



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:46 AM BST

PDB ID : 1NP0
Title : Human lysosomal beta-hexosaminidase isoform B in complex with intermediate analogue NAG-thiazoline
Authors : Mark, B.L.; Mahuran, D.J.; Cherney, M.M.; Zhao, D.; Knapp, S.; James, M.N.G.
Deposited on : 2003-01-16
Resolution : 2.50 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:

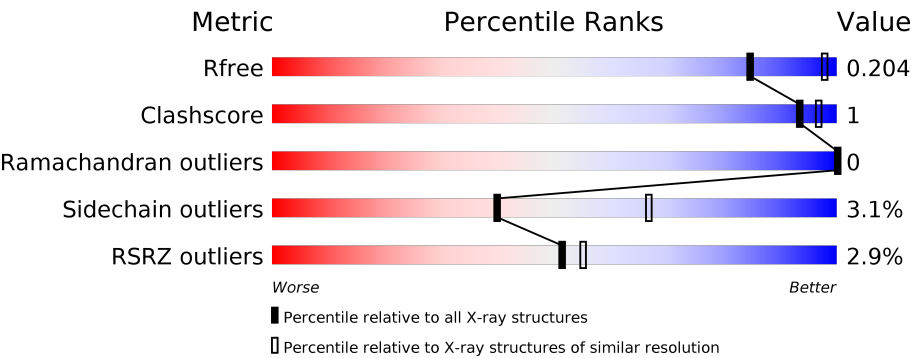
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	58	<div><div>5%</div><div>88%</div><div>9%</div></div>
1	B	58	<div><div>5%</div><div>86%</div><div>5%</div><div>9%</div></div>
2	C	190	<div><div>2%</div><div>92%</div><div>7%</div></div>
2	E	190	<div><div>3%</div><div>91%</div><div>8%</div></div>
3	D	241	<div><div>3%</div><div>90%</div><div>8%</div></div>
3	F	241	<div><div>2%</div><div>89%</div><div>9%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	2	 50%50%
4	H	2	 50%50%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8107 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 Beta-hexosaminidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			421	276	70	73	2			
1	B	53	Total	C	N	O	S	0	0	0
			421	276	70	73	2			

- Molecule 2 is a protein called Beta-hexosaminidase subunit beta chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			
2	E	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			

- Molecule 3 is a protein called Beta-hexosaminidase subunit beta chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	237	Total	C	N	O	S	0	0	0
			1929	1248	317	357	7			
3	F	237	Total	C	N	O	S	0	0	0
			1929	1248	317	357	7			

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



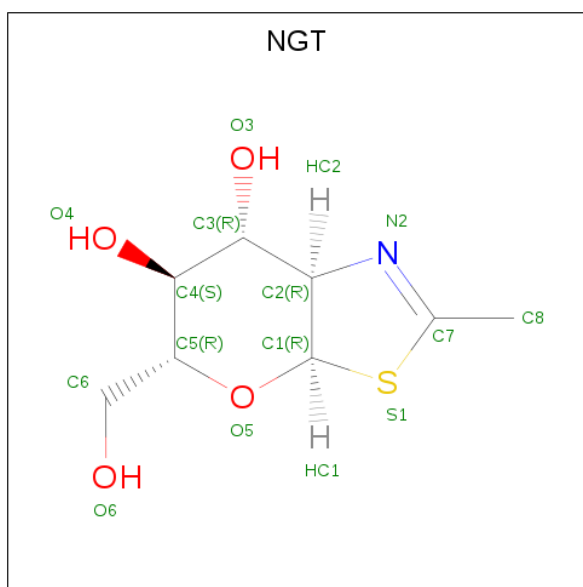
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O		0	0	0
			28	16	2	10				

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: $C_8H_{13}NO_4S$).



