:ASP:O	2.21	0.41
2:B:87:ALA:O	2:B:98:GLN:HB2	2.20	0.40
1:A:277:GLN:HG3	2:B:47:LEU:HD22	2.04	0.40
1:A:355:PHE:O	1:A:356:ASP:HB2	2.21	0.40
2:B:83:TRP:CH2	2:B:123:GLN:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	204/225 (91%)	192 (94%)	11 (5%)	1 (0%)	29	47
2	B	158/166 (95%)	135 (85%)	22 (14%)	1 (1%)	25	41
All	All	362/391 (93%)	327 (90%)	33 (9%)	2 (1%)	25	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	165	HIS
1	A	407	CYS

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	166/191 (87%)	160 (96%)	6 (4%)	35	59
2	B	117/136 (86%)	104 (89%)	13 (11%)	6	10
All	All	283/327 (86%)	264 (93%)	19 (7%)	16	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	SER
1	A	266	VAL
1	A	320	SER
1	A	349	THR
1	A	449	VAL
1	A	461	CYS
2	B	28	ASP
2	B	34	THR
2	B	67	ARG
2	B	73	GLN
2	B	93	CYS
2	B	115	VAL
2	B	149	SER
2	B	151	THR
2	B	152	CYS
2	B	153	SER
2	B	156	THR
2	B	170	CYS
2	B	184	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	GLN
2	B	73	GLN
2	B	98	GLN
2	B	125	GLN
2	B	130	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](#)

6 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	FUC	C	1	1,3	10,10,11	0.84	0	14,14,16	1.29	1 (7%)
3	BGC	C	2	3	11,11,12	1.08	1 (9%)	15,15,17	2.02	3 (20%)
4	NAG	D	1	1,4	14,14,15	0.67	0	17,19,21	1.53	4 (23%)
4	NAG	D	2	4	14,14,15	0.41	0	17,19,21	1.25	3 (17%)
3	FUC	E	1	3,2	10,10,11	0.23	0	14,14,16	1.07	1 (7%)
3	BGC	E	2	3	11,11,12	0.91	0	15,15,17	1.43	3 (20%)

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	FUC	C	1	1,3	-	-	0/1/1/1
3	BGC	C	2	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
3	FUC	E	1	3,2	-	-	0/1/1/1
3	BGC	E	2	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	BGC	C2-C3	2.29	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BGC	O5-C1-C2	-4.66	103.57	110.77
3	E	2	BGC	O5-C5-C6	3.49	112.67	107.20
3	C	2	BGC	C2-C3-C4	3.22	116.47	110.89
4	D	1	NAG	C2-N2-C7	3.00	127.17	122.90
4	D	1	NAG	O5-C1-C2	-2.92	106.67	111.29
3	C	1	FUC	C2-C3-C4	-2.76	106.12	110.89
4	D	2	NAG	C2-N2-C7	2.51	126.48	122.90
3	E	2	BGC	C2-C3-C4	2.44	115.12	110.89
3	E	2	BGC	O3-C3-C4	-2.41	104.77	110.35
3	C	2	BGC	O5-C5-C4	-2.40	105.00	110.83
4	D	1	NAG	O4-C4-C5	-2.38	103.38	109.30
4	D	2	NAG	C8-C7-N2	2.28	119.96	116.10
3	E	1	FUC	O3-C3-C2	-2.17	105.83	109.99
4	D	1	NAG	C4-C3-C2	2.10	114.09	111.02
4	D	2	NAG	C3-C4-C5	2.07	113.94	110.24

There are no chirality outliers.

