



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:54 AM UTC

PDB ID : 1E8T / pdb_00001e8t
Title : Structure of the multifunctional paramyxovirus hemagglutinin-neuraminidase
Authors : Crennell, S.; Takimoto, T.; Portner, A.; Taylor, G.
Deposited on : 2000-10-01
Resolution : 2.50 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

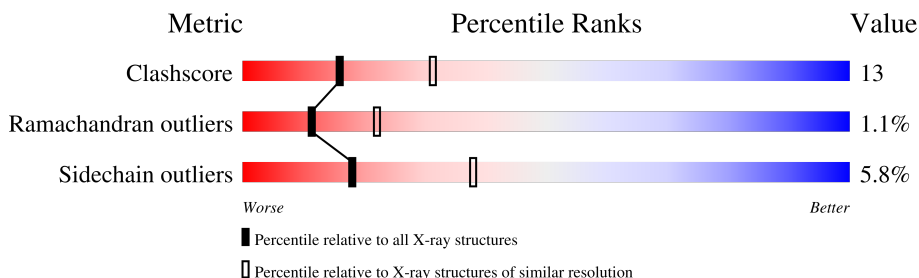
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	454	
1	B	454	
2	C	2	
2	D	2	

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	GOL	A	1003	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7214 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 HEMAGGLUTININ-NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	1
			3446	2172	588	667	19			
1	B	450	Total	C	N	O	S	0	0	1
			3468	2185	594	670	19			

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

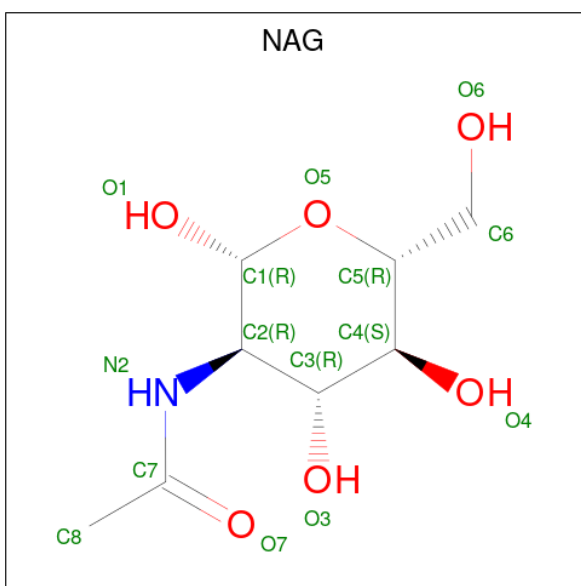
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total	O	0	0
			140	140		
6	B	71	Total	O	0	0
			71	71		

Chain C:  100%

MAG1
MAG2

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

Chain D:  50%  50%

MAG1
MAG2

4 Data and refinement statistics

Xtriage (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	71.71Å 77.91Å 198.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.0 (6.00-2.50)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7214	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: GOL, NAG, CA

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	0.47	1/3531 (0.0%)	0.97	15/4804 (0.3%)
1	B	0.43	2/3553 (0.1%)	0.89	8/4833 (0.2%)
All	All	0.45	3/7084 (0.0%)	0.93	23/9637 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	MET	SD-CE	-6.29	1.63	1.79
1	B	572	ARG	C-N	-5.59	1.25	1.33
1	A	569	ASP	C-N	-5.42	1.25	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	ASN	N-CA-C	7.39	120.28	111.33
1	A	173	THR	N-CA-C	-7.11	97.81	109.40
1	A	440	SER	CA-C-N	6.67	126.59	119.85
1	A	440	SER	C-N-CA	6.67	126.59	119.85
1	B	440	SER	CA-C-N	6.58	126.50	119.85
1	B	440	SER	C-N-CA	6.58	126.50	119.85
1	A	394	THR	N-CA-C	-6.58	105.25	113.28
1	B	394	THR	N-CA-C	-6.52	105.32	113.28
1	A	442	TYR	N-CA-C	-6.38	100.12	110.20
1	B	140	LEU	N-CA-C	6.22	117.85	111.14
1	A	472	ASP	N-CA-C	6.17	119.25	110.24
1	A	510	SER	N-CA-C	6.15	118.75	109.41
1	A	140	LEU	N-CA-C	5.98	117.47	111.07
1	A	370	GLN	N-CA-C	5.77	118.87	109.59
1	A	553	PHE	N-CA-C	5.70	119.22	112.72
1	B	173	THR	N-CA-C	-5.66	100.17	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	PRO	N-CA-C	5.60	120.28	111.38
1	B	499	LEU	N-CA-C	5.59	116.76	108.60
1	B	370	GLN	N-CA-C	5.59	118.92	109.76
1	A	150	SER	N-CA-C	-5.55	106.01	112.89
1	A	514	ILE	N-CA-C	5.45	116.98	109.46
1	B	442	TYR	N-CA-C	-5.41	101.65	110.20
1	A	275	LEU	N-CA-C	-5.11	100.41	108.73

