



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:25 AM UTC

PDB ID : 1P2B / pdb_00001p2b
Title : Crystal Structure of Glycogen Phosphorylase B in Complex with Maltoheptaose
Authors : Pinotsis, N.; Leonidas, D.D.; Chrysina, E.D.; Oikonomakos, N.G.; Mavridis, I.M.
Deposited on : 2003-04-15
Resolution : 2.20 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

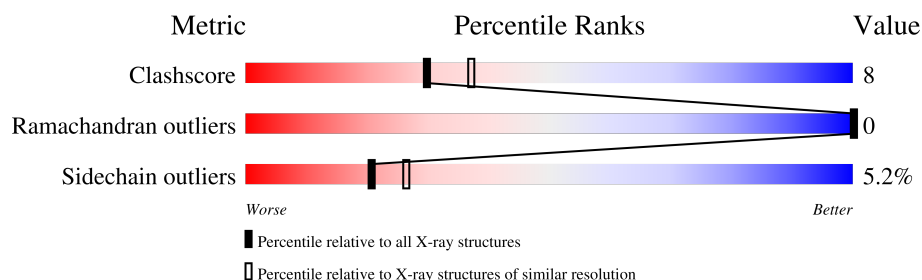
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	842	
2	B	5	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6945 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.

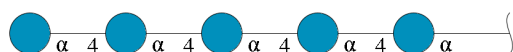
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	0	0
			6570	4188	1157	1196	29			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

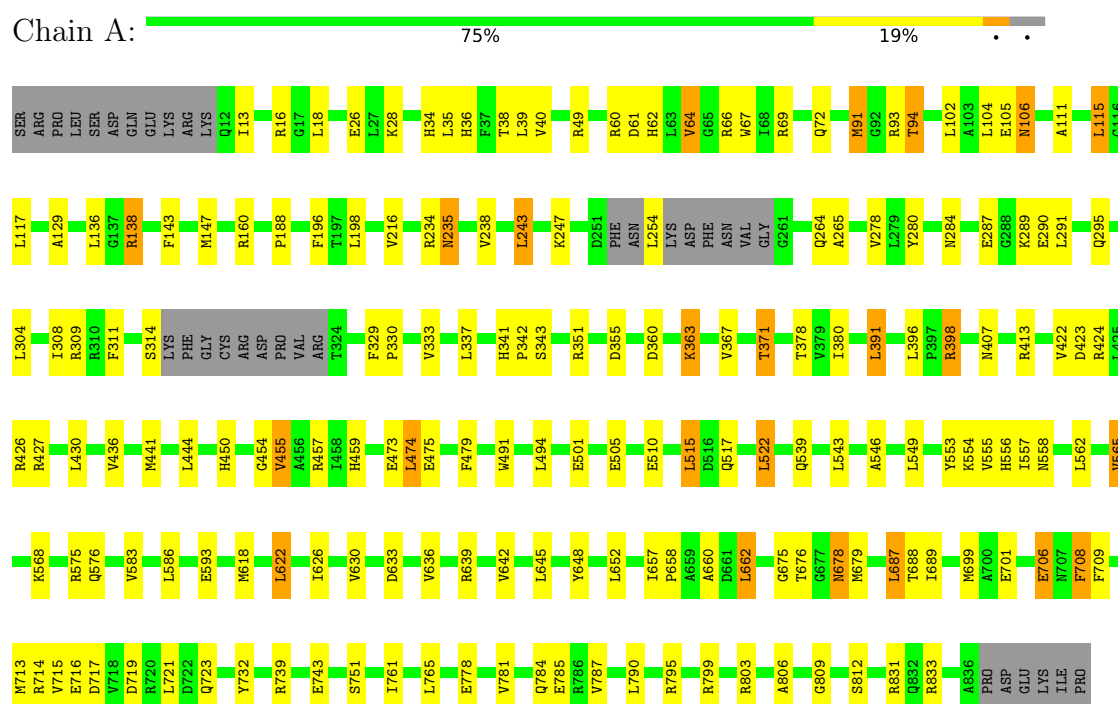
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total	O	0	0
			304	304		

