



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:53 PM UTC

PDB ID : 1HA0 / pdb_00001ha0
Title : HEMAGGLUTININ PRECURSOR HA0
Authors : Chen, J.; Ho Lee, K.; Steinhauer, D.A.; Stevens, D.J.; Skehel, J.J.; Wiley, D.C.
Deposited on : 1998-10-08
Resolution : 2.80 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

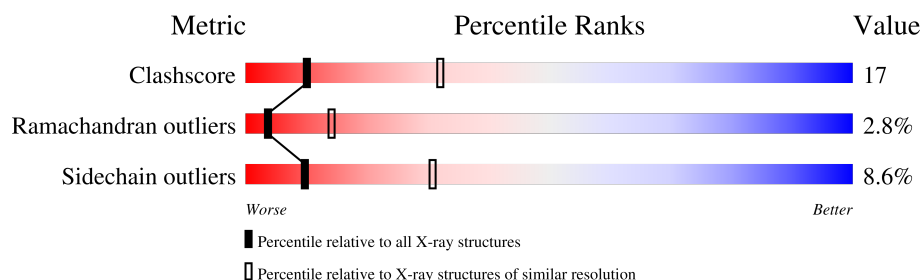
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

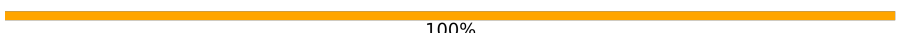
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	494	 62% 32% 5%
2	B	3	 67% 33%
2	C	3	 33% 67%
3	D	3	 100%

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
4	NAG	A	1440	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4070 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.

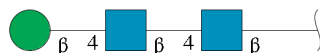
- Molecule 1 is a protein called PROTEIN (HEMAGGLUTININ PRECURSOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3888	2426	684	759	19			

There are 2 discrepancies between the modelled and reference sequences:

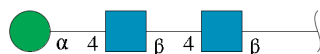
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	GLN	ARG	engineered mutation	UNP P03437
A	493	ASN	ASP	conflict	UNP P03437

- 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	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

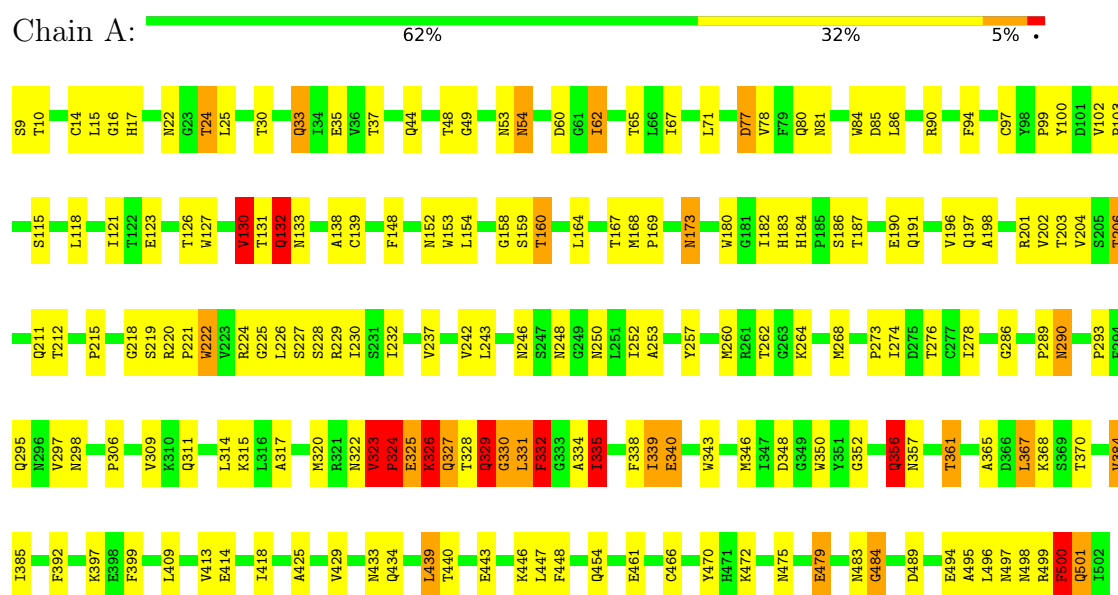
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	37	Total O 37 37	0	0

