Full wwPDB X-ray Structure Validation Report (i)

Sep 21, 2020 – 04:52 PM BST

PDB ID	:	3NSN
Title	:	Crystal Structure of insect beta-N-acetyl-D-hexosaminidase OfHex1 complexed with TMG-chitotriomycin
Authors	:	Zhang, H.; Liu, T.; Liu, F.; Yang, Q.; Shen, X.
Deposited on	:	2010-07-02
Resolution	:	2.10 Å(reported)

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	:	2.14.6
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)	:	2.14.6

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 2.10 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.
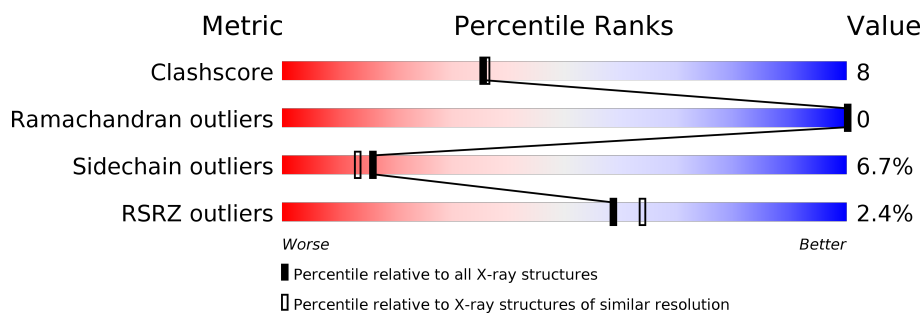
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	572	2% · 78% · 17% · ·
2	B	4	50% · 25% · 25%

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	1	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5097 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 N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4615	2944	776	870	25			

- Molecule 2 is an oligosaccharide called 2-deoxy-2-(trimethylammonio)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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	B	4	Total	C	N	O	0	0	0
			57	33	4	20			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	425	Total	O	0	0
			425	425		