3 Residue-property plots

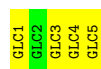
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.60 Å 128.60 Å 116.31 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 2.20	Depositor
% Data completeness (in resolution range)	95.7 (29.33-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6945	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: GLC, PLP

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	0.40	0/6715	0.93	32/9086 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	MET	N-CA-C	8.11	120.20	111.36
1	A	575	ARG	N-CA-C	6.68	120.87	111.52
1	A	556	HIS	CA-CB-CG	6.24	120.04	113.80
1	A	630	VAL	N-CA-C	6.17	116.33	110.53
1	A	714	ARG	N-CA-C	-6.15	101.67	110.59
1	A	64	VAL	N-CA-C	6.11	116.86	110.62
1	A	675	GLY	N-CA-C	-5.98	105.25	112.48
1	A	396	LEU	CA-C-N	5.97	125.45	119.24
1	A	396	LEU	C-N-CA	5.97	125.45	119.24
1	A	454	GLY	N-CA-C	-5.79	103.75	112.60
1	A	515	LEU	N-CA-C	5.73	119.08	111.75
1	A	278	VAL	N-CA-C	5.72	116.60	108.42
1	A	455	VAL	N-CA-C	5.71	117.59	112.17
1	A	565	VAL	N-CA-C	5.62	116.83	108.46
1	A	491	TRP	N-CA-C	5.59	119.73	113.02
1	A	430	LEU	N-CA-C	-5.46	106.12	112.89
1	A	751	SER	CA-C-N	5.40	124.86	119.24
1	A	751	SER	C-N-CA	5.40	124.86	119.24
1	A	576	GLN	N-CA-C	-5.40	105.50	111.71
1	A	676	THR	N-CA-C	-5.40	108.47	114.62
1	A	688	THR	N-CA-C	5.35	117.68	109.07
1	A	105	GLU	N-CA-C	5.32	117.50	111.11
1	A	333	VAL	N-CA-C	5.32	115.93	108.17
1	A	479	PHE	N-CA-C	5.25	118.11	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	GLU	CA-C-N	5.25	125.30	119.32
1	A	593	GLU	C-N-CA	5.25	125.30	119.32
1	A	558	ASN	CA-C-N	5.18	126.31	119.84
1	A	558	ASN	C-N-CA	5.18	126.31	119.84
1	A	422	VAL	N-CA-C	5.15	115.87	110.62
1	A	216	VAL	N-CA-C	5.10	116.24	108.80
1	A	633	ASP	CA-C-N	5.08	125.11	119.32
1	A	633	ASP	C-N-CA	5.08	125.11	119.32

There are no chirality outliers.

There are no planarity outliers.

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	6570	0	6517	111	0
2	B	56	0	48	2	0
3	A	15	0	7	0	0
4	A	304	0	0	9	0
All	All	6945	0	6572	112	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 8.

