



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 08:05 AM EDT

PDB ID : 7R86
Title : Structure of mouse BAI1 (ADGRB1) in complex with mouse Nogo receptor (RTN4R)
Authors : Miao, Y.; Jude, K.M.; Garcia, K.C.
Deposited on : 2021-06-26
Resolution : 1.65 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 : 2.23.2
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) : 2.23.2

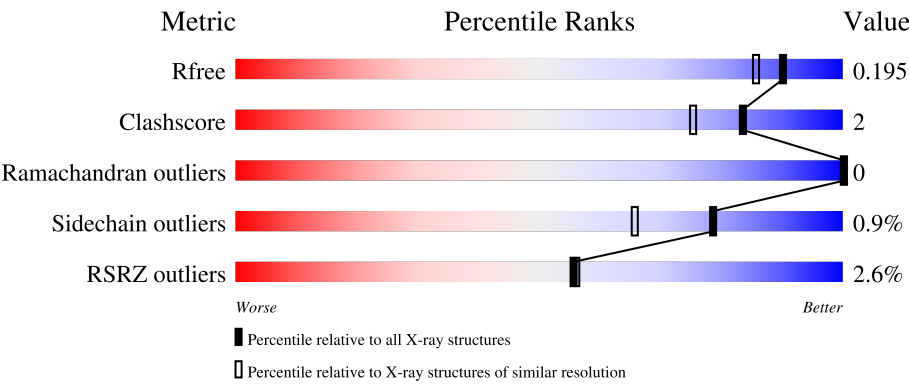
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	285	<div><div></div><div>94%6%</div></div>
1	B	285	<div><div>%</div><div>95%5%</div></div>
2	C	54	<div><div>15%</div><div>76%6%19%</div></div>
2	D	54	<div><div>9%</div><div>70%.26%</div></div>
3	E	2	<div><div></div><div>50%50%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	2	<div><div></div><div>50%</div><div></div><div>50%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6133 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 Reticulon-4 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	10	0
			2305	1456	433	402	14			
1	B	285	Total	C	N	O	S	0	9	0
			2310	1458	437	402	13			

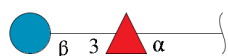
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	-	expression tag	UNP Q99PI8
A	26	SER	-	expression tag	UNP Q99PI8
B	25	ALA	-	expression tag	UNP Q99PI8
B	26	SER	-	expression tag	UNP Q99PI8

- Molecule 2 is a protein called Vasculostatin-120.

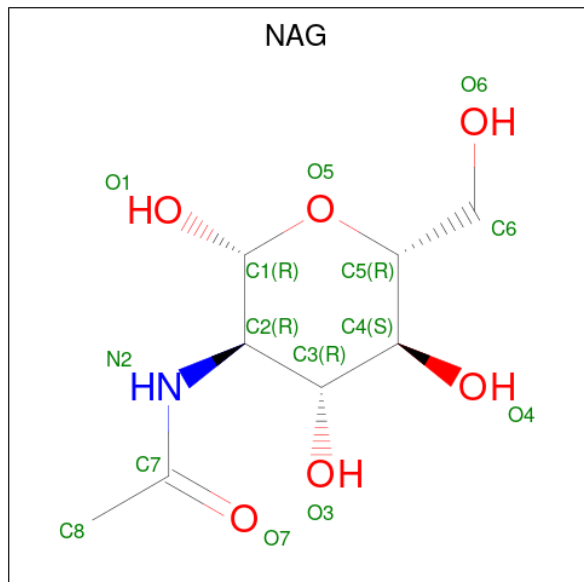
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	44	Total	C	N	O	S	0	0	0
			352	216	66	64	6			
2	D	40	Total	C	N	O	S	0	0	0
			322	200	59	58	5			

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



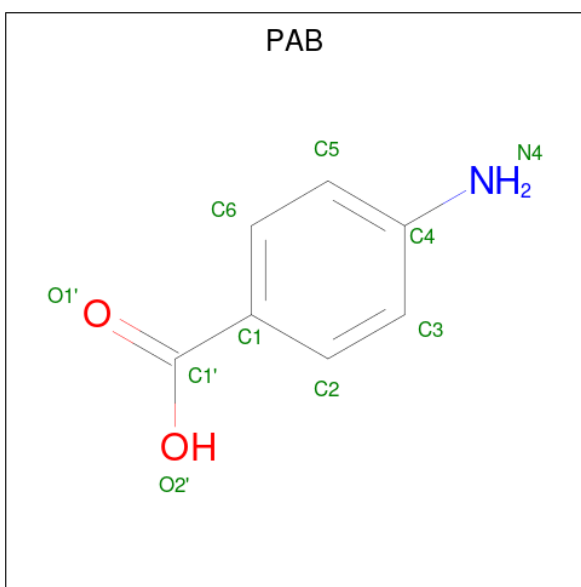
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			21	12	9			
3	F	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