3 Residue-property plots

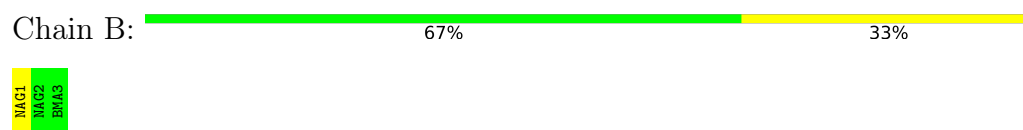
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PROTEIN (HEMAGGLUTININ PRECURSOR)



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



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



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

Chain D:  100%

MAG1
MAG2
MAG3

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	153.00Å 153.00Å 153.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.5 (8.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.224 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4070	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.51	1/3969 (0.0%)	1.04	17/5381 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	VAL	CA-CB	5.04	1.60	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	GLY	N-CA-C	11.85	124.05	112.08
1	A	323	VAL	CA-C-N	11.62	134.37	119.84
1	A	323	VAL	C-N-CA	11.62	134.37	119.84
1	A	326	LYS	N-CA-C	8.84	129.62	110.80
1	A	85	ASP	N-CA-C	-8.15	102.94	113.12
1	A	334	ALA	N-CA-C	-7.71	103.21	114.39
1	A	329	GLN	N-CA-C	7.22	118.07	107.88
1	A	327	GLN	N-CA-C	7.22	126.18	110.80
1	A	328	THR	N-CA-C	6.83	125.36	110.80
1	A	206	THR	N-CA-C	-6.76	99.59	109.18
1	A	115	SER	N-CA-C	-6.61	104.16	111.36
1	A	132	GLN	N-CA-C	6.22	124.05	110.80
1	A	356	GLN	N-CA-C	-5.78	98.66	108.26
1	A	65	THR	N-CA-C	-5.72	101.53	110.17
1	A	286	GLY	N-CA-C	-5.66	105.85	111.85
1	A	500	PHE	N-CA-C	5.21	121.89	110.80
1	A	78	VAL	N-CA-C	-5.17	106.03	113.07

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	3888	0	3757	133	0
2	B	39	0	34	0	0
2	C	39	0	34	2	0
3	D	39	0	34	3	0
4	A	28	0	26	1	0
5	A	37	0	0	9	0
All	All	4070	0	3885	137	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 17.

