Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 07:43 pm GMT

PDB ID	:	6I6R
Title	:	New Irreversible a-l-Iduronidase Inhibitors and Activity-Based Probes
Authors	:	Gloster, T.M.; McMahon, S.A.; Oehler, V.
Deposited on	:	2018-11-15
Resolution	:	2.02 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 (1)) were used in the production of this report:

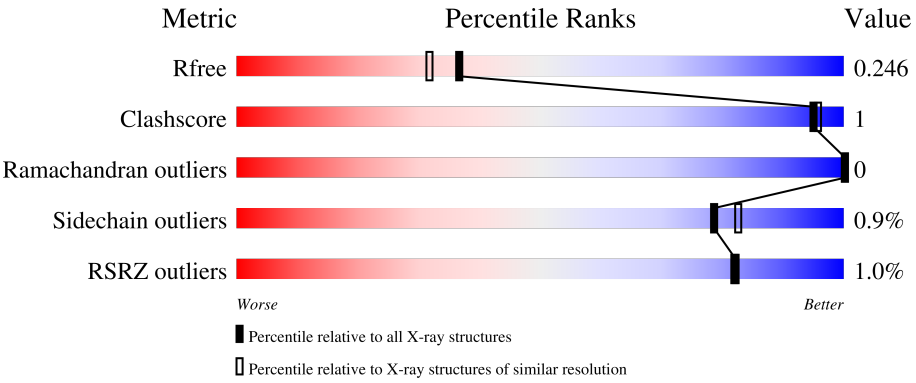
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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% 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	627	93% · 5%
1	B	627	92% · ·
2	C	3	100%
2	D	3	33% 67%

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
7	CL	A	710	-	-	X	-
7	CL	B	708	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9957 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.

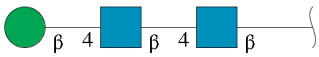
- Molecule 1 is a protein called Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	2	0
			4765	3052	860	841	12			
1	B	599	Total	C	N	O	S	0	0	0
			4759	3051	856	840	12			

There are 6 discrepancies between the modelled and reference sequences:

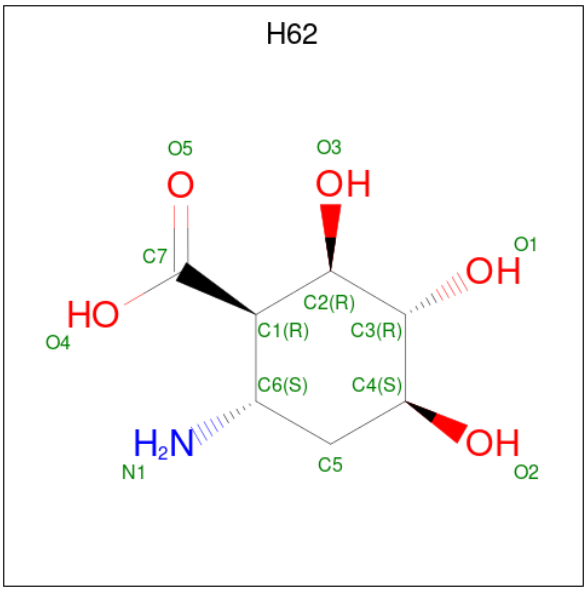
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLN	HIS	conflict	UNP P35475
A	63	PRO	GLN	conflict	UNP P35475
A	105	GLN	ARG	conflict	UNP P35475
B	33	GLN	HIS	conflict	UNP P35475
B	63	PRO	GLN	conflict	UNP P35475
B	105	GLN	ARG	conflict	UNP P35475

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



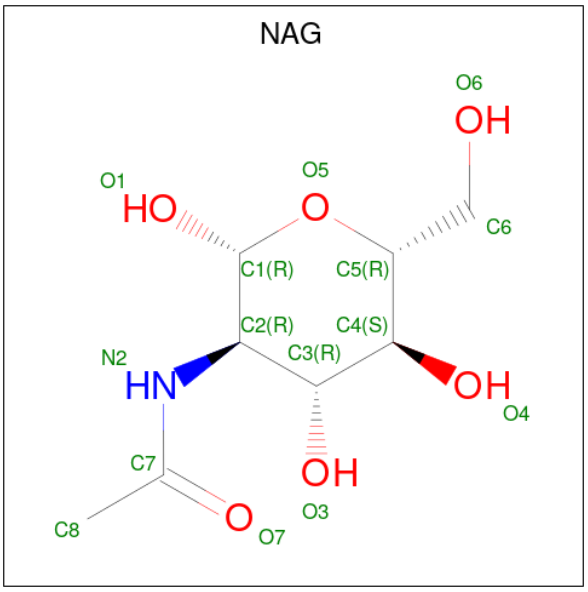
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is (1 {R},2 {R},3 {R},4 {S},6 {S})-6-azanyl-2,3,4-tris(oxidanyl)cyclohexane-1-carboxylic acid (three-letter code: H62) (formula: $C_7H_{13}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 13 7 1 5	0	0
3	B	1	Total C N O 13 7 1 5	0	0