All (112) 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:549:LEU:HG	1:A:555:VAL:HG21	1.48	0.95
1:A:455:VAL:H	1:A:459:HIS:HD2	1.23	0.87
1:A:474:LEU:HD13	1:A:475:GLU:HG3	1.58	0.85
1:A:716:GLU:HB2	4:A:1257:HOH:O	1.88	0.73
1:A:678:ASN:HD22	1:A:679:MET:H	1.36	0.73
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.73	0.71
2:B:4:GLC:H61	2:B:5:GLC:H5	1.72	0.70
1:A:546:ALA:HA	1:A:557:ILE:HD11	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:O	1:A:64:VAL:HG22	1.91	0.70
1:A:831:ARG:HA	1:A:831:ARG:HE	1.58	0.68
1:A:378:THR:OG1	1:A:380:ILE:HG12	1.94	0.67
1:A:355:ASP:OD1	1:A:398:ARG:HD3	1.93	0.67
1:A:49:ARG:HG2	1:A:49:ARG:HH21	1.59	0.67
1:A:138:ARG:O	1:A:138:ARG:HD3	1.95	0.66
1:A:367:VAL:O	1:A:371:THR:HG23	1.96	0.66
1:A:719:ASP:O	1:A:723:GLN:HG2	1.97	0.65
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.63	0.64
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.80	0.64
1:A:549:LEU:CG	1:A:555:VAL:HG21	2.25	0.64
1:A:13:ILE:HG12	1:A:16:ARG:HG3	1.79	0.63
1:A:235:ASN:H	1:A:235:ASN:HD22	1.46	0.62
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.82	0.61
1:A:678:ASN:ND2	1:A:679:MET:H	1.98	0.61
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.85	0.59
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.84	0.58
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.85	0.58
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.12	0.57
1:A:678:ASN:HD22	1:A:678:ASN:N	2.01	0.57
1:A:450:HIS:HD2	4:A:1091:HOH:O	1.87	0.57
1:A:35:LEU:HA	1:A:39:LEU:HD23	1.88	0.56
1:A:196:PHE:O	1:A:198:LEU:HD13	2.06	0.55
1:A:284:ASN:HB3	1:A:380:ILE:HD11	1.89	0.55
1:A:28:LYS:HD2	1:A:115:LEU:HD13	1.88	0.55
1:A:636:VAL:O	1:A:639:ARG:HD3	2.07	0.54
1:A:94:THR:HG21	4:A:1040:HOH:O	2.09	0.53
1:A:304:LEU:O	1:A:308:ILE:HG12	2.07	0.53
1:A:407:ASN:HB3	2:B:3:GLC:O6	2.08	0.53
1:A:94:THR:CG2	4:A:1139:HOH:O	2.58	0.52
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.40	0.52
1:A:706:GLU:H	1:A:706:GLU:CD	2.18	0.52
1:A:549:LEU:HG	1:A:555:VAL:CG2	2.33	0.51
1:A:13:ILE:HG12	1:A:16:ARG:CG	2.40	0.51
1:A:351:ARG:O	1:A:355:ASP:HB2	2.11	0.51
1:A:549:LEU:O	1:A:555:VAL:HG22	2.11	0.51
1:A:254:LEU:N	1:A:254:LEU:HD23	2.25	0.51
1:A:111:ALA:O	1:A:115:LEU:HD22	2.10	0.50
1:A:618:MET:HB3	1:A:761:ILE:HD11	1.92	0.50
1:A:549:LEU:CD2	1:A:557:ILE:HD13	2.41	0.50
1:A:739:ARG:O	1:A:743:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LYS:O	1:A:363:LYS:HD3	2.12	0.49
1:A:565:VAL:HG11	1:A:660:ALA:HB2	1.94	0.49
1:A:72:GLN:NE2	1:A:72:GLN:HA	2.27	0.49
1:A:501:GLU:O	1:A:505:GLU:HG3	2.12	0.49
1:A:678:ASN:HD22	1:A:679:MET:N	2.06	0.49
1:A:455:VAL:H	1:A:459:HIS:CD2	2.15	0.48
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.96	0.48
