



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 06:42 AM BST

PDB ID : 6GPB
Title : REFINED CRYSTAL STRUCTURE OF THE PHOSPHORYLASE-HEPTULOSE 2-PHOSPHATE-OLIGOSACCHARIDE-AMP COMPLEX
Authors : Acharya, K.R.; Johnson, L.N.
Deposited on : 1990-06-04
Resolution : 2.86 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

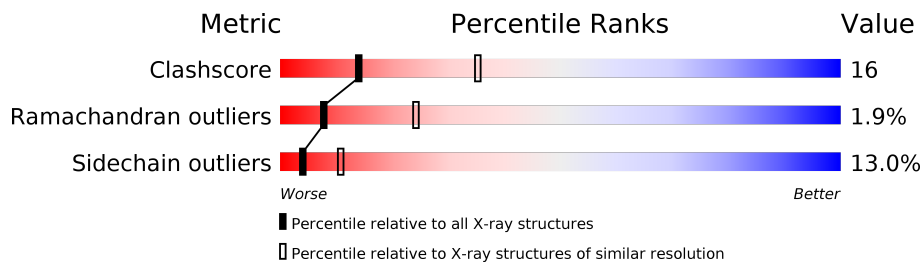
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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 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	

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
3	H2P	A	998	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7469 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 B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	828	6727	4286	1186	1225	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

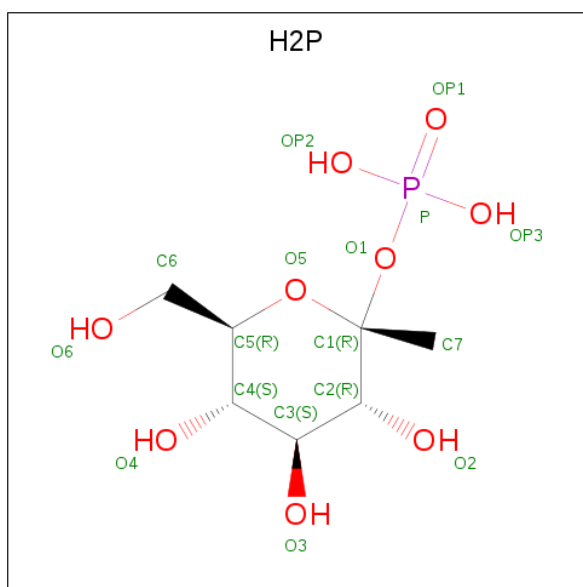
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489

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



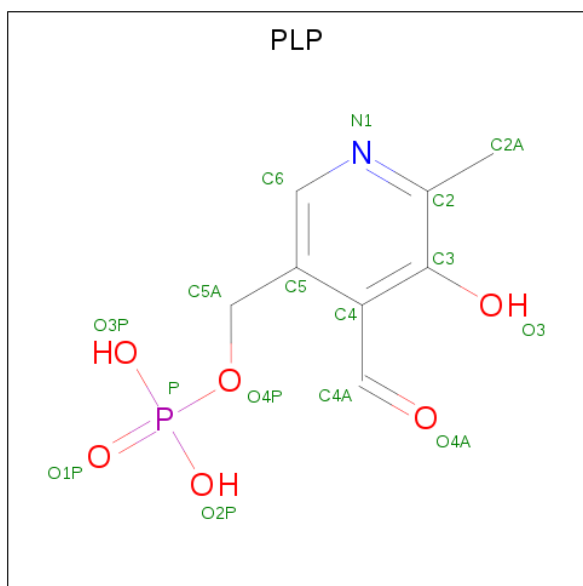
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	5	56	30	26	0	0	0

- Molecule 3 is 1-deoxy-2-O-phosphono-alpha-D-gluco-hept-2-ulopyranose (three-letter code: H2P) (formula: C₇H₁₅O₉P).