- 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 14 8 1 5	0	0

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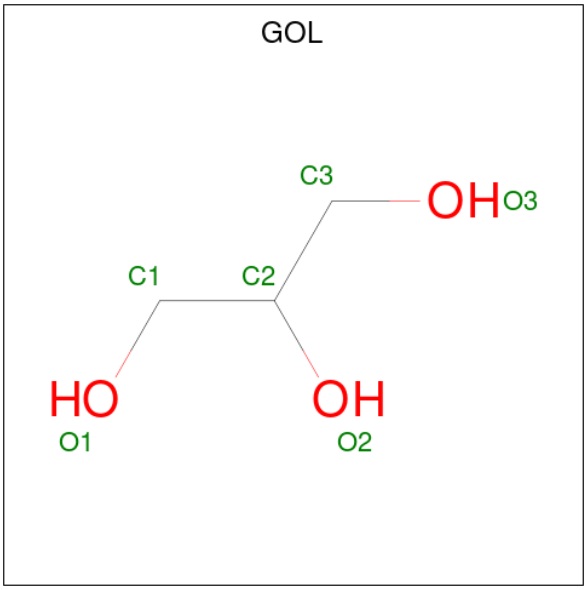
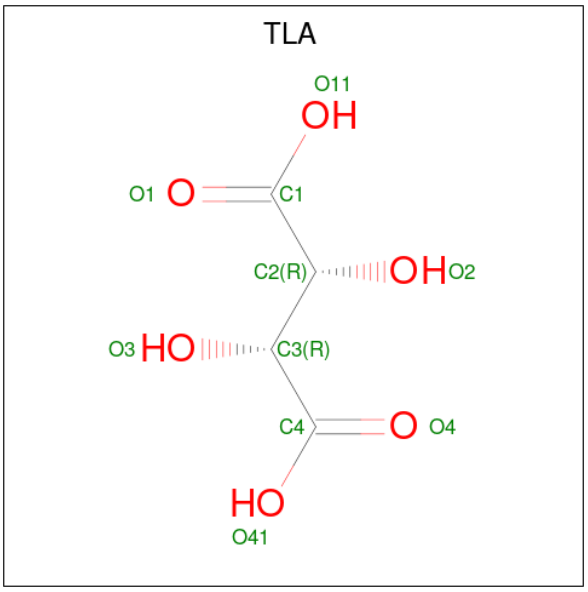
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is water.

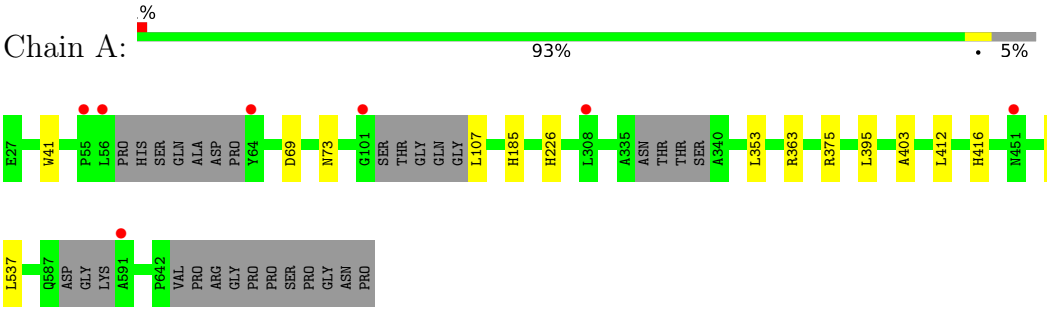
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	139	Total O 139 139	0	0
8	B	104	Total O 104 104	0	0

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.