3 Residue-property plots ⓘ

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: N-acetylglucosaminidase
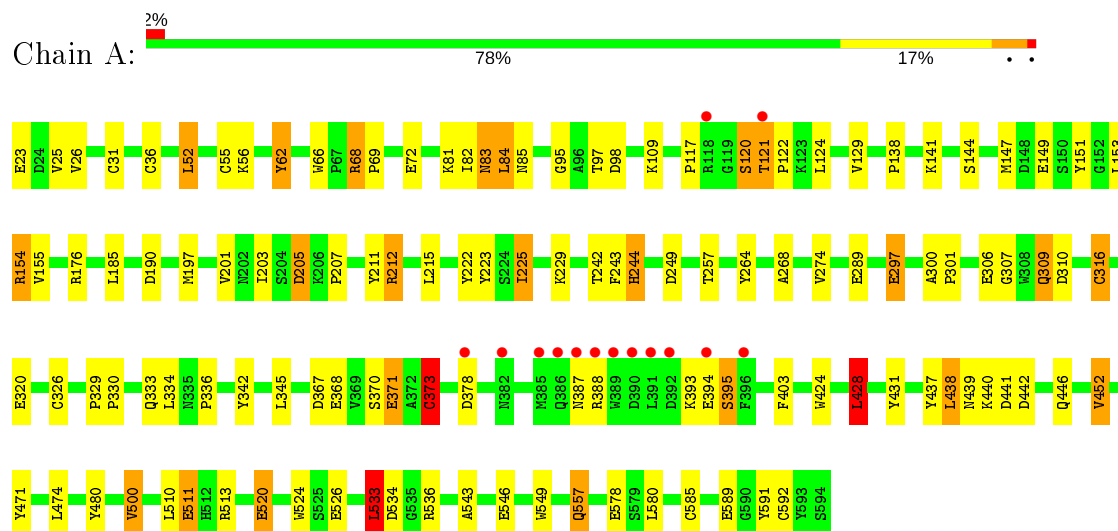
• Molecule 2: 2-deoxy-2-(trimethylammonio)-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.50Å 108.50Å 175.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.13 – 2.10 28.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.13-2.10) 79.3 (28.13-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.10Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0072	Depositor
R, R_{free}	0.202 , (Not available) 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.6	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5097	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TMX, 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	1.71	36/4737 (0.8%)	0.91	12/6432 (0.2%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	CYS	CB-SG	-9.42	1.66	1.82
1	A	316	CYS	CB-SG	-9.12	1.66	1.82
1	A	480	TYR	CD2-CE2	-8.41	1.26	1.39
1	A	585	CYS	CB-SG	-8.14	1.68	1.82
1	A	31	CYS	CB-SG	-7.51	1.69	1.82
1	A	326	CYS	CB-SG	-7.00	1.70	1.82
1	A	480	TYR	CD1-CE1	-6.85	1.29	1.39
1	A	222	TYR	CD1-CE1	-6.85	1.29	1.39
1	A	243	PHE	CD2-CE2	-6.67	1.25	1.39
1	A	592	CYS	CB-SG	-6.50	1.71	1.82
1	A	243	PHE	CD1-CE1	-6.45	1.26	1.39
1	A	289	GLU	CD-OE2	-5.98	1.19	1.25
1	A	526	GLU	CD-OE1	-5.85	1.19	1.25
1	A	480	TYR	CZ-OH	-5.74	1.28	1.37
1	A	591	TYR	CD2-CE2	-5.66	1.30	1.39
1	A	306	GLU	CD-OE1	-5.61	1.19	1.25
1	A	471	TYR	CD2-CE2	-5.61	1.30	1.39
1	A	526	GLU	CD-OE2	-5.57	1.19	1.25
1	A	66	TRP	CE3-CZ3	-5.55	1.29	1.38
1	A	212	ARG	CZ-NH2	-5.54	1.25	1.33
1	A	431	TYR	CD2-CE2	-5.48	1.31	1.39
1	A	212	ARG	CD-NE	-5.43	1.37	1.46
1	A	452	VAL	CB-CG1	-5.40	1.41	1.52
1	A	520	GLU	CD-OE2	-5.39	1.19	1.25
1	A	480	TYR	CE1-CZ	-5.38	1.31	1.38
1	A	26	VAL	CB-CG1	-5.30	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE2	-5.28	1.19	1.25
1	A	578	GLU	CD-OE1	-5.25	1.19	1.25
1	A	62	TYR	CD2-CE2	-5.18	1.31	1.39
1	A	297	GLU	CD-OE2	-5.14	1.20	1.25
1	A	264	TYR	CD2-CE2	-5.14	1.31	1.39
1	A	511	GLU	CD-OE2	-5.08	1.20	1.25
1	A	268	ALA	CA-CB	-5.05	1.41	1.52
1	A	320	GLU	CD-OE1	-5.03	1.20	1.25
1	A	342	TYR	CD1-CE1	-5.03	1.31	1.39
1	A	524	TRP	CG-CD1	-5.00	1.29	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	A	534	ASP	CB-CG-OD1	8.62	126.06	118.30
1	A	212	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	68	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	536	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	190	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	205	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	428	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	68	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	98	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	395	SER	N-CA-CB	-5.12	102.82	110.50
1	A	533	LEU	CA-CB-CG	-5.08	103.61	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4615	0	4448	71	0
2	B	57	0	56	1	0
3	A	425	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5097	0	4504	71	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 8.

