wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:47 PM GMT

PDB ID	:	1QM5
Title	:	PHOSPHORYLASE RECOGNITION AND PHOSPHORYLYSIS OF ITS OLIGOSACCHARIDE SUBSTRATE: ANSWERS TO A LONG OUTSTANDING QUESTION
Authors	:	Watson, K.A.; Mccleverty, C.; Geremia, S.; Cottaz, S.; Driguez, H.; Johnson, L.N.
Deposited on	:	1999-09-20
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

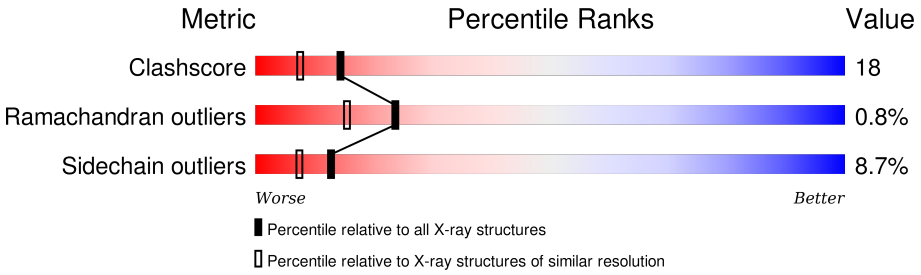
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 <=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	796	68% 27% ·
1	B	796	67% 28% 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
2	PO4	A	900	-	-	X	-
2	PO4	B	900	-	-	X	-
3	GLC	A	994	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	B	994	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13662 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.

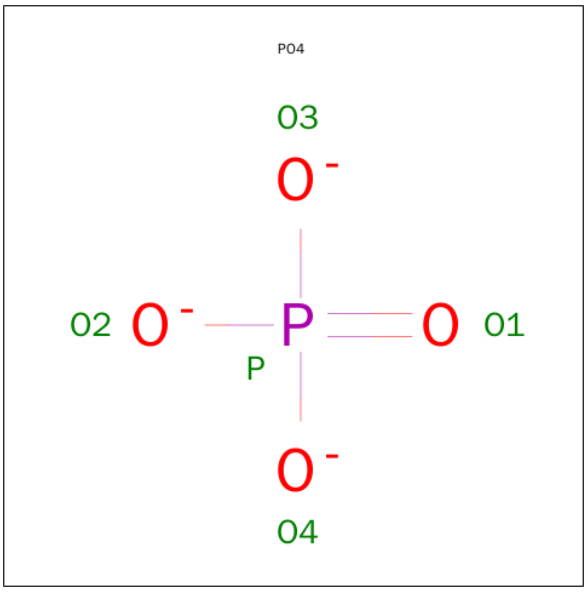
- Molecule 1 is a protein called MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6378	4068	1127	1163	20			
1	B	796	Total	C	N	O	S	0	0	0
			6378	4068	1127	1163	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	LYS	GLU	CONFLICT	UNP P00490
A	487	GLU	VAL	CONFLICT	UNP P00490
A	489	PHE	LEU	CONFLICT	UNP P00490
A	497	ASP	GLN	CONFLICT	UNP P00490
A	498	GLN	LEU	CONFLICT	UNP P00490
A	501	GLU	VAL	CONFLICT	UNP P00490
A	521	GLU	ASP	CONFLICT	UNP P00490
A	547	HIS	ARG	CONFLICT	UNP P00490
B	293	LYS	GLU	CONFLICT	UNP P00490
B	487	GLU	VAL	CONFLICT	UNP P00490
B	489	PHE	LEU	CONFLICT	UNP P00490
B	497	ASP	GLN	CONFLICT	UNP P00490
B	498	GLN	LEU	CONFLICT	UNP P00490
B	501	GLU	VAL	CONFLICT	UNP P00490
B	521	GLU	ASP	CONFLICT	UNP P00490
B	547	HIS	ARG	CONFLICT	UNP P00490

