Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 11:18 AM EDT

PDB ID	:	8DFX
Title	:	Crystal structure of Human BTN2A1-BTN3A1 Ectodomain Complex
Authors	:	Fulford, T.S.; Soliman, C.; Castle, R.G.; Rigau, M.; Ruan, Z.; Dolezal, O.; Seneviratna, R.; Brown, H.G.; Hanssen, E.; Hammet, A.; Li, S.; Redmond, S.J.; Chung, A.; Gorman, M.A.; Parker, M.W.; Patel, O.; Peat, T.S.; Newman, J.; Behren, A.; Gherardin, N.A.; Godfrey, D.I.; Uldrich, A.P.
Deposited on	:	2022-06-22
Resolution	:	5.55 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 (i) 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 (i)) were used in the production of this report:

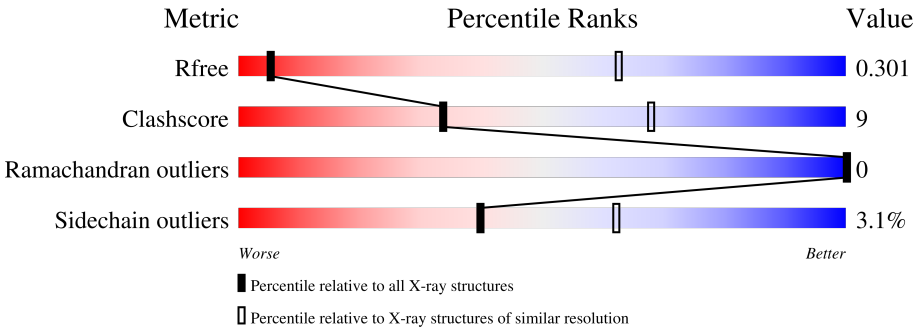
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.55 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	1000 (7.20-3.84)
Clashscore	141614	1012 (7.20-3.90)
Ramachandran outliers	138981	1015 (7.20-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	226	71% 23%
2	B	301	62% 7% 31%
3	C	2	50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3305 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 Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1695	1069	297	318	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	expression tag	UNP Q7KYR7
A	-1	THR	-	expression tag	UNP Q7KYR7
A	0	GLY	-	expression tag	UNP Q7KYR7
A	218	HIS	-	expression tag	UNP Q7KYR7
A	219	HIS	-	expression tag	UNP Q7KYR7
A	220	HIS	-	expression tag	UNP Q7KYR7
A	221	HIS	-	expression tag	UNP Q7KYR7
A	222	HIS	-	expression tag	UNP Q7KYR7
A	223	HIS	-	expression tag	UNP Q7KYR7