All (71) 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:510:LEU:O	1:A:513:ARG:HG3	1.54	1.08
1:A:333:GLN:NE2	1:A:370:SER:H	1.59	1.00
1:A:333:GLN:HE22	1:A:370:SER:N	1.70	0.88
1:A:36:CYS:HG	1:A:55:CYS:HG	1.02	0.87
1:A:333:GLN:HE22	1:A:370:SER:H	0.90	0.87
1:A:371:GLU:H	1:A:371:GLU:CD	1.82	0.82
1:A:52:LEU:HD21	1:A:56:LYS:HE2	1.64	0.79
1:A:371:GLU:HG3	1:A:393:LYS:HE2	1.65	0.78
1:A:307:GLY:H	1:A:309:GLN:HE22	1.32	0.74
1:A:129:VAL:HG21	1:A:197:MET:HE1	1.70	0.74
1:A:424:TRP:CZ3	1:A:446:GLN:HG2	2.23	0.73
1:A:309:GLN:H	1:A:309:GLN:HE21	1.35	0.73
1:A:52:LEU:CD2	1:A:56:LYS:HE2	2.19	0.73
1:A:387:ASN:O	1:A:388:ARG:HG2	1.92	0.70
1:A:316:CYS:HG	1:A:373:CYS:HG	1.41	0.69
1:A:149:GLU:OE1	1:A:212:ARG:NH2	2.27	0.68
1:A:82:ILE:HG13	1:A:197:MET:HE2	1.77	0.65
1:A:367:ASP:N	1:A:367:ASP:OD1	2.29	0.64
1:A:129:VAL:CG2	1:A:197:MET:HE1	2.28	0.63
1:A:83:ASN:HD22	1:A:84:LEU:N	2.00	0.60
1:A:82:ILE:HG13	1:A:197:MET:CE	2.33	0.59
1:A:83:ASN:C	1:A:83:ASN:HD22	2.05	0.58
1:A:215:LEU:C	1:A:215:LEU:HD23	2.23	0.57
1:A:225:ILE:CD1	1:A:229:LYS:HE3	2.36	0.56
1:A:511:GLU:H	1:A:511:GLU:CD	2.09	0.55
1:A:371:GLU:N	1:A:371:GLU:CD	2.56	0.55
1:A:316:CYS:HG	1:A:373:CYS:CB	2.19	0.54
1:A:155:VAL:HB	1:A:201:VAL:HB	1.89	0.54
1:A:439:ASN:HD22	1:A:441:ASP:H	1.54	0.54
1:A:244:HIS:HD2	1:A:520:GLU:OE1	1.91	0.53
1:A:307:GLY:H	1:A:309:GLN:NE2	2.02	0.52
1:A:52:LEU:HD22	1:A:56:LYS:HD2	1.90	0.52
1:A:95:GLY:HA3	1:A:138:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASN:O	1:A:388:ARG:CG	2.57	0.51
1:A:439:ASN:ND2	1:A:442:ASP:H	2.09	0.51
1:A:211:TYR:CZ	1:A:242:THR:HG21	2.47	0.50
1:A:121:THR:HG22	1:A:122:PRO:HD2	1.93	0.50
1:A:83:ASN:ND2	1:A:85:ASN:H	2.11	0.49
1:A:81:LYS:O	1:A:82:ILE:HD13	2.12	0.49
1:A:154:ARG:HB3	1:A:154:ARG:HH21	1.79	0.48
1:A:334:LEU:O	1:A:336:PRO:HD3	2.16	0.46
1:A:223:TYR:HE1	1:A:533:LEU:HB2	1.80	0.46
1:A:151:TYR:CE2	1:A:205:ASP:HB3	2.51	0.45
1:A:72:GLU:O	1:A:203:ILE:HA	2.16	0.45
1:A:117:PRO:O	1:A:120:SER:HB2	2.16	0.45
1:A:185:LEU:HD13	1:A:201:VAL:HG21	1.97	0.45
1:A:336:PRO:HB3	1:A:403:PHE:HB2	1.99	0.45
1:A:500:VAL:HG22	1:A:543:ALA:HB3	1.98	0.45
1:A:309:GLN:O	1:A:310:ASP:HB2	2.17	0.44
1:A:36:CYS:HG	1:A:55:CYS:CB	2.30	0.44
1:A:207:PRO:HB3	1:A:549:TRP:CE3	2.53	0.43
1:A:52:LEU:HD22	1:A:56:LYS:HE2	2.00	0.43
1:A:129:VAL:HG21	1:A:197:MET:CE	2.45	0.43
1:A:244:HIS:HE1	1:A:297:GLU:OE1	2.02	0.43
1:A:56:LYS:NZ	1:A:589:GLU:OE1	2.47	0.43
1:A:62:TYR:CE2	1:A:68:ARG:HD2	2.53	0.43
1:A:300:ALA:HB1	1:A:301:PRO:HA	2.01	0.43
1:A:97:THR:HG22	1:A:141:LYS:HB3	2.01	0.43
1:A:244:HIS:CE1	1:A:297:GLU:OE1	2.73	0.42
1:A:368:GLU:CD	2:B:4:TMX:H27	2.39	0.42
1:A:329:PRO:HA	1:A:330:PRO:HA	1.77	0.42
1:A:83:ASN:HD22	1:A:85:ASN:H	1.68	0.42
1:A:309:GLN:NE2	1:A:309:GLN:H	2.11	0.42
1:A:428:LEU:HD22	1:A:437:TYR:CD2	2.55	0.42
1:A:557:GLN:NE2	1:A:557:GLN:H	2.18	0.41
1:A:225:ILE:HD11	1:A:229:LYS:HE3	2.00	0.41
1:A:437:TYR:C	1:A:438:LEU:HD13	2.40	0.41
1:A:82:ILE:HA	1:A:82:ILE:HD13	1.76	0.41
1:A:68:ARG:HA	1:A:69:PRO:HD3	1.87	0.41
1:A:144:SER:O	1:A:147:MET:HG2	2.21	0.40
1:A:215:LEU:HD12	1:A:244:HIS:CD2	2.56	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	570/572 (100%)	560 (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	495/495 (100%)	462 (93%)	33 (7%)	16 13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	25	VAL
1	A	52	LEU
1	A	83	ASN
1	A	84	LEU
1	A	109	LYS
1	A	120	SER
1	A	121	THR
1	A	124	LEU
1	A	153	LEU
1	A	154	ARG
1	A	176	ARG
1	A	225	ILE