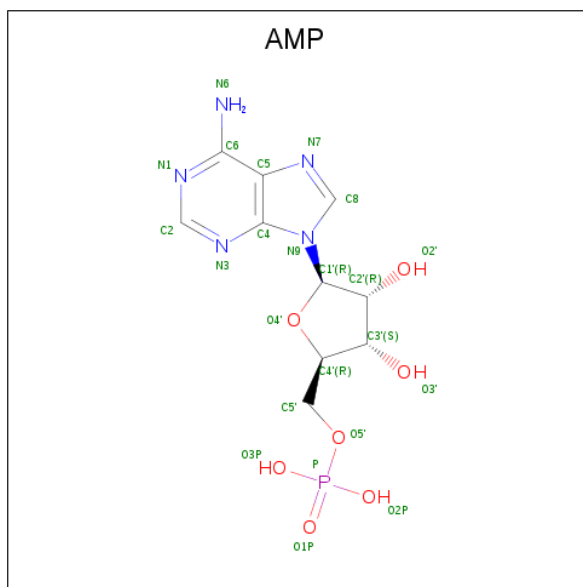
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			17	7	9	1		

- 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		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 6 is water.

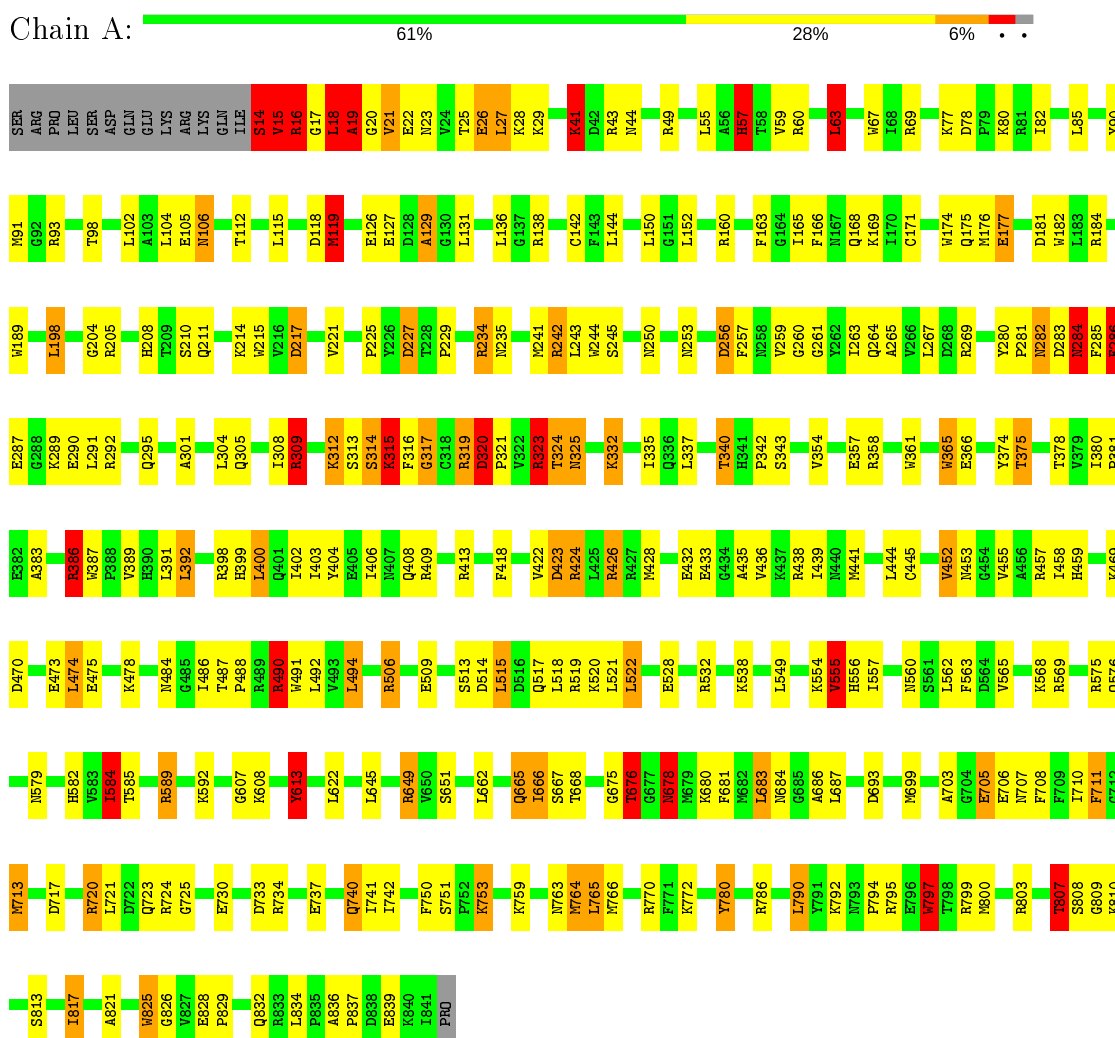
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	608	Total	O	0	0
			608	608		