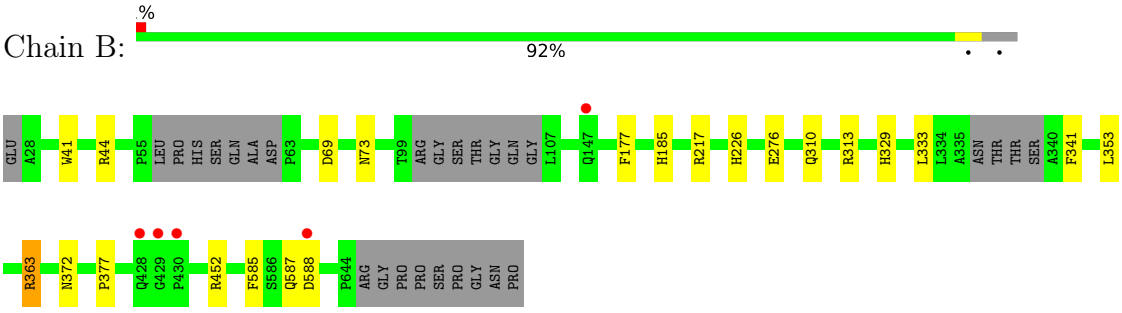
• Molecule 1: Alpha-L-iduronidase

Chain A:



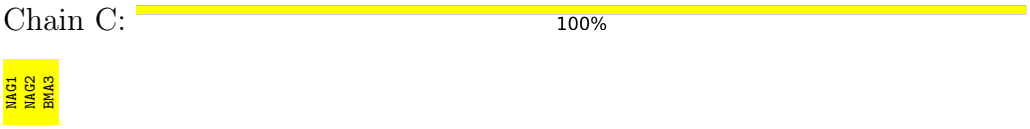
• Molecule 1: Alpha-L-iduronidase

Chain B:



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

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	206.86Å 69.89Å 93.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.21 – 2.02 66.21 – 2.02	Depositor EDS
% Data completeness (in resolution range)	94.3 (66.21-2.02) 94.3 (66.21-2.02)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.213 , 0.240 0.220 , 0.246	Depositor DCC
R_{free} test set	4232 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9957	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: H62, TLA, GOL, NAG, CL, BMA

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	0.42	0/4911	0.62	0/6707
1	B	0.40	0/4907	0.62	2/6705 (0.0%)
All	All	0.41	0/9818	0.62	2/13412 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	363	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	B	363	ARG	NE-CZ-NH1	5.30	122.95	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	4765	0	4666	10	0
1	B	4759	0	4668	12	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	13	0	0	1	0
3	B	13	0	0	1	0
4	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	26	0	0
5	A	12	0	16	2	0
5	B	6	0	8	0	0
6	A	10	0	4	0	0
7	A	1	0	0	2	0
7	B	1	0	0	3	0
8	A	139	0	0	0	0
8	B	104	0	0	0	0
All	All	9957	0	9482	22	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 (22) 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:363:ARG:NH2	3:A:704:H62:O3	2.20	0.73
1:A:403:ALA:HB3	5:A:707:GOL:H11	1.71	0.72
1:A:403:ALA:HB3	5:A:707:GOL:C1	2.30	0.60
1:B:310:GLN:HB2	1:B:313:ARG:HD2	1.86	0.56
1:B:185:HIS:NE2	1:B:226:HIS:CD2	2.76	0.53
1:A:185:HIS:NE2	1:A:226:HIS:CD2	2.76	0.53
1:B:363:ARG:NH2	3:B:704:H62:O3	2.42	0.52
1:B:363:ARG:HD3	7:B:708:CL:CL	2.51	0.48
1:A:363:ARG:HD2	7:A:710:CL:CL	2.50	0.47
1:B:333:LEU:HD11	1:B:341:PHE:CE2	2.50	0.47
1:B:585:PHE:CZ	1:B:587:GLN:HG2	2.50	0.46
1:B:313:ARG:NH2	7:B:708:CL:CL	2.83	0.46
1:A:412:LEU:HD13	1:A:416[B]:HIS:CD2	2.52	0.45
1:A:395:LEU:HD12	1:A:537:LEU:CD2	2.48	0.43
1:A:501:PHE:HA	1:A:504:MET:HE3	2.00	0.43
1:A:363:ARG:CD	7:A:710:CL:CL	3.04	0.42
1:B:363:ARG:CD	7:B:708:CL:CL	3.05	0.42
1:A:73:ASN:HB2	1:A:353:LEU:HD21	2.01	0.42
1:B:276:GLU:OE1	1:B:329:HIS:NE2	2.38	0.41
1:B:73:ASN:HB2	1:B:353:LEU:HD21	2.02	0.41
1:B:177:PHE:HB2	1:B:217:ARG:O	2.20	0.41
1:B:372:ASN:HA	1:B:377:PRO:HB3	2.03	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	589/627 (94%)	568 (96%)	21 (4%)	0	100	100
1	B	591/627 (94%)	572 (97%)	19 (3%)	0	100	100
All	All	1180/1254 (94%)	1140 (97%)	40 (3%)	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	505/527 (96%)	501 (99%)	4 (1%)	81	85
1	B	505/527 (96%)	500 (99%)	5 (1%)	76	80
All	All	1010/1054 (96%)	1001 (99%)	9 (1%)	78	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	69	ASP
1	A	107	LEU
1	A	375	ARG
1	B	41	TRP
1	B	44	ARG
1	B	69	ASP
1	B	452	ARG