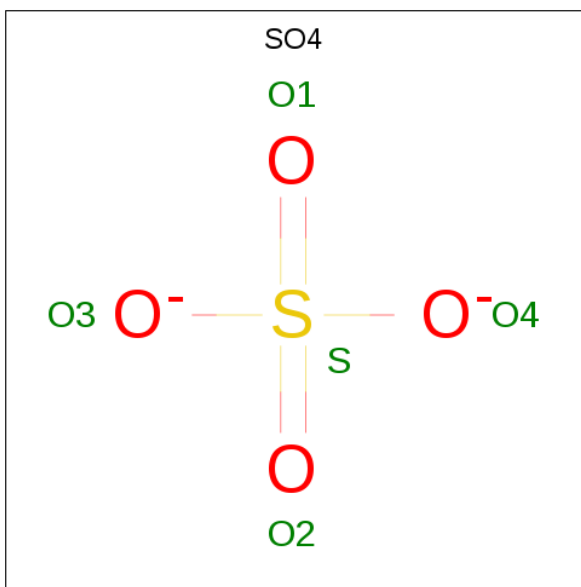
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

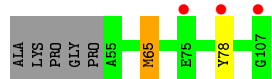
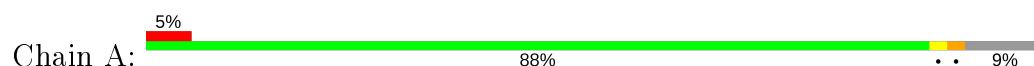
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	123	Total 123	O 123	0	0
8	B	121	Total 121	O 121	0	0

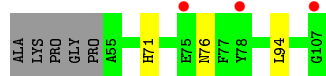
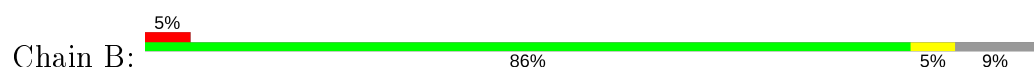
3 Residue-property plots [i](#)

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

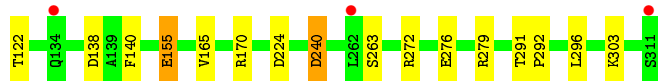
- Molecule 1: Beta-hexosaminidase subunit beta



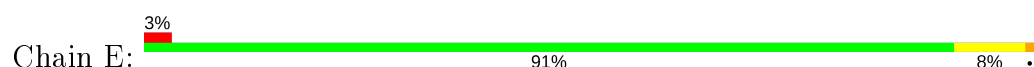
- Molecule 1: Beta-hexosaminidase subunit beta



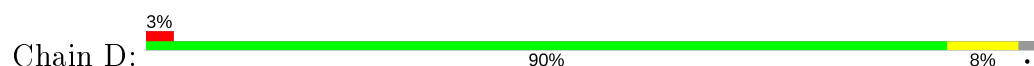
- Molecule 2: Beta-hexosaminidase subunit beta chain B




- Molecule 2: Beta-hexosaminidase subunit beta chain B



- Molecule 3: Beta-hexosaminidase subunit beta chain A



- Molecule 3: Beta-hexosaminidase subunit beta chain A

Chain F:  2% 89% 9% ..



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

Chain G:  50% 50%



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

Chain H:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.41Å 112.41Å 397.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.76 – 2.50 36.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.76-2.50) 99.6 (36.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.198 , 0.227 0.202 , 0.204	Depositor DCC
R_{free} test set	2661 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.0	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	0.94	EDS
Total number of atoms	8107	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: NGT, GOL, NAG, SO4