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.94	0.48
1:A:94:THR:HG23	4:A:1139:HOH:O	2.14	0.48
1:A:93:ARG:NH1	4:A:1010:HOH:O	2.45	0.48
1:A:436:VAL:O	1:A:436:VAL:HG13	2.14	0.48
1:A:16:ARG:HB2	1:A:106:ASN:CG	2.39	0.47
1:A:330:PRO:HG3	1:A:371:THR:HG22	1.96	0.47
1:A:235:ASN:H	1:A:235:ASN:ND2	2.12	0.47
1:A:510:GLU:HB3	1:A:517:GLN:HE22	1.78	0.47
1:A:761:ILE:O	1:A:765:LEU:HD23	2.15	0.46
1:A:367:VAL:O	1:A:371:THR:CG2	2.61	0.46
1:A:781:VAL:O	1:A:785:GLU:HG3	2.15	0.46
1:A:67:TRP:HA	1:A:238:VAL:HB	1.98	0.45
1:A:34:HIS:HE1	1:A:61:ASP:OD1	1.99	0.45
1:A:49:ARG:HH21	1:A:49:ARG:CG	2.29	0.45
1:A:136:LEU:C	1:A:136:LEU:HD23	2.42	0.45
1:A:622:LEU:O	1:A:626:ILE:HG13	2.16	0.45
1:A:831:ARG:HA	1:A:831:ARG:NE	2.30	0.45
1:A:424:ARG:NH1	1:A:473:GLU:OE2	2.43	0.45
1:A:450:HIS:HE1	4:A:1095:HOH:O	1.99	0.45
1:A:522:LEU:HD13	1:A:806:ALA:HB3	1.99	0.45
1:A:562:LEU:HD21	1:A:662:LEU:HB2	1.97	0.45
1:A:69:ARG:HG3	4:A:1036:HOH:O	2.16	0.45
1:A:678:ASN:ND2	1:A:678:ASN:N	2.62	0.45
1:A:494:LEU:C	1:A:494:LEU:HD23	2.42	0.44
1:A:553:TYR:O	1:A:554:LYS:C	2.60	0.44
1:A:360:ASP:OD1	1:A:363:LYS:HB2	2.18	0.44
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.82	0.44
1:A:143:PHE:O	1:A:147:MET:HG3	2.17	0.44
1:A:423:ASP:O	1:A:427:ARG:HG3	2.17	0.43
1:A:291:LEU:O	1:A:295:GLN:HG3	2.18	0.43
1:A:363:LYS:HD3	1:A:363:LYS:C	2.44	0.43
1:A:60:ARG:HD2	1:A:188:PRO:O	2.18	0.43
1:A:343:SER:OG	1:A:441:MET:HE3	2.18	0.43
1:A:784:GLN:O	1:A:787:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:HG2	1:A:309:ARG:HH21	1.83	0.43
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.19	0.43
1:A:539:GLN:HE21	1:A:543:LEU:HG	1.84	0.43
1:A:62:HIS:O	1:A:66:ARG:NH1	2.52	0.42
1:A:329:PHE:HD1	1:A:371:THR:HG21	1.84	0.42
1:A:423:ASP:O	1:A:426:ARG:HG2	2.19	0.42
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.99	0.42
1:A:290:GLU:HG3	1:A:391:LEU:HD21	2.01	0.42
1:A:678:ASN:ND2	1:A:679:MET:N	2.63	0.42
1:A:311:PHE:O	1:A:314:SER:HB3	2.19	0.42
1:A:795:ARG:O	1:A:799:ARG:HG3	2.19	0.42
1:A:515:LEU:HD12	1:A:812:SER:HB2	2.02	0.42
1:A:254:LEU:HB3	1:A:265:ALA:HB1	2.02	0.41
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.55	0.41
1:A:583:VAL:HG11	1:A:642:VAL:HG21	2.02	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.20	0.41
1:A:689:ILE:HA	1:A:709:PHE:HB2	2.03	0.41
1:A:18:LEU:HD12	1:A:18:LEU:N	2.35	0.41
1:A:522:LEU:HD12	1:A:522:LEU:HA	1.92	0.41
1:A:329:PHE:CD1	1:A:371:THR:HG21	2.57	0.40
1:A:715:VAL:HG23	4:A:1256:HOH:O	2.22	0.40
1:A:91:MET:HB2	1:A:129:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	801/842 (95%)	768 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	699/731 (96%)	663 (95%)	36 (5%)	21	26