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

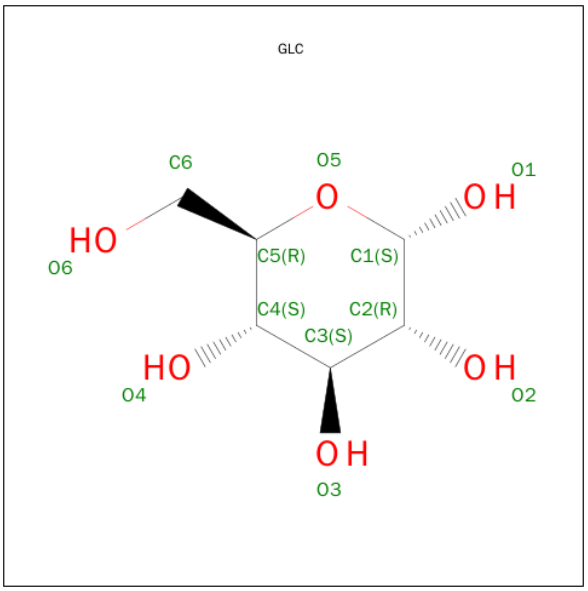


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

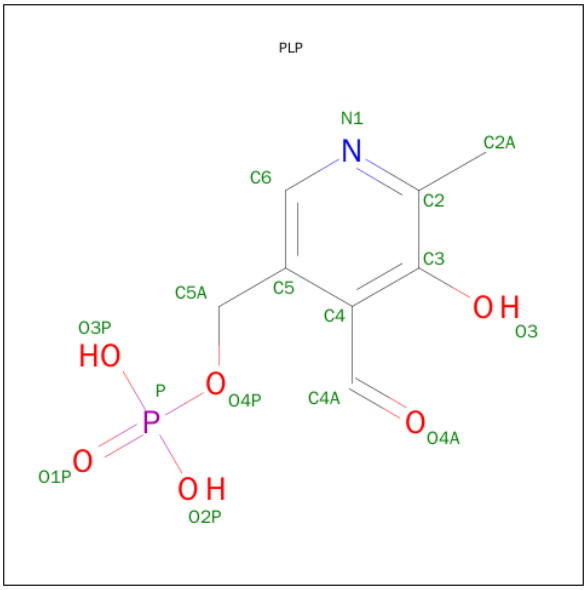
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total C O S 45 24 20 1	0	0
3	B	4	Total C O S 45 24 20 1	0	0

- Molecule 4 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	377	Total O 377 377	0	0
6	B	377	Total O 377 377	0	0

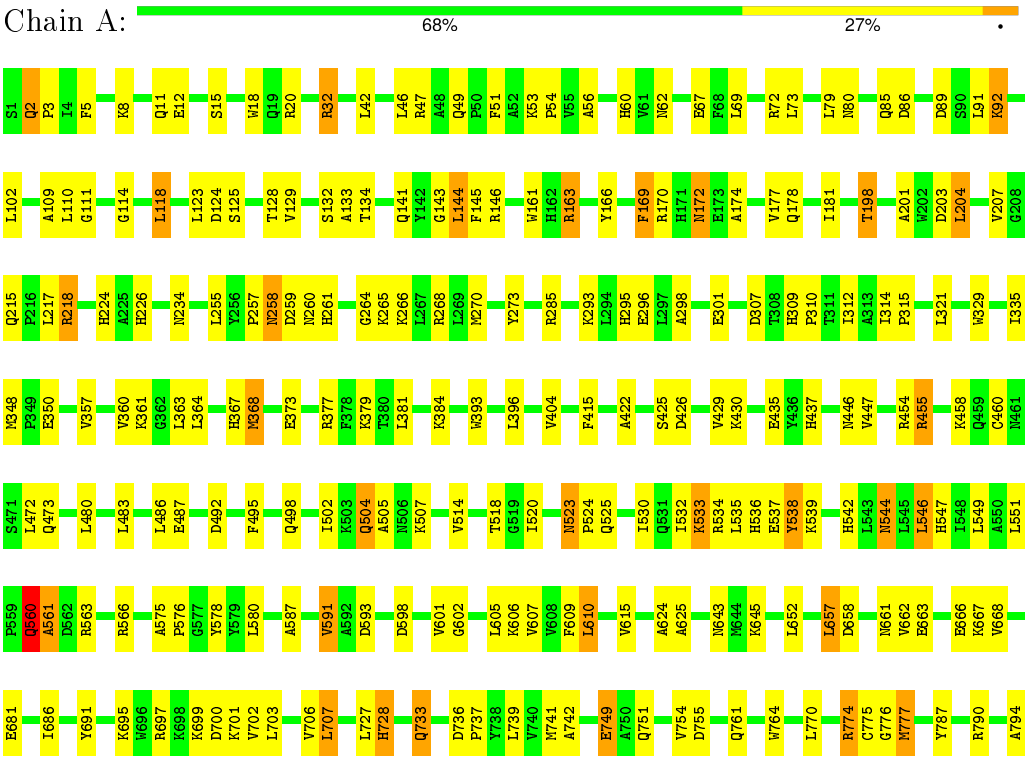
3 Residue-property plots (i)

