



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:11 AM UTC

PDB ID : 1DHK / pdb_00001dhk
Title : STRUCTURE OF PORCINE PANCREATIC ALPHA-AMYLASE
Authors : Bompard-Gilles, C.; Payan, F.
Deposited on : 1996-10-14
Resolution : 1.85 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

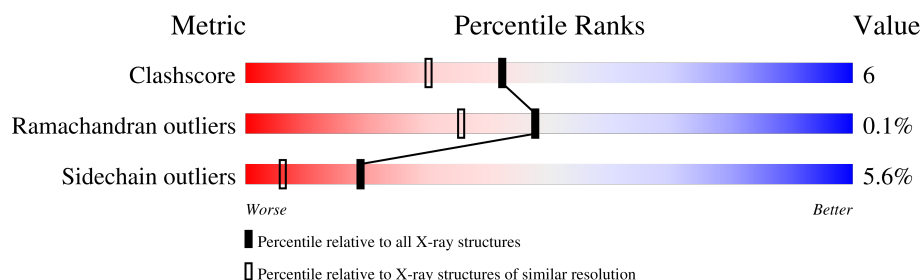
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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	496	 83% 14% .
2	B	223	 67% 17% . . 13%
3	C	2	 100%
3	D	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7712 atoms, of which 1887 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 PORCINE PANCREATIC ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	H	N	O	S	0	0	0
			4791	2468	885	687	730	21			

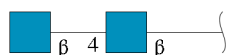
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	VAL	ILE	conflict	UNP P00690
A	404	GLN	GLU	conflict	UNP P00690

- Molecule 2 is a protein called BEAN LECTIN-LIKE INHIBITOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	195	Total	C	H	N	O	S	0	0	0
			1863	957	340	247	317	2			

- 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
3	C	2	Total	C	H	N	O		0	0	0
			35	16	7	2	10				
3	D	2	Total	C	H	N	O		0	0	0
			35	16	7	2	10				

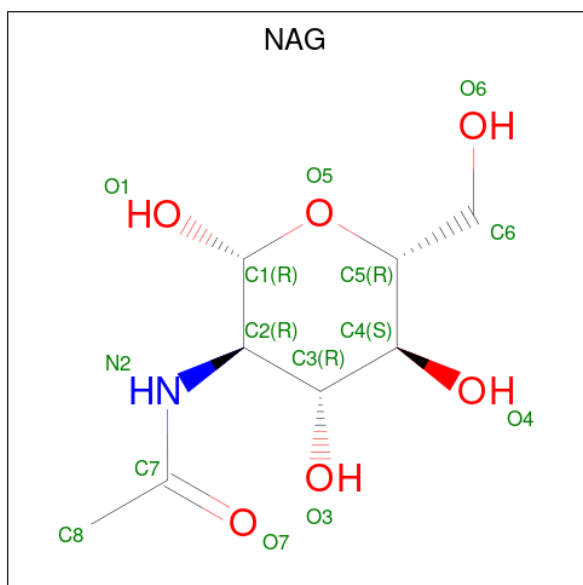
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	2	Total	Ca	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			18	8	4	1	5		

- Molecule 7 is water.

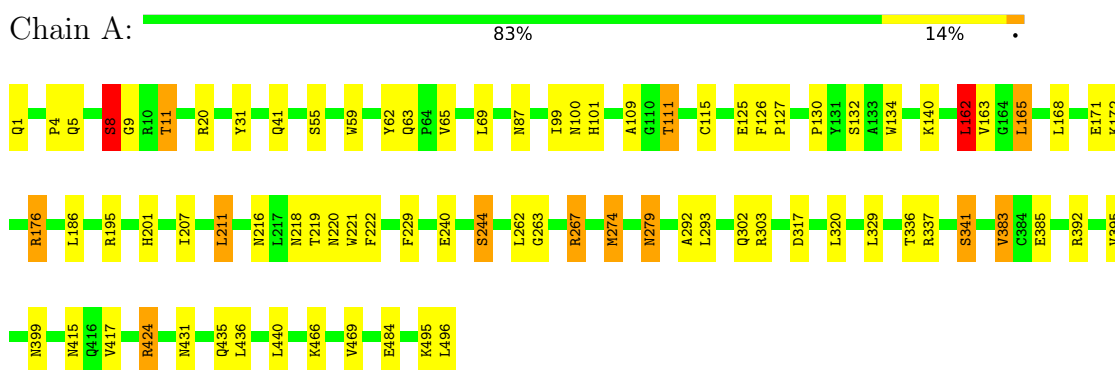
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	257	Total	H	O	0	0
			771	514	257		
7	B	65	Total	H	O	0	0
			195	130	65		