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	0.51	0/437	0.79	0/598
1	B	0.48	0/437	0.75	0/598
2	C	0.50	0/1567	0.93	5/2134 (0.2%)
2	E	0.50	0/1567	0.92	4/2134 (0.2%)
3	D	0.50	0/1984	0.93	12/2691 (0.4%)
3	F	0.51	0/1984	0.96	14/2691 (0.5%)
All	All	0.50	0/7976	0.92	35/10846 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	505	ARG	NE-CZ-NH2	-9.66	115.47	120.30
3	F	505	ARG	NE-CZ-NH1	8.41	124.51	120.30
3	D	505	ARG	NE-CZ-NH2	-8.06	116.27	120.30
3	D	346	ASP	CB-CG-OD2	8.01	125.51	118.30
3	F	354	ASP	CB-CG-OD2	7.60	125.14	118.30
3	D	354	ASP	CB-CG-OD2	7.24	124.81	118.30
3	F	346	ASP	CB-CG-OD2	6.99	124.59	118.30
3	D	505	ARG	NE-CZ-NH1	6.98	123.79	120.30
3	D	520	ARG	NE-CZ-NH1	6.70	123.65	120.30
3	D	411	ASP	CB-CG-OD2	6.68	124.31	118.30
2	C	240	ASP	CB-CG-OD2	6.64	124.28	118.30
3	D	521	ASP	CB-CG-OD2	6.60	124.24	118.30
3	F	459	ASP	CB-CG-OD2	6.53	124.18	118.30
3	F	372	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	C	224	ASP	CB-CG-OD2	6.24	123.92	118.30
3	F	524	ASP	CB-CG-OD2	6.24	123.92	118.30
2	C	170	ARG	NE-CZ-NH1	6.20	123.40	120.30
3	F	369	ASP	CB-CG-OD2	6.06	123.75	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	411	ASP	CB-CG-OD2	6.03	123.72	118.30
3	D	524	ASP	CB-CG-OD2	5.99	123.69	118.30
2	E	170	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	C	138	ASP	CB-CG-OD2	5.63	123.37	118.30
2	C	272	ARG	NE-CZ-NH1	5.54	123.07	120.30
3	F	520	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	E	272	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	D	535	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	E	240	ASP	CB-CG-OD2	5.31	123.08	118.30
3	F	521	ASP	CB-CG-OD2	5.24	123.02	118.30
3	F	512	ARG	NE-CZ-NH1	5.19	122.89	120.30
3	F	528	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	D	512	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	E	182	ASP	CB-CG-OD1	5.05	122.84	118.30
3	F	535	ARG	NE-CZ-NH1	5.02	122.81	120.30
3	D	459	ASP	CB-CG-OD2	5.01	122.81	118.30
3	D	528	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	421	0	408	1	0
1	B	421	0	408	3	0
2	C	1528	0	1510	3	0
2	E	1528	0	1510	9	0
3	D	1929	0	1868	4	0
3	F	1929	0	1868	7	0
4	G	28	0	25	1	0
4	H	28	0	25	0	0
5	A	14	0	13	1	0