All (137) 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:14:CYS:SG	1:A:335:ILE:HG22	1.86	1.14
1:A:25:LEU:HD13	1:A:33:GLN:HG3	1.47	0.96
1:A:132:GLN:HB3	1:A:152:ASN:HD21	1.30	0.94
1:A:123:GLU:HB3	1:A:168:MET:HE3	1.54	0.90
1:A:331:LEU:O	1:A:332:PHE:HB3	1.80	0.78
1:A:173:ASN:H	1:A:173:ASN:HD22	1.31	0.77
1:A:132:GLN:HB3	1:A:152:ASN:ND2	1.99	0.76
1:A:10:THR:HG22	1:A:470:TYR:HA	1.68	0.75
1:A:182:ILE:HD11	1:A:215:PRO:HD3	1.67	0.75
1:A:335:ILE:HD12	1:A:356:GLN:HB2	1.71	0.72
1:A:293:PRO:HD3	1:A:385:ILE:HG22	1.72	0.72
1:A:187:THR:HG23	1:A:190:GLU:H	1.56	0.70
1:A:17:HIS:HE1	1:A:324:PRO:HD3	1.58	0.69
1:A:14:CYS:SG	1:A:335:ILE:CG2	2.74	0.68
1:A:500:PHE:O	1:A:501:GLN:HB2	1.93	0.68
1:A:357:ASN:HD21	1:A:475:ASN:HD22	1.44	0.66
1:A:357:ASN:HD21	1:A:475:ASN:ND2	1.94	0.66
1:A:138:ALA:HB2	1:A:226:LEU:HD11	1.79	0.65
1:A:399:PHE:HB2	5:A:1474:HOH:O	1.94	0.65
1:A:346:MET:SD	1:A:365:ALA:HB2	2.36	0.65
1:A:53:ASN:OD1	1:A:276:THR:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:A:154:LEU:HB3	1.82	0.61
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.83	0.61
1:A:77:ASP:O	1:A:80:GLN:HG3	2.02	0.60
1:A:262:THR:HA	5:A:1486:HOH:O	2.02	0.58
1:A:325:GLU:O	1:A:326:LYS:HB2	2.03	0.58
1:A:133:ASN:H	1:A:152:ASN:HD21	1.51	0.57
1:A:203:THR:HA	1:A:211:GLN:O	2.05	0.57
1:A:290:ASN:HD22	1:A:290:ASN:H	1.51	0.57
1:A:384:VAL:HG12	1:A:385:ILE:HG23	1.88	0.56
1:A:339:ILE:HG22	1:A:340:GLU:N	2.20	0.56
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.42	0.54
1:A:201:ARG:HB3	1:A:248:ASN:OD1	2.08	0.54
1:A:16:GLY:HA2	1:A:338:PHE:HB3	1.89	0.54
1:A:222:TRP:HA	1:A:226:LEU:O	2.08	0.53
1:A:17:HIS:CE1	1:A:324:PRO:HD3	2.41	0.53
1:A:329:GLN:HG2	1:A:330:GLY:N	2.22	0.53
1:A:121:ILE:HD12	1:A:257:TYR:OH	2.09	0.53
1:A:206:THR:HA	1:A:242:VAL:O	2.08	0.53
1:A:323:VAL:HG22	1:A:323:VAL:O	2.08	0.53
1:A:67:ILE:HG12	5:A:1463:HOH:O	2.08	0.53
1:A:317:ALA:H	1:A:433:ASN:ND2	2.07	0.52
1:A:152:ASN:C	1:A:152:ASN:HD22	2.16	0.52
1:A:97:CYS:O	1:A:224:ARG:NH1	2.41	0.52
1:A:60:ASP:HB2	1:A:274:ILE:HD12	1.91	0.51
1:A:62:ILE:O	1:A:90:ARG:HB2	2.10	0.51
1:A:203:THR:OG1	1:A:212:THR:HG23	2.11	0.51
1:A:222:TRP:CZ3	1:A:225:GLY:HA2	2.45	0.50
1:A:309:VAL:HB	1:A:311:GLN:OE1	2.11	0.50
1:A:439:LEU:C	1:A:439:LEU:HD23	2.37	0.50
1:A:24:THR:HG21	1:A:315:LYS:HE2	1.93	0.49
1:A:97:CYS:HA	1:A:139:CYS:HA	1.94	0.49
1:A:290:ASN:HD22	1:A:290:ASN:N	2.06	0.48
1:A:352:GLY:HA3	1:A:365:ALA:HA	1.95	0.48
1:A:202:VAL:O	1:A:212:THR:HA	2.13	0.48
1:A:297:VAL:HG13	3:D:1:NAG:H82	1.94	0.48
1:A:103:PRO:HD2	1:A:232:ILE:O	2.14	0.48
1:A:446:LYS:HD2	5:A:1467:HOH:O	2.14	0.48
1:A:182:ILE:HD11	1:A:215:PRO:CD	2.39	0.48
1:A:186:SER:HA	1:A:218:GLY:O	2.13	0.48
1:A:184:HIS:HB3	1:A:220:ARG:NH2	2.29	0.48