3 Residue-property plots [i](#)

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 B



- 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

Xtrriage (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	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.86	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.86)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7469	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: AMP, GLC, H2P, 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	1.41	29/6880 (0.4%)	1.73	148/9313 (1.6%)

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	1	9

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	ARG	C-O	49.23	2.16	1.23
1	A	18	LEU	CG-CD1	38.26	2.93	1.51
1	A	312	LYS	CE-NZ	34.45	2.35	1.49
1	A	18	LEU	CA-C	18.30	2.00	1.52
1	A	282	ASN	C-N	-17.31	0.94	1.34

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	C-N-CA	16.65	163.32	121.70
1	A	16	ARG	CA-CB-CG	16.62	149.96	113.40
1	A	15	VAL	CA-C-N	-15.55	82.98	117.20
1	A	19	ALA	N-CA-CB	15.31	131.53	110.10
1	A	14	SER	N-CA-CB	14.19	131.78	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	19	ALA	CA

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	SER	Mainchain
1	A	15	VAL	Mainchain
1	A	16	ARG	Sidechain
1	A	18	LEU	Peptide
1	A	57	HIS	Mainchain

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	6727	0	6652	203	1
2	B	56	0	48	11	0
3	A	17	0	13	9	0
4	A	15	0	7	2	0
5	A	46	0	22	1	0
6	A	608	0	0	27	1
All	All	7469	0	6742	212	1

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 16.

The worst 5 of 212 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:SER:CB	1:A:14:SER:CA	1.76	1.57
1:A:18:LEU:CD2	1:A:18:LEU:CG	1.84	1.51
1:A:332:LYS:CE	1:A:332:LYS:NZ	1.74	1.46
1:A:15:VAL:CA	1:A:15:VAL:C	1.86	1.41
1:A:18:LEU:C	1:A:18:LEU:CA	2.00	1.30

All (1) 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)
1:A:319:ARG:NH1	6:A:1229:HOH:O[5_545]	1.79	0.41

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	826/842 (98%)	766 (93%)	44 (5%)	16 (2%)	8 24

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	284	ASN
1	A	320	ASP
1	A	323	ARG
1	A	315	LYS

5.3.2 Protein sidechains [i](#)

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	715/731 (98%)	622 (87%)	93 (13%)	4 11

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	LEU
1	A	441	MET

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Mol	Chain	Res	Type
1	A	765	LEU
1	A	340	THR
1	A	398	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	481	ASN
1	A	678	ASN
1	A	484	ASN
1	A	264	GLN
1	A	576	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	1.09	1 (8%)	17,17,17	1.72	2 (11%)
2	GLC	B	2	2	11,11,12	0.58	0	15,15,17	0.91	0
2	GLC	B	3	2	11,11,12	1.97	1 (9%)	15,15,17	1.59	2 (13%)
2	GLC	B	4	2	11,11,12	0.79	0	15,15,17	1.01	1 (6%)
2	GLC	B	5	2	11,11,12	0.48	0	15,15,17	0.90	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	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1
2	GLC	B	4	2	-	0/2/19/22	0/1/1/1
2	GLC	B	5	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	GLC	O5-C1	-6.24	1.33	1.43
2	B	1	GLC	O1-C1	2.53	1.47	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O1-C1-O5	5.36	126.45	110.38
2	B	3	GLC	O5-C1-C2	4.35	117.48	110.77
2	B	1	GLC	O3-C3-C2	-3.20	102.95	110.35
2	B	3	GLC	C1-O5-C5	2.54	115.63	112.19
2	B	4	GLC	C2-C3-C4	-2.27	106.96	110.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

