



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 03:25 PM EDT

PDB ID : 1ZU8
Title : Crystal structure of the goat signalling protein with a bound trisaccharide reveals that Trp78 reduces the carbohydrate binding site to half
Authors : Ethayathulla, A.S.; Kumar, J.; Srivastava, D.B.; Singh, N.; Sharma, S.; Bhushan, A.; Singh, T.P.
Deposited on : 2005-05-30
Resolution : 3.05 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

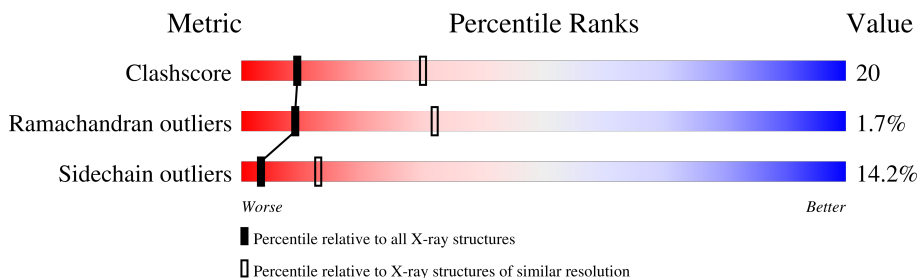
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	
2	B	3	
3	C	3	

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	NDG	B	2	-	X	-	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3002 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 Chitinase-3 like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2877	1836	508	524	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

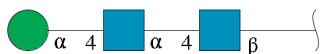
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	VAL	ILE	SEE REMARK 999	UNP Q8SPQ0
A	131	ALA	GLY	SEE REMARK 999	UNP Q8SPQ0
A	205	ASN	GLN	SEE REMARK 999	UNP Q8SPQ0
A	206	SER	GLU	SEE REMARK 999	UNP Q8SPQ0
A	?	-	ASP	SEE REMARK 999	UNP Q8SPQ0
A	361	ARG	GLU	SEE REMARK 999	UNP Q8SPQ0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	42	24	3	15	0	0	0

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



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

- Molecule 4 is water.

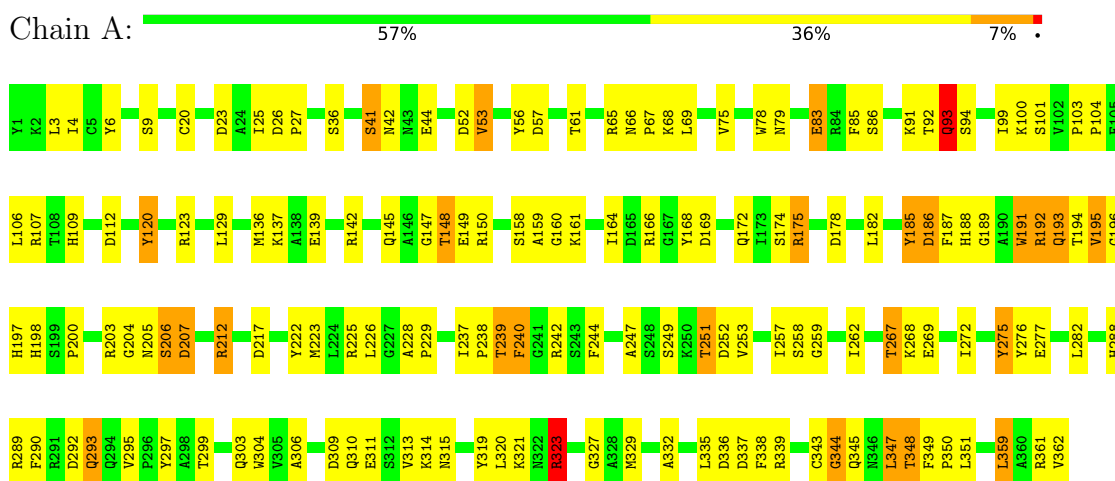
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		