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.

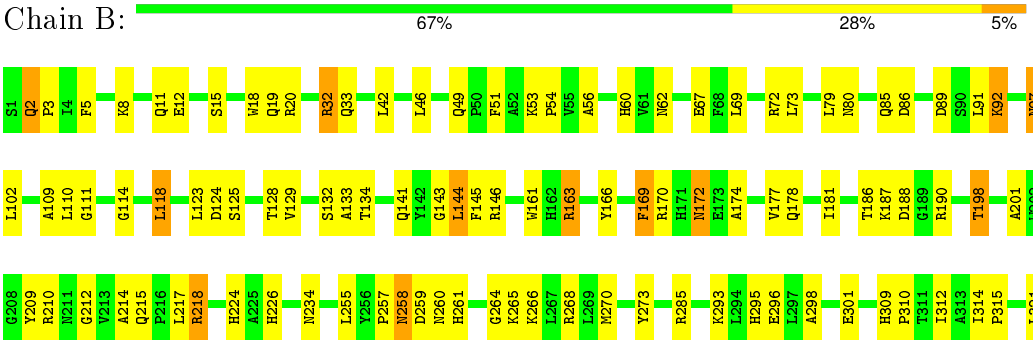
- Molecule 1: MALTODEXTRIN PHOSPHORYLASE

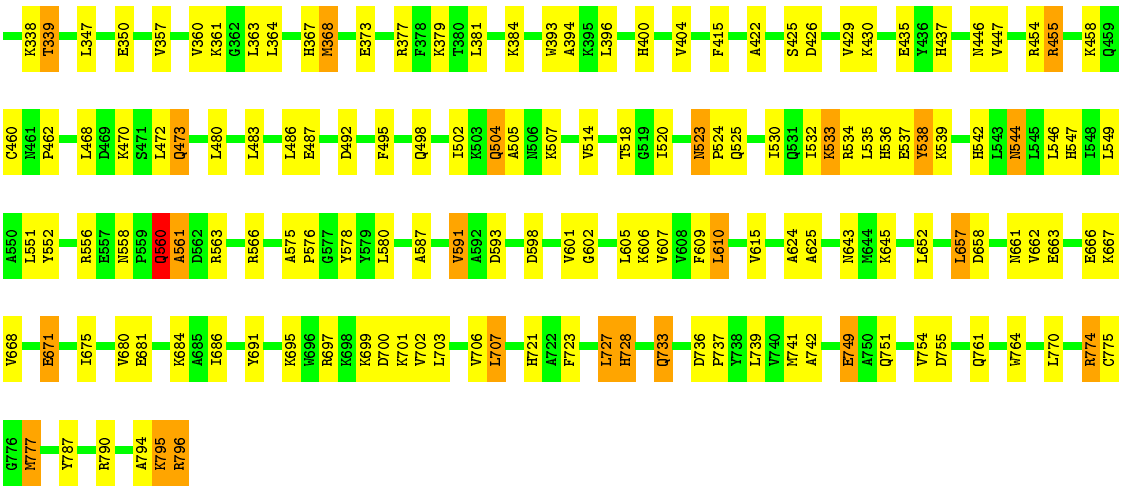
Chain A:



- Molecule 1: MALTODEXTRIN PHOSPHORYLASE

Chain B:




K338 T339 L347 E350 V357 V360 K361 G362 L363 L364 H367 M368 E373 R377 F378 K379 T380 L381 K384 W393 A394 K395 L396 H400 V404 F415 A422 S425 D426 V429 K430 E435 Y436 H437 N446 V447 R454 R455 K458 Q459
C460 N461 P462 L468 D469 K470 S471 L472 Q473 L480 L483 L486 E487 D492 F495 Q498 I502 K503 Q504 A505 N506 K507 V514 T518 G519 I520 N523 P524 Q525 I530 Q531 I532 K533 R534 L535 H536 E537 Y538 K539 H542 L543 N544 L545 L546 H547 I548 L549
A550 L551 Y552 R556 E557 N558 P559 Q560 A561 D562 R563 R566 A575 P576 G577 Y578 Y579 L580 A587 V591 A592 D593 D598 V601 G602 L605 K606 V607 V608 F609 L610 V615 A624 A625 N643 M644 K645 L652 L657 D658 N661 V662 E663 E666 K667
V668 E671 I675 V680 E681 K684 A685 I686 Y691 K695 W696 R697 K698 K699 D700 K701 V702 L703 V706 L707 H721 A722 F723 L727 H728 Q733 D736 F737 Y738 L739 V740 M741 A742 E749 A750 Q751 V754 D755 Q761 W764 L770 R774 C775
G776 M777 Y787 R790 A794 K795 R796

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.41Å 61.50Å 132.38Å 90.00° 105.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	80.0 (50.00-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.5	Depositor
R, R_{free}	0.228 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13662	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: PO4, GLC, SGC, 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	0.37	0/6528	0.60	0/8853
1	B	0.37	0/6528	0.60	0/8853
All	All	0.37	0/13056	0.60	0/17706

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
3	A	1	0
3	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	994	GLC	C1
3	B	994	GLC	C1

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	6378	0	6308	227	0
1	B	6378	0	6308	238	0
2	A	5	0	0	2	0
2	B	5	0	0	2	0
3	A	45	0	38	2	0
3	B	45	0	38	2	0
4	A	11	0	10	0	0
4	B	11	0	10	0	0
5	A	15	0	7	2	0
5	B	15	0	7	2	0
6	A	377	0	0	20	0
6	B	377	0	0	26	0
All	All	13662	0	12726	461	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 18.

The worst 5 of 461 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:473:GLN:CG	6:B:2227:HOH:O	1.91	1.15
1:A:728:HIS:HB3	1:A:733:GLN:NE2	1.72	1.04
1:B:657:LEU:HD13	1:B:662:VAL:HG12	1.41	1.03
1:B:728:HIS:HB3	1:B:733:GLN:NE2	1.72	1.02
1:A:657:LEU:HD13	1:A:662:VAL:HG12	1.41	1.01

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	794/796 (100%)	753 (95%)	35 (4%)	6 (1%)	24	15
1	B	794/796 (100%)	753 (95%)	35 (4%)	6 (1%)	24	15
All	All	1588/1592 (100%)	1506 (95%)	70 (4%)	12 (1%)	24	15

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ARG
1	A	795	LYS
1	B	795	LYS
1	A	2	GLN
1	B	2	GLN

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	665/667 (100%)	607 (91%)	58 (9%)	13	7
1	B	665/667 (100%)	607 (91%)	58 (9%)	13	7
All	All	1330/1334 (100%)	1214 (91%)	116 (9%)	13	7

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	749	GLU
1	B	97	ASN
1	B	727	LEU
1	A	761	GLN
1	B	32	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	678	HIS

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Mol	Chain	Res	Type
1	B	60	HIS
1	B	597	ASN
1	B	2	GLN
1	B	88	GLN

