Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:06 PM EDT

PDB ID	:	1JSM
Title	:	STRUCTURE OF H5 AVIAN HAEMAGGLUTININ
Authors	:	Ha, Y.; Stevens, D.J.; Skehel, J.J.; Wiley, D.C.
Deposited on	:	2001-08-17
Resolution	:	1.90 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 (i)) were used in the production of this report:

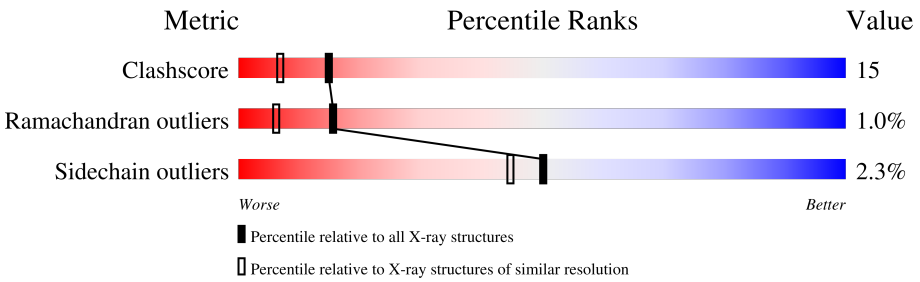
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	325	76% 21% • •
2	B	176	68% 21% • 9%
3	C	2	50% 50%
3	D	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4130 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 HAEMAGGLUTININ (HA1 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2509	1581	439	474	15	0	0	0

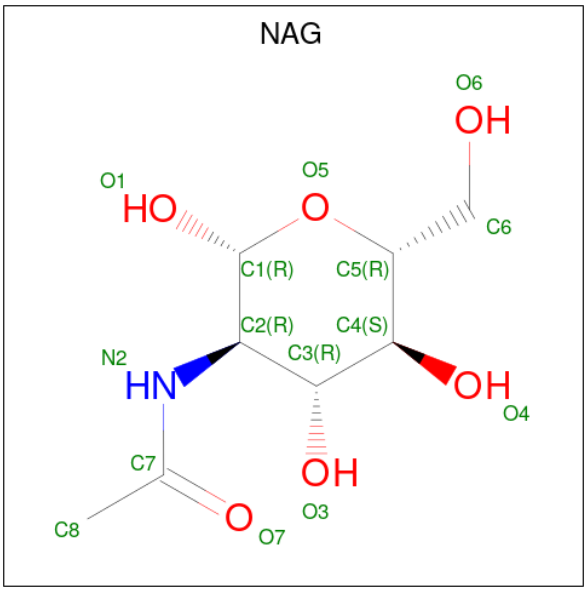
- Molecule 2 is a protein called HAEMAGGLUTININ (HA2 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	1227	766	211	242	8	0	0	0

- Molecule 3 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
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0
3	D	2	28	16	2	10	0	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
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	236	236	236	0	0
			Total	O		
5	B	60	60	60	0	0

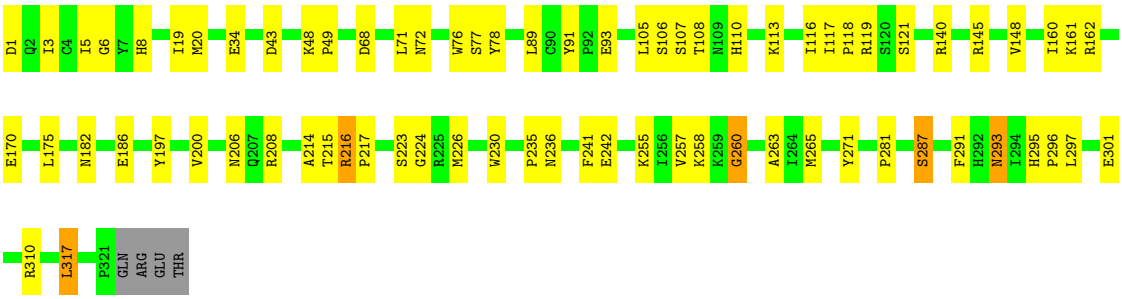
3 Residue-property plots (i)

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. 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.