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	3446	0	3340	96	0
1	B	3468	0	3366	87	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	1	0	0	0	0
4	A	12	0	16	5	0
4	B	6	0	8	1	0
5	A	14	0	13	2	0
6	A	140	0	0	3	0
6	B	71	0	0	4	0
All	All	7214	0	6793	182	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 13.

All (182) 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:511:ARG:HG2	1:A:511:ARG:HH11	1.30	0.96
1:B:156:PHE:HE2	1:B:517:VAL:HA	1.35	0.91
1:A:128:HIS:HA	1:A:210:VAL:HG13	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:CD2	1:A:211:LEU:H	1.96	0.83
1:B:156:PHE:CE2	1:B:517:VAL:HA	2.18	0.78
1:A:156:PHE:CE2	1:A:517:VAL:HA	2.23	0.73
1:A:404:ILE:HD13	1:A:413:LEU:HD23	1.71	0.73
1:B:284:LYS:HD3	1:B:382:LEU:O	1.90	0.72
1:B:128:HIS:CD2	1:B:211:LEU:H	2.08	0.71
1:B:128:HIS:HD2	1:B:211:LEU:H	1.40	0.70
1:B:549:SER:HB3	1:B:556:PHE:HA	1.74	0.69
1:A:511:ARG:HH11	1:A:511:ARG:CG	2.05	0.68
1:A:149:THR:HG21	1:A:510:SER:HB2	1.76	0.67
1:B:421:PHE:CE2	1:B:423:PRO:HG2	2.29	0.66
1:B:177:SER:HB3	1:B:188:THR:HG22	1.80	0.64
1:A:469:VAL:HG11	1:A:492:LEU:HD22	1.80	0.64
1:A:466:VAL:H	4:A:1003:GOL:H11	1.62	0.64
1:B:188:THR:OG1	1:B:249:MET:HE1	1.99	0.62
1:A:192:ILE:HD13	1:A:202:SER:HB3	1.80	0.62
1:A:462:PRO:HD2	6:A:2052:HOH:O	1.99	0.62
1:B:491:MET:HE2	1:B:506:PHE:CE2	2.35	0.61
1:A:154:SER:HB3	1:A:566:LEU:HD11	1.82	0.60
1:A:501:PRO:HG3	1:A:524:ALA:HB2	1.84	0.60
1:A:218:ARG:NE	1:A:218:ARG:HA	2.16	0.59
1:A:339:ARG:NH2	1:A:457:ALA:O	2.35	0.59
1:B:257:THR:HB	1:B:260:GLU:HB3	1.83	0.59
1:B:221:PHE:CE2	1:B:543:LEU:HD22	2.38	0.59
1:B:491:MET:HE2	1:B:506:PHE:HE2	1.68	0.59
1:B:430:THR:OG1	1:B:437:THR:HG23	2.03	0.58
1:B:238:CYS:HB3	1:B:249:MET:HE2	1.86	0.58
1:A:369:ILE:HB	1:A:398:MET:HG3	1.86	0.57
1:A:340:TYR:HE2	5:A:1570:NAG:H82	1.70	0.57
1:A:177:SER:HB3	1:A:188:THR:HG22	1.86	0.56
1:A:179:ASP:HA	6:A:2013:HOH:O	2.04	0.56
1:A:156:PHE:HE2	1:A:517:VAL:HA	1.69	0.55
1:B:297:ALA:O	1:B:318:GLY:HA3	2.07	0.54
1:A:156:PHE:CZ	1:A:517:VAL:HA	2.44	0.53
1:A:465:CYS:HA	4:A:1003:GOL:H32	1.91	0.53
1:B:421:PHE:CZ	1:B:423:PRO:HG2	2.43	0.53
1:B:237:SER:O	1:B:300:PRO:HB2	2.09	0.53