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Mol	Chain	Res	Type
1	B	588	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	B	226	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.38	0	17,19,21	1.10	1 (5%)
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	1.45	3 (17%)
2	BMA	C	3	2	11,11,12	0.42	0	15,15,17	0.91	1 (6%)
2	NAG	D	1	1,2	14,14,15	1.81	1 (7%)	17,19,21	1.86	4 (23%)
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	1.15	2 (11%)
2	BMA	D	3	2	11,11,12	0.27	0	15,15,17	0.81	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	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)
2	D	1	NAG	O5-C1	-6.18	1.33	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	-5.68	104.49	112.19
2	C	2	NAG	C1-O5-C5	3.67	117.17	112.19
2	D	2	NAG	O5-C1-C2	-3.11	106.37	111.29
2	C	1	NAG	O5-C1-C2	-2.74	106.96	111.29
2	C	2	NAG	C6-C5-C4	-2.53	107.09	113.00
2	C	2	NAG	C1-C2-N2	2.34	114.48	110.49
2	D	1	NAG	C4-C3-C2	-2.22	107.76	111.02
2	D	1	NAG	O5-C1-C2	-2.10	107.97	111.29
2	D	2	NAG	C1-O5-C5	2.09	115.02	112.19
2	C	3	BMA	O5-C5-C6	2.05	110.41	107.20
2	D	1	NAG	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

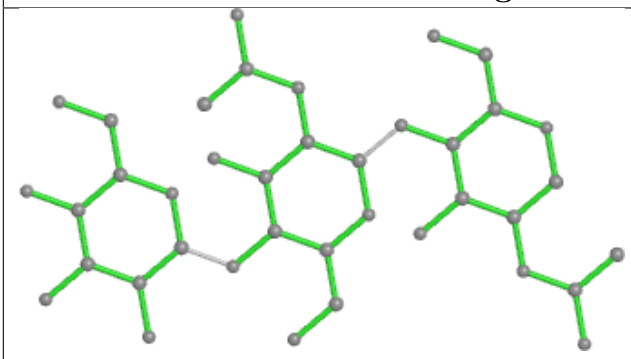
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

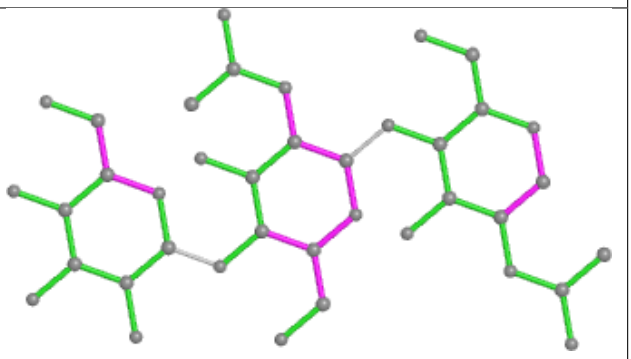
No monomer is involved in short contacts.