- Molecule 2 is a protein called Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1582	1000	269	305	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLU	-	expression tag	UNP O00481
B	-1	THR	-	expression tag	UNP O00481
B	0	GLY	-	expression tag	UNP O00481
B	218	SER	-	expression tag	UNP O00481
B	219	GLY	-	expression tag	UNP O00481
B	220	GLY	-	expression tag	UNP O00481
B	221	LEU	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	THR	-	expression tag	UNP O00481
B	223	PRO	-	expression tag	UNP O00481
B	224	ARG	-	expression tag	UNP O00481
B	225	GLY	-	expression tag	UNP O00481
B	226	VAL	-	expression tag	UNP O00481
B	227	ARG	-	expression tag	UNP O00481
B	228	LEU	-	expression tag	UNP O00481
B	229	GLY	-	expression tag	UNP O00481
B	230	GLY	-	expression tag	UNP O00481
B	231	LEU	-	expression tag	UNP O00481
B	232	GLU	-	expression tag	UNP O00481
B	233	ILE	-	expression tag	UNP O00481
B	234	ARG	-	expression tag	UNP O00481
B	235	ALA	-	expression tag	UNP O00481
B	236	ALA	-	expression tag	UNP O00481
B	237	PHE	-	expression tag	UNP O00481
B	238	LEU	-	expression tag	UNP O00481
B	239	ARG	-	expression tag	UNP O00481
B	240	ARG	-	expression tag	UNP O00481
B	241	ARG	-	expression tag	UNP O00481
B	242	ASN	-	expression tag	UNP O00481
B	243	THR	-	expression tag	UNP O00481
B	244	ALA	-	expression tag	UNP O00481
B	245	LEU	-	expression tag	UNP O00481
B	246	ARG	-	expression tag	UNP O00481
B	247	THR	-	expression tag	UNP O00481
B	248	ARG	-	expression tag	UNP O00481
B	249	VAL	-	expression tag	UNP O00481
B	250	ALA	-	expression tag	UNP O00481
B	251	GLU	-	expression tag	UNP O00481
B	252	LEU	-	expression tag	UNP O00481
B	253	ARG	-	expression tag	UNP O00481
B	254	GLN	-	expression tag	UNP O00481
B	255	ARG	-	expression tag	UNP O00481
B	256	VAL	-	expression tag	UNP O00481
B	257	GLN	-	expression tag	UNP O00481
B	258	ARG	-	expression tag	UNP O00481
B	259	LEU	-	expression tag	UNP O00481
B	260	ARG	-	expression tag	UNP O00481
B	261	ASN	-	expression tag	UNP O00481
B	262	ILE	-	expression tag	UNP O00481
B	263	VAL	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	SER	-	expression tag	UNP O00481
B	265	GLN	-	expression tag	UNP O00481
B	266	TYR	-	expression tag	UNP O00481
B	267	GLU	-	expression tag	UNP O00481
B	268	THR	-	expression tag	UNP O00481
B	269	ARG	-	expression tag	UNP O00481
B	270	TYR	-	expression tag	UNP O00481
B	271	GLY	-	expression tag	UNP O00481
B	272	PRO	-	expression tag	UNP O00481
B	273	LEU	-	expression tag	UNP O00481
B	274	GLY	-	expression tag	UNP O00481
B	275	GLY	-	expression tag	UNP O00481
B	276	THR	-	expression tag	UNP O00481
B	277	LEU	-	expression tag	UNP O00481
B	278	ASN	-	expression tag	UNP O00481
B	279	ASP	-	expression tag	UNP O00481
B	280	ILE	-	expression tag	UNP O00481
B	281	PHE	-	expression tag	UNP O00481
B	282	GLU	-	expression tag	UNP O00481
B	283	ALA	-	expression tag	UNP O00481
B	284	GLN	-	expression tag	UNP O00481
B	285	LYS	-	expression tag	UNP O00481
B	286	ILE	-	expression tag	UNP O00481
B	287	GLU	-	expression tag	UNP O00481
B	288	TRP	-	expression tag	UNP O00481
B	289	HIS	-	expression tag	UNP O00481
B	290	GLU	-	expression tag	UNP O00481
B	291	ASP	-	expression tag	UNP O00481
B	292	TYR	-	expression tag	UNP O00481
B	293	LYS	-	expression tag	UNP O00481
B	294	ASP	-	expression tag	UNP O00481
B	295	ASP	-	expression tag	UNP O00481
B	296	ASP	-	expression tag	UNP O00481
B	297	ASP	-	expression tag	UNP O00481
B	298	LYS	-	expression tag	UNP O00481

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

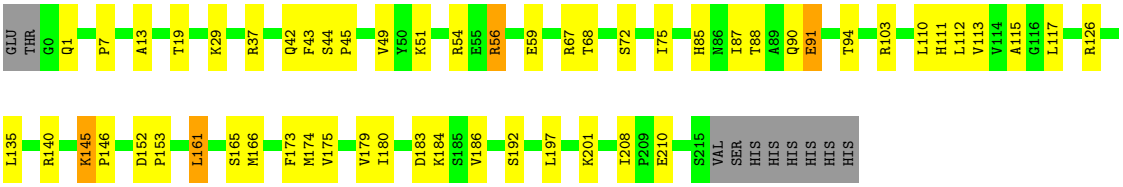
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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. 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. 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.