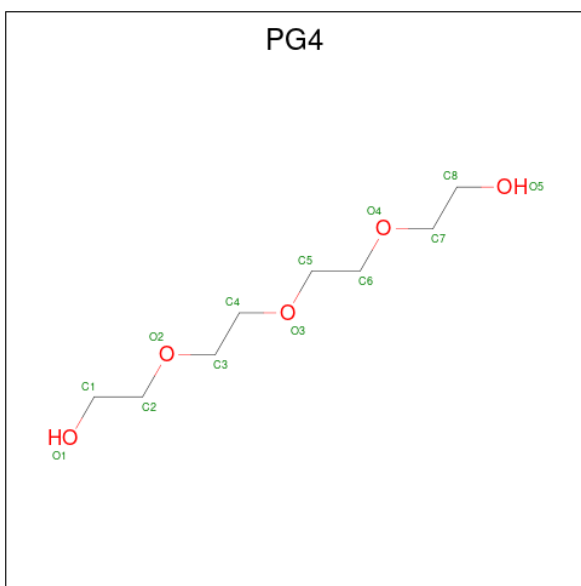
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 4-AMINOBENZOIC ACID (three-letter code: PAB) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			20	14	2	4		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

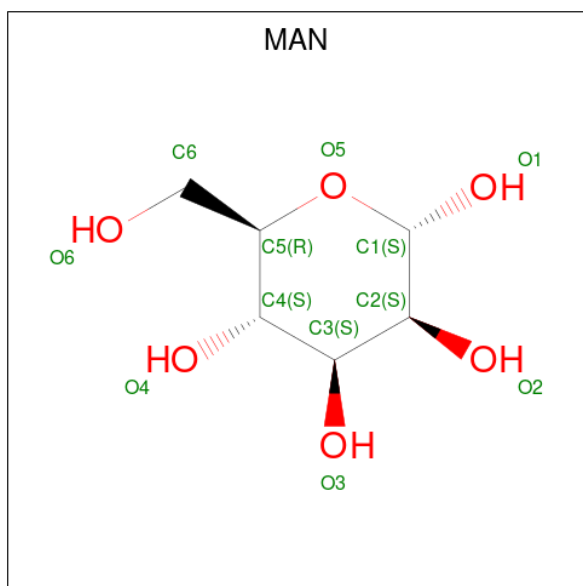
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0
8	B	1	Total Cl 1 1	0	0

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	291	Total	O	0	0
			291	291		
11	B	277	Total	O	0	0
			277	277		
11	C	33	Total	O	0	0
			33	33		
11	D	30	Total	O	0	0
			30	30		

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.

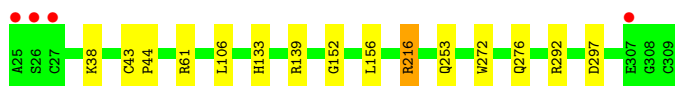
- Molecule 1: Reticulon-4 receptor

Chain A: 




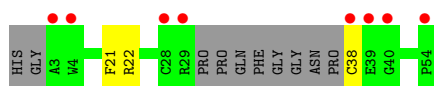
- Molecule 1: Reticulon-4 receptor

Chain B: 



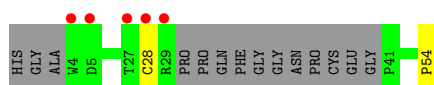
- Molecule 2: Vasculostatin-120

Chain C: 



- Molecule 2: Vasculostatin-120

Chain D: 



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

Chain E: 



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

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.47Å 95.31Å 69.68Å 90.00° 105.39° 90.00°	Depositor
Resolution (Å)	38.87 – 1.65 40.23 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.87-1.65) 89.5 (40.23-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.165 , 0.195 0.165 , 0.195	Depositor DCC
R_{free} test set	2000 reflections (2.13%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6133	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: NAG, FUC, PG4, CL, EDO, BGC, PAB, MAN, ACT

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	0.61	0/2378	0.75	0/3236
1	B	0.59	0/2380	0.75	3/3238 (0.1%)
2	C	0.57	0/361	0.66	0/486
2	D	0.54	0/331	0.68	0/446
All	All	0.59	0/5450	0.74	3/7406 (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	216[A]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	216[B]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	297	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2305	0	2294	11	0
1	B	2310	0	2297	13	0
2	C	352	0	321	2	0
2	D	322	0	294	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	21	0	19	0	0
3	F	21	0	19	0	0
4	A	28	0	26	0	0
4	B	28	0	26	1	0
5	A	20	0	12	2	0
6	A	13	0	18	3	0
7	A	20	0	30	1	0
7	B	8	0	12	1	0
7	C	4	0	6	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	4	0	3	1	0
10	C	22	0	20	0	0
10	D	22	0	20	0	0
11	A	291	0	0	3	0
11	B	277	0	0	5	0
11	C	33	0	0	0	0
11	D	30	0	0	0	0
All	All	6133	0	5417	26	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 2.