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

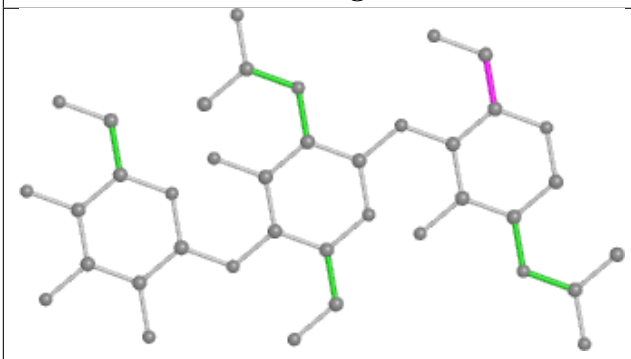
Oligosaccharide Chain C



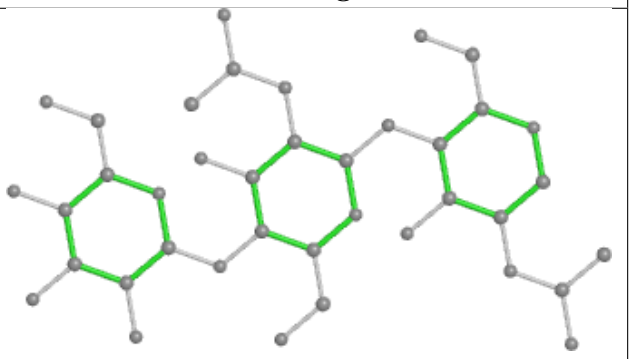
Bond lengths



Bond angles

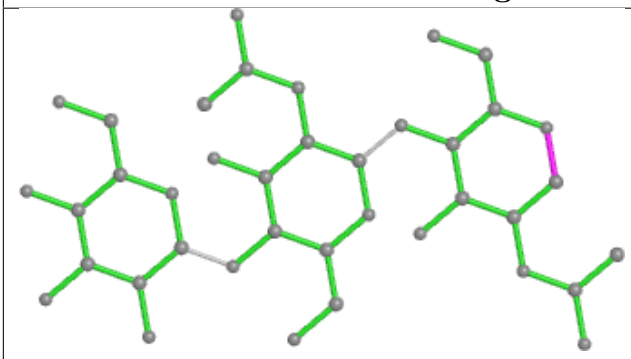


Torsions

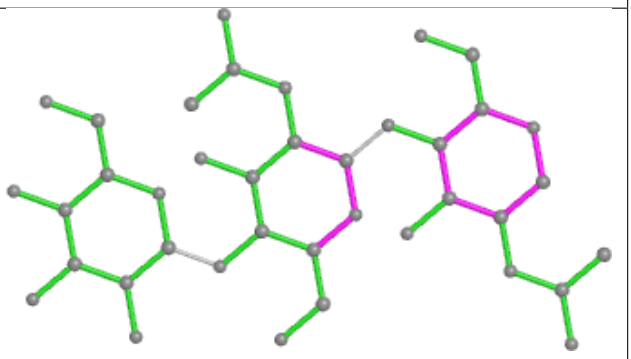


Rings

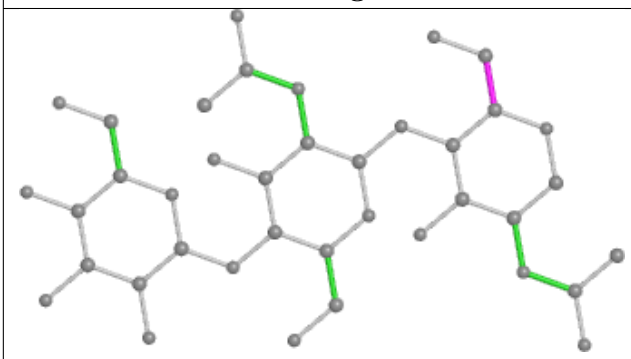
Oligosaccharide Chain D



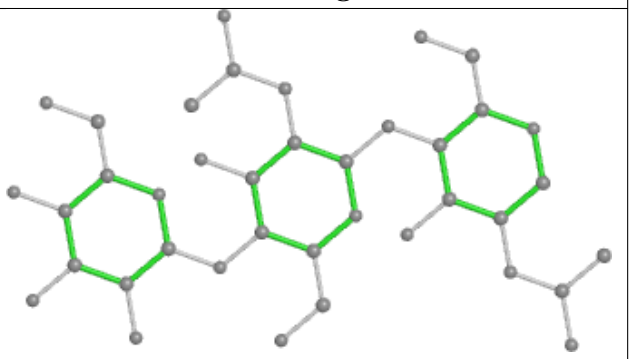
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	NAG	B	706	1	14,14,15	0.57	0	17,19,21	1.15	1 (5%)
3	H62	B	704	1	13,13,13	0.65	0	15,19,19	1.29	2 (13%)
5	GOL	A	707	-	5,5,5	0.40	0	5,5,5	0.36	0
3	H62	A	704	1	13,13,13	0.86	0	15,19,19	1.34	2 (13%)
5	GOL	B	707	-	5,5,5	0.20	0	5,5,5	0.63	0
4	NAG	B	705	1	14,14,15	0.34	0	17,19,21	0.97	1 (5%)
6	TLA	A	709	-	9,9,9	1.18	0	12,12,12	1.14	1 (8%)
4	NAG	A	706	1	14,14,15	0.38	0	17,19,21	1.07	0
5	GOL	A	708	-	5,5,5	0.62	0	5,5,5	0.73	0
4	NAG	A	705	1	14,14,15	0.36	0	17,19,21	1.44	3 (17%)

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	B	706	1	-	0/6/23/26	0/1/1/1
3	H62	B	704	1	-	2/4/24/24	0/1/1/1
5	GOL	A	707	-	-	4/4/4/4	-
3	H62	A	704	1	-	3/4/24/24	0/1/1/1
5	GOL	B	707	-	-	2/4/4/4	-
4	NAG	B	705	1	-	2/6/23/26	0/1/1/1
6	TLA	A	709	-	-	0/12/12/12	-
4	NAG	A	706	1	-	0/6/23/26	0/1/1/1
5	GOL	A	708	-	-	2/4/4/4	-
4	NAG	A	705	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	705	NAG	O5-C5-C6	3.78	113.14	107.20
4	B	706	NAG	C1-O5-C5	3.47	116.90	112.19
4	A	705	NAG	O5-C1-C2	-2.82	106.83	111.29