1:A:500:ASN:HD21	1:A:516:ARG:NH1	2.06	0.52
1:B:334:TYR:OH	1:B:352:ILE:HD12	2.10	0.52
1:B:420:TYR:CG	1:B:462:PRO:HA	2.45	0.52
1:A:265:ALA:O	1:A:321:LYS:HE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:HG11	1:B:526:TYR:CE2	2.45	0.52
1:A:218:ARG:HE	1:A:219:ILE:N	2.09	0.51
1:A:308:ILE:HG21	1:A:431:VAL:HG21	1.91	0.51
1:A:218:ARG:HE	1:A:219:ILE:H	1.58	0.51
1:A:511:ARG:HG2	1:A:511:ARG:NH1	2.08	0.51
1:A:339:ARG:HD2	1:A:445:ASN:OD1	2.11	0.50
1:B:451:GLY:O	1:B:456:GLN:HA	2.11	0.50
1:B:405:LEU:HD23	1:B:405:LEU:H	1.77	0.50
1:B:533:LYS:HG2	1:B:534:VAL:N	2.28	0.49
1:B:534:VAL:HG23	1:B:534:VAL:O	2.13	0.49
1:A:340:TYR:CE2	5:A:1570:NAG:H82	2.48	0.49
1:B:491:MET:CE	1:B:506:PHE:HE2	2.25	0.48
1:A:234:ASN:HB2	1:A:254:VAL:O	2.13	0.48
1:A:249:MET:HE3	1:A:251:CYS:SG	2.54	0.48
1:A:466:VAL:N	4:A:1003:GOL:H11	2.28	0.48
1:A:140:LEU:HG	1:A:540:THR:HG23	1.96	0.48
1:B:191:VAL:HG13	1:B:203:HIS:HB2	1.96	0.48
1:B:494:SER:HB2	1:B:499:LEU:HD12	1.94	0.48
1:A:132:PHE:CZ	1:A:211:LEU:HD22	2.49	0.48
1:A:173:THR:HB	1:A:558:ILE:HD12	1.96	0.48
1:A:518:SER:HB3	1:A:522:THR:OG1	2.13	0.48
1:B:405:LEU:HD23	1:B:405:LEU:N	2.29	0.48
1:A:133:ILE:O	1:A:535:VAL:HG21	2.14	0.48
1:A:160:LEU:HD13	1:A:221:PHE:CD1	2.49	0.48
1:B:548:ILE:HD11	1:B:559:VAL:HG21	1.95	0.47
1:B:148:VAL:HG13	1:B:477:ILE:HD12	1.96	0.47
1:A:567:LYS:C	1:A:569:ASP:H	2.23	0.47
1:A:411:HIS:HB2	1:A:429:MET:O	2.15	0.47
1:A:185:TYR:CZ	1:A:209:GLY:HA3	2.50	0.47
1:A:148:VAL:HG11	1:A:507:ASP:HB3	1.97	0.46
1:A:385:ASP:N	1:A:386:PRO:HD3	2.31	0.46
1:A:551:THR:OG1	1:A:552:LEU:HD22	2.14	0.46
1:B:140:LEU:HD13	1:B:540:THR:HG23	1.98	0.46
1:A:281:TYR:CE2	1:A:283:GLU:HB2	2.51	0.46
1:B:236:LYS:HB2	1:B:236:LYS:NZ	2.31	0.46
1:B:274:ARG:HH21	1:B:378:VAL:HG13	1.79	0.46
1:B:163:ILE:HD12	1:B:560:PRO:HB3	1.96	0.46
1:B:568:ASN:HB2	1:B:571:VAL:HG13	1.96	0.46
1:A:219:ILE:HD11	1:A:534:VAL:HG21	1.98	0.46
1:B:453:ILE:HG13	1:B:496:GLN:NE2	2.30	0.46
1:A:289:THR:O	1:A:293:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ASP:HB3	1:A:500:ASN:ND2	2.31	0.46
1:B:517:VAL:HG13	1:B:561:LEU:HD11	1.96	0.45
1:B:224:LEU:HD23	6:B:2020:HOH:O	2.16	0.45
1:A:511:ARG:CG	1:A:511:ARG:NH1	2.75	0.45