3 Residue-property plots

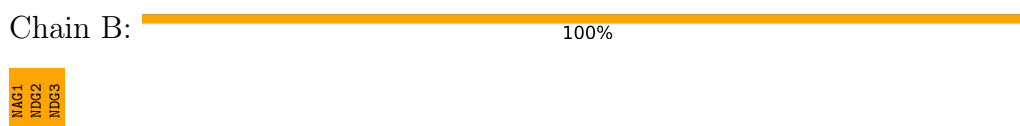
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: Chitinase-3 like protein 1



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



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



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.20Å 66.69Å 108.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.00 – 3.05	Depositor
% Data completeness (in resolution range)	98.6 (56.00-3.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.193 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3002	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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: MAN, NDG, 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	1.33	12/2953 (0.4%)	1.01	9/4001 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	TYR	CE2-CZ	-6.81	1.29	1.38
1	A	86	SER	CB-OG	-6.55	1.33	1.42
1	A	275	TYR	CG-CD1	-6.50	1.30	1.39
1	A	240	PHE	CG-CD1	-5.69	1.30	1.38
1	A	6	TYR	CD2-CE2	-5.48	1.31	1.39
1	A	93	GLN	CG-CD	5.33	1.63	1.51
1	A	9	SER	CB-OG	-5.30	1.35	1.42
1	A	276	TYR	CD2-CE2	-5.28	1.31	1.39
1	A	159	ALA	CA-CB	-5.23	1.41	1.52
1	A	275	TYR	CG-CD2	-5.18	1.32	1.39
1	A	313	VAL	CB-CG1	-5.04	1.42	1.52
1	A	56	TYR	CE2-CZ	-5.02	1.32	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	323	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	336	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	323	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	186	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	178	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	52	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	337	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	112	ASP	CB-CG-OD2	5.13	122.91	118.30

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	2877	0	2817	113	0
2	B	42	0	34	6	0
3	C	39	0	33	3	0
4	A	44	0	0	3	0
All	All	3002	0	2884	116	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 20.

