



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:04 PM BST

PDB ID : 3SI0
Title : Structure of glycosylated human glutaminyl cyclase
Authors : Parthier, C.; Carrillo, D.; Stubbs, M.T.
Deposited on : 2011-06-17
Resolution : 2.10 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

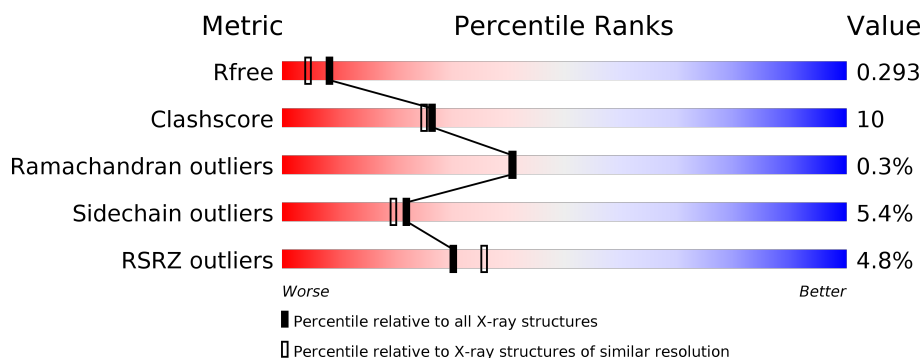
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	330	
2	B	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
2	NAG	B	2	-	-	-	X
5	CL	A	364	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2721 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2536	1623	437	467	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	HIS	-	expression tag	UNP Q16769
A	33	HIS	-	expression tag	UNP Q16769
A	34	HIS	-	expression tag	UNP Q16769
A	35	HIS	-	expression tag	UNP Q16769
A	36	HIS	-	expression tag	UNP Q16769
A	37	HIS	-	expression tag	UNP Q16769

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

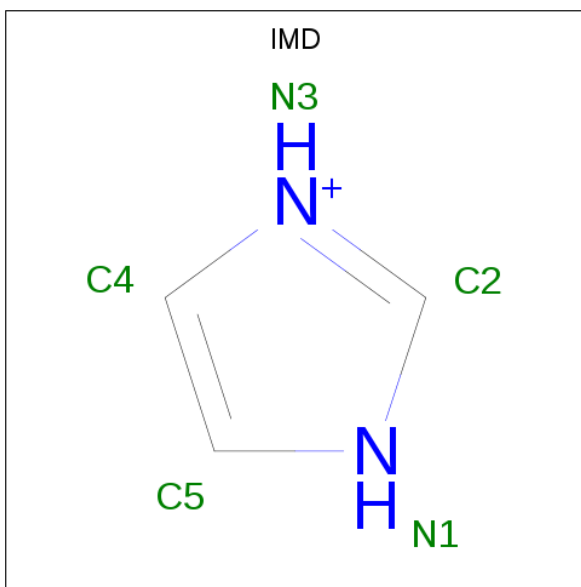


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		

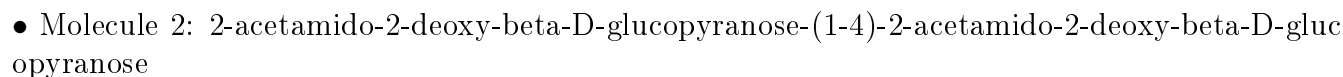
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	150	Total	O	0	0
			150	150		

- Molecule 1: Glutaminyl-peptide cyclotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.41Å 63.69Å 77.16Å 90.00° 105.76° 90.00°	Depositor
Resolution (Å)	11.98 – 2.10 11.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.4 (11.98-2.10) 95.4 (11.94-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.11Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.264 0.243 , 0.293	Depositor DCC
R_{free} test set	1073 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2721	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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: ZN, CL, IMD, 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	1.10	7/2605 (0.3%)	0.99	7/3539 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	TYR	CD1-CE1	9.64	1.53	1.39
1	A	105	GLU	CB-CG	6.65	1.64	1.52
1	A	214	TYR	CD2-CE2	6.53	1.49	1.39
1	A	215	GLY	N-CA	5.62	1.54	1.46
1	A	202	GLU	CB-CG	5.44	1.62	1.52
1	A	123	ILE	CB-CG2	5.28	1.69	1.52
1	A	109	PHE	CE1-CZ	5.26	1.47	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	238	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	77	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	332	MET	CG-SD-CE	-5.66	91.14	100.20
1	A	219	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	A	159	ASP	CB-CG-OD2	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	NE-CZ-NH2	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ASN	Peptide

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	2536	0	2463	52	0
2	B	28	0	25	0	0
3	A	1	0	0	0	0
4	A	5	0	4	2	0
5	A	1	0	0	2	0
6	A	150	0	0	7	0
All	All	2721	0	2492	52	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 10.

