



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2ATI
Title : Glycogen Phosphorylase Inhibitors
Authors : Klabunde, T.; Wendt, K.U.; Kadereit, D.; Brachvogel, V.; Burger, H.J.; Herling, A.W.; Oikonomakos, N.G.; Schmoll, D.; Sarubbi, E.; von Roedern, E.; Schoenafinger, K.; Defossa, E.
Deposited on : 2005-08-25
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

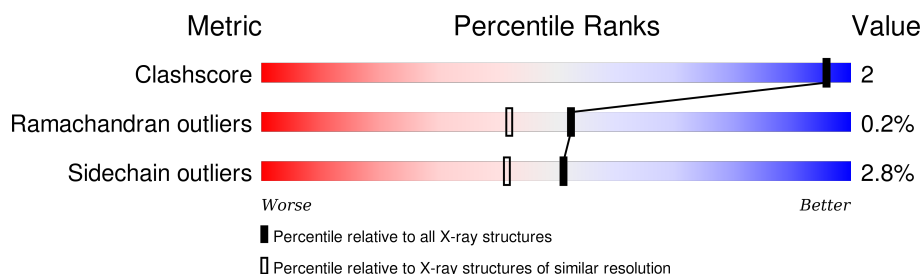
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	846	 87% 6% 7%
1	B	846	 88% 5% 7%

2 Entry composition [i](#)

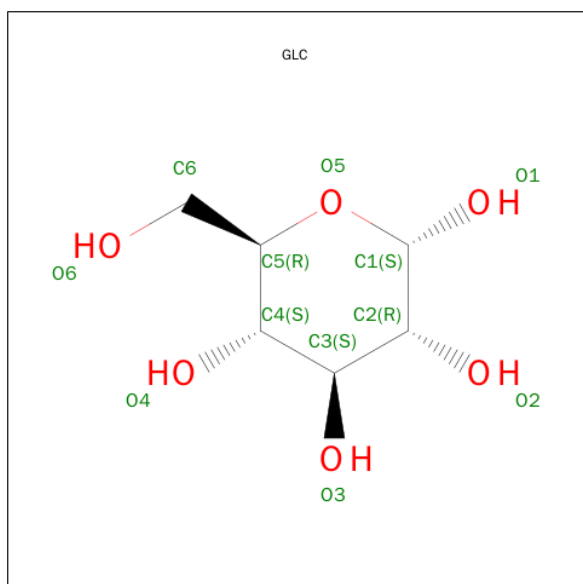
There are 5 unique types of molecules in this entry. The entry contains 13701 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, liver form.

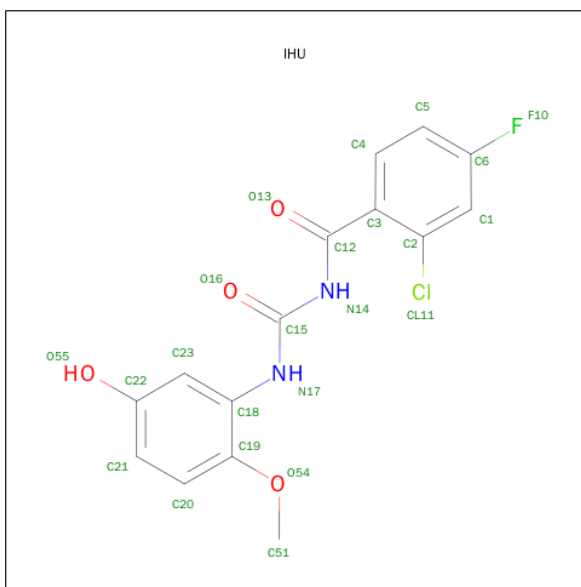
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6421	4127	1089	1176	29			
1	B	791	Total	C	N	O	S	0	0	0
			6421	4127	1089	1176	29			

- Molecule 2 is SUGAR (GLUCOSE) (three-letter code: GLC) (formula: C₆H₁₂O₆).