1:B:158:GLU:HG2	1:B:218:ARG:HG3	1.99	0.45
1:A:308:ILE:CG2	1:A:431:VAL:HG21	2.47	0.45
1:A:415:GLN:NE2	1:A:427:TYR:OH	2.49	0.45
1:B:452:SER:HB2	6:B:2061:HOH:O	2.17	0.45
1:B:467:THR:HG23	1:B:468:GLY:N	2.30	0.45
1:A:166:PRO:O	1:B:169:GLY:HA3	2.17	0.45
1:A:186:CYS:SG	1:A:242:ALA:HA	2.56	0.45
1:A:481:ASN:O	1:A:482:HIS:HB2	2.16	0.45
1:A:475:PRO:HA	1:A:487:VAL:HG12	1.99	0.45
1:B:136:ILE:HG23	1:B:180:MET:HE3	1.99	0.45
1:B:550:ASN:HB3	1:B:553:PHE:HD2	1.82	0.44
1:A:543:LEU:HD21	1:A:545:ILE:HD11	2.00	0.44
1:B:423:PRO:HB3	1:B:445:ASN:HA	1.98	0.44
1:B:272:HIS:CE1	1:B:382:LEU:HD23	2.52	0.44
1:B:470:TYR:C	1:B:470:TYR:CD1	2.96	0.44
1:B:325:PRO:O	1:B:329:VAL:HG23	2.17	0.44
1:B:403:ARG:HB2	1:B:470:TYR:OH	2.18	0.44
1:B:413:LEU:HD13	1:B:438:LEU:HD11	1.99	0.44
1:A:257:THR:O	1:A:261:ASP:HB2	2.17	0.44
1:B:174:ARG:NH2	1:B:190:ASN:OD1	2.48	0.44
1:B:211:LEU:HD21	1:B:221:PHE:CE1	2.53	0.44
1:B:475:PRO:HA	1:B:487:VAL:HG12	1.99	0.44
1:B:127:ILE:HG12	1:B:128:HIS:N	2.33	0.44
1:B:389:THR:HG21	1:B:436:ALA:O	2.18	0.43
1:A:363:ARG:H	4:A:1003:GOL:HO2	1.61	0.43
1:A:420:TYR:CG	1:A:462:PRO:HA	2.53	0.43
1:B:141:ILE:HD11	1:B:143:ASP:HB2	2.00	0.43
1:B:369:ILE:HB	1:B:398:MET:HG3	1.99	0.43
1:B:439:HIS:ND1	4:B:1004:GOL:H32	2.33	0.43
1:B:422:SER:N	1:B:423:PRO:HD2	2.33	0.43
1:A:187:TYR:OH	1:A:558:ILE:HG21	2.19	0.43
1:B:407:VAL:HG21	1:B:475:PRO:HB2	1.99	0.43
1:A:470:TYR:C	1:A:470:TYR:CD1	2.97	0.43
1:B:185:TYR:CD1	1:B:185:TYR:C	2.97	0.43
1:A:128:HIS:HD2	1:A:211:LEU:H	1.58	0.42
1:A:133:ILE:O	1:A:133:ILE:HG13	2.19	0.42
1:A:208:LEU:HD22	1:A:247:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:O	1:A:281:TYR:HA	2.19	0.42
1:A:447:PHE:C	1:A:447:PHE:CD1	2.97	0.42
1:A:154:SER:HB3	1:A:566:LEU:CD1	2.49	0.42
1:A:529:SER:HA	1:A:543:LEU:O	2.19	0.42
1:A:144:ASN:HD21	1:A:480:ARG:H	1.67	0.42
1:A:348:GLN:O	1:A:352:ILE:HG13	2.19	0.42
1:B:172:CYS:HB2	1:B:556:PHE:O	2.19	0.42
1:B:189:HIS:C	1:B:189:HIS:CD2	2.97	0.42
1:A:185:TYR:CE2	1:A:221:PHE:HD2	2.37	0.42
1:A:189:HIS:C	1:A:189:HIS:CD2	2.97	0.42
1:B:301:GLY:O	1:B:302:VAL:HB	2.20	0.42
1:A:308:ILE:HB	1:A:313:TRP:NE1	2.35	0.42
1:A:392:PRO:C	1:A:394:THR:H	2.27	0.42