All (26) 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:79:SER:H	7:A:407:EDO:H21	1.46	0.80
1:B:292[A]:ARG:NH1	11:B:501:HOH:O	2.22	0.73
2:C:22:ARG:HH21	7:C:203:EDO:H22	1.55	0.71
1:A:168:ALA:HB1	6:A:404:PG4:H62	1.80	0.63
1:A:61:ARG:HH22	5:A:403[A]:PAB:C1'	2.13	0.61
5:A:403[B]:PAB:C1'	1:B:61:ARG:HH22	2.21	0.54
1:A:170:PRO:HA	6:A:404:PG4:H61	1.89	0.53
1:B:216[B]:ARG:HD2	11:B:721:HOH:O	2.10	0.51
1:A:34:TYR:CE1	1:B:44:PRO:HG2	2.46	0.51
1:A:139:ARG:NH2	11:A:507:HOH:O	2.42	0.50
6:A:404:PG4:H81	11:A:734:HOH:O	2.13	0.49
1:B:152:GLY:HA3	7:B:403:EDO:H11	1.96	0.48
1:B:133[B]:HIS:HA	1:B:156:LEU:HA	1.96	0.47
1:B:253:GLN:HG2	11:B:727:HOH:O	2.14	0.47
1:A:133[B]:HIS:HA	1:A:156:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:401:NAG:H61	2:C:21:PHE:HB3	1.99	0.44
1:B:216[A]:ARG:CZ	1:B:216[A]:ARG:HB2	2.48	0.43
1:A:253:GLN:HG2	11:A:741:HOH:O	2.18	0.43
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.85	0.42
1:A:298:LEU:HD12	1:A:301:LEU:HD12	2.01	0.41
1:B:106:LEU:HD21	9:B:405:ACT:H2	2.02	0.41
1:B:139:ARG:CZ	2:D:54:PRO:HG2	2.50	0.41
1:A:242:PRO:HD2	1:A:245:VAL:HG21	2.03	0.41
1:B:139:ARG:NH2	11:B:521:HOH:O	2.54	0.41
1:B:272:TRP:O	1:B:276:GLN:HG2	2.21	0.41
1:B:38:LYS:NZ	11:B:519:HOH:O	2.54	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	292/285 (102%)	278 (95%)	14 (5%)	0	100	100
1	B	292/285 (102%)	278 (95%)	14 (5%)	0	100	100
2	C	40/54 (74%)	40 (100%)	0	0	100	100
2	D	36/54 (67%)	36 (100%)	0	0	100	100
All	All	660/678 (97%)	632 (96%)	28 (4%)	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	252/243 (104%)	250 (99%)	2 (1%)	81	70
1	B	251/243 (103%)	250 (100%)	1 (0%)	91	85
2	C	39/46 (85%)	38 (97%)	1 (3%)	46	21
2	D	36/46 (78%)	35 (97%)	1 (3%)	43	18
All	All	578/578 (100%)	573 (99%)	5 (1%)	78	66

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	CYS
1	A	165	ASN
1	B	43	CYS
2	C	38	CYS
2	D	28	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 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	E	1	2,3	10,10,11	1.26	1 (10%)	14,14,16	0.80	0
3	BGC	E	2	3	11,11,12	0.51	0	15,15,17	0.84	0
3	FUC	F	1	2,3	10,10,11	0.72	0	14,14,16	0.76	0
3	BGC	F	2	3	11,11,12	0.33	0	15,15,17	0.99	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	E	1	2,3	-	-	0/1/1/1
3	BGC	E	2	3	-	0/2/19/22	0/1/1/1
3	FUC	F	1	2,3	-	-	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	FUC	C2-C3	2.16	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	BGC	C1-O5-C5	2.34	115.37	112.19
3	F	2	BGC	O4-C4-C3	-2.07	105.56	110.35

There are no chirality outliers.