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Mol	Chain	Res	Type
1	A	244	HIS
1	A	249	ASP
1	A	257	THR
1	A	274	VAL
1	A	309	GLN
1	A	345	LEU
1	A	371	GLU
1	A	373	CYS
1	A	378	ASP
1	A	394	GLU
1	A	395	SER
1	A	428	LEU
1	A	438	LEU
1	A	440	LYS
1	A	452	VAL
1	A	474	LEU
1	A	500	VAL
1	A	533	LEU
1	A	557	GLN
1	A	580	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	83	ASN
1	A	137	ASN
1	A	170	ASN
1	A	244	HIS
1	A	309	GLN
1	A	333	GLN
1	A	381	GLN
1	A	408	GLN
1	A	439	ASN
1	A	515	GLN
1	A	557	GLN
1	A	588	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)

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	#$|Z| > 2$
2	NAG	B	1	2	15,15,15	1.64	3 (20%)	21,21,21	2.11	5 (23%)
2	NAG	B	2	2	14,14,15	0.72	0	17,19,21	1.03	0
2	NAG	B	3	2	14,14,15	0.68	0	17,19,21	0.88	0
2	TMX	B	4	2	12,14,15	1.06	1 (8%)	18,21,23	1.27	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
2	NAG	B	1	2	-	4/6/26/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	B	3	2	-	2/6/23/26	0/1/1/1
2	TMX	B	4	2	-	0/8/25/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	3.99	1.57	1.52
2	B	1	NAG	C3-C2	2.91	1.58	1.53
2	B	1	NAG	O4-C4	2.27	1.48	1.43
2	B	4	TMX	O5-C1	2.24	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O5-C1-C2	5.60	115.14	109.52
2	B	1	NAG	C1-C2-C3	4.80	117.09	110.54
2	B	4	TMX	C1-O5-C5	4.19	117.86	112.19
2	B	1	NAG	C4-C3-C2	3.13	114.93	110.34
2	B	1	NAG	C1-C2-N2	-2.74	107.55	110.73
2	B	1	NAG	C1-O5-C5	-2.13	109.64	113.66