All (52) 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:82:PRO:CG	1:A:82:PRO:CB	1.74	1.49
1:A:81:SER:HA	5:A:364:CL:CL	2.13	0.85
1:A:107:ASP:OD1	1:A:218:HIS:HE1	1.64	0.80
1:A:132:LYS:HD2	1:A:133:ARG:HG3	1.63	0.78
1:A:331:THR:HG23	1:A:333:ASP:H	1.51	0.75
1:A:289:LEU:O	1:A:292:ARG:HG2	1.90	0.71
1:A:107:ASP:OD1	1:A:218:HIS:CE1	2.44	0.70
1:A:64:GLU:HG3	6:A:468:HOH:O	1.97	0.63
1:A:272:GLN:HA	1:A:292:ARG:HH22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:CG	1:A:97:ARG:HH11	2.13	0.61
1:A:238:LEU:HD11	1:A:313:ARG:HD3	1.83	0.60
1:A:76:GLU:OE1	6:A:443:HOH:O	2.17	0.58
1:A:81:SER:CA	5:A:364:CL:CL	2.88	0.58
1:A:89:GLN:HE21	1:A:93:GLN:HE22	1.51	0.58
1:A:247:LEU:HD12	1:A:247:LEU:N	2.21	0.56
1:A:328:VAL:O	1:A:331:THR:HG22	2.06	0.55
1:A:166:MET:HG2	1:A:348:ASN:OD1	2.07	0.54
1:A:259:ASN:ND2	6:A:386:HOH:O	2.41	0.54
1:A:54:ARG:O	1:A:58:GLU:HG3	2.07	0.53
1:A:97:ARG:NH1	6:A:425:HOH:O	2.43	0.52
1:A:140:HIS:CB	1:A:201:GLU:HB2	2.39	0.52
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.75	0.51
1:A:159:ASP:OD2	4:A:363:IMD:H4	2.09	0.51
1:A:238:LEU:O	1:A:241:MET:HB2	2.11	0.51
1:A:207:TRP:CD1	1:A:207:TRP:C	2.83	0.51
1:A:140:HIS:HB2	1:A:201:GLU:HB2	1.92	0.50
1:A:67:GLN:HA	1:A:71:GLN:NE2	2.25	0.50
1:A:64:GLU:CG	6:A:468:HOH:O	2.57	0.50
1:A:279:HIS:NE2	1:A:289:LEU:HD12	2.27	0.49
1:A:134:HIS:CD2	1:A:192:SER:HB3	2.47	0.49
1:A:203:ALA:HB2	1:A:207:TRP:HA	1.95	0.49
1:A:222:LYS:NZ	6:A:435:HOH:O	2.41	0.47
1:A:199:ASP:OD1	1:A:200:GLY:N	2.48	0.47
1:A:331:THR:HG23	1:A:333:ASP:N	2.24	0.46
1:A:99:GLN:O	1:A:100:ALA:C	2.53	0.45
1:A:56:ILE:HD13	1:A:56:ILE:N	2.31	0.45
1:A:207:TRP:CZ2	1:A:304:GLN:HB3	2.52	0.45
1:A:207:TRP:HZ2	1:A:304:GLN:HB3	1.83	0.44
1:A:76:GLU:O	1:A:83:GLY:HA3	2.17	0.44
1:A:202:GLU:HB2	6:A:10:HOH:O	2.18	0.43
1:A:242:ASP:O	1:A:316:PRO:HG2	2.18	0.43
1:A:43:HIS:CE1	1:A:358:TYR:O	2.72	0.43
1:A:140:HIS:CG	1:A:140:HIS:O	2.72	0.42
1:A:67:GLN:HA	1:A:71:GLN:HE21	1.85	0.42
1:A:270:ARG:O	1:A:274:ILE:HG13	2.18	0.42
1:A:170:LEU:HG	1:A:174:LEU:HD12	2.02	0.41
1:A:247:LEU:N	1:A:247:LEU:CD1	2.84	0.41
1:A:248:ASP:OD2	4:A:363:IMD:H5	2.21	0.41
1:A:331:THR:CG2	1:A:333:ASP:HB2	2.50	0.41
1:A:43:HIS:HE1	1:A:358:TYR:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:HIS:HB2	1:A:237:GLN:HG3	2.03	0.41
1:A:272:GLN:HA	1:A:292:ARG:NH2	2.33	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	308/330 (93%)	290 (94%)	17 (6%)	1 (0%)	41 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	SER

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	277/293 (94%)	262 (95%)	15 (5%)	22 20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU

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Mol	Chain	Res	Type
1	A	51	SER
1	A	64	GLU
1	A	96	GLN
1	A	97	ARG
1	A	99	GLN
1	A	151	ASN
1	A	160	SER
1	A	192	SER
1	A	233	ARG
1	A	242	ASP
1	A	259	ASN
1	A	292	ARG
1	A	303	ILE
1	A	331	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	71	GLN
1	A	89	GLN
1	A	112	GLN
1	A	128	ASN
1	A	151	ASN
1	A	218	HIS
1	A	259	ASN
1	A	338	ASN