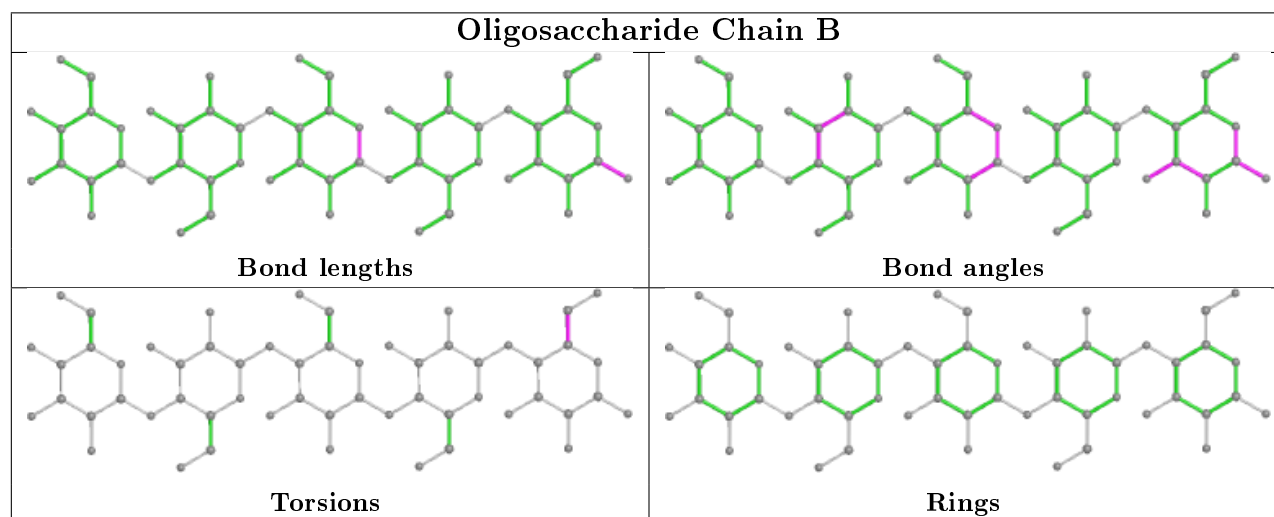
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

4 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	999	1	15,15,16	1.27	3 (20%)	20,22,23	1.01	1 (5%)
5	AMP	A	997	-	22,25,25	1.52	4 (18%)	25,38,38	1.95	9 (36%)
5	AMP	A	913	-	22,25,25	3.08	6 (27%)	25,38,38	2.45	11 (44%)
3	H2P	A	998	-	15,17,17	1.69	3 (20%)	19,27,27	1.03	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
4	PLP	A	999	1	-	0/6/6/8	0/1/1/1
5	AMP	A	997	-	-	2/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AMP	A	913	-	-	2/6/26/26	0/3/3/3
3	H2P	A	998	-	-	0/5/31/31	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	913	AMP	O4'-C1'	7.91	1.52	1.41
5	A	913	AMP	C2-N1	7.31	1.47	1.33
5	A	913	AMP	O4'-C4'	-5.11	1.33	1.45
5	A	913	AMP	C8-N7	4.97	1.43	1.34
5	A	913	AMP	C2-N3	4.13	1.38	1.32

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	913	AMP	O4'-C4'-C3'	5.64	116.27	105.11
5	A	913	AMP	C5-C6-N6	5.48	128.68	120.35
5	A	997	AMP	N3-C2-N1	-4.11	122.26	128.68
5	A	997	AMP	O3'-C3'-C4'	3.82	122.11	111.05
5	A	913	AMP	C5-C6-N1	-3.75	111.85	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	997	AMP	C5'-O5'-P-O1P
5	A	913	AMP	C5'-O5'-P-O2P
5	A	913	AMP	C5'-O5'-P-O3P
5	A	997	AMP	O4'-C4'-C5'-O5'