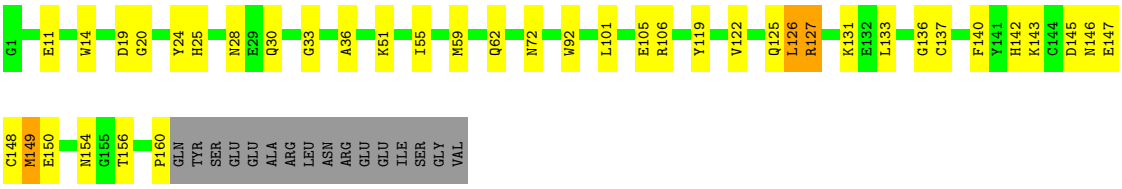
• Molecule 1: HAEMAGGLUTININ (HA1 CHAIN)

Chain A:



• Molecule 2: HAEMAGGLUTININ (HA2 CHAIN)

Chain B:

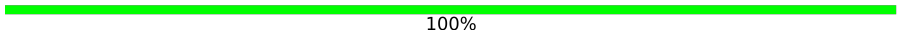


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	130.73Å 130.73Å 254.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4130	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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: 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	0.65	1/2572 (0.0%)	0.80	0/3501
2	B	0.63	1/1251 (0.1%)	0.66	1/1688 (0.1%)
All	All	0.65	2/3823 (0.1%)	0.76	1/5189 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	GLU	CB-CG	-5.81	1.41	1.52
2	B	11	GLU	CB-CG	-5.31	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	160	PRO	N-CA-CB	5.41	109.79	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	TYR	Sidechain

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	2509	0	2417	78	1
2	B	1227	0	1083	42	1
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	42	0	39	0	0
5	A	236	0	0	36	0
5	B	60	0	0	7	0
All	All	4130	0	3589	113	2

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 15.