3 Residue-property plots

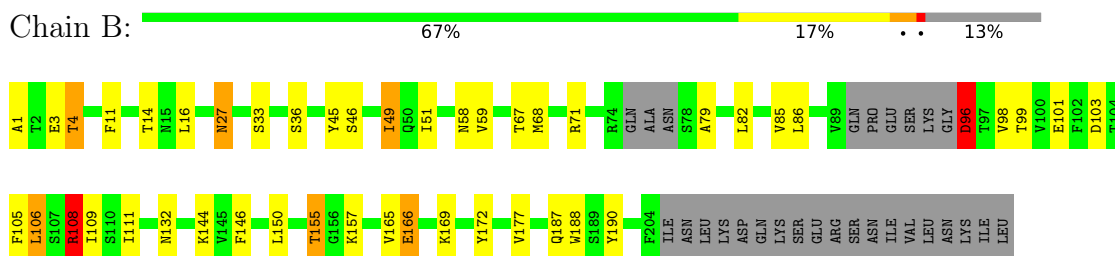
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

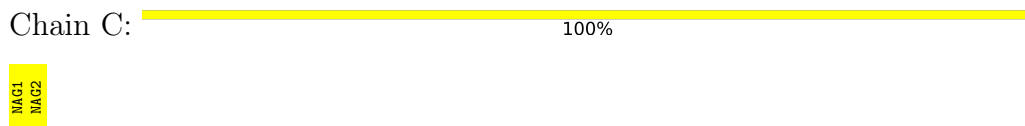
• Molecule 1: PORCINE PANCREATIC ALPHA-AMYLASE



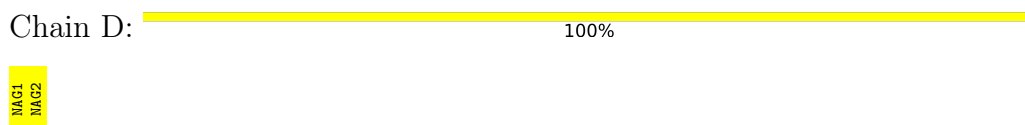
• Molecule 2: BEAN LECTIN-LIKE INHIBITOR



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



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



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.60Å 79.40Å 68.00Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	8.00 – 1.85	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7712	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: NAG, CL, CA, PCA

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	0.53	3/4009 (0.1%)	1.05	29/5450 (0.5%)
2	B	0.65	3/1555 (0.2%)	1.51	24/2120 (1.1%)
All	All	0.57	6/5564 (0.1%)	1.20	53/7570 (0.7%)