1:A:523:LYS:HG3	6:A:2114:HOH:O	2.20	0.42
1:B:413:LEU:C	1:B:413:LEU:HD23	2.45	0.42
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.88	0.42
1:B:126:PRO:HD3	6:B:2001:HOH:O	2.18	0.42
1:B:254:VAL:HG11	1:B:261:ASP:OD2	2.20	0.42
1:B:315:SER:HB3	1:B:404:ILE:HG13	2.02	0.42
1:B:160:LEU:HD13	1:B:221:PHE:CD1	2.55	0.41
1:A:125:ALA:HB1	1:A:183:THR:HG21	2.01	0.41
1:B:442:TYR:CZ	1:B:484:LEU:HB3	2.55	0.41
1:A:552:LEU:HD22	1:A:552:LEU:H	1.85	0.41
1:B:131:ASP:O	1:B:535:VAL:HG22	2.19	0.41
1:B:153:PRO:HG2	1:B:504:ALA:HA	2.02	0.41
1:B:403:ARG:HA	6:B:2035:HOH:O	2.20	0.41
1:A:312:VAL:O	1:A:375:SER:HA	2.20	0.41
1:A:523:LYS:HB3	1:A:556:PHE:CE1	2.56	0.41
1:B:186:CYS:SG	1:B:242:ALA:HA	2.60	0.41
1:B:203:HIS:ND1	1:B:230:ASP:HA	2.35	0.41
1:A:418:SER:HA	1:A:467:THR:O	2.20	0.41
1:B:304:GLY:N	1:B:403:ARG:HG3	2.36	0.41
1:A:148:VAL:CG1	1:A:507:ASP:HB3	2.50	0.41
1:A:447:PHE:C	1:A:447:PHE:HD1	2.29	0.41
1:B:336:ILE:CD1	1:B:352:ILE:HD13	2.51	0.41
1:A:174:ARG:HH12	1:A:198:ASP:HA	1.86	0.41
1:B:210:VAL:HG13	1:B:224:LEU:HD11	2.02	0.41
1:B:253:LYS:HE3	1:B:271:ALA:HB2	2.03	0.41
1:B:348:GLN:O	1:B:352:ILE:HG12	2.21	0.41
1:B:377:LYS:HD2	1:B:377:LYS:HA	1.94	0.41
1:B:506:PHE:CD1	1:B:506:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:CD1	1:A:221:PHE:HB2	2.56	0.41
1:A:163:ILE:HA	1:A:164:PRO:HD3	1.91	0.41
1:A:404:ILE:CD1	1:A:413:LEU:HD23	2.48	0.41
1:A:164:PRO:HG2	1:A:205:TYR:CZ	2.57	0.40
1:A:166:PRO:HD3	1:A:557:ARG:HG3	2.03	0.40
1:A:354:MET:HE2	1:A:463:ASN:ND2	2.36	0.40
1:B:157:GLN:O	1:B:158:GLU:C	2.64	0.40
1:A:126:PRO:HD3	1:A:277:PHE:CE1	2.56	0.40
1:A:344:CYS:HB2	1:A:460:ARG:O	2.21	0.40
1:A:465:CYS:HA	4:A:1003:GOL:C3	2.52	0.40
1:B:257:THR:HB	1:B:260:GLU:CB	2.49	0.40
1:A:272:HIS:ND1	1:A:376:ILE:HG21	2.36	0.40
1:B:334:TYR:CZ	1:B:352:ILE:HG23	2.56	0.40
1:A:567:LYS:HE3	1:A:570:GLY:N	2.37	0.40
1:B:338:LYS:CD	1:B:338:LYS:H	2.34	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	445/454 (98%)	406 (91%)	33 (7%)	6 (1%)	9	18
1	B	448/454 (99%)	410 (92%)	34 (8%)	4 (1%)	14	27
All	All	893/908 (98%)	816 (91%)	67 (8%)	10 (1%)	11	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	551	THR
1	B	158	GLU