5	B	14	0	13	1	0
6	A	12	0	16	0	0
6	B	6	0	8	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	5	0	0	1	0
8	A	123	0	0	1	0
8	B	121	0	0	0	0
All	All	8107	0	7672	21	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 1.

All (21) 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)
5:B:558:NGT:S1	3:F:450:TYR:OH	2.41	0.76
2:C:122:THR:N	2:C:155:GLU:OE1	2.32	0.62
2:E:311:SER:HG	3:F:316:LEU:N	1.98	0.60
2:E:122:THR:N	2:E:155:GLU:OE1	2.42	0.53
7:B:557:SO4:O3	3:F:372:ARG:NH2	2.45	0.49
2:C:140:PHE:CE1	2:C:279:ARG:HD3	2.49	0.48
1:B:94:LEU:HD11	2:E:131:ILE:CD1	2.43	0.48
1:B:71:HIS:N	2:E:122:THR:O	2.43	0.47
1:A:65:MET:HE2	4:G:1:NAG:H82	1.98	0.45
8:A:629:HOH:O	3:D:531:ARG:NH1	2.38	0.45
2:E:291:THR:HB	2:E:292:PRO:HA	1.99	0.45
2:E:125:GLN:HA	2:E:125:GLN:HE21	1.82	0.44
2:E:291:THR:HB	3:F:322:ILE:HD12	2.00	0.44
3:D:404:VAL:HG13	3:D:408:VAL:HB	2.00	0.44
6:B:559:GOL:H32	3:F:546:LEU:HD23	2.00	0.43
2:C:291:THR:HB	2:C:292:PRO:HA	2.00	0.43
2:E:311:SER:OG	3:F:316:LEU:N	2.50	0.43
5:A:557:NGT:S1	3:D:450:TYR:OH	2.62	0.41
1:B:76:ASN:ND2	2:E:125:GLN:HE22	2.19	0.41
3:D:369:ASP:OD1	3:D:372:ARG:NH2	2.54	0.40
3:F:404:VAL:HG13	3:F:408:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
1	B	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
2	C	188/190 (99%)	185 (98%)	3 (2%)	0	100	100
2	E	188/190 (99%)	186 (99%)	2 (1%)	0	100	100
3	D	235/241 (98%)	229 (97%)	6 (3%)	0	100	100
3	F	235/241 (98%)	231 (98%)	4 (2%)	0	100	100
All	All	948/978 (97%)	931 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	46/49 (94%)	44 (96%)	2 (4%)	29	53
1	B	46/49 (94%)	46 (100%)	0	100	100
2	C	174/174 (100%)	167 (96%)	7 (4%)	31	56
2	E	174/174 (100%)	167 (96%)	7 (4%)	31	56
3	D	206/210 (98%)	201 (98%)	5 (2%)	49	74
3	F	206/210 (98%)	201 (98%)	5 (2%)	49	74
All	All	852/866 (98%)	826 (97%)	26 (3%)	40	67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	78	TYR
2	C	155	GLU
2	C	165	VAL
2	C	240	ASP
2	C	263	SER
2	C	276	GLU
2	C	296	LEU
2	C	303	LYS
3	D	366	LYS
3	D	388	ILE
3	D	404	VAL
3	D	431	GLU
3	D	502	LEU
2	E	125	GLN
2	E	151	LEU
2	E	154	LYS
2	E	165	VAL
2	E	201	SER
2	E	217	LYS
2	E	276	GLU
3	F	317	ASP
3	F	366	LYS
3	F	404	VAL
3	F	427	SER
3	F	502	LEU