1:A:357:ASN:ND2	1:A:475:ASN:HD22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:CYS:HA	1:A:466:CYS:HA	1.96	0.47
1:A:317:ALA:H	1:A:433:ASN:HD21	1.61	0.47
1:A:343:TRP:HE3	1:A:346:MET:HE2	1.79	0.47
1:A:220:ARG:HB3	1:A:221:PRO:CD	2.45	0.47
3:D:2:NAG:O7	3:D:2:NAG:C1	2.63	0.47
1:A:500:PHE:O	1:A:501:GLN:CB	2.63	0.47
1:A:356:GLN:HG2	1:A:361:THR:HB	1.95	0.47
1:A:399:PHE:CD1	1:A:399:PHE:N	2.83	0.47
1:A:152:ASN:HD22	1:A:153:TRP:N	2.13	0.46
1:A:494:GLU:HG2	1:A:498:ASN:ND2	2.31	0.46
1:A:184:HIS:CE1	5:A:1487:HOH:O	2.67	0.46
1:A:290:ASN:H	1:A:290:ASN:ND2	2.13	0.46
1:A:338:PHE:HE1	1:A:448:PHE:CD1	2.34	0.46
1:A:221:PRO:O	1:A:229:ARG:NH2	2.49	0.46
1:A:260:MET:N	5:A:1480:HOH:O	2.45	0.46
1:A:331:LEU:O	1:A:332:PHE:CB	2.57	0.45
1:A:49:GLY:O	1:A:273:PRO:HD2	2.16	0.45
1:A:81:ASN:ND2	4:A:1440:NAG:C7	2.79	0.45
1:A:314:LEU:HB3	1:A:429:VAL:HG21	1.99	0.45
1:A:131:THR:HA	5:A:1495:HOH:O	2.15	0.45
1:A:461:GLU:HG3	5:A:1476:HOH:O	2.17	0.45
1:A:367:LEU:HA	1:A:370:THR:HB	1.99	0.45
1:A:17:HIS:HA	1:A:350:TRP:O	2.16	0.44
1:A:295:GLN:HB3	1:A:306:PRO:HB2	2.00	0.44
1:A:86:LEU:HD11	1:A:268:MET:HB2	1.99	0.44
1:A:322:ASN:O	1:A:323:VAL:C	2.61	0.44
1:A:24:THR:O	1:A:35:GLU:HA	2.17	0.44
1:A:448:PHE:HZ	1:A:461:GLU:HG3	1.82	0.44
2:C:1:NAG:H62	2:C:2:NAG:O5	2.17	0.44
1:A:167:THR:HA	1:A:243:LEU:O	2.17	0.44
1:A:173:ASN:H	1:A:173:ASN:ND2	2.08	0.43
1:A:237:VAL:HG21	1:A:243:LEU:HB2	2.00	0.43
1:A:320:MET:HE1	1:A:350:TRP:HB3	1.99	0.43
1:A:479:GLU:O	1:A:483:ASN:ND2	2.51	0.43
1:A:44:GLN:OE1	1:A:289:PRO:HG2	2.19	0.43
1:A:102:VAL:HG22	1:A:232:ILE:HB	2.00	0.43
1:A:197:GLN:HG3	1:A:248:ASN:O	2.18	0.43
1:A:15:LEU:CD1	1:A:447:LEU:HG	2.48	0.43
1:A:169:PRO:HA	1:A:242:VAL:HG23	2.01	0.43
1:A:220:ARG:HD2	1:A:220:ARG:N	2.34	0.43
1:A:10:THR:CG2	1:A:470:TYR:HA	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:O	1:A:126:THR:HG23	2.19	0.43
1:A:324:PRO:O	1:A:325:GLU:HB2	2.18	0.43
1:A:298:ASN:HA	5:A:1481:HOH:O	2.18	0.43
1:A:409:LEU:O	1:A:413:VAL:HG23	2.19	0.43
1:A:84:TRP:CZ3	1:A:118:LEU:HG	2.54	0.42
1:A:37:THR:HG22	1:A:322:ASN:OD1	2.19	0.42
1:A:54:ASN:O	1:A:278:ILE:HA	2.19	0.42
1:A:434:GLN:HE21	1:A:434:GLN:HA	1.85	0.42
1:A:494:GLU:HG2	1:A:498:ASN:HD22	1.84	0.42
1:A:218:GLY:O	1:A:220:ARG:NH1	2.53	0.42
1:A:94:PHE:CD1	1:A:94:PHE:C	2.98	0.42
1:A:164:LEU:O	1:A:246:ASN:HA	2.20	0.42
1:A:454:GLN:NE2	1:A:484:GLY:HA2	2.34	0.41
1:A:160:THR:HA	1:A:196:VAL:HG21	2.02	0.41
1:A:414:GLU:O	1:A:418:ILE:HG13	2.19	0.41
1:A:100:TYR:HB2	1:A:230:ILE:O	2.21	0.41
2:C:1:NAG:H3	2:C:1:NAG:O7	2.20	0.41
1:A:173:ASN:HD22	1:A:173:ASN:N	2.09	0.41
1:A:495:ALA:O	1:A:499:ARG:HG3	2.20	0.41
1:A:180:TRP:CZ2	1:A:204:VAL:HB	2.55	0.41
1:A:35:GLU:OE1	1:A:326:LYS:HD3	2.21	0.41
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.86	0.41
1:A:99:PRO:O	1:A:229:ARG:HD3	2.21	0.41
1:A:191:GLN:HG2	1:A:198:ALA:O	2.20	0.41