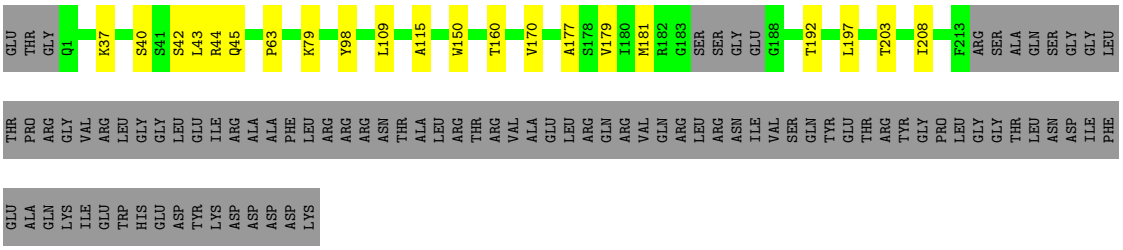
• Molecule 1: Butyrophilin subfamily 2 member A1

Chain A:



• Molecule 2: Butyrophilin subfamily 3 member A1

Chain B:



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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	114.63Å 138.93Å 336.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 5.55 47.35 – 5.55	Depositor EDS
% Data completeness (in resolution range)	56.5 (47.35-5.55) 56.5 (47.35-5.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 5.39Å)	Xtriage
Refinement program	BUSTER 2.10.4 (3-FEB-2022)	Depositor
R, R_{free}	0.290 , 0.336 0.313 , 0.301	Depositor DCC
R_{free} test set	255 reflections (10.20%)	wwPDB-VP
Wilson B-factor (Å^2)	186.2	Xtriage
Anisotropy	1.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 374.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	3305	wwPDB-VP
Average B, all atoms (Å^2)	277.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.38	0/1732	0.58	0/2343
2	B	0.35	0/1614	0.53	0/2189
All	All	0.36	0/3346	0.56	0/4532

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

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	1695	0	1677	44	0
2	B	1582	0	1561	16	0
3	C	28	0	25	0	0
All	All	3305	0	3263	56	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 9.