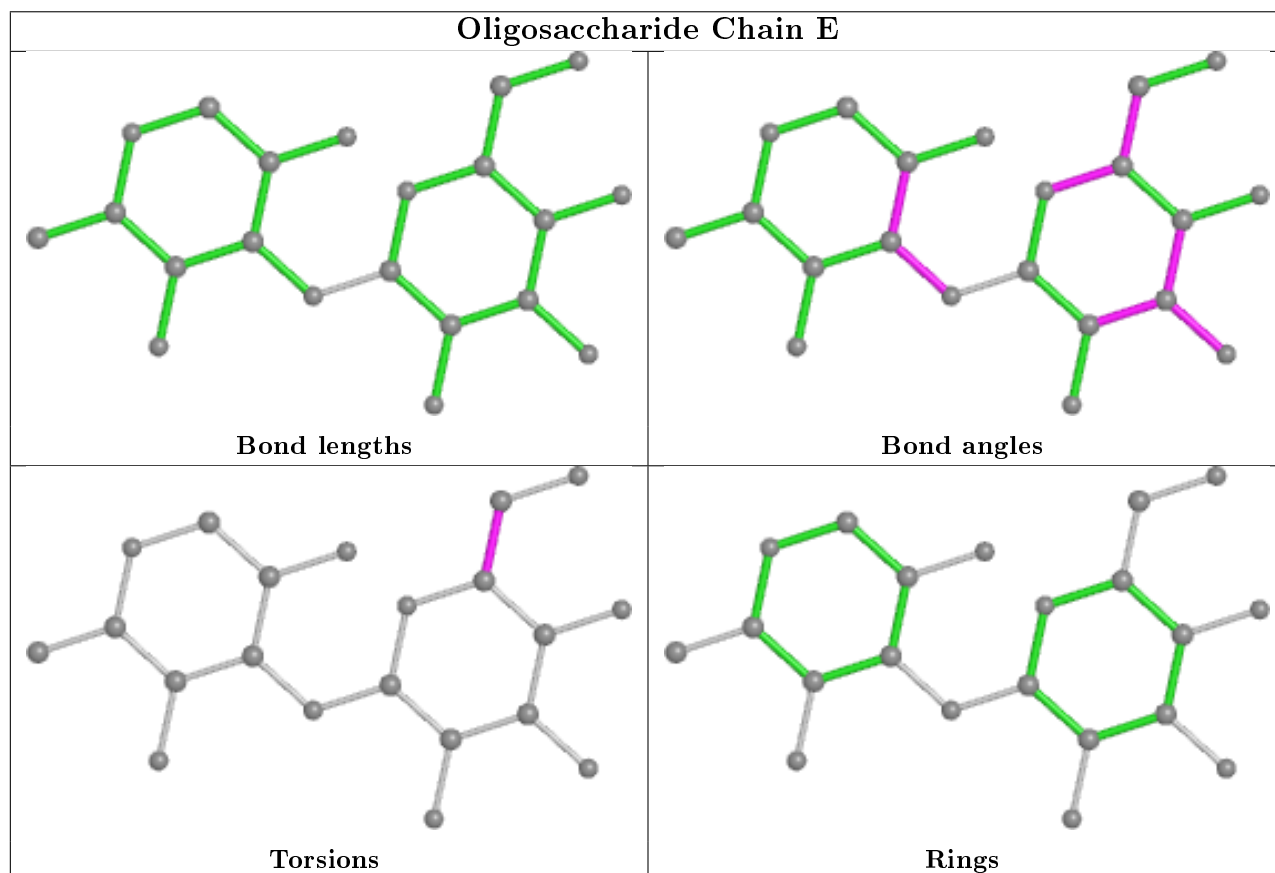
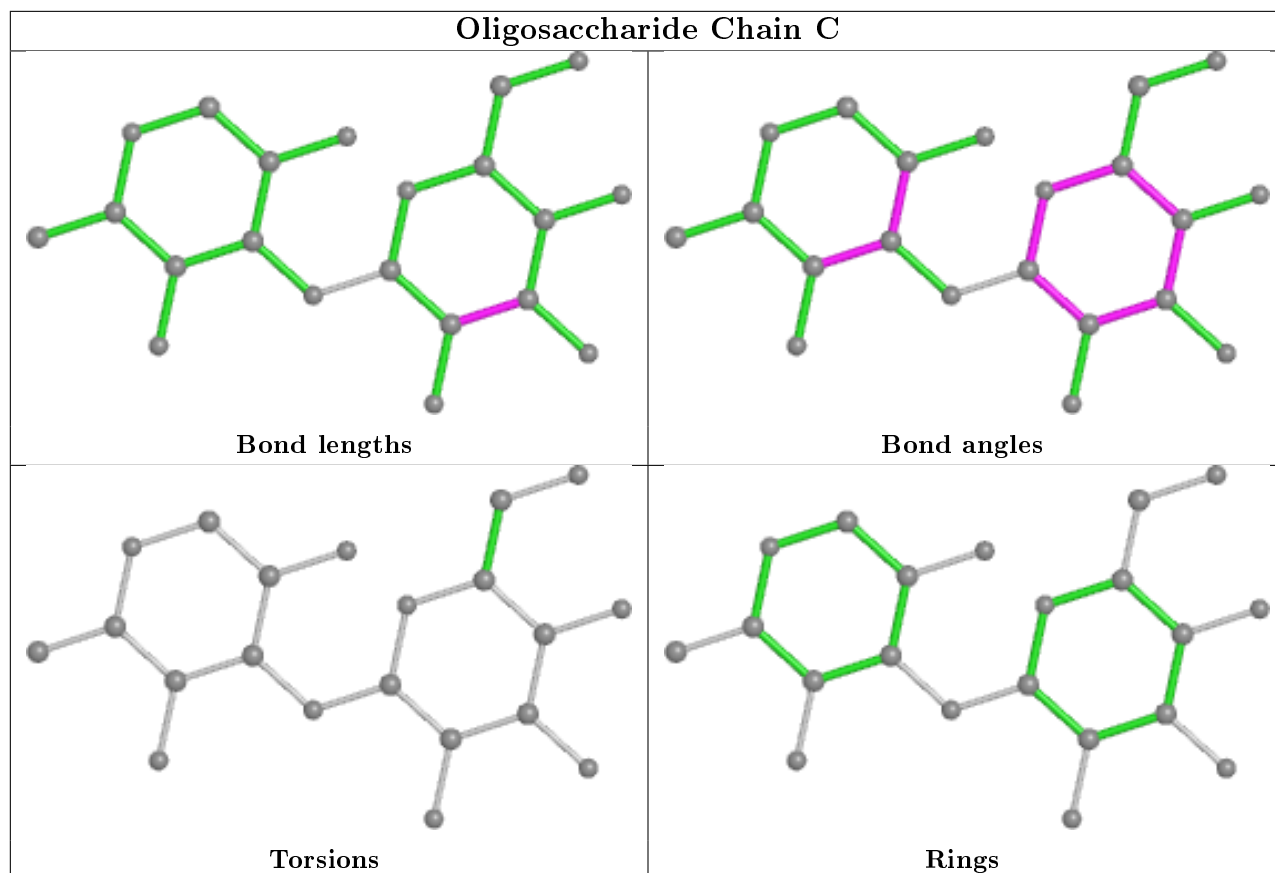
All (8) torsion outliers are listed below:

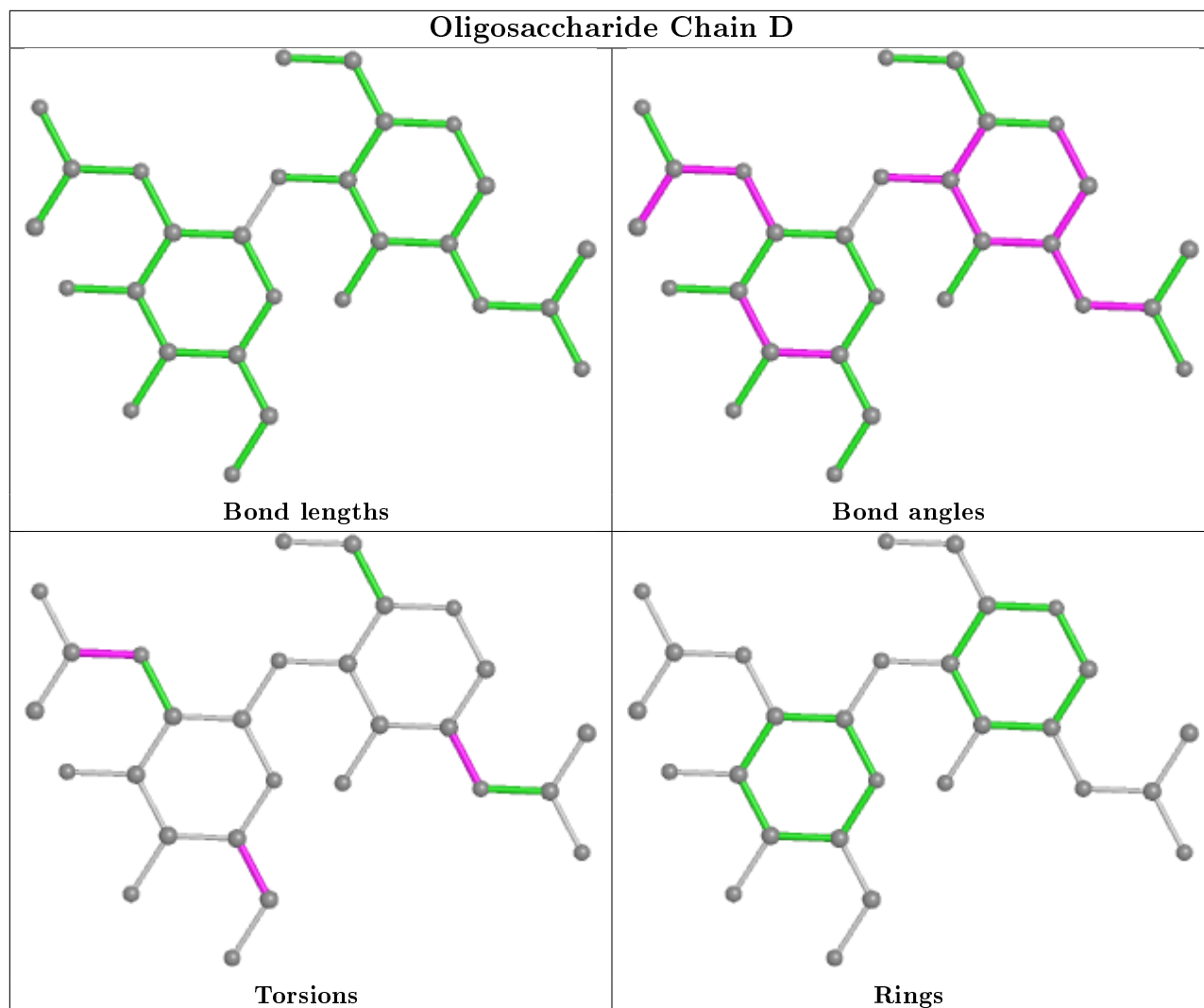
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
3	E	2	BGC	O5-C5-C6-O6
3	E	2	BGC	C4-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

11 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
5	MAN	A	501	-	11,11,12	0.39	0	15,15,17	1.74	4 (26%)
5	MAN	A	504	-	11,11,12	0.44	0	15,15,17	2.36	4 (26%)
5	MAN	B	204	-	11,11,12	0.65	0	15,15,17	1.72	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	509	-	11,11,12	0.81	1 (9%)	15,15,17	1.95	3 (20%)
5	MAN	B	203	-	11,11,12	0.29	0	15,15,17	1.32	2 (13%)
5	MAN	A	503	-	11,11,12	0.49	0	15,15,17	1.61	4 (26%)
5	MAN	A	506	-	11,11,12	0.38	0	15,15,17	1.41	1 (6%)
5	MAN	A	502	-	11,11,12	0.40	0	15,15,17	1.86	5 (33%)
6	FUC	B	205	2	10,10,11	0.61	0	14,14,16	2.35	5 (35%)
5	MAN	A	505	-	11,11,12	0.40	0	15,15,17	1.32	2 (13%)