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	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.69	0	17,19,21	1.46	1 (5%)
2	NAG	B	2	2	14,14,15	0.66	0	17,19,21	1.09	2 (11%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1	NAG	C1-O5-C5	4.79	118.68	112.19
2	B	2	NAG	O5-C1-C2	-2.02	108.10	111.29
2	B	2	NAG	C1-C2-N2	2.02	113.93	110.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

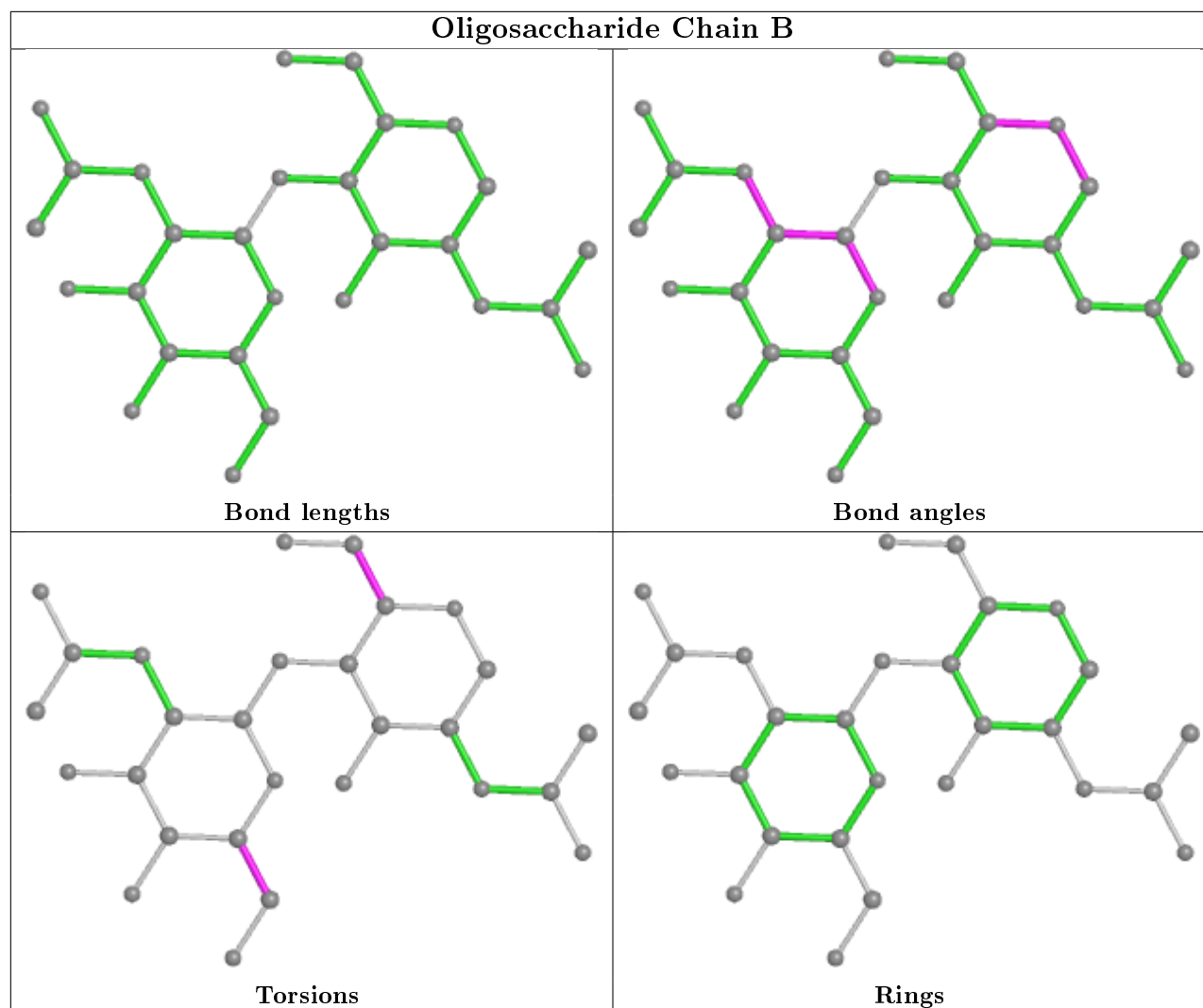
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
4	IMD	A	363	3	3,5,5	0.67	0	4,5,5	0.88	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
4	IMD	A	363	3	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	363	IMD	2	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	314/330 (95%)	0.47	15 (4%) 30 36	18, 35, 66, 77	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	TYR	6.6
1	A	151	ASN	5.5
1	A	297	TYR	4.4
1	A	296	ASN	3.2
1	A	298	SER	3.0
1	A	176	LYS	3.0
1	A	282	GLY	2.7
1	A	233	ARG	2.6
1	A	150	ASN	2.4
1	A	292	ARG	2.2
1	A	295	GLN	2.2
1	A	182	LYS	2.2
1	A	230	PRO	2.2
1	A	284	LEU	2.1
1	A	120	PHE	2.1