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
2	B	1	1
All	All	1	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	96	ASP	CA-CB	-13.48	1.26	1.53
1	A	216	ASN	CA-CB	-11.39	1.34	1.53
1	A	8	SER	CA-C	-11.02	1.38	1.52
2	B	108	ARG	CD-NE	-10.77	1.31	1.46
1	A	424	ARG	CD-NE	-9.60	1.32	1.46
2	B	96	ASP	CA-C	5.39	1.64	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	ASP	CA-CB-CG	44.49	157.09	112.60
2	B	96	ASP	CB-CA-C	13.73	136.18	110.10
2	B	67	THR	CA-CB-CG2	13.68	133.76	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	VAL	CA-CB-CG1	11.83	130.51	110.40
1	A	176	ARG	NE-CZ-NH2	11.63	129.66	119.20
1	A	176	ARG	NE-CZ-NH1	-10.56	110.94	121.50
1	A	9	GLY	CA-C-O	-10.28	107.55	119.07
2	B	108	ARG	NE-CZ-NH1	9.87	131.37	121.50
1	A	424	ARG	CD-NE-CZ	9.66	137.92	124.40
1	A	8	SER	CA-C-O	-9.53	106.88	120.51
1	A	165	LEU	CB-CG-CD2	9.20	138.29	110.70
2	B	108	ARG	NE-CZ-NH2	-9.04	111.06	119.20
2	B	190	TYR	N-CA-C	8.99	124.48	112.88
2	B	71	ARG	CG-CD-NE	-8.89	92.44	112.00
1	A	240	GLU	N-CA-C	8.59	119.98	108.38
1	A	9	GLY	O-C-N	7.85	131.94	122.60
1	A	216	ASN	CA-CB-CG	7.28	119.88	112.60
1	A	162	LEU	CB-CG-CD2	7.13	132.08	110.70
2	B	98	VAL	CA-CB-CG1	7.01	122.32	110.40
2	B	132	ASN	CA-CB-CG	6.90	119.50	112.60
1	A	292	ALA	N-CA-C	6.58	120.55	109.76
2	B	108	ARG	CD-NE-CZ	6.50	133.50	124.40
2	B	14	THR	N-CA-C	6.39	118.78	111.11
1	A	162	LEU	CB-CG-CD1	-6.33	91.72	110.70
1	A	244	SER	CA-CB-OG	-6.31	98.47	111.10
2	B	96	ASP	CA-C-O	6.27	131.45	120.80
2	B	111	ILE	N-CA-C	-6.15	98.27	107.37
1	A	216	ASN	N-CA-C	-6.08	102.68	110.53
1	A	8	SER	N-CA-C	6.01	123.61	110.80
2	B	46	SER	N-CA-C	5.87	118.46	111.71
1	A	99	ILE	N-CA-C	5.74	118.67	113.10
2	B	59	VAL	CA-CB-CG2	5.70	120.09	110.40
1	A	293	LEU	N-CA-C	-5.69	99.14	108.41
1	A	341	SER	N-CA-C	5.69	118.14	109.95
1	A	195	ARG	N-CA-C	-5.68	99.48	108.73
1	A	111	THR	N-CA-CB	-5.66	101.86	111.20
2	B	45	TYR	N-CA-C	-5.57	102.04	110.28
1	A	336	THR	N-CA-C	5.55	119.29	109.96
1	A	109	ALA	CA-C-N	-5.49	112.91	121.97
1	A	109	ALA	C-N-CA	-5.49	112.91	121.97
1	A	65	VAL	N-CA-C	-5.44	108.54	113.71
2	B	79	ALA	N-CA-C	-5.43	105.44	111.36
2	B	11	PHE	N-CA-C	5.40	117.84	110.55
2	B	108	ARG	CG-CD-NE	-5.29	100.35	112.00
1	A	395	VAL	CB-CA-C	-5.22	103.81	112.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	CG-CD-NE	5.19	123.42	112.00
2	B	3	GLU	CA-C-N	-5.17	113.76	122.29
2	B	3	GLU	C-N-CA	-5.17	113.76	122.29
1	A	11	THR	N-CA-C	5.10	121.26	113.61
2	B	67	THR	CA-CB-OG1	5.07	117.21	109.60
1	A	55	SER	N-CA-C	5.04	116.69	108.63
2	B	36	SER	N-CA-C	5.03	115.96	108.86
2	B	96	ASP	N-CA-CB	-5.01	101.98	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	67	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	ARG	Sidechain
2	B	108	ARG	Sidechain

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	3906	885	3680	45	1
2	B	1523	340	1424	21	1
3	C	28	7	25	0	0
3	D	28	7	25	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	1	0
6	B	14	4	13	0	0
7	A	257	514	0	12	1
7	B	65	130	0	1	1
All	All	5825	1887	5167	65	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 6.