5	MAN	B	200	-	11,11,12	0.43	0	15,15,17	1.59	4 (26%)

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	MAN	A	501	-	-	1/2/19/22	0/1/1/1
5	MAN	A	504	-	-	0/2/19/22	0/1/1/1
5	MAN	B	204	-	-	2/2/19/22	0/1/1/1
5	MAN	A	509	-	-	0/2/19/22	0/1/1/1
5	MAN	B	203	-	-	0/2/19/22	0/1/1/1
5	MAN	A	503	-	-	0/2/19/22	0/1/1/1
5	MAN	A	506	-	-	0/2/19/22	0/1/1/1
5	MAN	A	502	-	-	0/2/19/22	0/1/1/1
6	FUC	B	205	2	-	-	0/1/1/1
5	MAN	A	505	-	-	1/2/19/22	0/1/1/1
5	MAN	B	200	-	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	509	MAN	C2-C3	2.27	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	MAN	C1-O5-C5	7.60	122.50	112.19
6	B	205	FUC	C1-C2-C3	5.53	116.47	109.67
5	A	509	MAN	C1-C2-C3	5.03	115.85	109.67
5	B	204	MAN	C1-C2-C3	4.09	114.70	109.67
5	A	506	MAN	O5-C5-C6	4.09	113.61	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	MAN	O5-C5-C6	3.76	113.11	107.20
5	B	203	MAN	C1-O5-C5	3.74	117.26	112.19
