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PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:22 am GMT

PDB ID : 2PYI

Title : Crystal structure of Glycogen Phosphorylase in complex with glucosyl triazoleacetamide

Authors : Alexacou, K.M.; Tiraidis, C.; Zographos, S.E.; Chrysina, E.D.; Hayes, J.; Oikonomakos, N.G.

Deposited on : 2007-05-16

Resolution : 1.88 Å(reported)

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

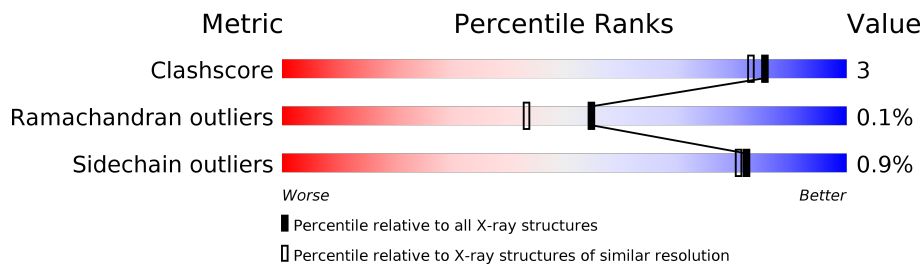|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 1.88 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		0.9%

Worse   *Better*

▪ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)

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 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	843	90% 6% ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7542 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	807	Total 6598	C 4202	N 1167	O 1199	P 1	S 29	0	3	0

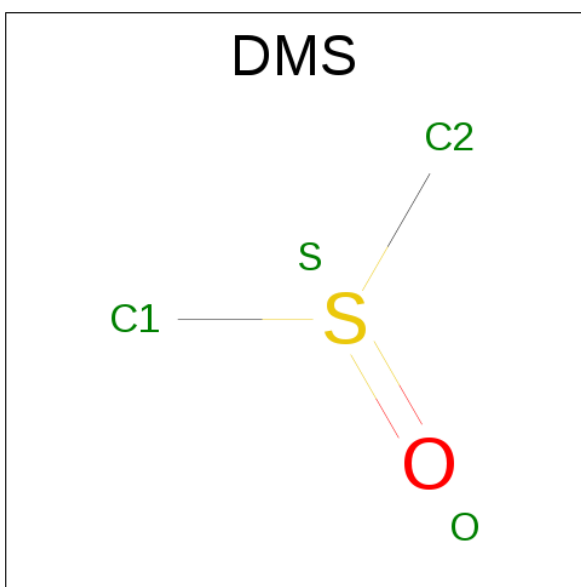There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LLP	LYS	MODIFIED RESIDUE	UNP P00489

- Molecule 2 is N-[(4-PHENYL-1H-1,2,3-TRIAZOL-1-YL)ACETYL]-BETA-D-GLUCOPYR ANOSYLAMINE (three-letter code: DL8) (formula: $C_{16}H_{20}N_4O_6$).
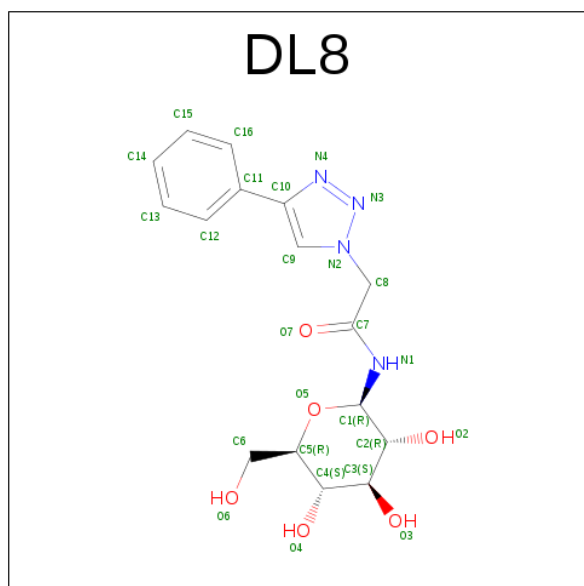
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 26	C 16	N 4	O 6	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

```
                    DMS


                            C2

                     S
            C1              S

                            O

                               O
```

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	878	Total 878	O 878	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 the various outlier classes 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, muscle form

Chain A:
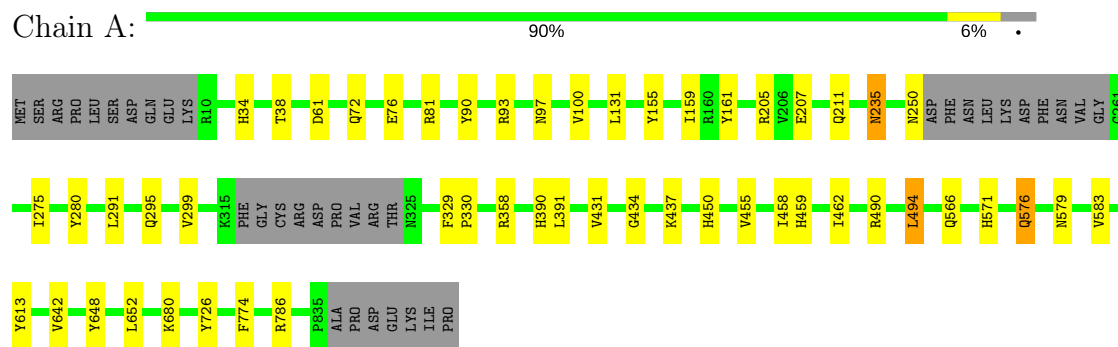
4 Data and refinement statistics (i)