All (113) 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:20:MET:SD	1:A:20:MET:CE	2.01	1.46
1:A:214:ALA:HB2	5:A:542:HOH:O	1.44	1.16
1:A:215:THR:HA	5:A:449:HOH:O	1.55	1.06
1:A:182:ASN:HB3	5:A:625:HOH:O	1.56	1.02
1:A:76:TRP:HB2	5:A:603:HOH:O	1.67	0.93
1:A:148:VAL:HA	5:A:586:HOH:O	1.71	0.89
1:A:263:ALA:HA	5:A:611:HOH:O	1.73	0.89
1:A:295:HIS:HD2	1:A:297:LEU:H	1.20	0.88
1:A:258:LYS:C	1:A:260:GLY:H	1.73	0.86
1:A:223:SER:HB2	5:A:483:HOH:O	1.77	0.84
1:A:19:ILE:HG12	5:B:224:HOH:O	1.77	0.83
1:A:258:LYS:C	1:A:260:GLY:N	2.30	0.82
1:A:49:PRO:HA	5:A:603:HOH:O	1.83	0.78
1:A:5:ILE:HD11	2:B:122:VAL:HG21	1.66	0.77
1:A:182:ASN:HA	1:A:214:ALA:O	1.88	0.74
1:A:77:SER:N	5:A:603:HOH:O	2.20	0.73
2:B:28:ASN:HD21	2:B:146:ASN:ND2	1.86	0.73
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.55	0.71
1:A:224:GLY:HA2	5:A:537:HOH:O	1.90	0.70
2:B:62:GLN:HG2	2:B:92:TRP:CE3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD21	5:A:616:HOH:O	1.91	0.70
1:A:118:PRO:O	1:A:121:SER:HB3	1.92	0.70
2:B:28:ASN:HD21	2:B:146:ASN:HD22	1.39	0.70
1:A:182:ASN:HB3	5:A:483:HOH:O	1.90	0.70
2:B:150:GLU:O	2:B:154:ASN:HB2	1.91	0.70
1:A:295:HIS:CD2	1:A:297:LEU:H	2.08	0.69
1:A:257:VAL:HG23	5:A:561:HOH:O	1.91	0.69
1:A:215:THR:HG22	5:A:564:HOH:O	1.92	0.69
1:A:121:SER:OG	1:A:162:ARG:NH2	2.26	0.69
1:A:1:ASP:OD1	5:A:433:HOH:O	2.11	0.68
2:B:133:LEU:N	2:B:133:LEU:HD12	2.10	0.66
1:A:3:ILE:HB	2:B:149:MET:HE3	1.79	0.65
1:A:258:LYS:O	1:A:260:GLY:N	2.30	0.65
1:A:78:TYR:N	5:A:603:HOH:O	2.31	0.64
1:A:161:LYS:HG2	5:A:595:HOH:O	1.98	0.64
1:A:107:SER:HB3	5:A:588:HOH:O	1.99	0.63
1:A:3:ILE:HB	2:B:149:MET:CE	2.29	0.62
1:A:265:MET:HG3	1:A:281:PRO:HG3	1.81	0.62
1:A:106:SER:HB2	5:A:611:HOH:O	2.00	0.62
2:B:133:LEU:HD12	2:B:133:LEU:H	1.65	0.61
1:A:91:TYR:CD2	1:A:226:MET:HG2	2.35	0.61
2:B:105:GLU:OE2	5:B:238:HOH:O	2.17	0.60
1:A:43:ASP:OD1	1:A:271:TYR:OH	2.08	0.59
1:A:224:GLY:CA	5:A:625:HOH:O	2.51	0.59
1:A:78:TYR:O	5:A:603:HOH:O	2.15	0.59
2:B:145:ASP:OD2	2:B:147:GLU:HG2	2.04	0.58
1:A:119:ARG:NH1	5:A:586:HOH:O	2.34	0.58
1:A:110:HIS:HD2	5:A:647:HOH:O	1.87	0.57
2:B:30:GLN:OE1	2:B:145:ASP:HB2	2.03	0.57
1:A:68:ASP:OD1	5:A:616:HOH:O	2.16	0.57
2:B:19:ASP:HB3	2:B:36:ALA:CB	2.34	0.57
1:A:72:ASN:HA	5:A:655:HOH:O	2.05	0.56
2:B:72:ASN:HB3	5:B:211:HOH:O	2.04	0.56
1:A:113:LYS:HB2	5:A:655:HOH:O	2.06	0.55
1:A:317:LEU:H	1:A:317:LEU:HD23	1.71	0.55
1:A:110:HIS:CD2	5:A:647:HOH:O	2.60	0.55
2:B:28:ASN:ND2	2:B:145:ASP:HA	2.20	0.54
1:A:20:MET:HB2	5:B:238:HOH:O	2.08	0.54
1:A:116:ILE:HG13	1:A:117:ILE:HG13	1.89	0.54
2:B:106:ARG:HD2	5:B:230:HOH:O	2.08	0.53
1:A:216:ARG:HB2	1:A:217:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HD3	5:A:548:HOH:O	2.10	0.51
1:A:175:LEU:HD23	1:A:230:TRP:HB3	1.94	0.50
1:A:161:LYS:O	1:A:162:ARG:HD3	2.11	0.50
1:A:293:ASN:C	1:A:293:ASN:HD22	2.15	0.50
1:A:224:GLY:N	5:A:625:HOH:O	2.45	0.50
2:B:131:LYS:O	2:B:133:LEU:HD12	2.12	0.49
2:B:125:GLN:O	2:B:127:ARG:N	2.39	0.49
1:A:216:ARG:HB2	1:A:217:PRO:HD2	1.94	0.49
1:A:235:PRO:O	1:A:236:ASN:HB2	2.11	0.49
1:A:291:PHE:HZ	2:B:59:MET:HG3	1.77	0.49
1:A:8:HIS:HB2	2:B:20:GLY:O	2.12	0.49
2:B:147:GLU:HG3	2:B:148:CYS:N	2.27	0.49
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.48	0.49
1:A:281:PRO:HD3	1:A:297:LEU:O	2.14	0.47
2:B:154:ASN:C	2:B:156:THR:H	2.17	0.47
1:A:310:ARG:NH1	5:A:629:HOH:O	2.47	0.47
2:B:19:ASP:HB3	2:B:36:ALA:HB2	1.97	0.47
1:A:216:ARG:N	5:A:449:HOH:O	2.39	0.47
2:B:19:ASP:HB3	2:B:36:ALA:HB3	1.96	0.46
1:A:5:ILE:HG13	2:B:119:TYR:HA	1.97	0.46
2:B:133:LEU:H	2:B:133:LEU:CD1	2.27	0.46
2:B:145:ASP:CG	2:B:147:GLU:HG2	2.35	0.46
2:B:126:LEU:O	2:B:127:ARG:C	2.54	0.46
2:B:147:GLU:CG	2:B:148:CYS:N	2.79	0.45
1:A:1:ASP:N	5:A:433:HOH:O	2.45	0.44
1:A:200:VAL:HG22	1:A:241:PHE:CD2	2.53	0.44
1:A:215:THR:O	1:A:215:THR:HG23	2.18	0.44
2:B:133:LEU:N	2:B:133:LEU:CD1	2.79	0.43
1:A:296:PRO:HG2	1:A:297:LEU:HD13	1.99	0.43
2:B:140:PHE:HE1	2:B:149:MET:HE1	1.82	0.43
2:B:72:ASN:CB	5:B:211:HOH:O	2.63	0.43
1:A:3:ILE:O	1:A:3:ILE:HG23	2.17	0.43
1:A:145:ARG:HD2	5:A:616:HOH:O	2.18	0.43
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.84	0.43
2:B:105:GLU:HB2	5:B:224:HOH:O	2.19	0.43
1:A:34:GLU:OE2	1:A:287:SER:HB2	2.19	0.43
1:A:293:ASN:C	1:A:293:ASN:ND2	2.73	0.42
1:A:310:ARG:NE	5:A:626:HOH:O	2.49	0.42
2:B:51:LYS:O	2:B:55:ILE:HG13	2.20	0.42
2:B:126:LEU:O	2:B:127:ARG:O	2.38	0.42
1:A:182:ASN:CB	5:A:483:HOH:O	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:O	1:A:242:GLU:HA	2.21	0.41
1:A:6:GLY:HA3	2:B:14:TRP:CH2	2.55	0.41
1:A:105:LEU:O	1:A:108:THR:HG22	2.20	0.41
2:B:154:ASN:C	2:B:156:THR:N	2.73	0.41
2:B:25:HIS:HA	2:B:33:GLY:O	2.20	0.41
1:A:71:LEU:CG	5:A:616:HOH:O	2.69	0.41
1:A:170:GLU:OE1	1:A:255:LYS:HE3	2.21	0.41
2:B:133:LEU:HD13	2:B:137:CYS:O	2.20	0.41
1:A:182:ASN:OD1	1:A:186:GLU:OE1	2.39	0.41
2:B:140:PHE:CE1	2:B:149:MET:HE1	2.56	0.40
1:A:48:LYS:HG3	1:A:49:PRO:HD2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:OD1	1:A:216:ARG:NH1[3_655]	2.11	0.09
2:B:142:HIS:NE2	2:B:142:HIS:NE2[11_446]	2.12	0.08