6	B	205	FUC	O5-C1-C2	3.73	116.53	110.77
5	A	509	MAN	O5-C5-C6	3.66	112.94	107.20
5	B	204	MAN	O5-C5-C6	3.54	112.75	107.20
5	A	502	MAN	C1-O5-C5	3.28	116.64	112.19
6	B	205	FUC	O2-C2-C3	-3.19	103.75	110.14
6	B	205	FUC	C3-C4-C5	-2.96	105.16	109.77
5	A	505	MAN	O5-C5-C6	2.95	111.84	107.20
5	A	509	MAN	C1-O5-C5	2.90	116.12	112.19
5	A	502	MAN	C1-C2-C3	2.83	113.15	109.67
5	A	502	MAN	O5-C5-C6	2.81	111.62	107.20
5	A	504	MAN	C1-C2-C3	2.79	113.09	109.67
5	B	200	MAN	O5-C5-C6	2.76	111.53	107.20
5	A	502	MAN	C3-C4-C5	2.75	115.14	110.24
5	A	502	MAN	C2-C3-C4	2.64	115.46	110.89
5	B	200	MAN	O2-C2-C1	2.63	114.54	109.15
5	A	504	MAN	O3-C3-C2	2.47	114.72	109.99
5	A	503	MAN	C1-O5-C5	2.47	115.54	112.19
5	B	200	MAN	C1-O5-C5	2.44	115.50	112.19
5	A	504	MAN	O6-C6-C5	-2.43	102.95	111.29
5	A	501	MAN	C2-C3-C4	2.43	115.09	110.89
5	B	204	MAN	C2-C3-C4	2.37	115.00	110.89
5	B	200	MAN	O2-C2-C3	-2.36	105.41	110.14