All (116) 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:204:GLY:HA2	1:A:292:ASP:HB3	1.39	1.05
3:C:2:NDG:H6C1	3:C:3:MAN:O5	1.68	0.92
1:A:206:SER:O	1:A:207:ASP:HB2	1.80	0.81
1:A:192:ARG:HA	1:A:192:ARG:HE	1.46	0.79
1:A:57:ASP:O	1:A:61:THR:HG23	1.84	0.77
1:A:103:PRO:HB2	1:A:104:PRO:CD	2.16	0.76
3:C:2:NDG:C6	3:C:3:MAN:C1	2.65	0.74
1:A:103:PRO:HB2	1:A:104:PRO:HD3	1.72	0.72
1:A:319:TYR:CZ	1:A:323:ARG:HD2	2.24	0.72
1:A:192:ARG:HA	1:A:192:ARG:NE	2.05	0.71
3:C:2:NDG:H6C1	3:C:3:MAN:C1	2.21	0.71
1:A:239:THR:CG2	1:A:335:LEU:HB2	2.21	0.70
1:A:188:HIS:CD2	1:A:196:GLY:HA3	2.26	0.70
1:A:239:THR:HG23	1:A:239:THR:O	1.91	0.69
1:A:200:PRO:HB3	1:A:293:GLN:HG2	1.74	0.68
1:A:239:THR:HG21	1:A:332:ALA:O	1.93	0.67
1:A:332:ALA:HB1	1:A:335:LEU:HG	1.75	0.67
1:A:191:TRP:CE3	1:A:192:ARG:HG2	2.29	0.67
1:A:267:THR:HB	1:A:277:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:CG2	1:A:239:THR:O	2.46	0.64
1:A:79:ASN:OD1	2:B:1:NAG:H62	1.98	0.64
1:A:269:GLU:OE1	2:B:2:NDG:H6C2	1.98	0.63
1:A:160:GLY:HA2	4:A:404:HOH:O	1.98	0.63
1:A:25:ILE:O	1:A:27:PRO:HD3	1.98	0.63
1:A:185:TYR:CB	1:A:238:PRO:HG3	2.30	0.62
1:A:79:ASN:HB2	2:B:2:NDG:O7	1.99	0.62
1:A:212:ARG:O	1:A:212:ARG:HD2	2.01	0.61
1:A:189:GLY:HA3	1:A:191:TRP:NE1	2.16	0.60
1:A:195:VAL:HG23	1:A:257:ILE:HD11	1.84	0.59
1:A:239:THR:HG22	1:A:335:LEU:HB2	1.82	0.59
1:A:185:TYR:HB3	1:A:238:PRO:HG3	1.85	0.58
1:A:203:ARG:HB3	1:A:212:ARG:HD3	1.85	0.57
1:A:251:THR:HG23	4:A:389:HOH:O	2.04	0.57
1:A:289:ARG:NH2	1:A:309:ASP:OD2	2.35	0.57
1:A:361:ARG:O	1:A:362:VAL:HB	2.05	0.56
1:A:362:VAL:HG22	1:A:362:VAL:O	2.05	0.56
1:A:304:TRP:CZ3	1:A:306:ALA:HB2	2.40	0.56
1:A:41:SER:O	1:A:42:ASN:HB2	2.04	0.56
1:A:349:PHE:N	1:A:350:PRO:CD	2.70	0.55
1:A:103:PRO:CB	1:A:104:PRO:CD	2.82	0.54
1:A:343:CYS:O	1:A:344:GLY:C	2.45	0.54
1:A:310:GLN:O	1:A:314:LYS:HG3	2.07	0.54
1:A:164:ILE:HA	1:A:168:TYR:HD2	1.73	0.54
1:A:137:LYS:HE3	1:A:150:ARG:NH2	2.22	0.54
1:A:320:LEU:HD11	1:A:327:GLY:C	2.28	0.54
1:A:83:GLU:H	1:A:83:GLU:CD	2.11	0.54
1:A:222:TYR:CE2	1:A:226:LEU:HD21	2.44	0.53
1:A:257:ILE:CG2	1:A:259:GLY:H	2.22	0.53
1:A:262:ILE:H	1:A:303:GLN:HE22	1.56	0.53
1:A:321:LYS:NZ	1:A:362:VAL:OXT	2.40	0.52
1:A:91:LYS:HB2	1:A:94:SER:OG	2.10	0.51
1:A:347:LEU:HD23	1:A:348:THR:H	1.77	0.50
1:A:120:TYR:CE1	1:A:158:SER:HB2	2.47	0.50
1:A:293:GLN:HE21	1:A:293:GLN:H	1.57	0.50
1:A:78:TRP:CE3	2:B:1:NAG:O5	2.65	0.49
1:A:187:PHE:HB2	1:A:198:HIS:O	2.13	0.49
1:A:148:THR:OG1	1:A:149:GLU:N	2.45	0.49
1:A:4:ILE:HD12	1:A:4:ILE:N	2.28	0.49
1:A:323:ARG:HH11	1:A:323:ARG:CG	2.26	0.49