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

Mol	Chain	Res	Type
1	A	76	ASN
2	C	123	GLN
2	C	125	GLN
2	E	125	GLN

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$
4	NAG	G	1	2,4	14,14,15	0.72	0	17,19,21	1.15	3 (17%)
4	NAG	G	2	4	14,14,15	1.01	2 (14%)	17,19,21	0.66	0
4	NAG	H	1	2,4	14,14,15	0.57	0	17,19,21	1.04	0
4	NAG	H	2	4	14,14,15	1.00	1 (7%)	17,19,21	0.66	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	NAG	G	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NAG	C2-N2	2.39	1.50	1.46
4	G	2	NAG	C2-N2	2.23	1.50	1.46
4	G	2	NAG	O5-C1	-2.15	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C4-C3-C2	-2.38	107.53	111.02
4	G	1	NAG	O7-C7-C8	-2.29	117.80	122.06
4	G	1	NAG	O5-C5-C6	2.01	110.36	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

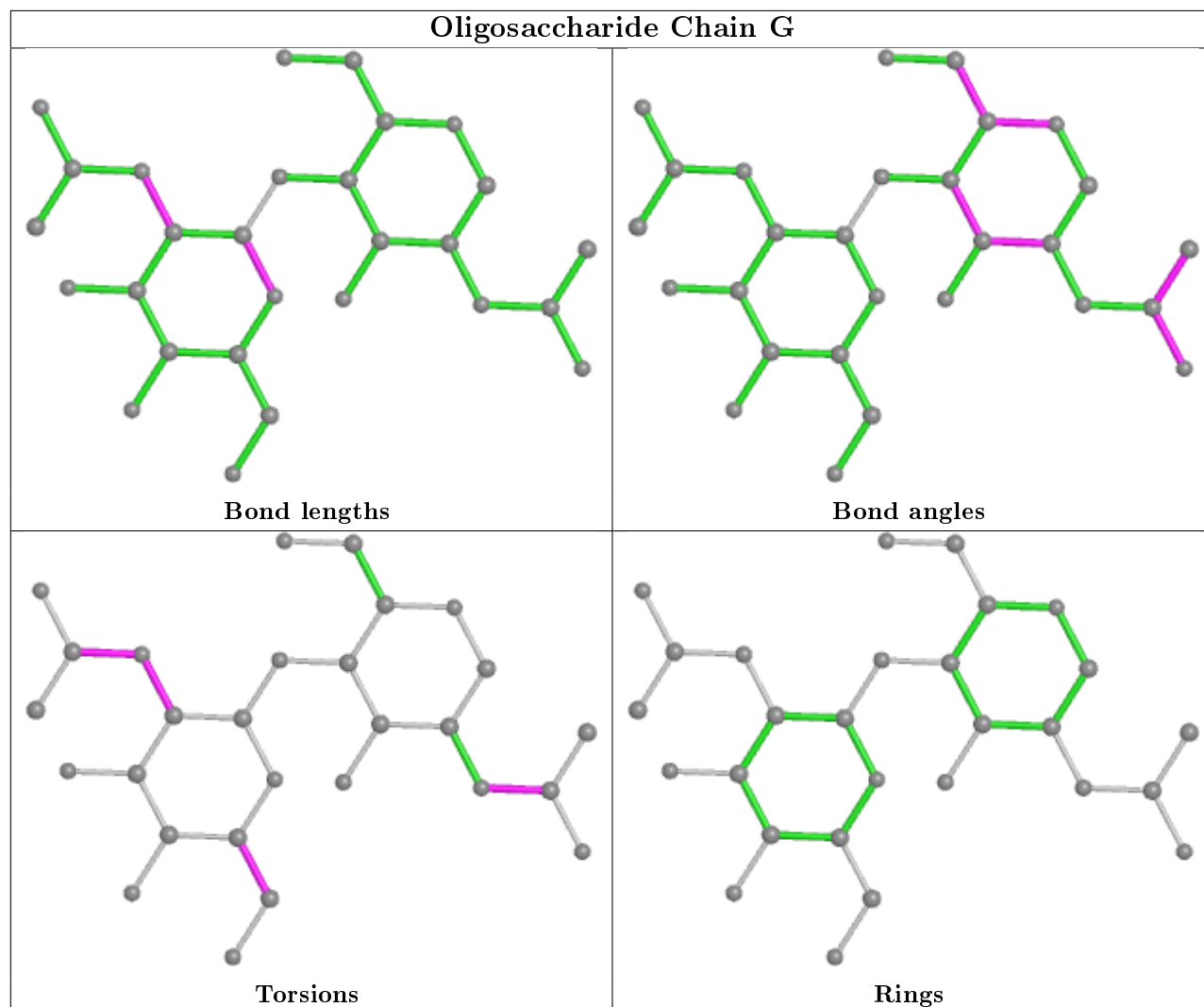
Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C8-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	2	NAG	C3-C2-N2-C7
4	H	1	NAG	O7-C7-N2-C2