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	319/325 (98%)	303 (95%)	14 (4%)	2 (1%)	25 15
2	B	158/176 (90%)	144 (91%)	11 (7%)	3 (2%)	8 1
All	All	477/501 (95%)	447 (94%)	25 (5%)	5 (1%)	15 6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLU

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Mol	Chain	Res	Type
1	A	260	GLY
2	B	127	ARG
2	B	143	LYS
2	B	126	LEU

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	279/289 (96%)	273 (98%)	6 (2%)	52	47
2	B	118/150 (79%)	115 (98%)	3 (2%)	47	41
All	All	397/439 (90%)	388 (98%)	9 (2%)	50	45

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

Mol	Chain	Res	Type
1	A	89	LEU
1	A	140	ARG
1	A	216	ARG
1	A	287	SER
1	A	293	ASN
1	A	317	LEU
2	B	24	TYR
2	B	101	LEU
2	B	149	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	207	GLN
1	A	293	ASN
1	A	295	HIS
2	B	62	GLN

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Mol	Chain	Res	Type
2	B	146	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	$\#\|Z\| > 2$
3	NAG	C	1	3,1	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
3	NAG	C	2	3	14,14,15	0.60	0	17,19,21	0.65	0
3	NAG	D	1	2,3	14,14,15	0.71	0	17,19,21	0.59	0
3	NAG	D	2	3	14,14,15	0.64	0	17,19,21	0.69	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
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