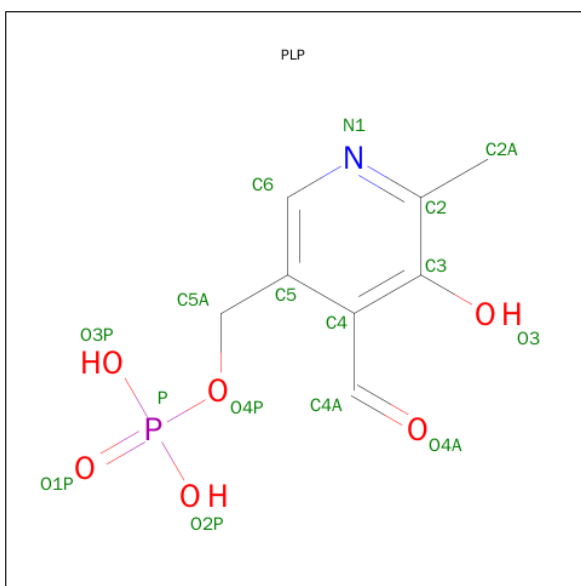
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is N-(2-CHLORO-4-FLUOROBENZOYL)-N'-(5-HYDROXY-2-METHOXYPHENYL)UREA (three-letter code: IHU) (formula: C₁₅H₁₂ClFN₂O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			23	15	1	1	2	4		
3	B	1	Total	C	Cl	F	N	O	0	0
			23	15	1	1	2	4		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 5 is water.

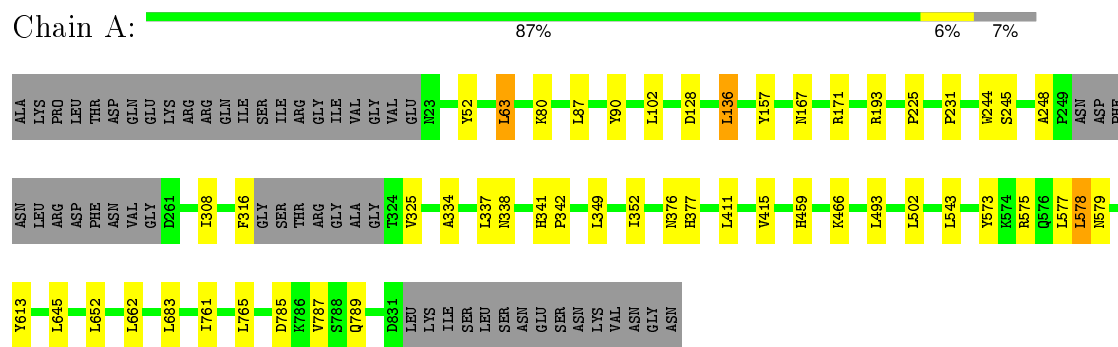
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	392	Total 392	O 392	0	0
5	B	367	Total 367	O 367	0	0

3 Residue-property plots

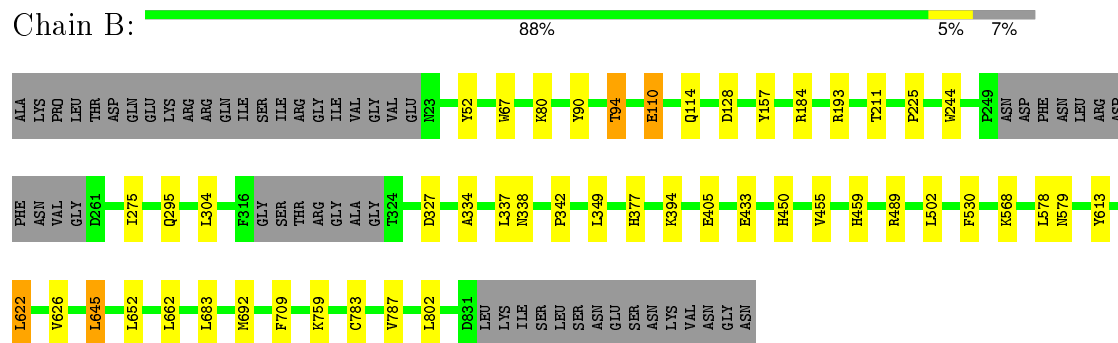
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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, liver form



- Molecule 1: Glycogen phosphorylase, liver form



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.50 Å 124.50 Å 123.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	99.6 ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.232 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13701	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: IHU, 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	0.67	0/6565	0.72	2/8879 (0.0%)
1	B	0.67	0/6565	0.72	0/8879
All	All	0.67	0/13130	0.72	2/17758 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	136	LEU	CA-CB-CG	6.35	129.90	115.30
1	A	63	LEU	CA-CB-CG	5.29	127.46	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	TYR	Sidechain
1	B	52	TYR	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	6421	0	6416	18	0
1	B	6421	0	6416	18	0
2	A	12	0	12	0	0
2	B	12	0	12	1	0
3	A	23	0	11	3	0
3	B	23	0	11	1	0
4	A	15	0	7	0	0
4	B	15	0	6	0	0
5	A	392	0	0	1	0
5	B	367	0	0	4	0
All	All	13701	0	12891	39	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 2.