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Mol	Chain	Res	Type
1	A	127	ILE
1	A	156	PHE
1	A	340	TYR
1	A	493	ASP
1	B	342	ASP
1	B	302	VAL
1	B	473	PRO

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	387/392 (99%)	365 (94%)	22 (6%)	18	39
1	B	389/392 (99%)	366 (94%)	23 (6%)	18	37
All	All	776/784 (99%)	731 (94%)	45 (6%)	18	38

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	158	GLU
1	A	189	HIS
1	A	193	LEU
1	A	198	ASP
1	A	199	HIS
1	A	208	LEU
1	A	210	VAL
1	A	211	LEU
1	A	216	THR
1	A	233	GLN
1	A	261	ASP
1	A	275	LEU
1	A	343	THR
1	A	347	GLU
1	A	349	ASP

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Mol	Chain	Res	Type
1	A	463	ASN
1	A	511	ARG
1	A	517	VAL
1	A	523	LYS
1	A	550	ASN
1	A	552	LEU
1	B	130	PRO
1	B	141	ILE
1	B	143	ASP
1	B	147	ASP
1	B	167	THR
1	B	189	HIS
1	B	199	HIS
1	B	236	LYS
1	B	245	LEU
1	B	254	VAL
1	B	259	GLU
1	B	338	LYS
1	B	343	THR
1	B	405	LEU
1	B	410	SER
1	B	434	LYS
1	B	437	THR
1	B	454	PRO
1	B	456	GLN
1	B	491	MET
1	B	506	PHE
1	B	552	LEU
1	B	568	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	128	HIS
1	A	203	HIS
1	A	233	GLN
1	A	323	ASN
1	A	371	GLN
1	A	415	GLN
1	A	463	ASN
1	A	500	ASN
1	A	568	ASN

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Mol	Chain	Res	Type
1	B	128	HIS
1	B	157	GLN
1	B	161	ASN
1	B	263	ASN
1	B	280	GLN
1	B	282	HIS
1	B	351	GLN
1	B	496	GLN
1	B	550	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 ⓘ

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	C	1	1,2	14,14,15	0.44	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.45	0	17,19,21	0.59	0
2	NAG	D	1	1,2	14,14,15	0.43	0	17,19,21	0.65	0
2	NAG	D	2	2	14,14,15	0.42	0	17,19,21	0.71	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	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	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(°)	Ideal(°)
2	D	2	NAG	C2-N2-C7	-2.06	120.14	122.90

There are no chirality outliers.