All (56) 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:54:ARG:NE	1:A:56:ARG:HE	1.50	1.09
1:A:54:ARG:HE	1:A:56:ARG:NE	1.66	0.93
1:A:161:LEU:HD11	1:A:180:ILE:HG13	1.53	0.90
1:A:7:PRO:CD	1:A:110:LEU:HG	2.02	0.89
1:A:54:ARG:HE	1:A:56:ARG:HE	0.90	0.89
1:A:7:PRO:HD3	1:A:110:LEU:HG	1.64	0.79
1:A:184:LYS:HG2	1:A:210:GLU:HG3	1.64	0.77
2:B:181:MET:HE1	2:B:208:ILE:HD12	1.67	0.74
1:A:88:THR:HG22	1:A:91:GLU:OE1	1.90	0.72
1:A:161:LEU:CD1	1:A:180:ILE:HG13	2.21	0.71
1:A:161:LEU:HG	1:A:179:VAL:HA	1.76	0.67
1:A:54:ARG:NE	1:A:56:ARG:NE	2.31	0.65
1:A:94:THR:HG22	1:A:111:HIS:CE1	2.36	0.61
1:A:135:LEU:HD11	1:A:208:ILE:HD11	1.83	0.60
1:A:54:ARG:HH21	1:A:56:ARG:HH21	1.51	0.59
1:A:54:ARG:CD	1:A:56:ARG:HE	2.15	0.58
2:B:181:MET:CE	2:B:208:ILE:HD12	2.32	0.58
1:A:42:GLN:HG3	2:B:42:SER:HA	1.86	0.57
1:A:7:PRO:CG	1:A:110:LEU:HG	2.33	0.57
1:A:1:GLN:HB2	1:A:29:LYS:NZ	2.20	0.56
2:B:115:ALA:HB2	2:B:197:LEU:HD23	1.88	0.55
2:B:45:GLN:HE22	2:B:63:PRO:HG2	1.72	0.55
1:A:54:ARG:HH21	1:A:56:ARG:NH2	2.06	0.54
1:A:115:ALA:HB2	1:A:197:LEU:HD12	1.89	0.54
1:A:145:LYS:HD2	1:A:146:PRO:HD2	1.88	0.53
1:A:145:LYS:HD3	1:A:165:SER:HB2	1.89	0.52
1:A:59:GLU:HA	2:B:109:LEU:HD11	1.93	0.51
1:A:186:VAL:O	1:A:186:VAL:HG23	2.10	0.51
1:A:140:ARG:NH1	1:A:174:MET:SD	2.85	0.50
1:A:1:GLN:CB	1:A:29:LYS:NZ	2.74	0.50
1:A:37:ARG:HG3	1:A:49:VAL:HG22	1.93	0.50
1:A:7:PRO:HG3	1:A:110:LEU:HG	1.95	0.49
2:B:150:TRP:CD1	2:B:179:VAL:HG13	2.48	0.48
1:A:145:LYS:HG2	1:A:173:PHE:CE2	2.49	0.48
2:B:43:LEU:HB3	2:B:45:GLN:HG3	1.96	0.48
1:A:88:THR:HG23	1:A:90:GLN:HB2	1.95	0.47
1:A:152:ASP:HB2	1:A:153:PRO:HD2	1.95	0.47
1:A:51:LYS:HB3	1:A:56:ARG:HD3	1.96	0.47
1:A:94:THR:CG2	1:A:111:HIS:CE1	2.98	0.47
1:A:44:SER:HA	1:A:45:PRO:C	2.36	0.46
1:A:19:THR:HG22	1:A:87:ILE:HD11	1.98	0.46
1:A:165:SER:HB3	1:A:175:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LYS:HZ2	2:B:79:LYS:HB2	1.80	0.46
1:A:7:PRO:HD3	1:A:110:LEU:CG	2.41	0.45
2:B:160:THR:CG2	2:B:177:ALA:HB1	2.47	0.45
1:A:42:GLN:NE2	2:B:42:SER:OG	2.50	0.44
1:A:43:PHE:CZ	2:B:44:ARG:NH2	2.86	0.44
1:A:192:SER:HB3	1:A:201:LYS:HD3	1.99	0.44
1:A:72:SER:HB2	1:A:75:ILE:HB	2.00	0.43
1:A:13:ALA:HB2	1:A:112:LEU:HD11	2.00	0.43
2:B:40:SER:O	2:B:44:ARG:HA	2.19	0.42
1:A:54:ARG:HE	1:A:56:ARG:CZ	2.28	0.42
2:B:37:LYS:HB3	2:B:98:TYR:HB2	2.02	0.41
1:A:67:ARG:HG2	1:A:85:HIS:O	2.21	0.41
2:B:192:THR:HG23	2:B:203:THR:HG22	2.03	0.41
2:B:170:VAL:O	2:B:170:VAL:HG22	2.21	0.41

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	214/226 (95%)	207 (97%)	7 (3%)	0	100	100
2	B	205/301 (68%)	202 (98%)	3 (2%)	0	100	100
All	All	419/527 (80%)	409 (98%)	10 (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	186/196 (95%)	175 (94%)	11 (6%)	19 46
2	B	170/246 (69%)	170 (100%)	0	100 100
All	All	356/442 (80%)	345 (97%)	11 (3%)	40 62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	68	THR
1	A	91	GLU
1	A	103	ARG
1	A	113	VAL
1	A	117	LEU
1	A	126	ARG
1	A	145	LYS
1	A	161	LEU
1	A	166	MET
1	A	183	ASP

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	42	GLN
2	B	45	GLN
2	B	147	GLN
2	B	149	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)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	3,1	14,14,15	0.27	0	17,19,21	0.64	0
3	NAG	C	2	3	14,14,15	0.28	0	17,19,21	0.75	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
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