1:A:103:PRO:HB2	1:A:104:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG12	1:A:290:PHE:CE1	2.47	0.48
1:A:204:GLY:O	1:A:206:SER:N	2.46	0.48
1:A:332:ALA:CB	1:A:335:LEU:HG	2.41	0.48
1:A:257:ILE:HG22	1:A:259:GLY:H	1.77	0.48
1:A:339:ARG:HB2	4:A:372:HOH:O	2.13	0.47
1:A:137:LYS:HE3	1:A:150:ARG:CZ	2.45	0.47
1:A:142:ARG:HB2	1:A:142:ARG:NH1	2.28	0.47
1:A:185:TYR:HB3	1:A:238:PRO:CG	2.45	0.47
1:A:323:ARG:HH11	1:A:323:ARG:HB3	1.80	0.47
1:A:145:GLN:C	1:A:147:GLY:H	2.18	0.47
1:A:66:ASN:HA	1:A:67:PRO:HD2	1.75	0.46
1:A:139:GLU:HA	1:A:139:GLU:OE1	2.15	0.46
1:A:169:ASP:OD2	1:A:172:GLN:HG3	2.16	0.46
1:A:240:PHE:HB3	1:A:335:LEU:HD13	1.97	0.46
1:A:44:GLU:HG2	1:A:101:SER:HB2	1.97	0.45
1:A:268:LYS:O	2:B:3:NDG:H8C3	2.17	0.45
1:A:288:HIS:HB2	1:A:297:TYR:CE1	2.51	0.45
1:A:53:VAL:HG12	1:A:109:HIS:CE1	2.51	0.44
1:A:222:TYR:CZ	1:A:226:LEU:HD21	2.52	0.44
1:A:321:LYS:CE	1:A:362:VAL:OXT	2.65	0.44
1:A:195:VAL:HG13	1:A:304:TRP:CZ2	2.51	0.44
1:A:257:ILE:HD13	1:A:257:ILE:HA	1.86	0.44
1:A:361:ARG:O	1:A:362:VAL:CB	2.65	0.44
1:A:123:ARG:HA	1:A:166:ARG:O	2.17	0.44
1:A:120:TYR:CD1	1:A:120:TYR:N	2.82	0.44
1:A:253:VAL:HG12	1:A:290:PHE:HE1	1.82	0.43
1:A:332:ALA:HB3	1:A:335:LEU:HD12	1.99	0.43
1:A:321:LYS:HE2	1:A:362:VAL:OXT	2.17	0.43
1:A:189:GLY:HA3	1:A:191:TRP:CD1	2.53	0.43
1:A:323:ARG:HH11	1:A:323:ARG:CB	2.31	0.43
1:A:26:ASP:OD1	1:A:26:ASP:C	2.55	0.43
1:A:348:THR:O	1:A:349:PHE:HB2	2.19	0.43
1:A:20:CYS:HB2	1:A:338:PHE:CZ	2.54	0.43
1:A:197:HIS:CD2	1:A:295:VAL:CG2	3.01	0.43
1:A:237:ILE:N	1:A:329:MET:O	2.43	0.42
1:A:175:ARG:H	1:A:175:ARG:HG2	1.62	0.42
1:A:192:ARG:CZ	1:A:193:GLN:HG2	2.49	0.42
1:A:160:GLY:O	1:A:161:LYS:C	2.56	0.42
1:A:79:ASN:OD1	2:B:2:NDG:H2	2.19	0.42
1:A:257:ILE:HG22	1:A:259:GLY:N	2.35	0.42
1:A:269:GLU:OE2	1:A:272:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:HB2	1:A:258:SER:HB3	2.02	0.42
1:A:347:LEU:HD23	1:A:348:THR:N	2.35	0.42
1:A:252:ASP:O	1:A:253:VAL:C	2.58	0.42
1:A:93:GLN:HG2	1:A:94:SER:N	2.33	0.41
1:A:182:LEU:HD21	1:A:223:MET:HG3	2.02	0.41
1:A:99:ILE:HD13	1:A:136:MET:HA	2.03	0.41
1:A:145:GLN:C	1:A:147:GLY:N	2.74	0.41
1:A:244:PHE:HB3	1:A:257:ILE:HD12	2.02	0.41
1:A:257:ILE:CG2	1:A:258:SER:N	2.83	0.41
1:A:197:HIS:NE2	1:A:295:VAL:HB	2.35	0.41
1:A:228:ALA:HA	1:A:229:PRO:HD3	1.81	0.41
1:A:359:LEU:HD12	1:A:359:LEU:HA	1.88	0.41
1:A:275:TYR:CE2	1:A:351:LEU:HD13	2.55	0.41
1:A:323:ARG:CG	1:A:323:ARG:NH1	2.84	0.41
1:A:253:VAL:O	1:A:253:VAL:HG23	2.20	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	359/361 (99%)	325 (90%)	28 (8%)	6 (2%)	9 32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	207	ASP
1	A	345	GLN
1	A	120	TYR
1	A	191	TRP
1	A	344	GLY