3	B	704	H62	C1-C2-C3	2.47	113.66	110.43
3	B	704	H62	C5-C4-C3	-2.45	107.13	110.69
3	A	704	H62	C5-C4-C3	-2.41	107.18	110.69
6	A	709	TLA	O11-C1-C2	2.38	119.72	113.27
3	A	704	H62	C2-C1-C7	-2.22	106.67	110.45
4	B	705	NAG	C1-O5-C5	2.15	115.11	112.19
4	A	705	NAG	C8-C7-N2	2.09	119.64	116.10

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	707	GOL	O1-C1-C2-C3
5	A	707	GOL	C1-C2-C3-O3
5	A	708	GOL	O1-C1-C2-C3
4	A	705	NAG	O5-C5-C6-O6
4	A	705	NAG	C4-C5-C6-O6
4	A	705	NAG	C8-C7-N2-C2
4	A	705	NAG	O7-C7-N2-C2
5	A	707	GOL	O2-C2-C3-O3
4	B	705	NAG	O5-C5-C6-O6
5	B	707	GOL	O1-C1-C2-C3
5	A	707	GOL	O1-C1-C2-O2
5	B	707	GOL	O1-C1-C2-O2
4	B	705	NAG	C4-C5-C6-O6
3	A	704	H62	C6-C1-C7-O5
3	A	704	H62	C6-C1-C7-O4
3	B	704	H62	C6-C1-C7-O5
3	B	704	H62	C6-C1-C7-O4
5	A	708	GOL	O1-C1-C2-O2
3	A	704	H62	C2-C1-C7-O4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	704	H62	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	707	GOL	2	0
3	A	704	H62	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, 95^{th} 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	597/627 (95%)	0.07	7 (1%)	79 78	25, 33, 50, 71	0
1	B	599/627 (95%)	0.06	5 (0%)	86 85	28, 39, 58, 87	0
All	All	1196/1254 (95%)	0.06	12 (1%)	82 82	25, 36, 55, 87	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	GLY	4.4
1	B	588	ASP	4.2
1	A	451	ASN	4.0
1	B	429	GLY	3.7
1	A	55	PRO	2.9
1	A	591	ALA	2.8
1	B	428	GLN	2.6
1	A	64	TYR	2.4
1	B	430	PRO	2.4
1	A	56	LEU	2.2
1	A	308	LEU	2.2
1	B	147	GLN	2.1