5	A	505	MAN	C1-O5-C5	2.35	115.37	112.19
5	A	501	MAN	C3-C4-C5	2.33	114.40	110.24
5	A	503	MAN	O5-C5-C6	2.26	110.74	107.20
5	A	501	MAN	C1-O5-C5	2.25	115.24	112.19
6	B	205	FUC	C1-O5-C5	2.25	117.87	112.78
5	B	204	MAN	C3-C4-C5	2.20	114.16	110.24
5	A	503	MAN	C3-C4-C5	2.15	114.08	110.24
5	A	503	MAN	O4-C4-C5	-2.15	103.95	109.30
5	B	203	MAN	O5-C5-C6	2.10	110.49	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	204	MAN	O5-C5-C6-O6
5	A	501	MAN	C4-C5-C6-O6
5	B	204	MAN	C4-C5-C6-O6
5	A	505	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	200	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	MAN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	208/225 (92%)	0.37	1 (0%) 91 92	29, 47, 78, 104	0
2	B	160/166 (96%)	1.01	27 (16%) 1 1	40, 78, 117, 126	0
All	All	368/391 (94%)	0.65	28 (7%) 13 14	29, 57, 114, 126	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	147	PRO	5.2
2	B	146	GLU	5.1
2	B	143	GLY	4.6
2	B	141	GLY	4.4