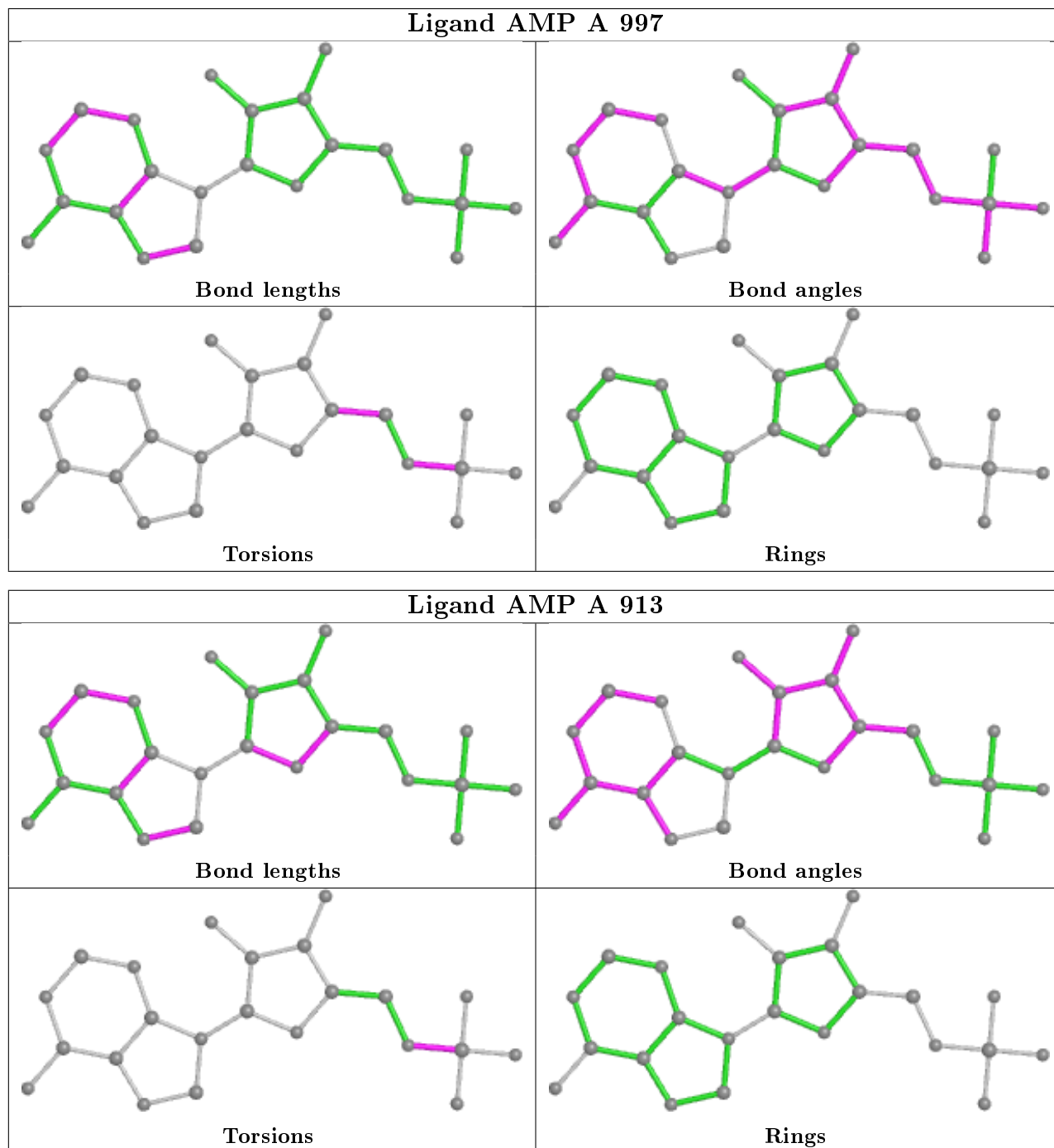
There are no ring outliers.