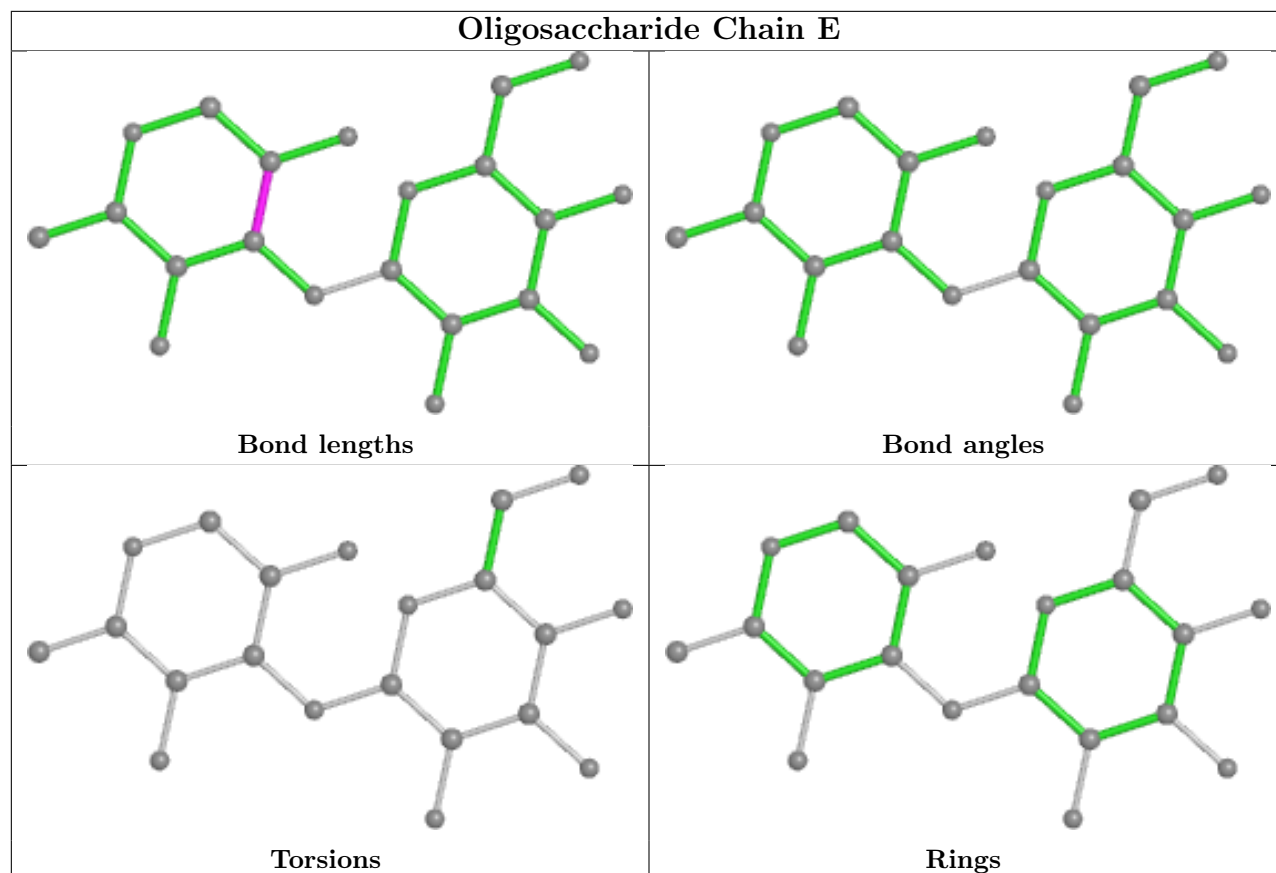
There are no torsion outliers.

There are no ring outliers.