2	B	150	VAL	4.1
2	B	144	PRO	4.1
2	B	140	SER	4.0
2	B	158	THR	3.5
2	B	107	TRP	3.5
2	B	142	TRP	3.5
2	B	181	SER	3.4
2	B	178	ALA	3.3
2	B	101	TYR	3.3
2	B	105	VAL	3.3
2	B	78	PRO	3.1
2	B	82	LEU	3.1
2	B	148	CYS	2.9
2	B	27	SER	2.9
2	B	153	SER	2.6
2	B	164	ASN	2.4
2	B	138	GLY	2.1
2	B	122	TRP	2.1
2	B	114	LYS	2.1
1	A	461	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	160	ARG	2.1
2	B	93	CYS	2.1
2	B	184	CYS	2.1
2	B	151	THR	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](#)

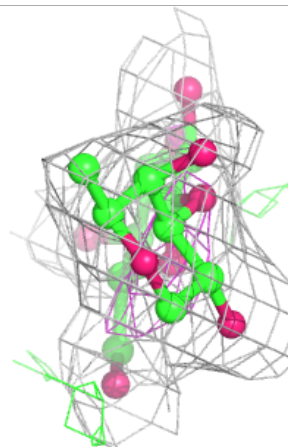
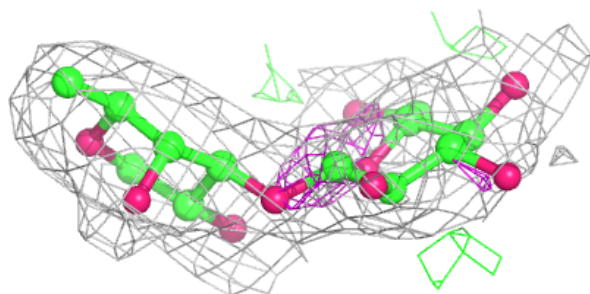
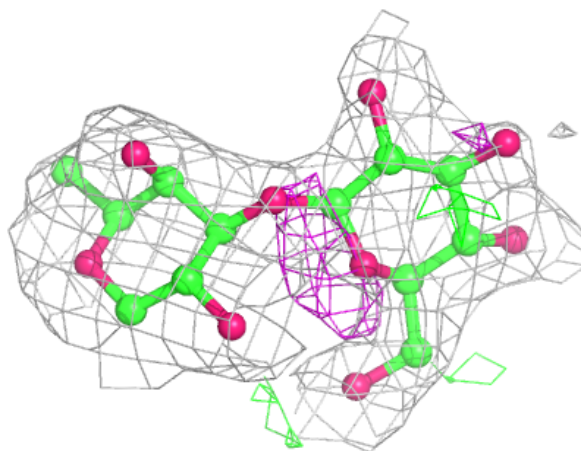
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	2	14/15	0.71	0.46	129,132,142,144	0
4	NAG	D	1	14/15	0.76	0.42	104,109,117,122	0
3	BGC	C	2	11/12	0.81	0.21	52,55,58,62	0
3	BGC	E	2	11/12	0.89	0.13	72,76,79,81	0
3	FUC	C	1	10/11	0.93	0.18	42,45,47,51	0
3	FUC	E	1	10/11	0.98	0.12	76,77,79,79	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.