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	302/302 (100%)	259 (86%)	43 (14%)	3 13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	23	ASP
1	A	36	SER
1	A	41	SER
1	A	53	VAL
1	A	65	ARG
1	A	68	LYS
1	A	69	LEU
1	A	75	VAL
1	A	83	GLU
1	A	85	PHE
1	A	92	THR
1	A	93	GLN
1	A	100	LYS
1	A	106	LEU
1	A	107	ARG
1	A	129	LEU
1	A	148	THR
1	A	174	SER
1	A	175	ARG
1	A	185	TYR
1	A	186	ASP
1	A	192	ARG
1	A	193	GLN
1	A	194	THR
1	A	195	VAL
1	A	206	SER
1	A	212	ARG
1	A	225	ARG
1	A	239	THR

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Mol	Chain	Res	Type
1	A	242	ARG
1	A	249	SER
1	A	251	THR
1	A	267	THR
1	A	282	LEU
1	A	293	GLN
1	A	299	THR
1	A	311	GLU
1	A	315	ASN
1	A	323	ARG
1	A	347	LEU
1	A	348	THR
1	A	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	60	ASN
1	A	109	HIS
1	A	188	HIS
1	A	193	GLN
1	A	198	HIS
1	A	293	GLN
1	A	303	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	B	1	2	14,14,15	1.99	5 (35%)	17,19,21	3.11	10 (58%)
2	NDG	B	2	2	14,14,15	3.10	9 (64%)	17,19,21	3.27	13 (76%)
2	NDG	B	3	2	14,14,15	2.63	10 (71%)	17,19,21	2.46	7 (41%)
3	NAG	C	1	1,3	14,14,15	1.17	1 (7%)	17,19,21	2.76	8 (47%)
3	NDG	C	2	3	14,14,15	1.19	1 (7%)	17,19,21	3.76	9 (52%)
3	MAN	C	3	3	11,11,12	1.14	2 (18%)	15,15,17	3.73	9 (60%)

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	-	0/6/23/26	0/1/1/1
2	NDG	B	2	2	-	4/6/23/26	0/1/1/1
2	NDG	B	3	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NDG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	2/2/19/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NDG	C8-C7	5.71	1.62	1.50
2	B	2	NDG	C1-C2	4.76	1.59	1.52
2	B	2	NDG	O3-C3	4.44	1.53	1.43
2	B	3	NDG	C1-C2	3.78	1.58	1.52
2	B	3	NDG	O7-C7	3.67	1.31	1.23
2	B	2	NDG	C4-C5	3.60	1.60	1.53
2	B	3	NDG	C2-N2	3.47	1.52	1.46
2	B	1	NAG	C1-C2	3.46	1.57	1.52
2	B	1	NAG	O5-C1	3.27	1.48	1.43
2	B	3	NDG	O5-C1	3.17	1.48	1.43
2	B	2	NDG	O5-C1	3.15	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NDG	O7-C7	3.11	1.30	1.23
3	C	1	NAG	C2-N2	-3.07	1.41	1.46
2	B	3	NDG	C4-C5	3.02	1.59	1.53
2	B	1	NAG	O3-C3	2.88	1.49	1.43
2	B	3	NDG	C8-C7	2.87	1.56	1.50
2	B	2	NDG	C3-C2	2.79	1.58	1.52
2	B	2	NDG	C4-C3	2.74	1.59	1.52
3	C	3	MAN	C2-C3	2.72	1.56	1.52
2	B	3	NDG	O5-C5	2.61	1.48	1.43
2	B	1	NAG	C4-C3	2.41	1.58	1.52
3	C	3	MAN	O2-C2	-2.39	1.38	1.43
2	B	3	NDG	O4-C4	2.36	1.48	1.43
2	B	3	NDG	C4-C3	2.25	1.58	1.52
2	B	3	NDG	O3-C3	2.20	1.48	1.43
2	B	2	NDG	C6-C5	2.14	1.59	1.51
3	C	2	NDG	O4-C4	-2.13	1.38	1.43
2	B	1	NAG	O7-C7	2.03	1.27	1.23