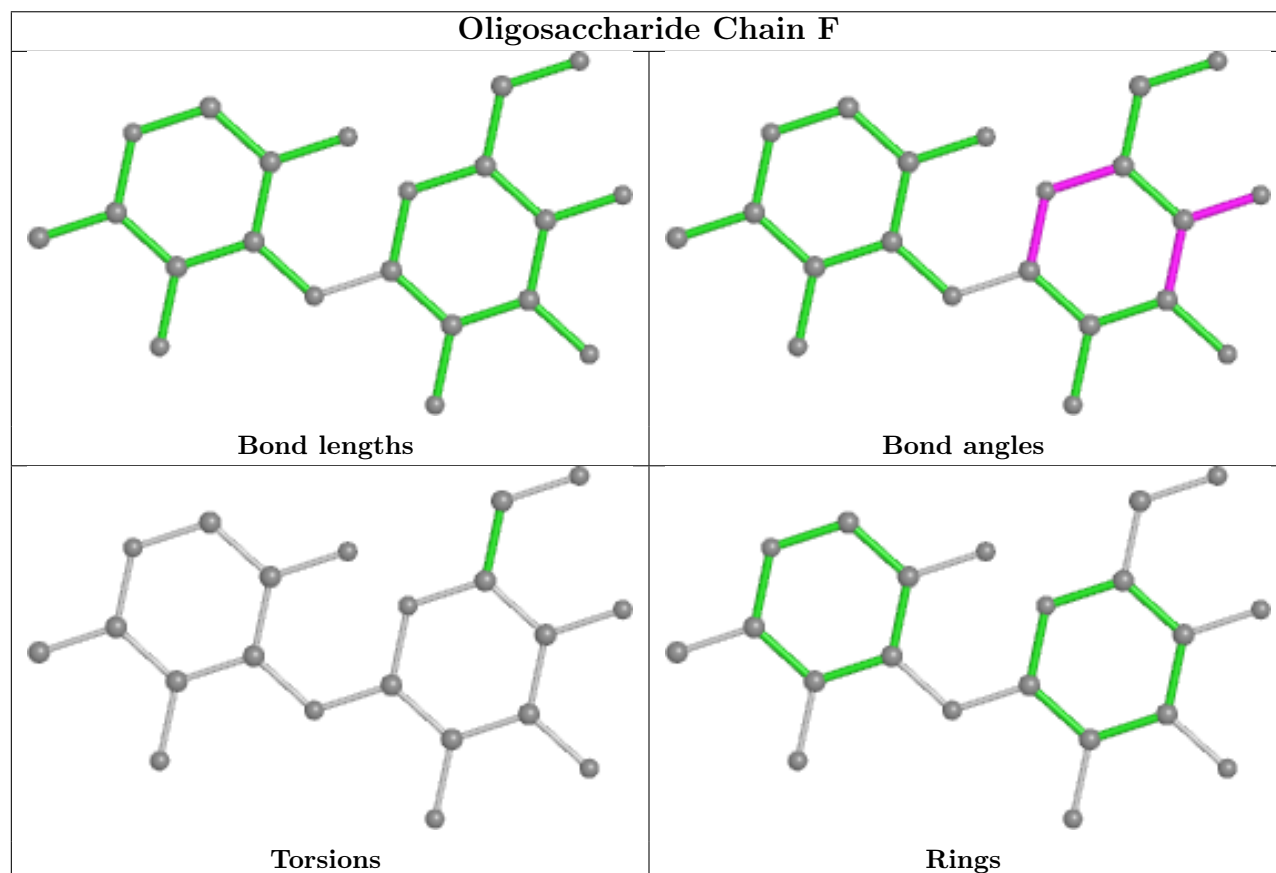
No monomer is involved in short contacts.