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

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

6.3 Carbohydrates

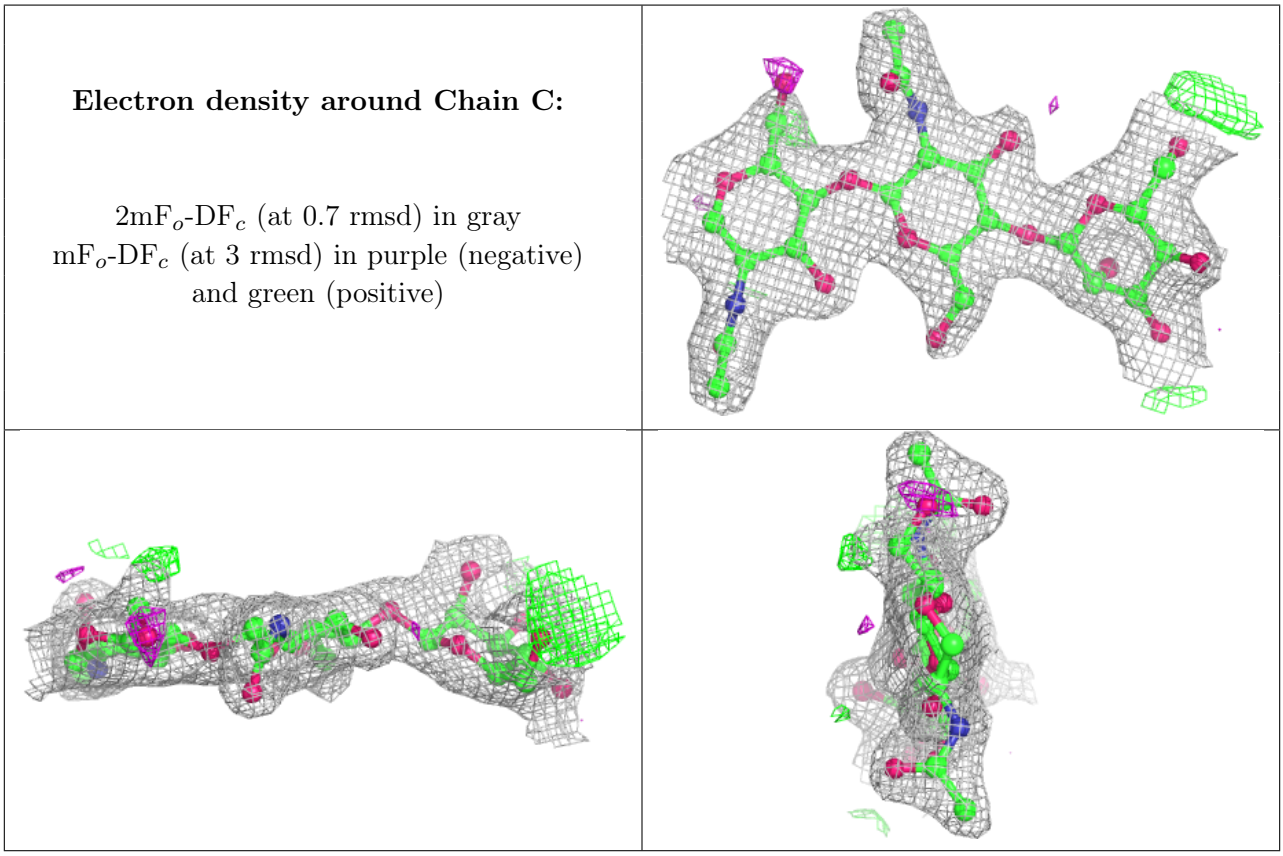
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