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NDG	C1-C2-N2	7.92	124.02	110.49
3	C	3	MAN	C1-C2-C3	7.53	118.93	109.67
3	C	2	NDG	O5-C5-C6	7.08	118.31	107.20
3	C	2	NDG	C2-N2-C7	-6.81	113.21	122.90
2	B	1	NAG	C3-C4-C5	6.43	121.70	110.24
3	C	1	NAG	C2-N2-C7	-6.35	113.86	122.90
3	C	3	MAN	O2-C2-C1	-6.10	96.67	109.15
3	C	3	MAN	C1-O5-C5	5.99	120.30	112.19
2	B	2	NDG	C1-C2-N2	5.59	120.04	110.49
2	B	3	NDG	C2-N2-C7	5.57	130.84	122.90
2	B	2	NDG	O4-C4-C3	-5.55	97.52	110.35
3	C	3	MAN	O5-C1-C2	5.31	118.96	110.77
3	C	1	NAG	C3-C4-C5	-5.15	101.06	110.24
2	B	2	NDG	C4-C3-C2	-5.06	103.60	111.02
2	B	1	NAG	O4-C4-C3	4.92	121.71	110.35
2	B	2	NDG	O7-C7-N2	-4.82	113.10	121.95
2	B	3	NDG	O5-C5-C6	4.28	113.91	107.20
2	B	1	NAG	O5-C1-C2	4.22	117.95	111.29
3	C	2	NDG	C1-O5-C5	-4.22	106.48	112.19
3	C	1	NAG	O5-C1-C2	-4.21	104.64	111.29
3	C	2	NDG	C3-C4-C5	3.80	117.01	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	NDG	C1-C2-N2	3.79	116.97	110.49
3	C	2	NDG	O3-C3-C2	-3.75	101.71	109.47
2	B	1	NAG	C4-C3-C2	-3.60	105.74	111.02
2	B	2	NDG	C8-C7-N2	3.50	122.03	116.10
2	B	2	NDG	O5-C5-C6	-3.40	101.88	107.20
3	C	2	NDG	C6-C5-C4	-3.36	105.14	113.00
3	C	3	MAN	C2-C3-C4	-3.24	105.28	110.89
2	B	1	NAG	C1-O5-C5	-3.17	107.89	112.19
3	C	1	NAG	O3-C3-C2	-3.15	102.95	109.47
2	B	3	NDG	O5-C1-C2	3.15	116.26	111.29
3	C	2	NDG	O7-C7-N2	3.06	127.58	121.95
2	B	1	NAG	C2-N2-C7	-3.05	118.57	122.90
3	C	1	NAG	O6-C6-C5	-3.02	100.92	111.29
2	B	2	NDG	O5-C1-C2	3.01	116.05	111.29
3	C	3	MAN	C3-C4-C5	2.99	115.57	110.24
2	B	1	NAG	O3-C3-C4	2.99	117.25	110.35
2	B	1	NAG	C6-C5-C4	-2.96	106.06	113.00
2	B	1	NAG	C1-C2-N2	2.90	115.44	110.49
3	C	3	MAN	O5-C5-C4	2.89	117.86	110.83
2	B	2	NDG	O3-C3-C4	2.84	116.91	110.35
2	B	1	NAG	O4-C4-C5	-2.62	102.80	109.30
2	B	2	NDG	C6-C5-C4	2.61	119.12	113.00
3	C	3	MAN	O2-C2-C3	2.47	115.09	110.14
3	C	1	NAG	C1-O5-C5	-2.46	108.86	112.19
2	B	3	NDG	C4-C3-C2	2.46	114.62	111.02
3	C	3	MAN	O3-C3-C2	2.42	114.64	109.99
2	B	3	NDG	C8-C7-N2	-2.34	112.14	116.10
3	C	2	NDG	O4-C4-C3	-2.32	104.99	110.35
2	B	3	NDG	O3-C3-C2	-2.25	104.81	109.47
3	C	1	NAG	C4-C3-C2	2.22	114.27	111.02
2	B	2	NDG	O4-C4-C5	2.17	114.70	109.30
3	C	1	NAG	C8-C7-N2	2.14	119.72	116.10
2	B	2	NDG	O3-C3-C2	2.13	113.87	109.47
2	B	2	NDG	C3-C4-C5	2.09	113.98	110.24
2	B	2	NDG	C2-N2-C7	2.07	125.85	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NDG	C8-C7-N2-C2
2	B	2	NDG	O7-C7-N2-C2