1:A:220:ARG:HD3	1:A:227:SER:O	2.21	0.41
1:A:443:GLU:HA	1:A:446:LYS:HE3	2.01	0.41
3:D:2:NAG:H62	3:D:3:MAN:C1	2.51	0.41
1:A:71:LEU:O	1:A:148:PHE:HB3	2.21	0.40
1:A:138:ALA:CB	1:A:226:LEU:HD11	2.49	0.40
1:A:314:LEU:CD1	1:A:425:ALA:HB1	2.51	0.40
1:A:320:MET:HB3	1:A:440:THR:HB	2.03	0.40
1:A:215:PRO:HG3	1:A:250:ASN:ND2	2.36	0.40
1:A:132:GLN:HB3	1:A:152:ASN:CG	2.47	0.40
1:A:264:LYS:O	1:A:392:PHE:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/494 (100%)	426 (87%)	52 (11%)	14 (3%)	4	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	324	PRO
1	A	327	GLN
1	A	331	LEU
1	A	332	PHE
1	A	339	ILE
1	A	501	GLN
1	A	326	LYS
1	A	62	ILE
1	A	484	GLY
1	A	500	PHE
1	A	335	ILE
1	A	130	VAL
1	A	158	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/431 (100%)	394 (91%)	37 (9%)	10	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	22	ASN
1	A	24	THR
1	A	30	THR
1	A	33	GLN
1	A	48	THR
1	A	54	ASN
1	A	77	ASP
1	A	130	VAL
1	A	159	SER
1	A	160	THR
1	A	173	ASN
1	A	219	SER
1	A	222	TRP
1	A	228	SER
1	A	290	ASN
1	A	323	VAL
1	A	324	PRO
1	A	325	GLU
1	A	326	LYS
1	A	329	GLN
1	A	332	PHE
1	A	335	ILE
1	A	340	GLU
1	A	348	ASP
1	A	356	GLN
1	A	361	THR
1	A	367	LEU
1	A	368	LYS
1	A	384	VAL
1	A	397	LYS
1	A	439	LEU
1	A	472	LYS
1	A	479	GLU
1	A	489	ASP
1	A	496	LEU
1	A	497	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	96	ASN
1	A	152	ASN
1	A	173	ASN
1	A	211	GLN
1	A	246	ASN
1	A	250	ASN
1	A	290	ASN
1	A	357	ASN
1	A	378	ASN
1	A	424	ASN
1	A	433	ASN
1	A	434	GLN
1	A	454	GLN
1	A	475	ASN
1	A	483	ASN
1	A	498	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	2,1	14,14,15	0.67	0	17,19,21	1.64	3 (17%)
2	NAG	B	2	2	14,14,15	0.45	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	B	3	2	11,11,12	0.43	0	15,15,17	0.47	0
2	NAG	C	1	2,1	14,14,15	0.88	1 (7%)	17,19,21	1.77	2 (11%)
2	NAG	C	2	2	14,14,15	0.75	0	17,19,21	1.56	3 (17%)
2	BMA	C	3	2	11,11,12	0.47	0	15,15,17	0.42	0
3	NAG	D	1	3,1	14,14,15	0.82	1 (7%)	17,19,21	0.70	0
3	NAG	D	2	3	14,14,15	0.75	0	17,19,21	1.46	3 (17%)
3	MAN	D	3	3	11,11,12	0.78	1 (9%)	15,15,17	1.00	1 (6%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.61	1.55	1.52
2	C	1	NAG	C1-C2	2.13	1.55	1.52
3	D	3	MAN	O5-C5	2.05	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C4-C3-C2	-5.72	102.64	111.02
2	C	2	NAG	C4-C3-C2	-5.05	103.61	111.02
2	B	1	NAG	C4-C3-C2	-4.75	104.06	111.02
3	D	2	NAG	C4-C3-C2	-3.77	105.49	111.02
3	D	2	NAG	C1-C2-N2	3.12	115.35	110.43
3	D	3	MAN	C1-O5-C5	3.02	116.24	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-C2-N2	2.60	114.53	110.43
2	C	1	NAG	C1-O5-C5	2.50	115.54	112.19
3	D	2	NAG	O5-C1-C2	-2.32	107.71	111.29
2	B	1	NAG	O5-C1-C2	-2.29	107.75	111.29
2	C	2	NAG	C1-C2-N2	2.16	113.84	110.43
2	C	2	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