All (39) 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:B:455:VAL:H	1:B:459:HIS:HD2	1.48	0.61
3:B:848:IHU:H23	3:B:848:IHU:O16	2.06	0.55
3:A:848:IHU:O16	3:A:848:IHU:H23	2.05	0.55
1:B:193:ARG:HB2	1:B:225:PRO:HG2	1.91	0.52
1:B:530:PHE:HE2	1:B:802:LEU:HD13	1.76	0.51
1:B:450:HIS:HE1	5:B:2162:HOH:O	1.94	0.50
1:A:761:ILE:O	1:A:765:LEU:HD23	2.14	0.48
1:A:87:LEU:HD23	5:A:2568:HOH:O	2.13	0.48
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.95	0.48
1:B:304:LEU:HD22	1:B:349:LEU:HD13	1.96	0.47
1:A:575:ARG:HB3	1:A:578:LEU:HB2	1.96	0.47
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.97	0.47
1:A:136:LEU:HD21	1:A:341:HIS:HE1	1.79	0.47
2:B:847:GLC:H3	5:B:2468:HOH:O	2.15	0.46
1:A:63:LEU:HG	1:A:102:LEU:HD11	1.97	0.46
1:B:94:THR:HG22	5:B:2070:HOH:O	2.15	0.46
1:B:338:ASN:ND2	1:B:377:HIS:NE2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:ND2	1:A:377:HIS:NE2	2.64	0.45
1:A:376:ASN:HD22	1:A:459:HIS:CE1	2.35	0.45
1:A:248:ALA:O	1:B:184:ARG:NH2	2.50	0.43
1:B:80:LYS:HE2	1:B:334:ALA:HB2	2.00	0.43
1:B:110:GLU:OE1	1:B:114:GLN:NE2	2.51	0.43
1:A:136:LEU:HD21	1:A:341:HIS:CE1	2.54	0.43
1:A:785:ASP:O	1:A:789:GLN:HG2	2.19	0.43
1:A:662:LEU:HD22	1:A:787:VAL:HG11	2.01	0.42
1:B:157:TYR:HD2	1:B:244:TRP:HE1	1.66	0.42
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.68	0.41
1:B:622:LEU:O	1:B:626:VAL:HG23	2.20	0.41
1:B:211:THR:HG21	5:B:2842:HOH:O	2.20	0.41
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.02	0.41
1:B:645:LEU:HD22	1:B:652:LEU:HD21	2.02	0.41
1:A:411:LEU:O	1:A:415:VAL:HG23	2.21	0.41
1:B:662:LEU:HD22	1:B:787:VAL:HG11	2.02	0.41
1:A:167:ASN:HD22	1:A:167:ASN:HA	1.77	0.41
1:A:63:LEU:HD21	1:A:231:PRO:HB3	2.02	0.41
1:B:275:ILE:O	1:B:295:GLN:HG2	2.21	0.41
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.61	0.40
3:A:848:IHU:H1	1:B:67:TRP:CZ2	2.57	0.40
3:A:848:IHU:C23	3:A:848:IHU:O16	2.70	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	785/846 (93%)	753 (96%)	30 (4%)	2 (0%)	46	35
1	B	785/846 (93%)	759 (97%)	25 (3%)	1 (0%)	56	46
All	All	1570/1692 (93%)	1512 (96%)	55 (4%)	3 (0%)	52	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	VAL
1	A	342	PRO
1	B	342	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	693/739 (94%)	674 (97%)	19 (3%)	52	43
1	B	693/739 (94%)	673 (97%)	20 (3%)	50	40
All	All	1386/1478 (94%)	1347 (97%)	39 (3%)	51	41

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TYR
1	A	128	ASP
1	A	171	ARG
1	A	245	SER
1	A	316	PHE
1	A	337	LEU
1	A	349	LEU
1	A	466	LYS
1	A	493	LEU
1	A	502	LEU
1	A	543	LEU
1	A	573	TYR
1	A	577	LEU
1	A	578	LEU
1	A	579	ASN
1	A	613	TYR
1	A	645	LEU
1	A	652	LEU
1	A	683	LEU
1	B	90	TYR

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Mol	Chain	Res	Type
1	B	94	THR
1	B	110	GLU
1	B	128	ASP
1	B	327	ASP
1	B	337	LEU
1	B	394	LYS
1	B	405	GLU
1	B	433	GLU
1	B	489	ARG
1	B	502	LEU
1	B	568	LYS
1	B	578	LEU
1	B	579	ASN
1	B	613	TYR
1	B	622	LEU
1	B	645	LEU
1	B	683	LEU
1	B	692	MET
1	B	759	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	71	GLN
1	A	72	GLN
1	A	167	ASN
1	A	208	HIS
1	A	270	ASN
1	A	338	ASN
1	A	376	ASN
1	A	450	HIS
1	A	453	ASN
1	A	481	ASN
1	A	566	GLN
1	A	571	HIS
1	A	579	ASN
1	B	32	ASN
1	B	72	GLN
1	B	167	ASN
1	B	270	ASN
1	B	338	ASN