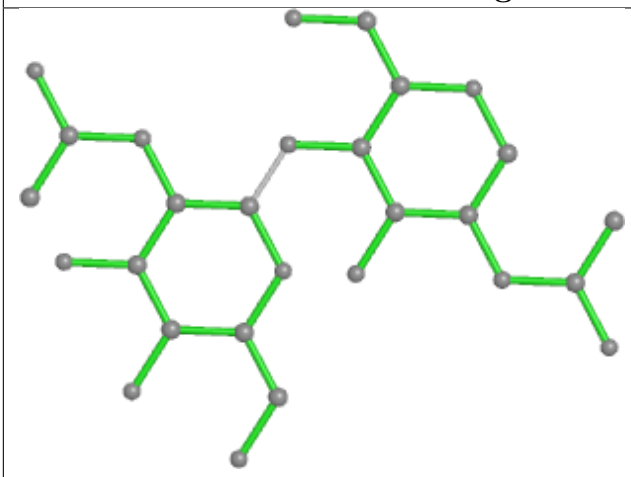
There are no torsion outliers.

There are no ring outliers.

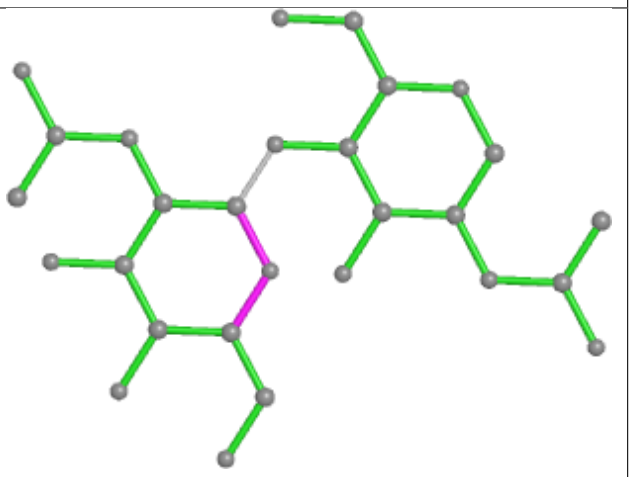
No monomer is involved in short contacts.

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

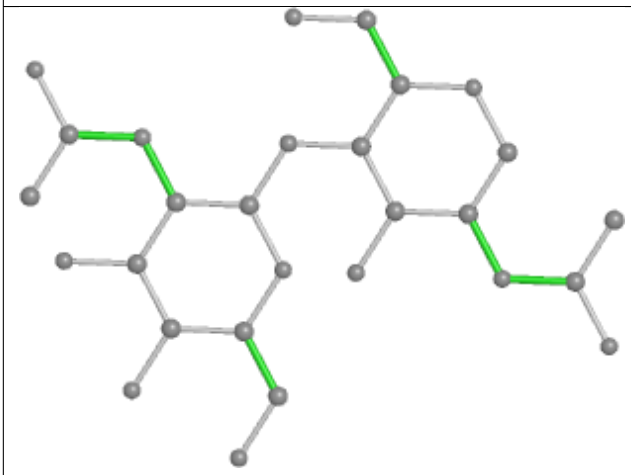
Oligosaccharide Chain C



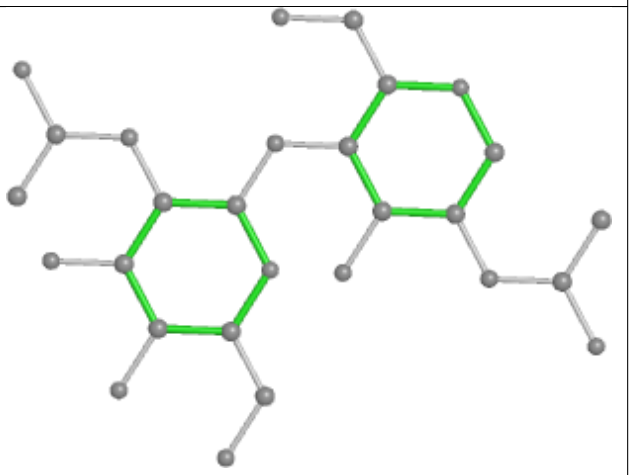
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