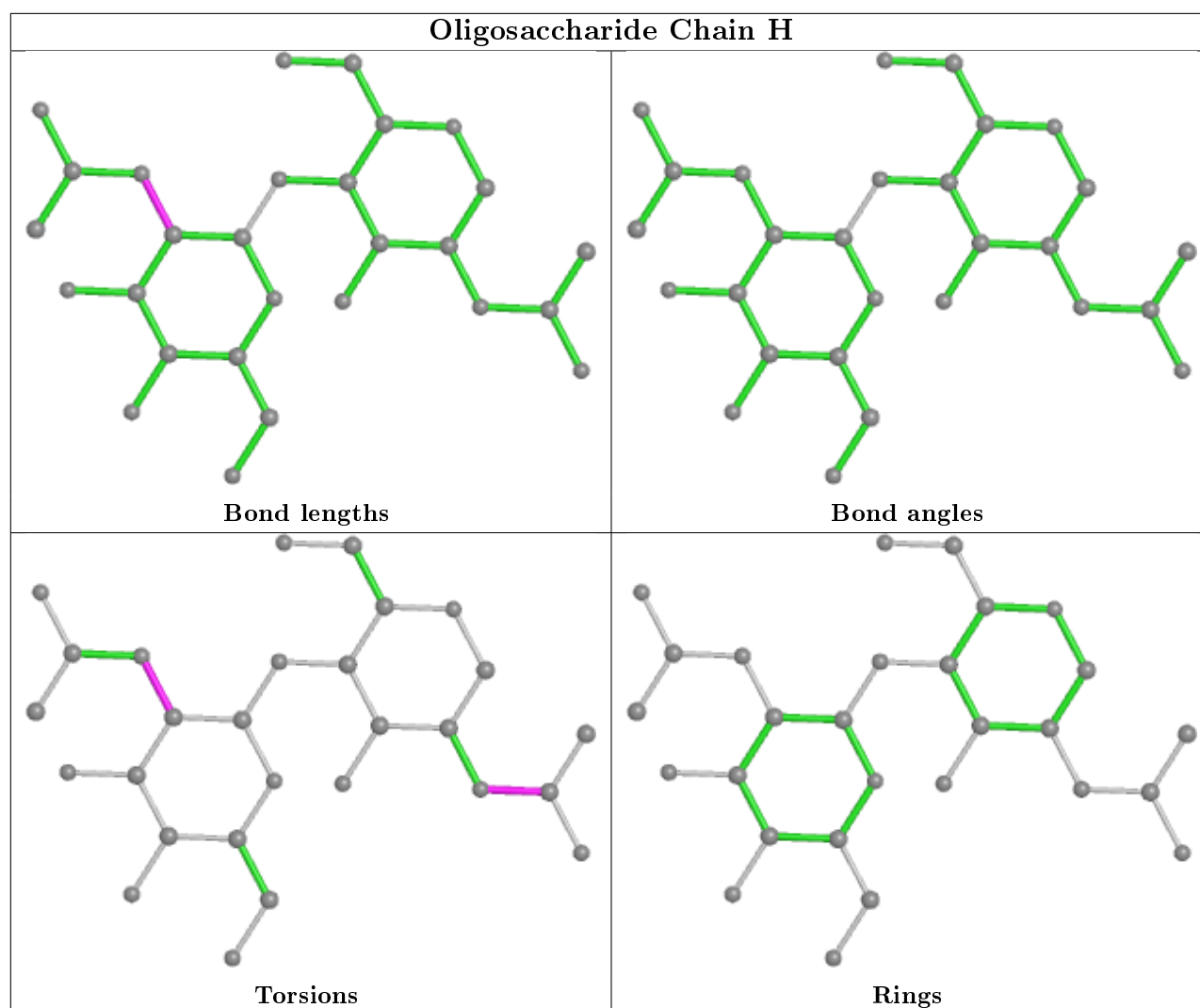
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

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 ⓘ

6 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	NGT	B	558	-	13,15,15	1.44	2 (15%)	12,22,22	0.85	1 (8%)
5	NGT	A	557	-	13,15,15	1.42	2 (15%)	12,22,22	0.85	1 (8%)
7	SO4	B	557	-	4,4,4	0.28	0	6,6,6	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	559	-	5,5,5	0.48	0	5,5,5	0.61	0
6	GOL	B	559	-	5,5,5	0.44	0	5,5,5	0.50	0
6	GOL	A	558	-	5,5,5	0.41	0	5,5,5	0.29	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
5	NGT	B	558	-	-	1/2/30/30	0/2/2/2
6	GOL	B	559	-	-	0/4/4/4	-
5	NGT	A	557	-	-	0/2/30/30	0/2/2/2
6	GOL	A	559	-	-	2/4/4/4	-
6	GOL	A	558	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	558	NGT	C2-N2	-3.82	1.43	1.47
5	A	557	NGT	C3-C2	3.55	1.59	1.53
5	A	557	NGT	C2-N2	-3.19	1.44	1.47
5	B	558	NGT	C3-C2	2.65	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	558	NGT	C1-O5-C5	2.28	116.78	112.58
5	A	557	NGT	C1-O5-C5	2.26	116.74	112.58