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

Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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	EDO	A	409	-	3,3,3	0.51	0	2,2,2	0.21	0
7	EDO	A	408	-	3,3,3	0.49	0	2,2,2	0.43	0
4	NAG	A	401	1	14,14,15	0.34	0	17,19,21	0.75	1 (5%)
10	MAN	C	202	2	11,11,12	0.68	0	15,15,17	1.97	3 (20%)
7	EDO	B	404	-	3,3,3	0.44	0	2,2,2	0.40	0
4	NAG	B	401	1	14,14,15	0.46	0	17,19,21	0.92	1 (5%)
5	PAB	A	403[B]	-	8,10,10	1.96	1 (12%)	10,13,13	1.59	2 (20%)
4	NAG	B	402	1	14,14,15	0.27	0	17,19,21	0.71	0
7	EDO	C	203	-	3,3,3	0.71	0	2,2,2	0.25	0
4	NAG	A	402	1	14,14,15	0.30	0	17,19,21	0.51	0
7	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.51	0
10	MAN	C	201	2	11,11,12	1.48	1 (9%)	15,15,17	1.79	3 (20%)
6	PG4	A	404	-	12,12,12	0.53	0	11,11,11	0.29	0
7	EDO	A	407	-	3,3,3	0.41	0	2,2,2	0.60	0
5	PAB	A	403[A]	-	8,10,10	1.62	1 (12%)	10,13,13	1.58	2 (20%)
7	EDO	A	405	-	3,3,3	0.58	0	2,2,2	0.49	0
10	MAN	D	202	2	11,11,12	0.89	1 (9%)	15,15,17	2.26	3 (20%)
10	MAN	D	201	2	11,11,12	1.26	1 (9%)	15,15,17	1.76	3 (20%)
9	ACT	B	405	-	1,3,3	6.77	1 (100%)	0,3,3	-	-
7	EDO	A	406	-	3,3,3	0.47	0	2,2,2	0.38	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
7	EDO	A	409	-	-	1/1/1/1	-
7	EDO	A	408	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
10	MAN	C	202	2	-	0/2/19/22	0/1/1/1
7	EDO	B	404	-	-	0/1/1/1	-
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
5	PAB	A	403[B]	-	-	0/0/4/4	0/1/1/1
4	NAG	B	402	1	-	0/6/23/26	0/1/1/1
7	EDO	C	203	-	-	1/1/1/1	-
4	NAG	A	402	1	-	0/6/23/26	0/1/1/1
7	EDO	B	403	-	-	1/1/1/1	-
10	MAN	C	201	2	-	0/2/19/22	0/1/1/1
6	PG4	A	404	-	-	8/10/10/10	-
7	EDO	A	407	-	-	1/1/1/1	-
5	PAB	A	403[A]	-	-	0/0/4/4	0/1/1/1
7	EDO	A	405	-	-	1/1/1/1	-
10	MAN	D	202	2	-	2/2/19/22	0/1/1/1
10	MAN	D	201	2	-	0/2/19/22	0/1/1/1
7	EDO	A	406	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	405	ACT	CH3-C	6.77	1.57	1.48
5	A	403[B]	PAB	C1-C1'	5.07	1.52	1.47
5	A	403[A]	PAB	C1-C1'	4.14	1.51	1.47
10	C	201	MAN	C2-C3	3.92	1.58	1.52
10	D	202	MAN	O5-C5	2.08	1.47	1.43
10	D	201	MAN	C2-C3	2.02	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	202	MAN	C1-O5-C5	7.20	121.94	112.19
10	C	202	MAN	C1-O5-C5	5.37	119.46	112.19
10	C	201	MAN	C1-O5-C5	5.12	119.13	112.19
10	D	201	MAN	C1-O5-C5	4.54	118.35	112.19
10	D	202	MAN	O5-C1-C2	3.27	115.82	110.77
10	C	202	MAN	O5-C1-C2	3.04	115.47	110.77
10	C	202	MAN	O2-C2-C3	-2.90	104.34	110.14
4	B	401	NAG	C1-O5-C5	2.89	116.10	112.19
10	D	202	MAN	O5-C5-C6	2.75	111.51	107.20
5	A	403[A]	PAB	C6-C1-C1'	-2.64	116.82	120.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403[B]	PAB	C6-C1-C1'	-2.61	116.87	120.37
10	D	201	MAN	O5-C5-C6	2.56	111.21	107.20
10	C	201	MAN	O5-C1-C2	2.36	114.42	110.77
10	D	201	MAN	O5-C1-C2	2.33	114.36	110.77
5	A	403[B]	PAB	C5-C4-C3	2.26	121.65	118.15
10	C	201	MAN	O5-C5-C6	2.26	110.74	107.20
4	A	401	NAG	C1-O5-C5	2.20	115.17	112.19
5	A	403[A]	PAB	C5-C4-C3	2.14	121.47	118.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	202	MAN	O5-C5-C6-O6
6	A	404	PG4	O3-C5-C6-O4
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
10	D	202	MAN	C4-C5-C6-O6
6	A	404	PG4	O2-C3-C4-O3
7	A	405	EDO	O1-C1-C2-O2
7	A	407	EDO	O1-C1-C2-O2
7	A	409	EDO	O1-C1-C2-O2
7	B	403	EDO	O1-C1-C2-O2
7	C	203	EDO	O1-C1-C2-O2
6	A	404	PG4	C6-C5-O3-C4
6	A	404	PG4	C4-C3-O2-C2
6	A	404	PG4	C5-C6-O4-C7
6	A	404	PG4	C1-C2-O2-C3
6	A	404	PG4	C8-C7-O4-C6
6	A	404	PG4	C3-C4-O3-C5
7	A	408	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	NAG	1	0
5	A	403[B]	PAB	1	0
7	C	203	EDO	1	0
7	B	403	EDO	1	0
6	A	404	PG4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	407	EDO	1	0
5	A	403[A]	PAB	1	0
9	B	405	ACT	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 [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	284/285 (99%)	-0.57	0 100 100	16, 22, 40, 66	0
1	B	285/285 (100%)	-0.33	4 (1%) 75 79	16, 24, 49, 91	0
2	C	44/54 (81%)	0.48	8 (18%) 1 1	20, 33, 79, 97	0
2	D	40/54 (74%)	0.46	5 (12%) 3 3	22, 37, 83, 92	0
All	All	653/678 (96%)	-0.33	17 (2%) 56 56	16, 24, 56, 97	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	28	CYS	9.2
1	B	25	ALA	8.7
2	C	38	CYS	8.1
2	D	4	TRP	5.6
2	C	39	GLU	5.4
2	C	3	ALA	5.3
2	C	40	GLY	3.7
2	D	5	ASP	3.6
2	C	4	TRP	3.4
2	D	27	THR	3.0
2	C	28	CYS	3.0
1	B	26	SER	2.7
2	C	29	ARG	2.6
2	D	29	ARG	2.3
1	B	27	CYS	2.2
1	B	307	GLU	2.2
2	C	54	PRO	2.1