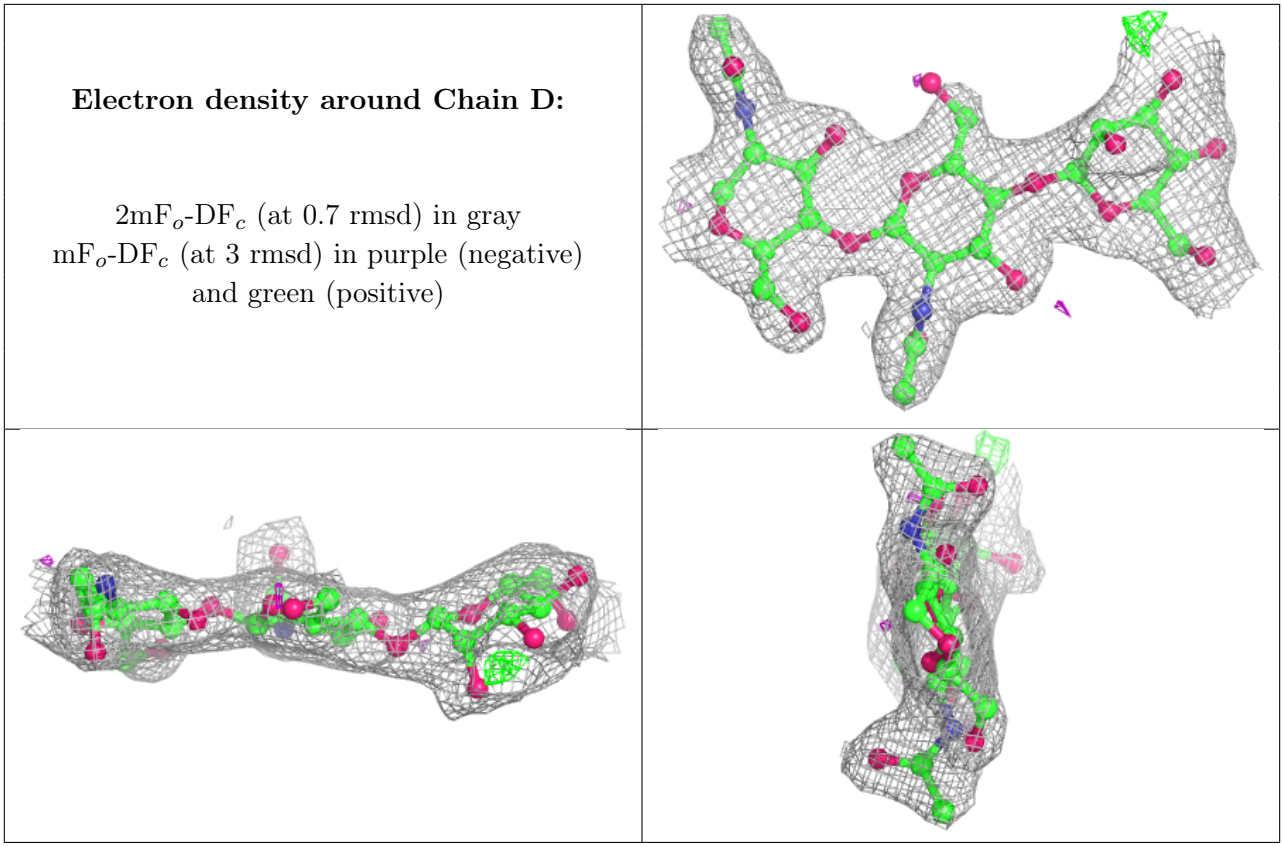
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	D	3	11/12	0.86	0.13	54,57,58,60	0
2	BMA	C	3	11/12	0.88	0.11	47,50,57,59	0
2	NAG	C	1	14/15	0.91	0.15	41,43,45,51	0
2	NAG	D	2	14/15	0.94	0.12	48,50,55,61	0
2	NAG	D	1	14/15	0.94	0.12	49,51,53,54	0
2	NAG	C	2	14/15	0.95	0.11	43,44,46,51	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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





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, 95^{th} 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	B	706	14/15	0.80	0.23	51,54,60,63	0
4	NAG	B	705	14/15	0.82	0.17	64,69,73,74	0
3	H62	A	704	13/13	0.83	0.17	35,41,47,48	0
3	H62	B	704	13/13	0.84	0.15	42,45,48,50	0
4	NAG	A	705	14/15	0.85	0.15	49,54,60,61	0
5	GOL	A	707	6/6	0.86	0.23	37,38,40,40	0
5	GOL	A	708	6/6	0.88	0.24	36,42,44,48	0
6	TLA	A	709	10/10	0.89	0.17	45,49,50,52	0
5	GOL	B	707	6/6	0.91	0.23	43,51,52,54	0
4	NAG	A	706	14/15	0.93	0.10	41,45,49,54	0
7	CL	A	710	1/1	0.99	0.11	28,28,28,28	0
7	CL	B	708	1/1	1.00	0.12	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.