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Mol	Chain	Res	Type
1	B	376	ASN
1	B	450	HIS
1	B	453	ASN
1	B	459	HIS
1	B	481	ASN
1	B	566	GLN
1	B	579	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	PLP	A	1001	1	15,15,16	2.05	6 (40%)	21,22,23	1.46	4 (19%)
2	GLC	A	847	-	12,12,12	0.36	0	17,17,17	0.39	0
3	IHU	A	848	-	24,24,24	1.32	4 (16%)	33,33,33	1.67	6 (18%)
4	PLP	B	1001	1	15,15,16	1.99	5 (33%)	21,22,23	1.43	5 (23%)
2	GLC	B	847	-	12,12,12	0.40	0	17,17,17	0.36	0
3	IHU	B	848	-	24,24,24	1.33	4 (16%)	33,33,33	1.58	6 (18%)

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	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
2	GLC	A	847	-	-	0/2/22/22	0/1/1/1
3	IHU	A	848	-	-	0/14/14/14	0/2/2/2
4	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
2	GLC	B	847	-	-	0/2/22/22	0/1/1/1
3	IHU	B	848	-	-	0/14/14/14	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	848	IHU	C18-N17	-4.23	1.33	1.41
3	A	848	IHU	C18-N17	-4.21	1.33	1.41
4	B	1001	PLP	C4A-C4	-3.42	1.44	1.51
4	A	1001	PLP	C4A-C4	-3.30	1.44	1.51
3	B	848	IHU	C15-N14	-2.72	1.33	1.39
3	A	848	IHU	C15-N14	-2.70	1.33	1.39
4	B	1001	PLP	C3-C2	-2.64	1.38	1.40
4	B	1001	PLP	P-O3P	-2.61	1.45	1.54
3	B	848	IHU	C12-N14	-2.37	1.33	1.37
3	A	848	IHU	C12-N14	-2.31	1.33	1.37
4	A	1001	PLP	P-O3P	-2.21	1.46	1.54
4	A	1001	PLP	C3-C2	-2.19	1.39	1.40
3	A	848	IHU	C15-N17	-2.12	1.33	1.37
3	B	848	IHU	C15-N17	-2.10	1.33	1.37
4	A	1001	PLP	C2-N1	2.17	1.38	1.34
4	A	1001	PLP	C3-C4	2.18	1.45	1.40
4	B	1001	PLP	C3-C4	2.21	1.45	1.40
4	B	1001	PLP	C5-C4	4.17	1.45	1.40
4	A	1001	PLP	C5-C4	5.26	1.46	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	848	IHU	C12-N14-C15	-5.98	121.90	128.09
3	B	848	IHU	C12-N14-C15	-5.03	122.89	128.09
3	A	848	IHU	C51-O54-C19	-2.48	113.78	117.54
3	B	848	IHU	C5-C6-C1	-2.46	120.17	123.35
4	A	1001	PLP	C5A-C5-C6	-2.43	114.69	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	848	IHU	C1-C2-C3	-2.42	119.97	121.59
3	A	848	IHU	C5-C6-C1	-2.42	120.23	123.35
3	A	848	IHU	C1-C2-C3	-2.33	120.03	121.59
4	B	1001	PLP	C5A-C5-C6	-2.24	115.03	119.28
3	B	848	IHU	C51-O54-C19	-2.23	114.17	117.54
4	B	1001	PLP	C5-C6-N1	-2.02	120.34	123.86
4	A	1001	PLP	C6-C5-C4	2.00	119.84	118.15
4	B	1001	PLP	C6-C5-C4	2.05	119.89	118.15
4	A	1001	PLP	O3P-P-O2P	2.06	115.24	107.38
4	B	1001	PLP	O3P-P-O2P	2.09	115.35	107.38
4	B	1001	PLP	C5A-C5-C4	2.59	125.08	121.65
3	B	848	IHU	O54-C19-C18	2.72	118.35	114.87
3	A	848	IHU	O54-C19-C18	2.83	118.48	114.87
4	A	1001	PLP	C5A-C5-C4	2.88	125.47	121.65
3	A	848	IHU	C2-C1-C6	3.80	120.08	117.81
3	B	848	IHU	C2-C1-C6	3.83	120.09	117.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	848	IHU	3	0
2	B	847	GLC	1	0
3	B	848	IHU	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.