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	125.93Å 125.93Å 115.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.88	Depositor
% Data completeness (in resolution range)	99.7 (30.00-1.88)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7542	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: DL8, DMS, LLP

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	0.35	0/6737	0.50	1/9112 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	494	LEU	CA-CB-CG	6.71	130.73	115.30

There are no chirality outliers.

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	6598	0	6536	34	0
2	A	26	0	20	0	0
3	A	40	0	60	1	0
4	A	878	0	0	4	0
All	All	7542	0	6616	34	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 3.

The worst 5 of 34 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:490:ARG:HA	1:A:494:LEU:HG	1.39	1.04
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.61	0.81
1:A:458:ILE:O	1:A:462:ILE:HG13	1.82	0.80
1:A:159:ILE:HG12	1:A:299:VAL:HG22	1.65	0.78
1:A:159:ILE:HG12	1:A:299:VAL:CG2	2.16	0.75

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	803/843 (95%)	782 (97%)	20 (2%)	1 (0%)	55	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLY

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	701/731 (96%)	695 (99%)	6 (1%)	82	81

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	613	TYR
1	A	576	GLN
1	A	235	ASN
1	A	579	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	HIS
1	A	459	HIS
1	A	566	GLN
1	A	325	ASN
1	A	576	GLN

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	LLP	A	680	1	24,24,25	1.74	5 (20%)	28,32,34	1.25	5 (17%)

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	LLP	A	680	1	-	0/15/17/19	0/1/1/1

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All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O3-C3	-5.55	1.24	1.37
1	A	680	LLP	C4'-NZ	2.30	1.34	1.27
1	A	680	LLP	C2-N1	2.33	1.38	1.33
1	A	680	LLP	CA-C	2.39	1.53	1.50
1	A	680	LLP	C4-C4'	2.99	1.51	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	CE-NZ-C4'	-2.86	110.72	119.03
1	A	680	LLP	C4-C4'-NZ	-2.65	111.79	124.66
1	A	680	LLP	OP4-P-OP1	-2.40	99.75	106.47
1	A	680	LLP	C5-C6-N1	-2.17	120.19	123.87
1	A	680	LLP	OP3-P-OP2	2.21	116.52	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	680	LLP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

11 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
3	DMS	A	931	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
3	DMS	A	936	-	3,3,3	2.57	1 (33%)	3,3,3	0.48	0
3	DMS	A	937	-	3,3,3	2.62	1 (33%)	3,3,3	0.50	0
3	DMS	A	938	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
3	DMS	A	939	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
3	DMS	A	940	-	3,3,3	2.62	1 (33%)	3,3,3	0.42	0
3	DMS	A	942	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
3	DMS	A	945	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
3	DMS	A	946	-	3,3,3	2.57	1 (33%)	3,3,3	0.45	0
3	DMS	A	972	-	3,3,3	2.60	1 (33%)	3,3,3	0.50	0
2	DL8	A	998	-	26,28,28	2.48	6 (23%)	35,39,39	1.45	5 (14%)

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	DMS	A	931	-	-	0/0/0/0	0/0/0/0
3	DMS	A	936	-	-	0/0/0/0	0/0/0/0
3	DMS	A	937	-	-	0/0/0/0	0/0/0/0
3	DMS	A	938	-	-	0/0/0/0	0/0/0/0
3	DMS	A	939	-	-	0/0/0/0	0/0/0/0
3	DMS	A	940	-	-	0/0/0/0	0/0/0/0
3	DMS	A	942	-	-	0/0/0/0	0/0/0/0
3	DMS	A	945	-	-	0/0/0/0	0/0/0/0
3	DMS	A	946	-	-	0/0/0/0	0/0/0/0
3	DMS	A	972	-	-	0/0/0/0	0/0/0/0
2	DL8	A	998	-	-	0/13/34/34	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	DL8	N4-N3	-7.19	1.24	1.34
2	A	998	DL8	C11-C10	-5.98	1.39	1.48
2	A	998	DL8	N3-N2	-5.30	1.24	1.34
2	A	998	DL8	C9-C10	-3.73	1.33	1.37
2	A	998	DL8	C9-N2	-2.26	1.33	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	998	DL8	C8-N2-C9	-4.79	123.09	129.19
2	A	998	DL8	O5-C1-N1	-2.09	104.52	107.98
2	A	998	DL8	C9-C10-N4	-2.06	106.13	109.90
2	A	998	DL8	N4-N3-N2	3.10	109.66	107.31
2	A	998	DL8	C11-C10-N4	3.82	126.94	120.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	939	DMS	1	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 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.