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	3	NAG	C8-C7-N2-C2
2	B	3	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
2	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	TMX	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.
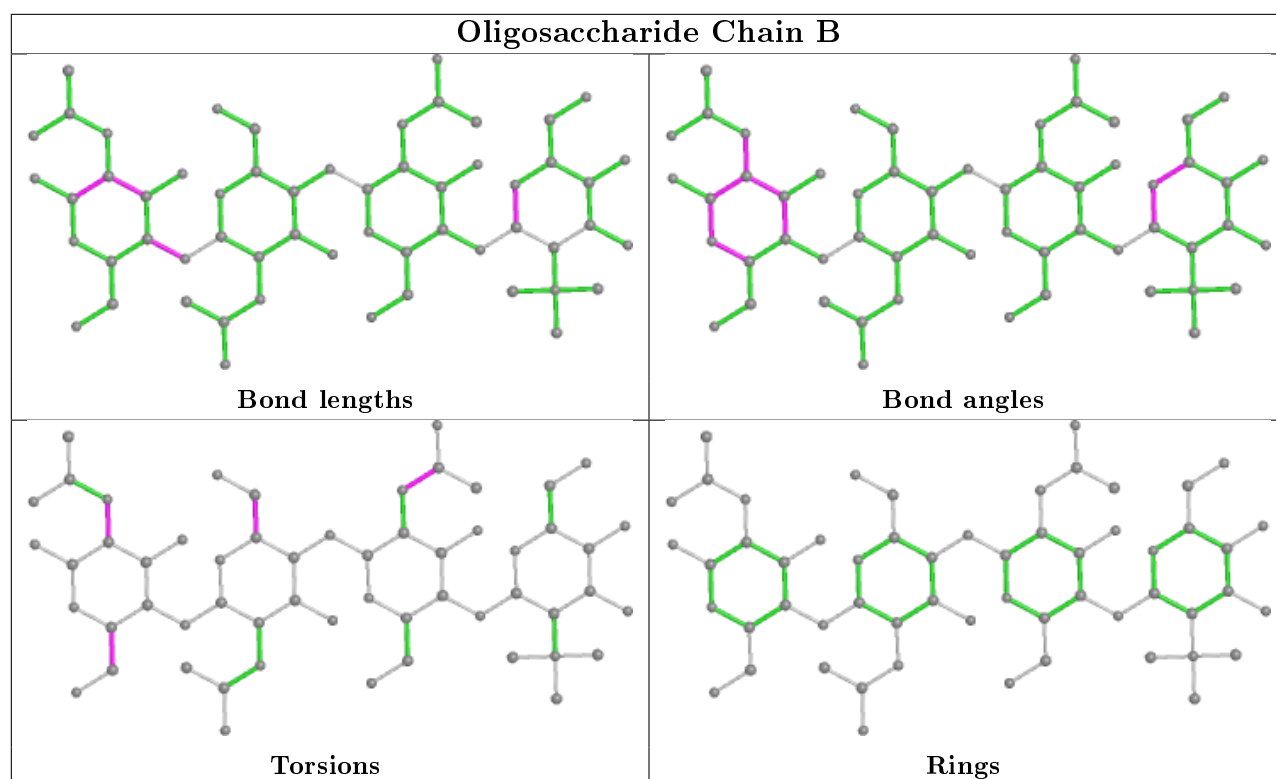
5.6 Ligand geometry (i)

There are no ligands in this entry.