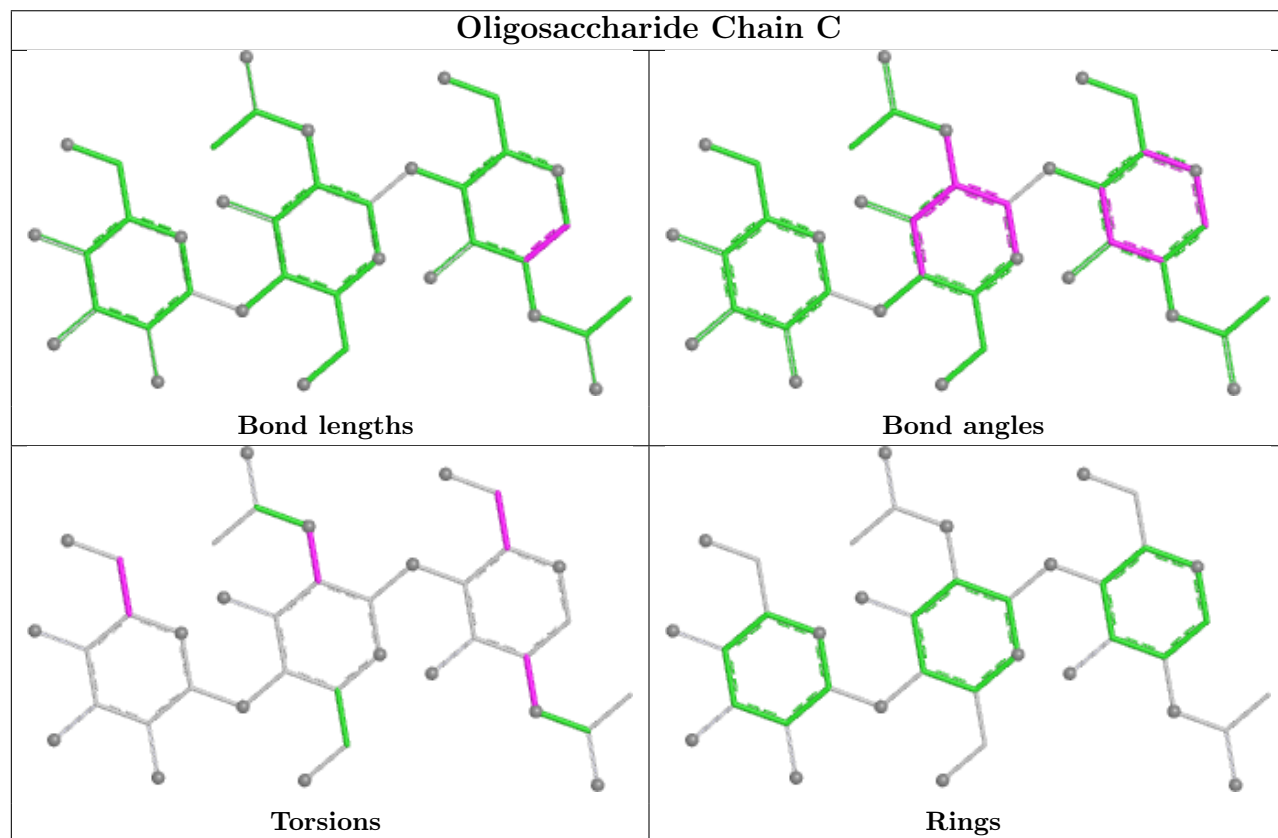
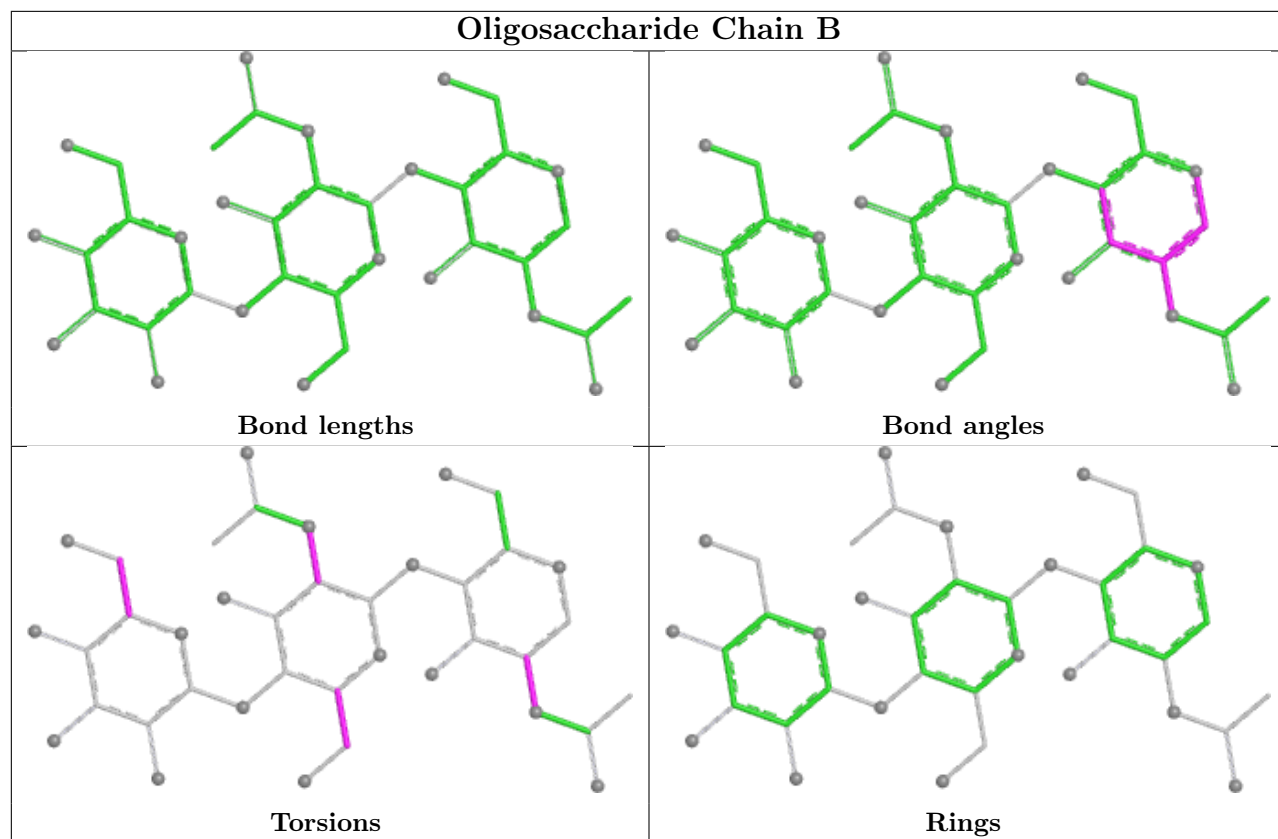
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
2	C	2	NAG	C1-C2-N2-C7
3	D	2	NAG	C1-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7