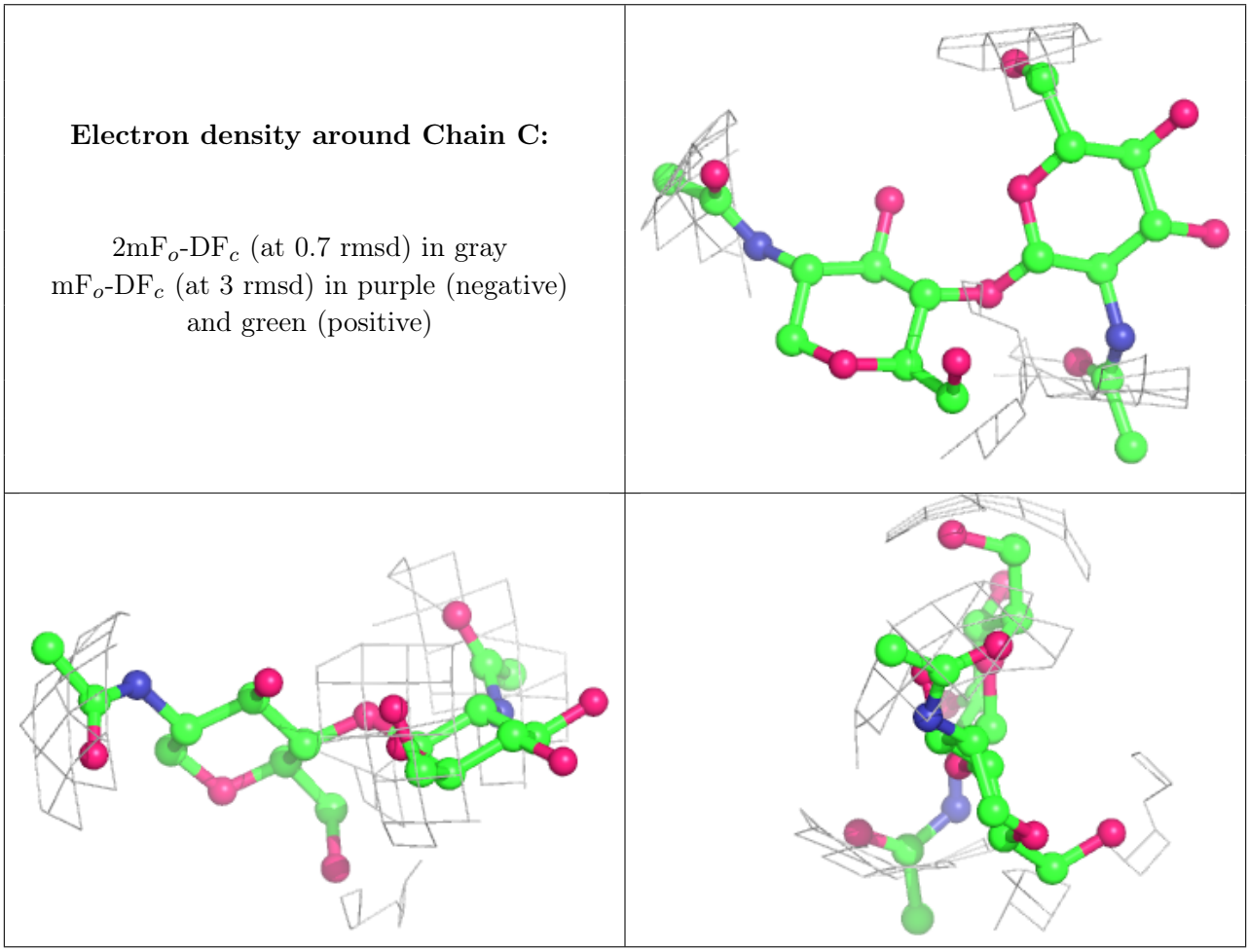
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.