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

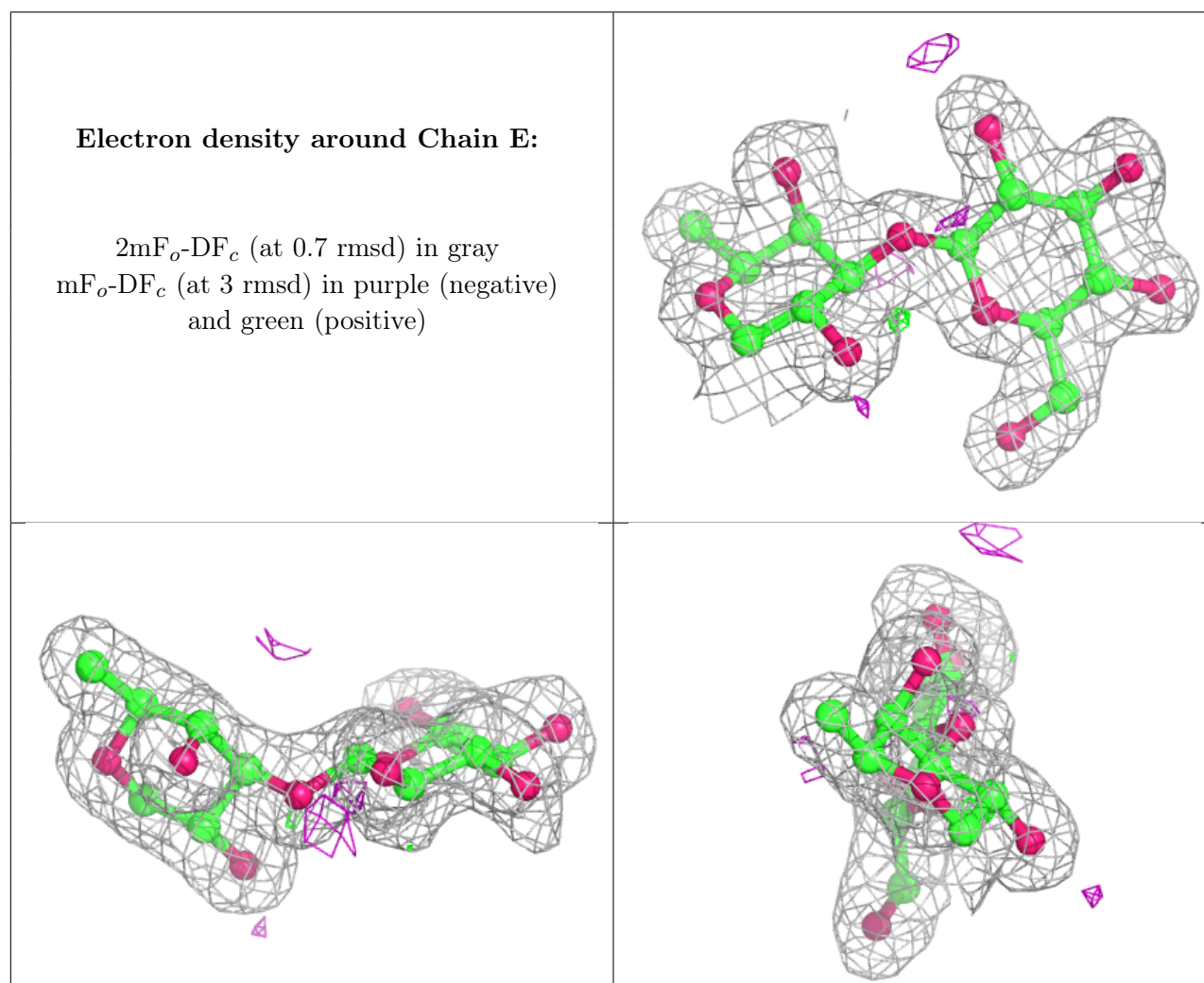
There are no non-standard protein/DNA/RNA residues in this entry.