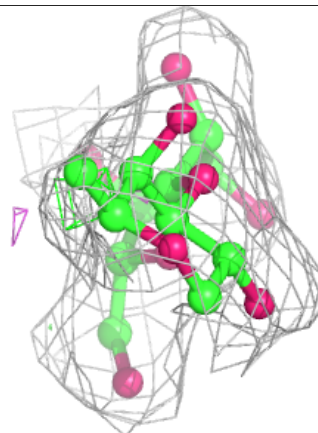
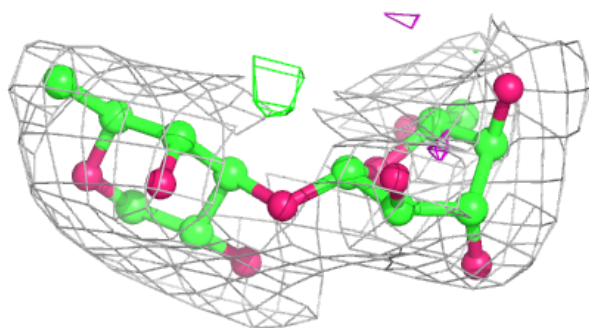
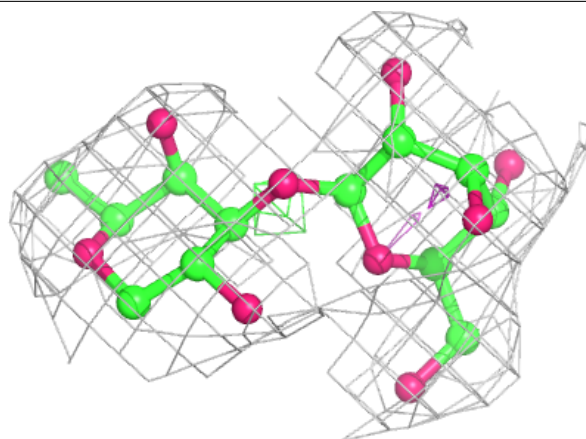
Electron density around Chain C:

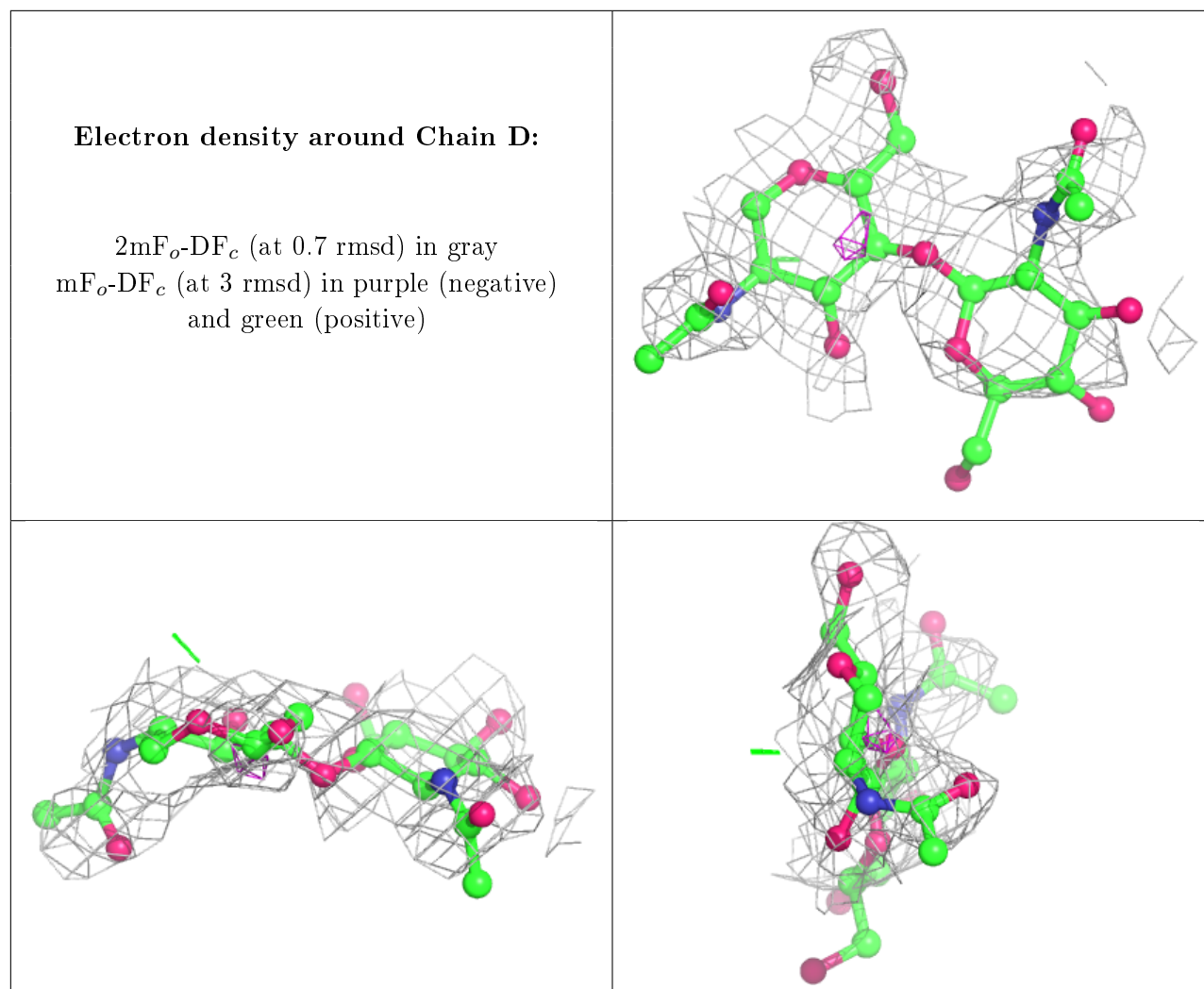
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (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
5	MAN	B	204	11/12	0.77	0.24	112,113,115,115	0
6	FUC	B	205	10/11	0.85	0.31	113,116,119,119	0
5	MAN	B	200	11/12	0.89	0.26	81,84,91,91	0
5	MAN	A	509	11/12	0.90	0.15	65,68,72,73	0
5	MAN	B	203	11/12	0.92	0.23	102,103,104,105	0
5	MAN	A	505	11/12	0.93	0.12	67,72,76,77	0
5	MAN	A	504	11/12	0.95	0.15	32,35,37,38	0
5	MAN	A	506	11/12	0.96	0.14	60,62,67,69	0
5	MAN	A	503	11/12	0.97	0.17	30,32,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	A	501	11/12	0.97	0.13	34,36,37,38	0
5	MAN	A	502	11/12	0.97	0.14	40,44,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.