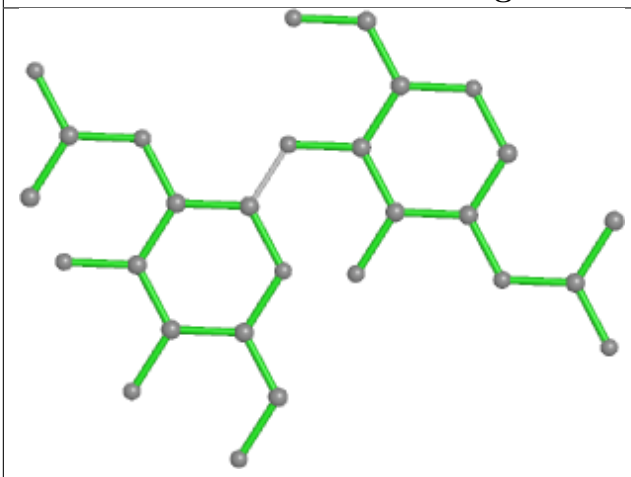
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C3-C2-N2-C7
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C1-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C3-C2-N2-C7

There are no ring outliers.

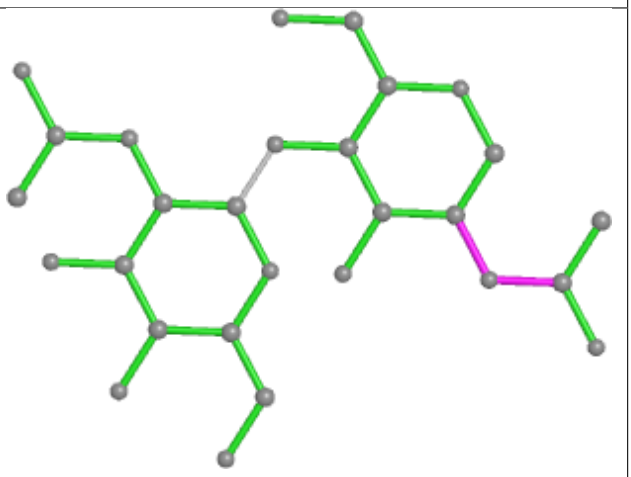
No monomer is involved in short contacts.