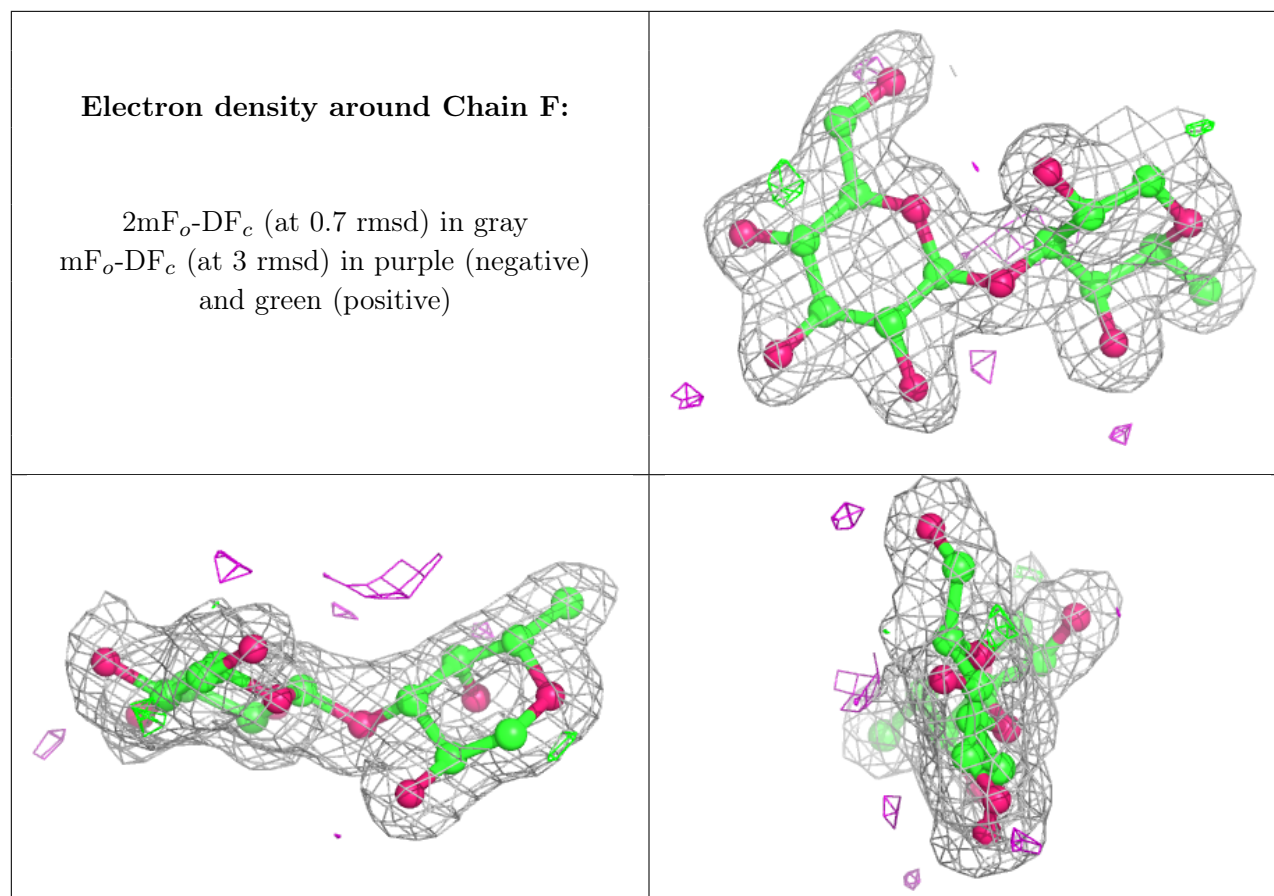
6.3 Carbohydrates [i](#)

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
3	BGC	E	2	11/12	0.92	0.17	27,33,41,41	0
3	FUC	E	1	10/11	0.96	0.08	20,23,25,26	0
3	FUC	F	1	10/11	0.97	0.06	19,22,26,27	0
3	BGC	F	2	11/12	0.97	0.12	29,33,41,42	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.





6.4 Ligands ⓘ

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	PAB	A	403[A]	10/10	0.49	0.29	40,47,51,52	10
5	PAB	A	403[B]	10/10	0.49	0.29	35,46,48,48	10
7	EDO	A	405	4/4	0.67	0.21	58,62,64,68	0
7	EDO	A	408	4/4	0.71	0.14	49,54,57,58	0
7	EDO	A	407	4/4	0.79	0.17	57,59,61,63	0
7	EDO	B	403	4/4	0.83	0.21	52,57,58,62	0
7	EDO	C	203	4/4	0.84	0.17	34,43,53,56	0
6	PG4	A	404	13/13	0.85	0.30	59,65,74,74	0
10	MAN	D	202	11/12	0.85	0.16	61,67,71,73	0
7	EDO	A	409	4/4	0.86	0.18	42,55,61,63	0
9	ACT	B	405	4/4	0.87	0.12	54,58,59,61	0
10	MAN	C	202	11/12	0.88	0.11	51,57,61,63	0
7	EDO	A	406	4/4	0.88	0.11	53,57,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	402	14/15	0.89	0.14	31,41,49,51	0
4	NAG	A	401	14/15	0.90	0.09	26,34,50,53	0
4	NAG	A	402	14/15	0.92	0.15	23,34,52,54	0
10	MAN	C	201	11/12	0.92	0.07	25,32,39,42	0
7	EDO	B	404	4/4	0.93	0.17	46,49,49,49	0
10	MAN	D	201	11/12	0.93	0.10	28,34,40,41	0
4	NAG	B	401	14/15	0.93	0.09	27,35,45,48	0
8	CL	A	410	1/1	0.99	0.05	21,21,21,21	0
8	CL	B	406	1/1	1.00	0.08	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.