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	94	THR
1	A	102	LEU
1	A	104	LEU
1	A	106	ASN
1	A	115	LEU
1	A	117	LEU
1	A	138	ARG
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	247	LYS
1	A	264	GLN
1	A	337	LEU
1	A	363	LYS
1	A	371	THR
1	A	391	LEU
1	A	398	ARG
1	A	413	ARG
1	A	444	LEU
1	A	474	LEU
1	A	522	LEU
1	A	568	LYS
1	A	586	LEU
1	A	622	LEU
1	A	645	LEU
1	A	662	LEU
1	A	678	ASN
1	A	687	LEU
1	A	706	GLU

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Mol	Chain	Res	Type
1	A	708	PHE
1	A	721	LEU
1	A	778	GLU
1	A	790	LEU
1	A	803	ARG
1	A	833	ARG

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	23	ASN
1	A	34	HIS
1	A	71	GLN
1	A	72	GLN
1	A	106	ASN
1	A	114	GLN
1	A	235	ASN
1	A	239	ASN
1	A	412	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	539	GLN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	A	727	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 ⓘ

5 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	GLC	B	1	2	12,12,12	0.67	0	17,17,17	0.82	1 (5%)
2	GLC	B	2	2	11,11,12	0.52	0	15,15,17	0.43	0
2	GLC	B	3	2	11,11,12	0.37	0	15,15,17	0.74	0
2	GLC	B	4	2	11,11,12	0.54	0	15,15,17	0.60	0
2	GLC	B	5	2	11,11,12	0.66	0	15,15,17	0.66	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
2	GLC	B	1	2	-	2/2/22/22	0/1/1/1
2	GLC	B	2	2	-	2/2/19/22	0/1/1/1
2	GLC	B	3	2	-	2/2/19/22	0/1/1/1
2	GLC	B	4	2	-	2/2/19/22	0/1/1/1
2	GLC	B	5	2	-	2/2/19/22	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	B	1	GLC	C1-C2-C3	-2.07	106.12	110.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	GLC	O5-C5-C6-O6
2	B	5	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6

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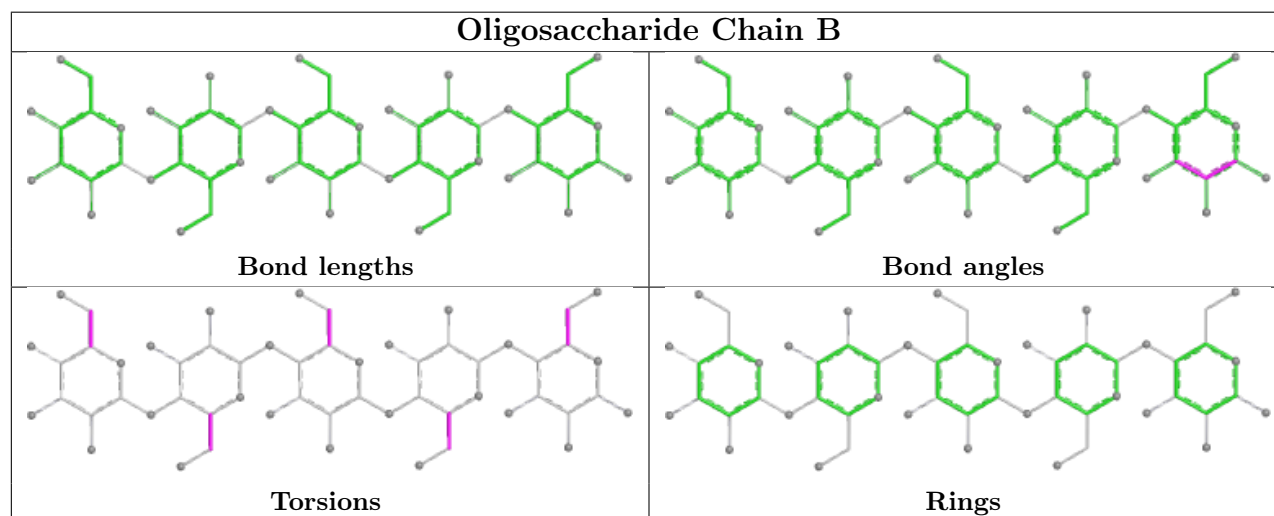
Mol	Chain	Res	Type	Atoms
2	B	4	GLC	O5-C5-C6-O6
2	B	2	GLC	O5-C5-C6-O6
2	B	4	GLC	C4-C5-C6-O6
2	B	3	GLC	C4-C5-C6-O6
2	B	3	GLC	O5-C5-C6-O6
2	B	2	GLC	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	GLC	1	0
2	B	4	GLC	1	0
2	B	5	GLC	1	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](#)

1 ligand 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
3	PLP	A	999	1	15,15,16	1.52	2 (13%)	21,22,23	1.10	1 (4%)

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	PLP	A	999	1	-	2/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C4A-C4	3.17	1.57	1.51
3	A	999	PLP	C5A-C5	3.17	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PLP	O3P-P-O1P	2.34	119.97	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C4-C5-C5A-O4P
3	A	999	PLP	C6-C5-C5A-O4P

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.