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

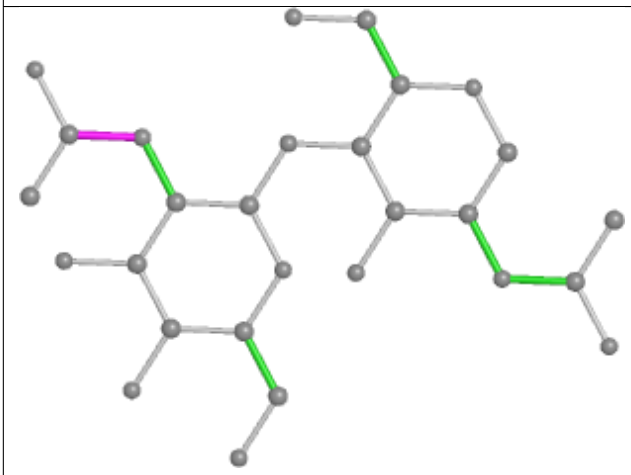
Oligosaccharide Chain C



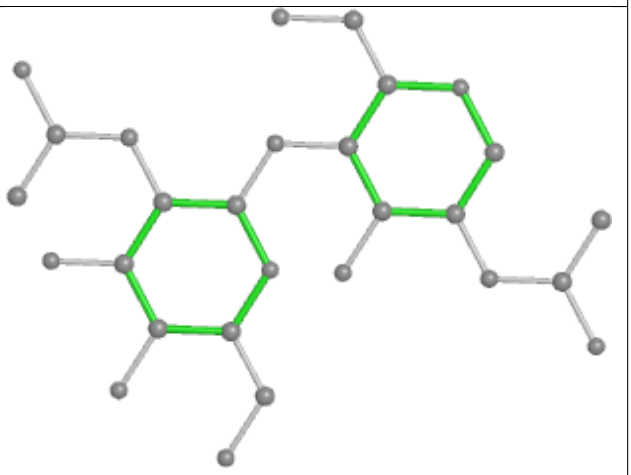
Bond lengths



Bond angles

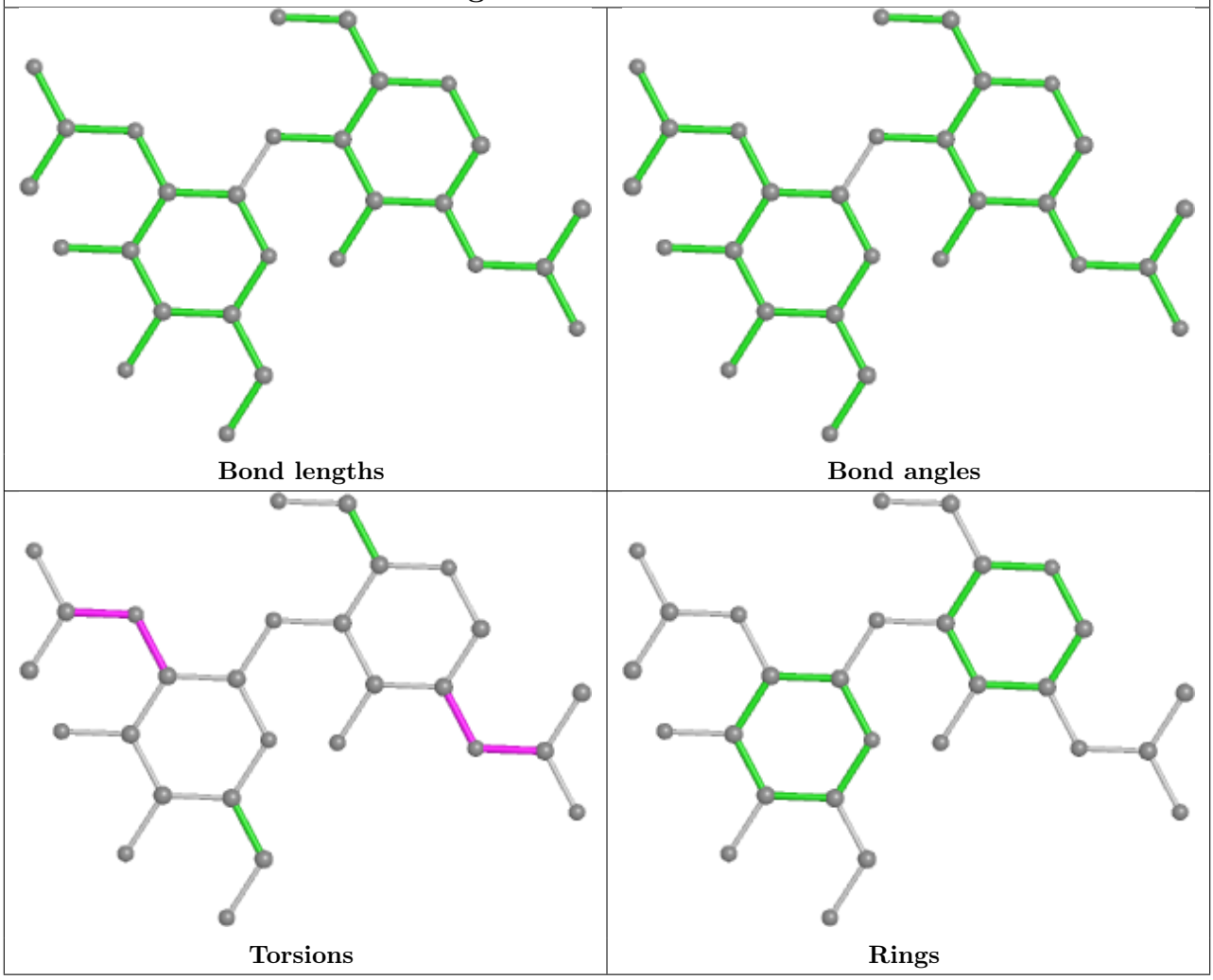


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
4	NAG	A	401	1	14,14,15	0.71	0	17,19,21	0.76	0
4	NAG	A	431	1	14,14,15	0.74	0	17,19,21	0.59	0
4	NAG	A	411	1	14,14,15	0.52	0	17,19,21	0.82	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
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	431	1	-	2/6/23/26	0/1/1/1
4	NAG	A	411	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	411	NAG	C2-N2-C7	-2.44	119.42	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	A	411	NAG	C8-C7-N2-C2
4	A	411	NAG	O7-C7-N2-C2
4	A	411	NAG	O5-C5-C6-O6
4	A	431	NAG	C8-C7-N2-C2
4	A	411	NAG	C4-C5-C6-O6
4	A	431	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.