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

8 carbohydrates 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	GLC	A	994	-	12,12,12	0.39	0	17,17,17	0.34	0
3	GLC	A	995	-	11,11,12	0.49	0	14,15,17	0.75	1 (7%)
3	GLC	A	996	-	11,11,12	0.44	0	14,15,17	0.70	1 (7%)
3	SGC	A	997	2,4	9,11,12	0.60	0	10,15,17	0.95	1 (10%)
3	GLC	B	994	-	12,12,12	0.40	0	17,17,17	0.34	0
3	GLC	B	995	-	11,11,12	0.50	0	14,15,17	0.75	1 (7%)
3	GLC	B	996	-	11,11,12	0.44	0	14,15,17	0.70	1 (7%)
3	SGC	B	997	2,4	9,11,12	0.59	0	10,15,17	0.95	1 (10%)

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	GLC	A	994	-	1/1/5/5	0/2/22/22	0/1/1/1
3	GLC	A	995	-	-	0/2/19/22	0/1/1/1
3	GLC	A	996	-	-	0/2/19/22	0/1/1/1
3	SGC	A	997	2,4	-	0/2/19/22	0/1/1/1
3	GLC	B	994	-	1/1/5/5	0/2/22/22	0/1/1/1
3	GLC	B	995	-	-	0/2/19/22	0/1/1/1
3	GLC	B	996	-	-	0/2/19/22	0/1/1/1
3	SGC	B	997	2,4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	997	SGC	C1-C2-C3	2.03	111.94	109.54
3	B	997	SGC	C1-C2-C3	2.04	111.95	109.54
3	B	996	GLC	C1-O5-C5	2.14	114.96	112.25
3	A	996	GLC	C1-O5-C5	2.16	114.99	112.25
3	A	995	GLC	C1-O5-C5	2.59	115.53	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	994	GLC	C1
3	B	994	GLC	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	995	GLC	1	0
3	A	997	SGC	1	0
3	B	995	GLC	1	0
3	B	997	SGC	1	0

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	PO4	A	900	3	4,4,4	1.85	2 (50%)	6,6,6	0.45	0
4	GLC	A	998	3	11,11,12	0.46	0	14,15,17	1.12	2 (14%)
5	PLP	A	999	-	15,15,16	2.39	6 (40%)	21,22,23	3.35	11 (52%)
2	PO4	B	900	3	4,4,4	1.84	2 (50%)	6,6,6	0.45	0
4	GLC	B	998	3	11,11,12	0.46	0	14,15,17	1.13	2 (14%)
5	PLP	B	999	-	15,15,16	2.39	6 (40%)	21,22,23	3.36	11 (52%)

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	PO4	A	900	3	-	0/0/0/0	0/0/0/0
4	GLC	A	998	3	-	0/2/19/22	0/1/1/1
5	PLP	A	999	-	-	0/6/6/8	0/1/1/1
2	PO4	B	900	3	-	0/0/0/0	0/0/0/0
4	GLC	B	998	3	-	0/2/19/22	0/1/1/1
5	PLP	B	999	-	-	0/6/6/8	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	B	999	PLP	C4A-C4	-4.98	1.41	1.51
5	A	999	PLP	C4A-C4	-4.98	1.41	1.51
5	A	999	PLP	P-O4P	-3.84	1.47	1.60
5	B	999	PLP	P-O4P	-3.82	1.47	1.60
2	B	900	PO4	P-O2	-2.43	1.44	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	999	PLP	C4A-C4-C5	-6.51	114.10	120.88
5	A	999	PLP	C4A-C4-C5	-6.48	114.13	120.88
5	A	999	PLP	C4A-C4-C3	-5.80	109.86	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	999	PLP	C4A-C4-C3	-5.76	109.93	120.36
5	A	999	PLP	C6-C5-C4	-3.82	114.91	118.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	PO4	2	0
5	A	999	PLP	2	0
2	B	900	PO4	2	0
5	B	999	PLP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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