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	559	GOL	C1-C2-C3-O3
6	A	559	GOL	O2-C2-C3-O3
6	A	558	GOL	O1-C1-C2-C3
5	B	558	NGT	O5-C5-C6-O6
6	A	558	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	558	NGT	1	0
5	A	557	NGT	1	0
7	B	557	SO4	1	0
6	B	559	GOL	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	53/58 (91%)	-0.05	3 (5%)	23 25	17, 25, 37, 45	0
1	B	53/58 (91%)	0.22	3 (5%)	23 25	21, 29, 40, 43	0
2	C	190/190 (100%)	-0.17	3 (1%)	72 74	16, 21, 30, 41	0
2	E	190/190 (100%)	-0.19	5 (2%)	56 59	18, 23, 34, 44	0
3	D	237/241 (98%)	0.10	8 (3%)	45 48	15, 24, 46, 55	0
3	F	237/241 (98%)	-0.12	6 (2%)	57 61	16, 24, 38, 51	0
All	All	960/978 (98%)	-0.07	28 (2%)	51 55	15, 24, 39, 55	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	316	LEU	9.9
3	D	316	LEU	8.2
2	C	311	SER	6.9
1	A	107	GLY	6.7
3	D	317	ASP	6.4
3	F	317	ASP	5.7
1	B	107	GLY	4.1
3	D	552	ASN	4.0
1	B	78	TYR	3.6
3	D	374	LYS	3.5
3	D	376	PHE	3.5
3	F	552	ASN	3.4
1	B	75	GLU	3.3
3	F	417	PRO	3.1
2	E	122	THR	2.9
3	F	475	GLN	2.8
3	D	373	GLN	2.7
1	A	78	TYR	2.7
2	C	262	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	134	GLN	2.4
2	E	310	TYR	2.3
2	E	311	SER	2.3
1	A	75	GLU	2.2
3	D	371	MET	2.1
3	F	476	LYS	2.1
2	C	134	GLN	2.1
3	D	386	PHE	2.0
2	E	303	LYS	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](#)

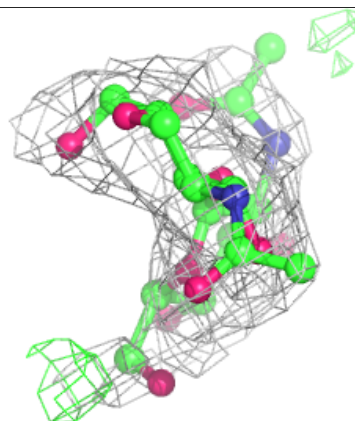
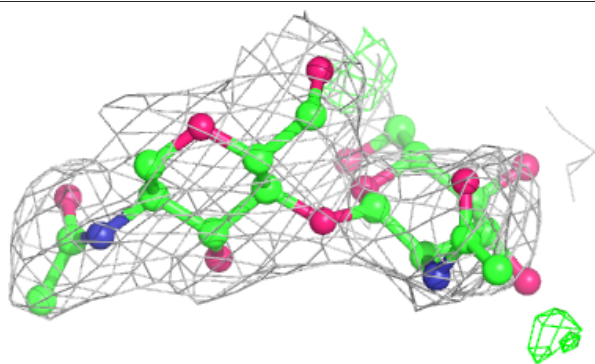
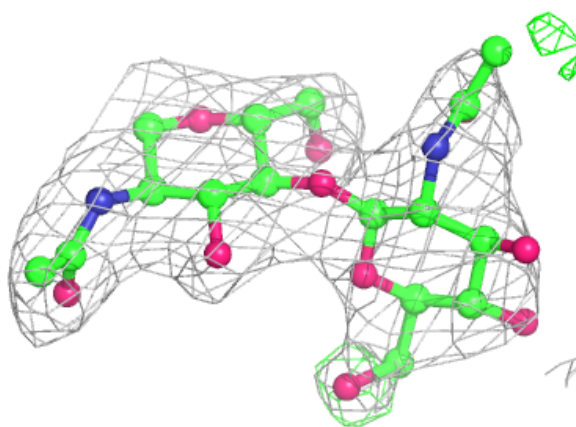
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