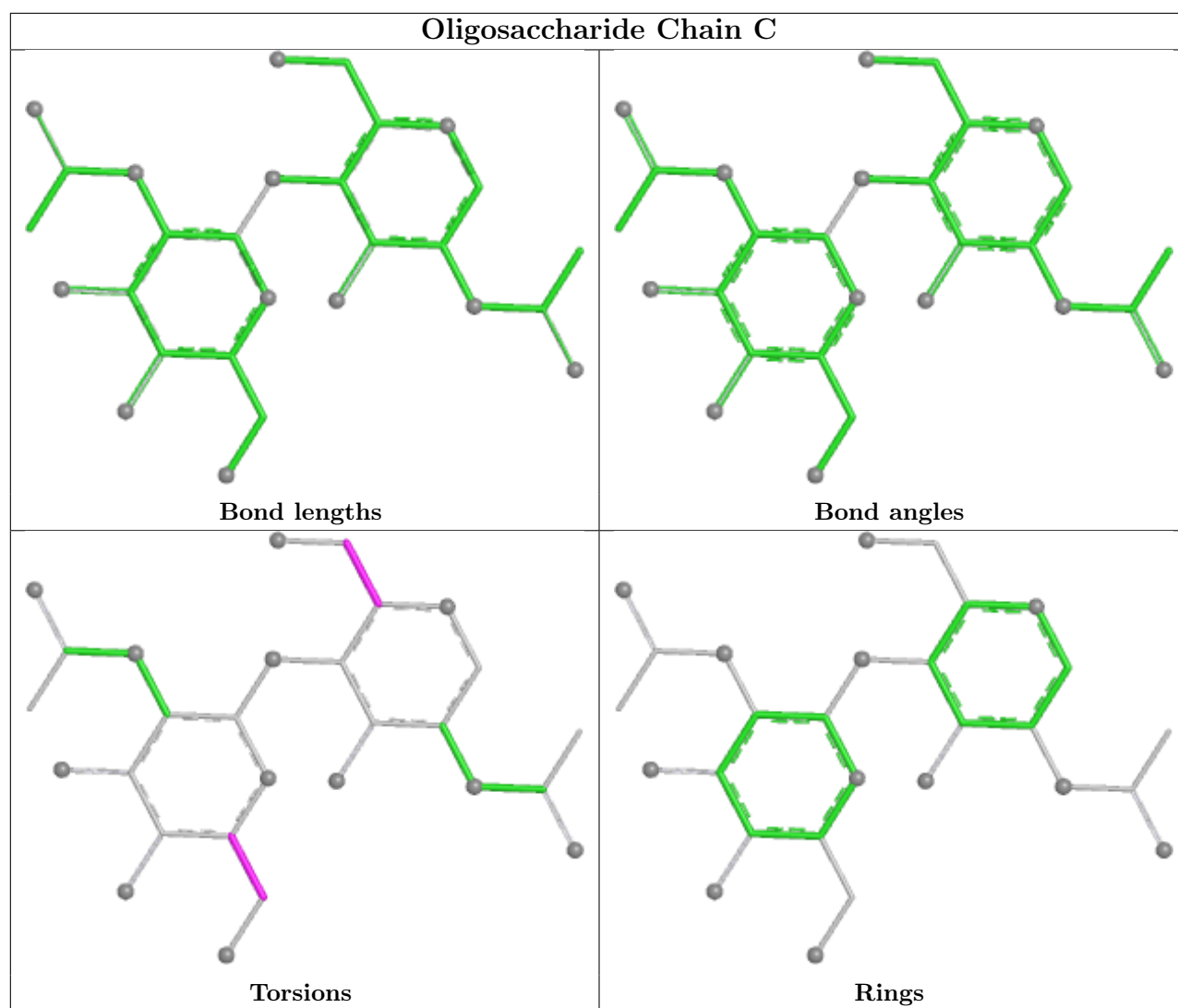
All (8) torsion outliers are listed below:

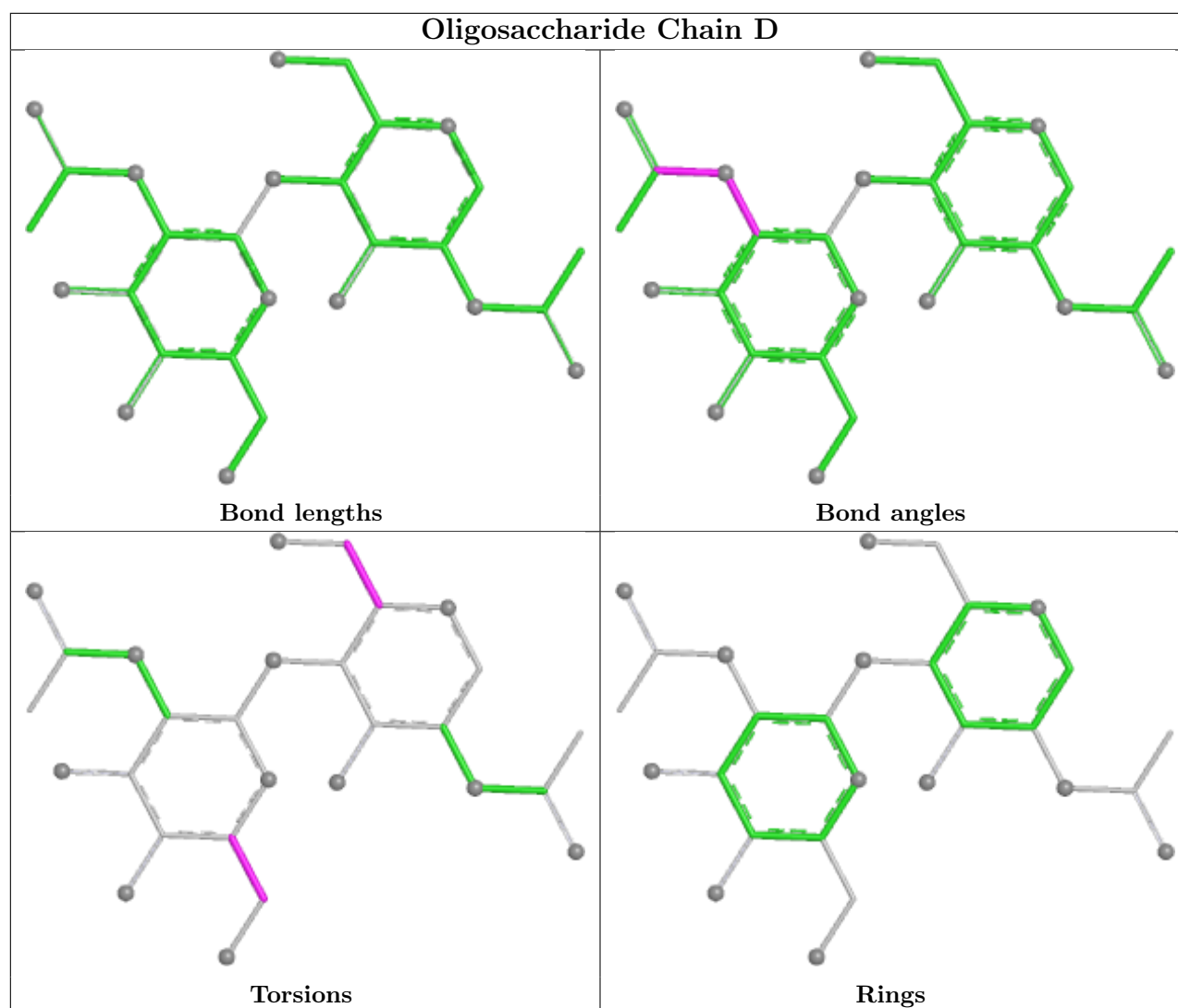
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
5	NAG	A	1570	1	14,14,15	0.43	0	17,19,21	0.71	1 (5%)
4	GOL	A	1003	-	5,5,5	1.22	1 (20%)	5,5,5	0.34	0
4	GOL	A	1002	-	5,5,5	0.58	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	1004	-	5,5,5	1.00	0	5,5,5	0.24	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
5	NAG	A	1570	1	-	0/6/23/26	0/1/1/1
4	GOL	A	1003	-	-	2/4/4/4	-
4	GOL	A	1002	-	-	2/4/4/4	-
4	GOL	B	1004	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	GOL	C1-C2	2.26	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1570	NAG	C2-N2-C7	-2.02	120.19	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	GOL	O1-C1-C2-C3
4	A	1003	GOL	O1-C1-C2-C3
4	B	1004	GOL	O1-C1-C2-C3
4	A	1002	GOL	O1-C1-C2-O2
4	B	1004	GOL	O1-C1-C2-O2
4	A	1003	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1570	NAG	2	0
4	A	1003	GOL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1004	GOL	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

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.