All (65) 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:125:GLU:HB3	7:A:741:HOH:O	1.34	1.26
1:A:132:SER:OG	1:A:134:TRP:CE2	2.25	0.90
2:B:155:THR:HG22	2:B:157:LYS:HG2	1.55	0.88
1:A:127:PRO:HD3	7:A:741:HOH:O	1.74	0.87
2:B:155:THR:CG2	2:B:157:LYS:HG2	2.11	0.80
1:A:100:ASN:HD22	1:A:101:HIS:HD2	1.30	0.79
2:B:4:THR:CG2	2:B:49:ILE:HD12	2.19	0.72
1:A:279:ASN:H	1:A:279:ASN:HD22	1.39	0.69
1:A:41:GLN:HE22	1:A:337:ARG:HH11	1.41	0.68
1:A:317:ASP:OD2	7:A:750:HOH:O	2.13	0.66
2:B:4:THR:HG23	2:B:49:ILE:HD12	1.78	0.66
1:A:172:LYS:O	1:A:176:ARG:HG3	1.95	0.66
1:A:484:GLU:HG2	7:A:706:HOH:O	1.96	0.64
2:B:27:ASN:H	2:B:27:ASN:HD22	1.47	0.62
2:B:86:LEU:HD22	2:B:177:VAL:HG12	1.81	0.60
1:A:125:GLU:CB	7:A:741:HOH:O	2.15	0.60
1:A:140:LYS:HE3	7:A:654:HOH:O	2.01	0.60
1:A:302:GLN:HE21	1:A:303:ARG:HH12	1.49	0.59
1:A:125:GLU:CA	7:A:741:HOH:O	2.49	0.57
2:B:4:THR:HG21	2:B:49:ILE:HD12	1.87	0.55
1:A:41:GLN:HE22	1:A:337:ARG:NH1	2.02	0.55
1:A:162:LEU:HD13	1:A:163:VAL:HG22	1.89	0.55
1:A:337:ARG:NH2	5:A:498:CL:CL	2.74	0.54
1:A:263:GLY:O	1:A:267:ARG:HG3	2.09	0.53
1:A:302:GLN:HE21	1:A:303:ARG:NH1	2.07	0.53
2:B:85:VAL:HG12	2:B:99:THR:HG23	1.91	0.53
1:A:125:GLU:C	7:A:741:HOH:O	2.52	0.52
1:A:383:VAL:HG22	1:A:385:GLU:OE1	2.10	0.52
2:B:86:LEU:CD2	2:B:177:VAL:HG12	2.41	0.52
1:A:140:LYS:HZ3	1:A:171:GLU:CD	2.18	0.51
1:A:100:ASN:HD22	1:A:101:HIS:CD2	2.20	0.51
2:B:96:ASP:O	2:B:172:TYR:HE1	1.94	0.51
2:B:4:THR:HG22	7:B:526:HOH:O	2.13	0.48
1:A:11:THR:H	1:A:399:ASN:HD21	1.61	0.48
2:B:51:ILE:HB	2:B:172:TYR:O	2.13	0.48
1:A:126:PHE:O	1:A:130:PRO:HA	2.13	0.48
1:A:62:TYR:O	1:A:101:HIS:HE1	1.96	0.48
1:A:274:MET:HG3	7:A:554:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TYR:OH	1:A:392:ARG:HG3	2.15	0.47
2:B:169:LYS:HD2	2:B:172:TYR:HE2	1.80	0.46
1:A:207:ILE:HG22	1:A:211:LEU:HD22	1.98	0.46
1:A:132:SER:OG	1:A:134:TRP:NE1	2.49	0.45
1:A:63:GLN:HG2	1:A:165:LEU:HD22	1.97	0.45
2:B:187:GLN:HG2	2:B:188:TRP:CD1	2.51	0.45
1:A:59:TRP:CE2	2:B:187:GLN:HB3	2.52	0.44
1:A:436:LEU:C	1:A:436:LEU:HD23	2.43	0.44
1:A:5:GLN:NE2	1:A:5:GLN:HA	2.32	0.44
1:A:5:GLN:HA	1:A:5:GLN:HE21	1.83	0.44
1:A:4:PRO:HA	1:A:229:PHE:CG	2.53	0.44
1:A:466:LYS:HE2	7:A:735:HOH:O	2.17	0.44
1:A:132:SER:OG	1:A:134:TRP:CD2	2.67	0.43
1:A:218:ASN:OD1	1:A:220:ASN:HB2	2.17	0.43
2:B:68:MET:SD	2:B:82:LEU:HD23	2.58	0.43
2:B:146:PHE:HB2	2:B:165:VAL:HG22	2.01	0.43
2:B:105:PHE:HD2	2:B:106:LEU:HD22	1.84	0.43
2:B:144:LYS:HE2	2:B:166:GLU:HG2	2.00	0.43
1:A:162:LEU:HD23	1:A:201:HIS:CE1	2.54	0.42
1:A:219:THR:HA	1:A:222:PHE:O	2.19	0.42
1:A:392:ARG:NH2	7:A:599:HOH:O	2.43	0.42
2:B:103:ASP:OD2	2:B:106:LEU:HD23	2.20	0.42
1:A:87:ASN:HB3	1:A:221:TRP:CD1	2.55	0.41
1:A:415:ASN:HB3	1:A:431:ASN:HB3	2.02	0.41
2:B:101:GLU:O	2:B:109:ILE:HA	2.21	0.41
1:A:140:LYS:CE	7:A:654:HOH:O	2.65	0.41
1:A:279:ASN:HD22	1:A:279:ASN:N	2.10	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)
2:B:1:ALA:H2	7:B:527:HOH:H1[2_655]	1.13	0.47
1:A:495:LYS:HZ1	7:A:751:HOH:H2[4_655]	1.14	0.46