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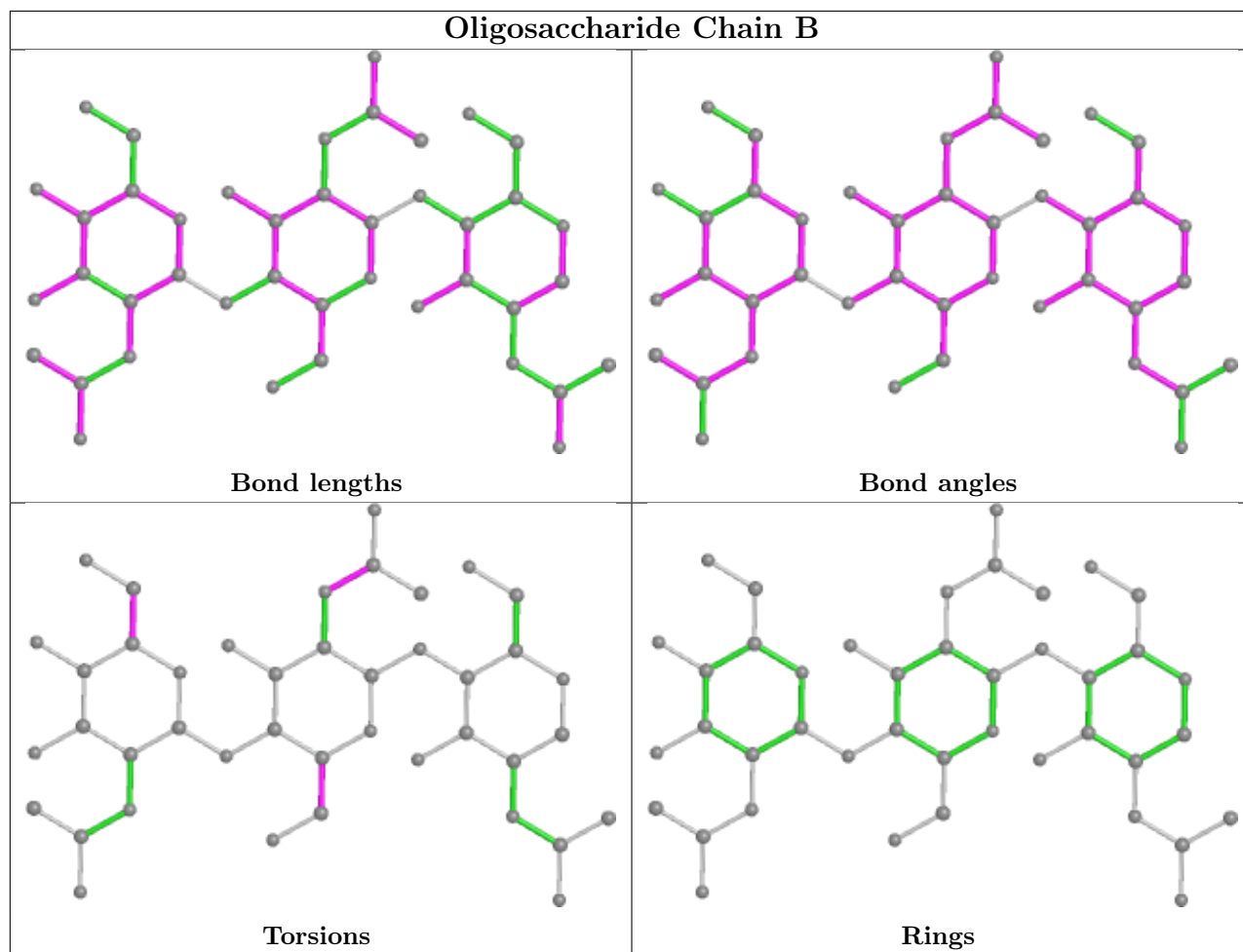
Mol	Chain	Res	Type	Atoms
2	B	3	NDG	O5-C5-C6-O6
2	B	3	NDG	C4-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
3	C	2	NDG	C8-C7-N2-C2
3	C	2	NDG	O7-C7-N2-C2
3	C	3	MAN	O5-C5-C6-O6
2	B	2	NDG	C4-C5-C6-O6
2	B	2	NDG	O5-C5-C6-O6