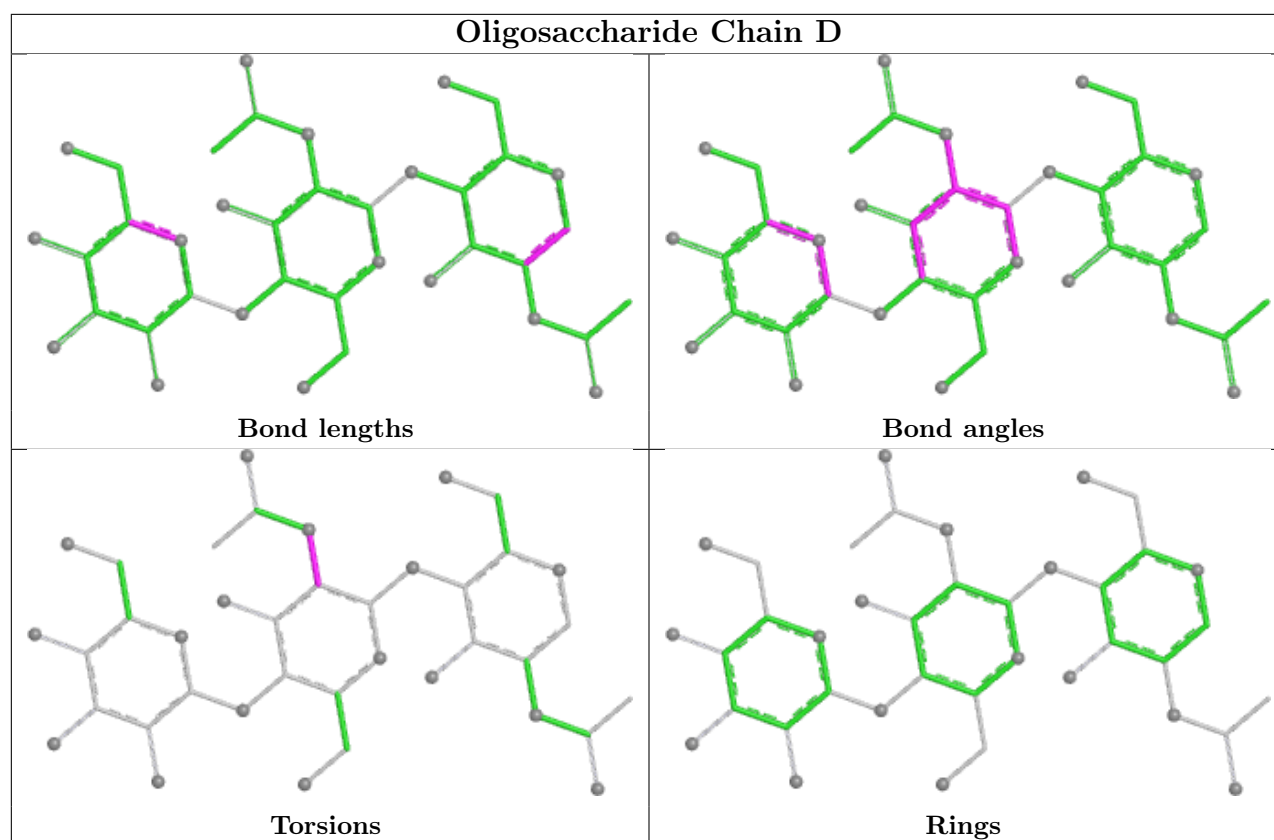
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	MAN	1	0
2	C	2	NAG	1	0
2	C	1	NAG	2	0
3	D	1	NAG	1	0
3	D	2	NAG	2	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](#)

2 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	1440	1	14,14,15	0.51	0	17,19,21	1.56	2 (11%)
4	NAG	A	1420	1	14,14,15	0.90	1 (7%)	17,19,21	1.62	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	A	1420	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1440	1	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1420	NAG	O5-C5	2.31	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1440	NAG	O5-C1-C2	5.25	119.42	111.29
4	A	1420	NAG	C1-O5-C5	4.71	118.50	112.19
4	A	1440	NAG	C2-N2-C7	-2.28	119.85	122.90
4	A	1420	NAG	O5-C1-C2	2.27	114.81	111.29
4	A	1420	NAG	C4-C3-C2	-2.03	108.04	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1440	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1420	NAG	O5-C5-C6-O6
4	A	1420	NAG	C4-C5-C6-O6
4	A	1440	NAG	C4-C5-C6-O6
4	A	1440	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1440	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.