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	494/496 (100%)	479 (97%)	14 (3%)	1 (0%)	43	31
2	B	189/223 (85%)	184 (97%)	5 (3%)	0	100	100
All	All	683/719 (95%)	663 (97%)	19 (3%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER

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	411/411 (100%)	390 (95%)	21 (5%)	21	7
2	B	176/203 (87%)	164 (93%)	12 (7%)	14	4
All	All	587/614 (96%)	554 (94%)	33 (6%)	19	6

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

Mol	Chain	Res	Type
1	A	8	SER
1	A	20	ARG
1	A	69	LEU
1	A	111	THR
1	A	115	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	LEU
1	A	168	LEU
1	A	186	LEU
1	A	211	LEU
1	A	244	SER
1	A	262	LEU
1	A	274	MET
1	A	279	ASN
1	A	320	LEU
1	A	329	LEU
1	A	341	SER
1	A	383	VAL
1	A	417	VAL
1	A	435	GLN
1	A	440	LEU
1	A	496	LEU
2	B	4	THR
2	B	16	LEU
2	B	27	ASN
2	B	33	SER
2	B	49	ILE
2	B	58	ASN
2	B	96	ASP
2	B	106	LEU
2	B	108	ARG
2	B	150	LEU
2	B	155	THR
2	B	166	GLU

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	15	HIS
1	A	41	GLN
1	A	101	HIS
1	A	220	ASN
1	A	279	ASN
1	A	302	GLN
1	A	355	ASN
1	A	399	ASN
1	A	460	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	19	GLN
2	B	27	ASN
2	B	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	PCA	A	1	1	7,8,9	1.29	1 (14%)	9,10,12	4.80	7 (77%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CG-CD	2.81	1.57	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-N	10.23	147.10	124.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CG-CD-N	-6.93	91.42	108.39
1	A	1	PCA	CB-CA-C	-3.72	107.56	112.66
1	A	1	PCA	CB-CG-CD	3.28	109.48	104.41
1	A	1	PCA	CA-N-CD	3.27	124.77	113.58
1	A	1	PCA	OE-CD-CG	-2.94	121.47	126.72
1	A	1	PCA	CG-CB-CA	-2.50	94.57	104.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	3,2	14,14,15	0.72	1 (7%)	17,19,21	1.01	1 (5%)
3	NAG	C	2	3	14,14,15	0.76	1 (7%)	17,19,21	2.47	2 (11%)
3	NAG	D	1	3,2	14,14,15	0.67	1 (7%)	17,19,21	1.03	1 (5%)
3	NAG	D	2	3	14,14,15	0.86	1 (7%)	17,19,21	1.09	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
3	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.44	1.55	1.52
3	C	1	NAG	C1-C2	2.29	1.55	1.52
3	D	1	NAG	C1-C2	2.12	1.55	1.52
3	D	2	NAG	C1-C2	2.10	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	-9.35	110.37	122.90
3	D	2	NAG	C1-O5-C5	-3.71	107.21	112.19
3	D	1	NAG	C1-O5-C5	-3.33	107.72	112.19
3	C	2	NAG	C1-O5-C5	-3.25	107.83	112.19
3	C	1	NAG	C1-O5-C5	-2.90	108.30	112.19

There are no chirality outliers.