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

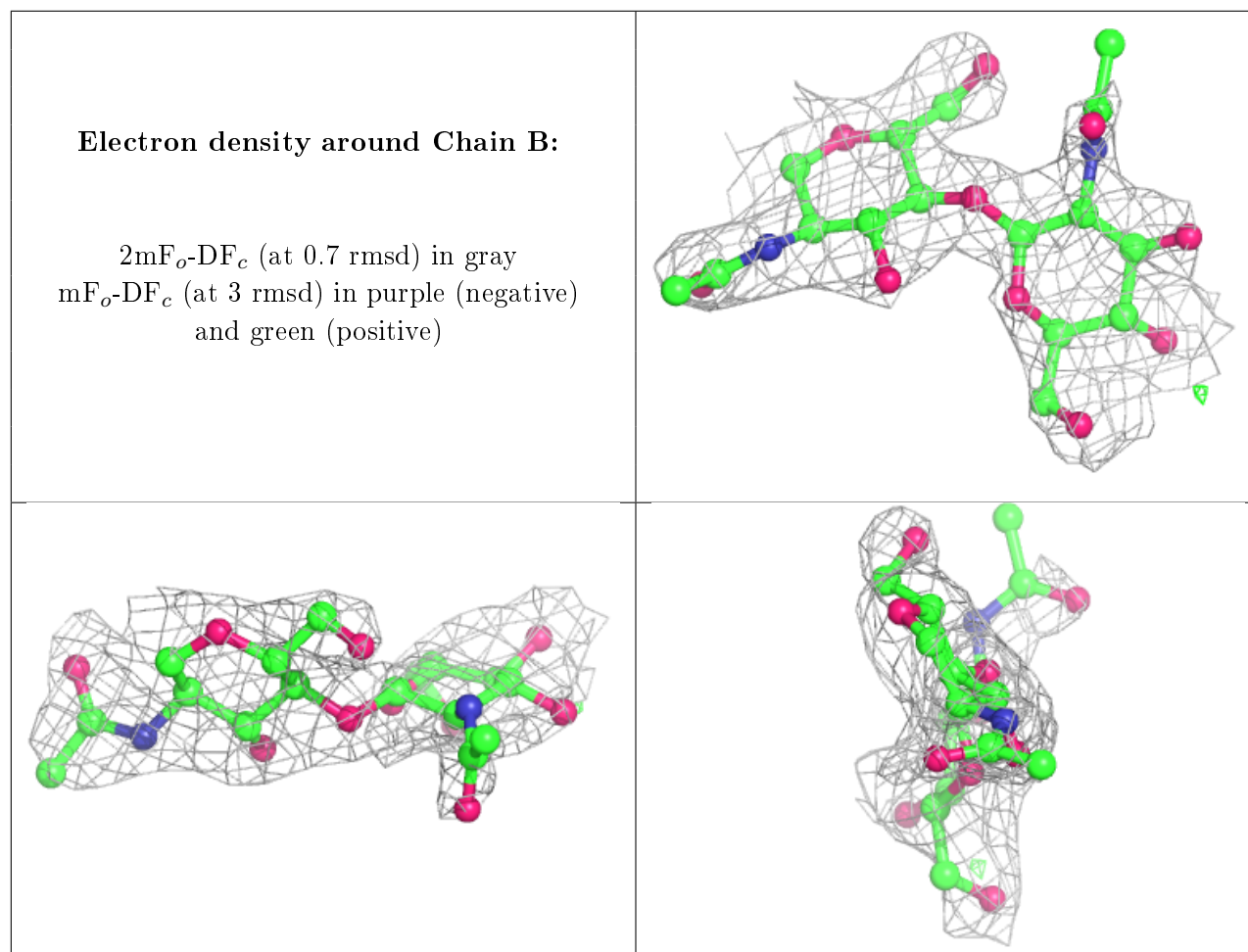
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	NAG	B	2	14/15	0.76	0.43	61,66,67,68	0
2	NAG	B	1	14/15	0.81	0.21	46,55,57,59	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
4	IMD	A	363	5/5	0.97	0.10	12,13,18,18	0
3	ZN	A	362	1/1	0.99	0.07	19,19,19,19	0
5	CL	A	364	1/1	0.99	0.08	25,25,25,25	1

6.5 Other polymers

There are no such residues in this entry.