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	572/572 (100%)	-0.24	14 (2%)	59	64	15, 27, 44, 72	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	ARG	6.3
1	A	385	MET	5.6
1	A	378	ASP	3.9
1	A	386	GLN	3.9
1	A	394	GLU	3.8
1	A	389	TRP	3.7
1	A	390	ASP	3.2
1	A	392	ASP	3.0
1	A	387	ASN	3.0
1	A	118	ARG	2.9
1	A	382	ASN	2.4
1	A	391	LEU	2.3
1	A	396	PHE	2.2
1	A	121	THR	2.1

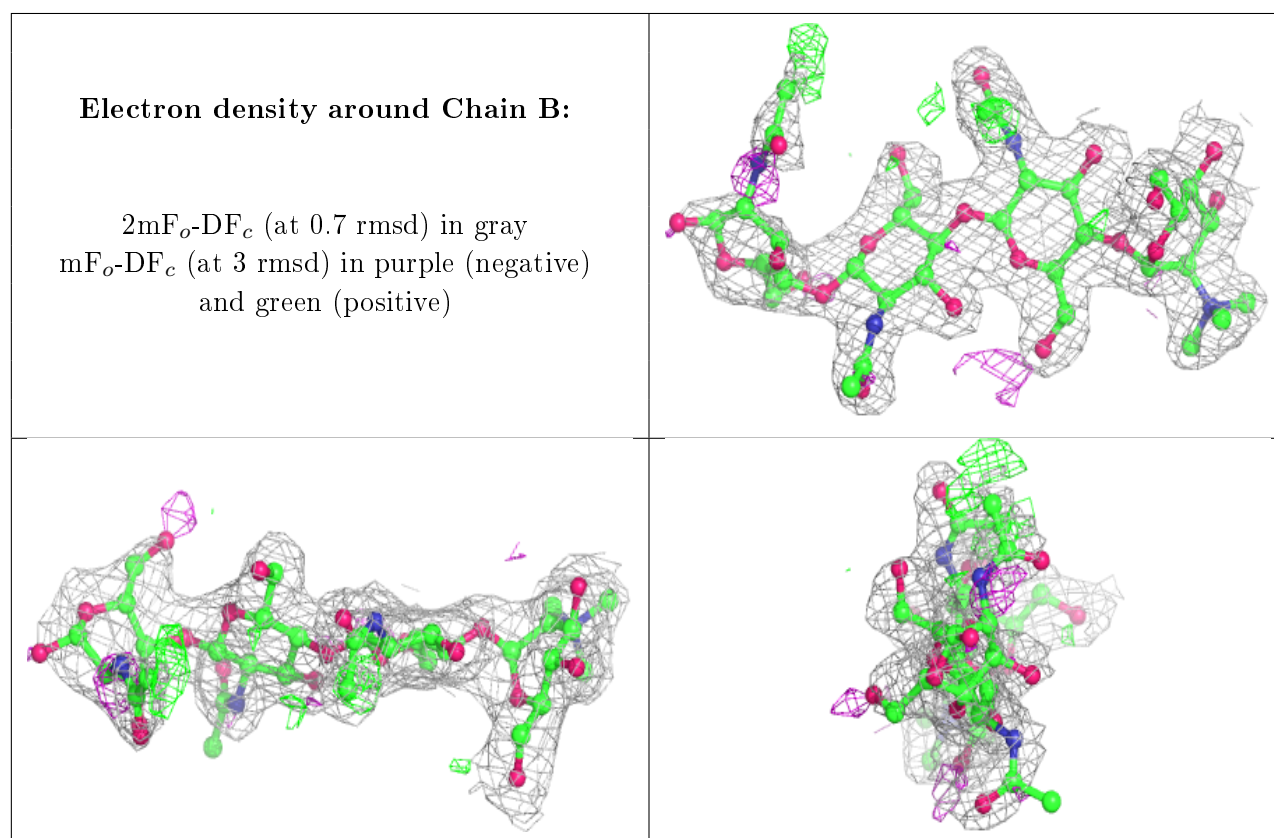## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	1	15/15	0.73	0.42	49,56,58,58	0
2	NAG	B	2	14/15	0.84	0.13	32,41,44,44	0
2	NAG	B	3	14/15	0.94	0.11	23,26,28,29	0
2	TMX	B	4	14/15	0.97	0.10	21,22,23,23	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 B:

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

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.