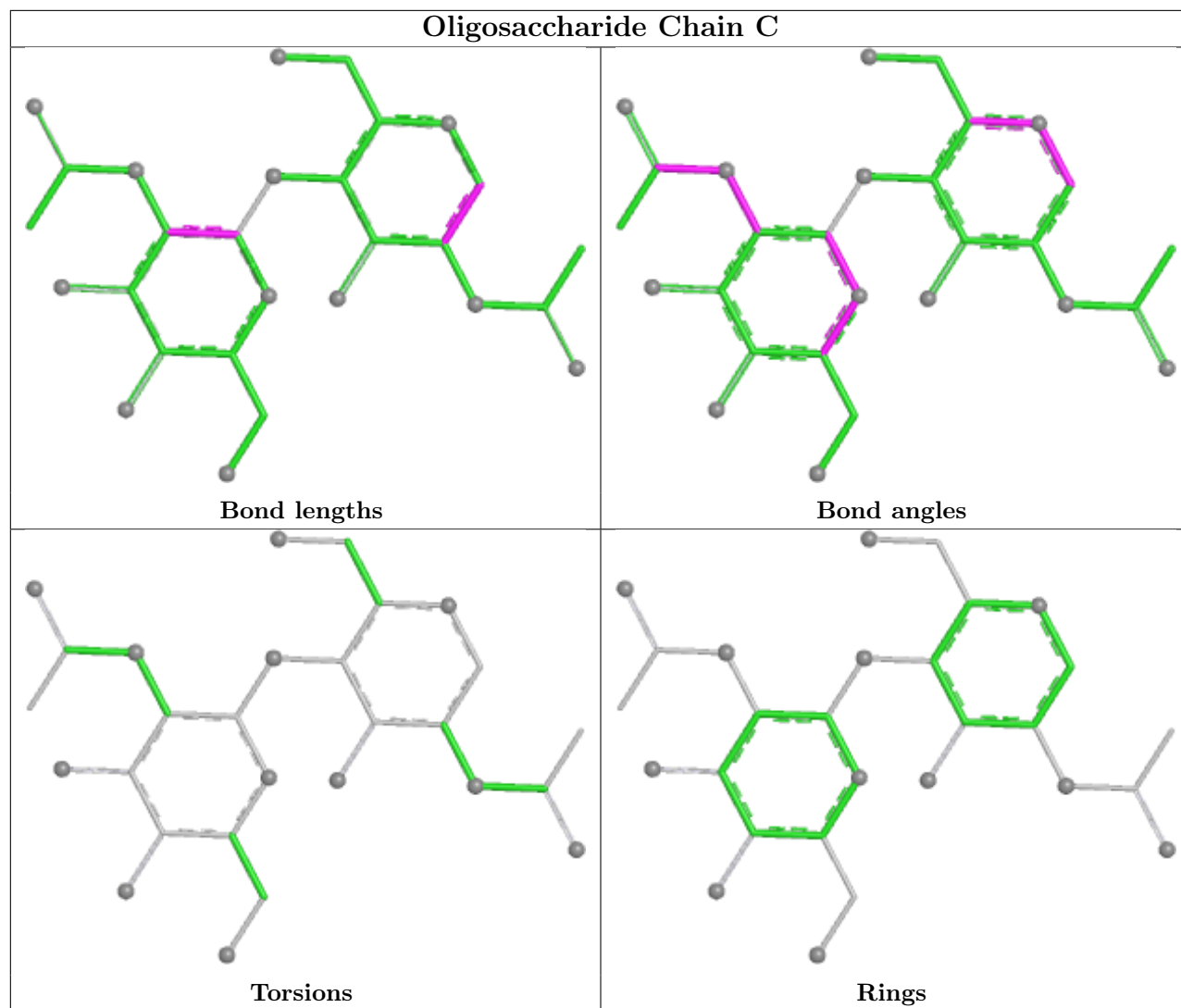
All (1) torsion outliers are listed below:

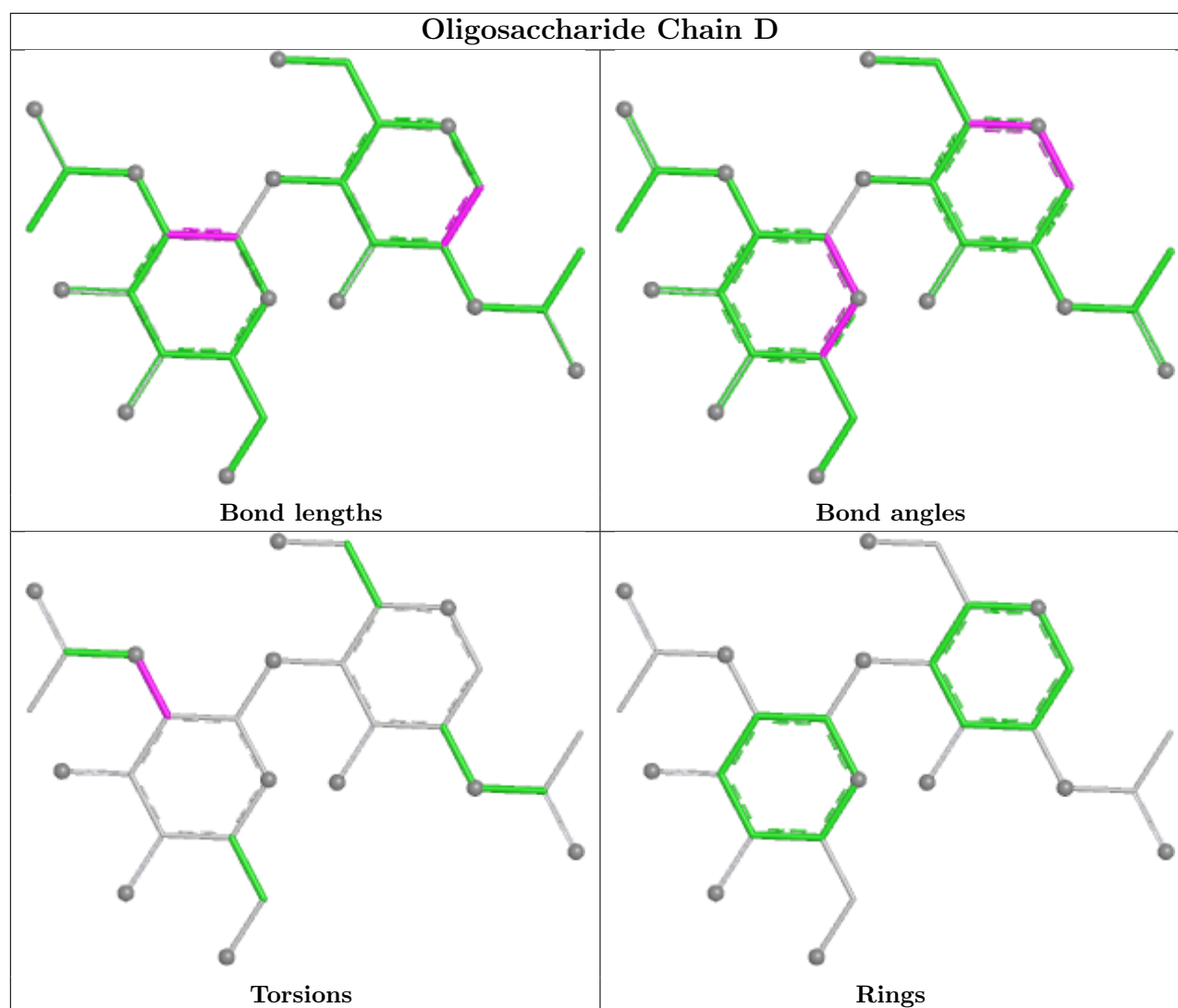
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C3-C2-N2-C7

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.





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
6	NAG	B	512	2	14,14,15	0.91	1 (7%)	17,19,21	1.08	2 (11%)

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
6	NAG	B	512	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	512	NAG	C1-C2	3.00	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	512	NAG	C1-O5-C5	-2.86	108.35	112.19
6	B	512	NAG	C3-C4-C5	-2.76	105.23	110.23

There are no chirality outliers.

There are no torsion outliers.

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

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.