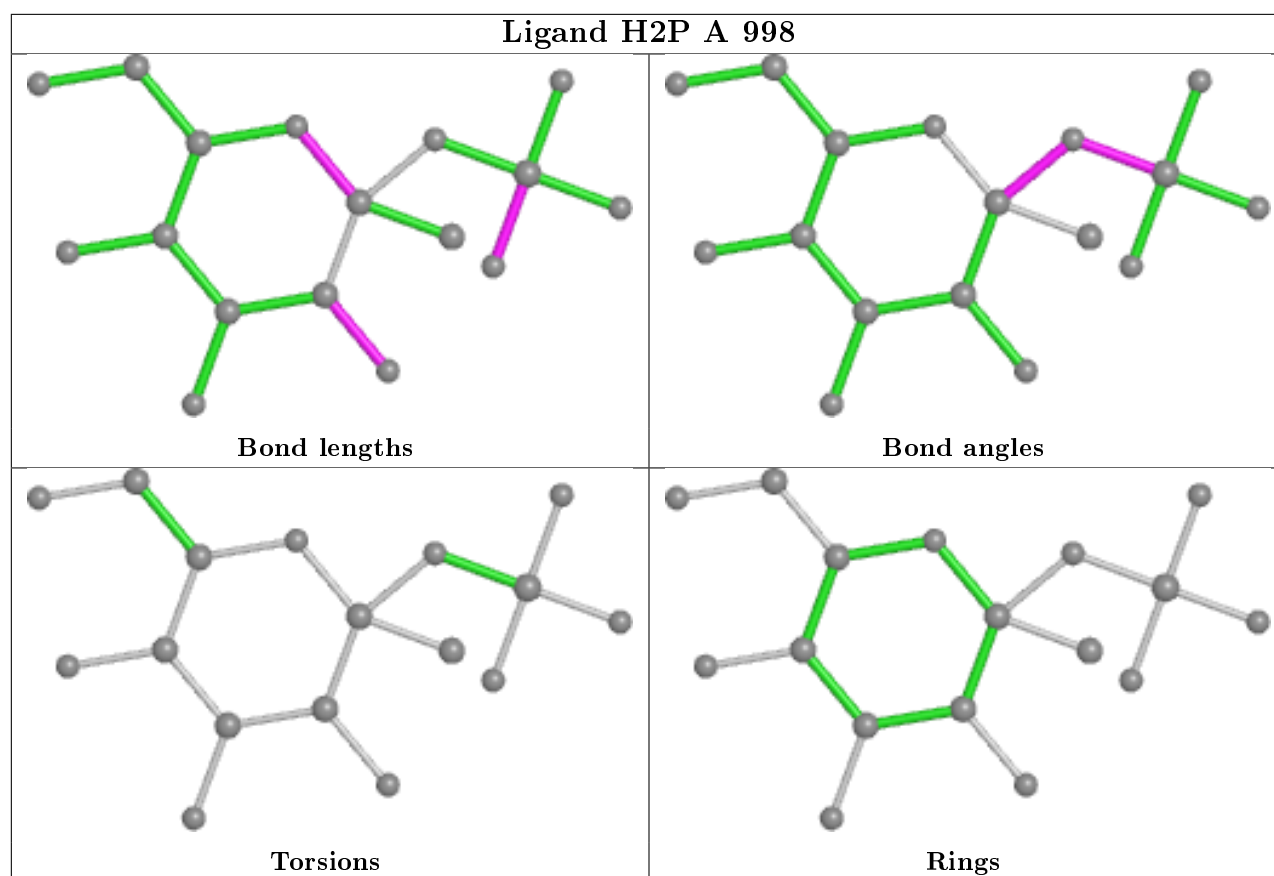
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	PLP	2	0
5	A	913	AMP	1	0
3	A	998	H2P	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	281:PRO	C	282:ASN	N	1.16
1	A	41:LYS	C	42:ASP	N	1.13
1	A	282:ASN	C	283:ASP	N	0.94

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.