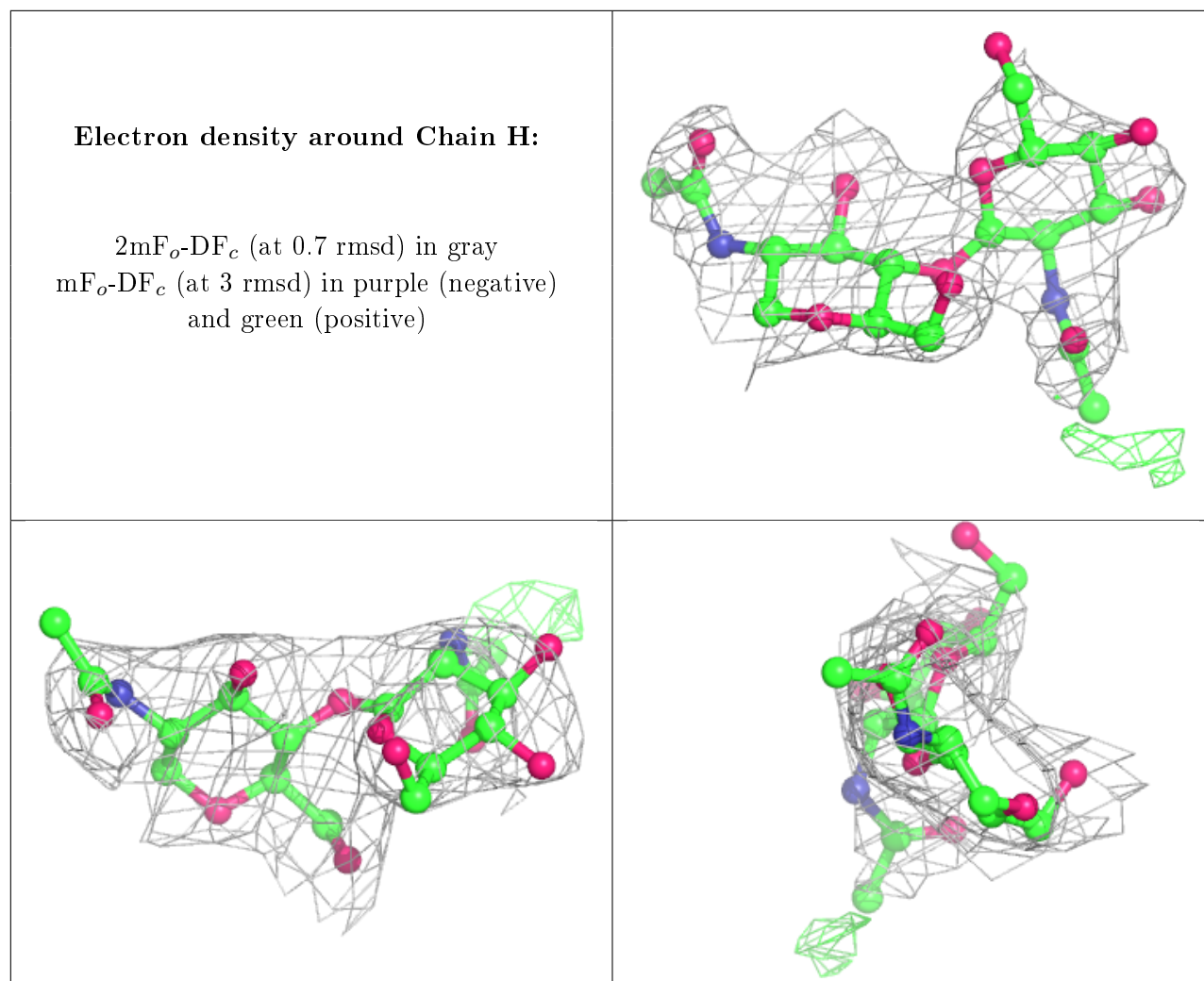
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	G	2	14/15	0.86	0.38	87,93,94,95	0
4	NAG	H	2	14/15	0.88	0.44	105,111,112,113	0
4	NAG	H	1	14/15	0.92	0.22	64,73,75,84	0
4	NAG	G	1	14/15	0.95	0.16	47,53,57,65	0

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 G:

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





6.4 Ligands ⓘ

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
6	GOL	A	558	6/6	0.76	0.29	61,63,64,64	0
5	NGT	B	558	14/14	0.90	0.21	48,51,52,52	0
5	NGT	A	557	14/14	0.91	0.16	43,46,48,49	0
6	GOL	B	559	6/6	0.96	0.14	38,39,39,40	0
6	GOL	A	559	6/6	0.97	0.11	35,37,37,37	0
7	SO4	B	557	5/5	0.99	0.11	37,37,39,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.