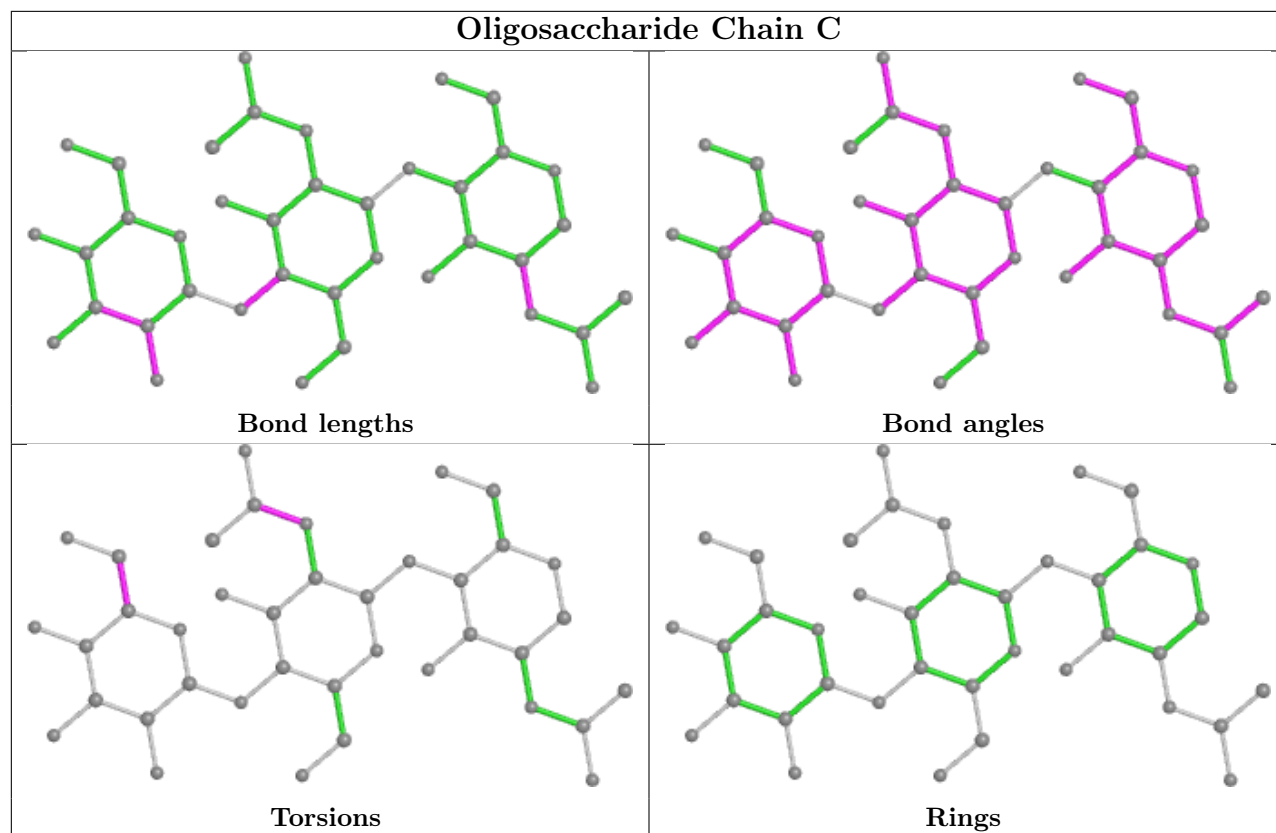
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	MAN	3	0
2	B	3	NDG	1	0
2	B	1	NAG	2	0
2	B	2	NDG	3	0
3	C	2	NDG	3	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.