



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 02:26 PM EDT

PDB ID : 2ZB2
Title : Human liver glycogen phosphorylase a complexed with glucose and 5-chloro-N-[4-(1,2-dihydroxyethyl)phenyl]-1H-indole-2-carboxamide
Authors : Katayama, N.; Onda, K.
Deposited on : unknown
Resolution : 2.45 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (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) : rb-20030345

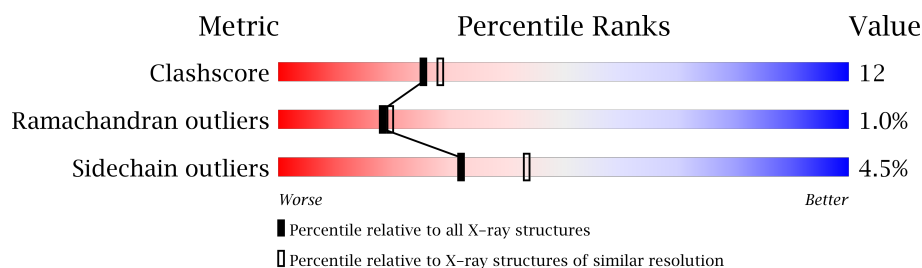
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)

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	849	
1	B	849	

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
6	MPD	B	852	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13413 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.

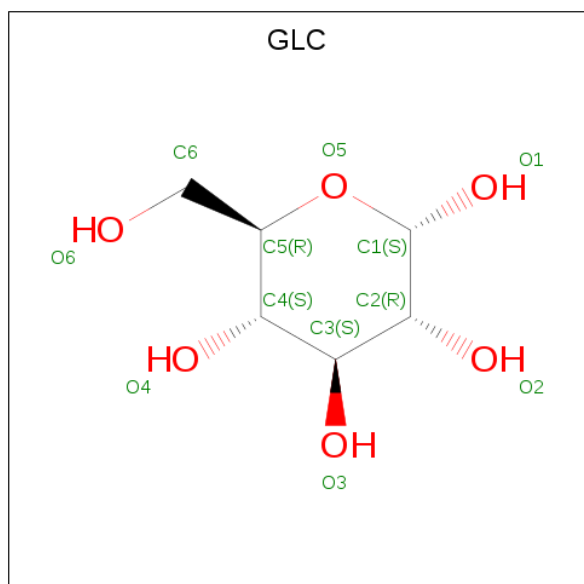
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	798	Total	C	N	O	S	0	0	0
			6466	4154	1097	1186	29			
1	B	791	Total	C	N	O	S	0	0	0
			6410	4116	1088	1177	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P06737
A	-1	SER	-	EXPRESSION TAG	UNP P06737
B	-2	GLY	-	EXPRESSION TAG	UNP P06737
B	-1	SER	-	EXPRESSION TAG	UNP P06737

- Molecule 2 is ALPHA-D-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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



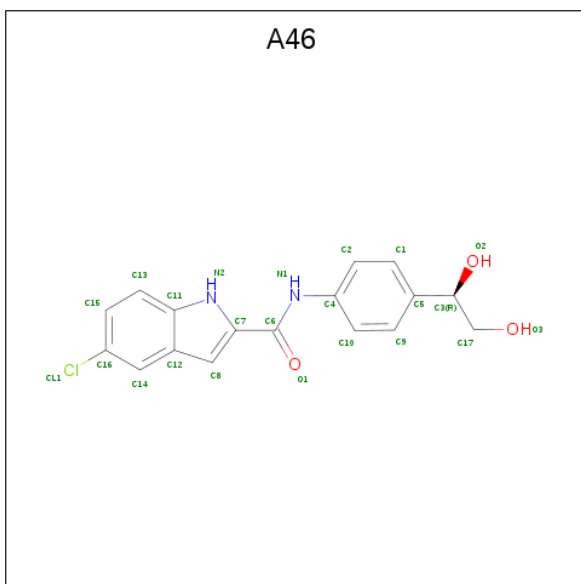
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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 5-chloro-N-{4-[(1R)-1,2-dihydroxyethyl]phenyl}-1H-indole-2-carboxamide (three-letter code: A46) (formula: $C_{17}H_{15}ClN_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			23	17	1	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	
			23	17	1	2	3	
								0
								0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O		
			8	6	2		
						0	0
6	B	1	Total	C	O		
			8	6	2		
						0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O		
			199	199		
					0	0
7	B	198	Total	O		
			198	198		
					0	0

D785	A673	V567	H440	ALA	V221
Q789	S674	K568	H441	GLY	L224
N793	N678	H571	A442	V325	P225
P794	N679	E572	H450	F326	Y226
K795	N680	Y573	V455	P329	V230
A796	N681	K574	A456	P330	I235
W797	N682	N575	K457	A334	I236
L802	L683	N579	H458	T340	T237
S808	L687	C580	H459	H341	R242
G809	N692	V583	V463	P342	L243
K810	D693	Y587	L474	A345	W244
S813	N696	K591	N481	D355	N250
R815	N697	P594	L492	PHE	ASP
T816	E701	L597	L493	ASN	PHE
K818	F709	L597	L494	LEU	ASN
E819	I710	V603	L499	ARG	ASP
V827	N713	I604	L502	ASP	PHE
E828	R714	L605	L503	ASN	ASN
P829	I715	G606	A504	VAL	VAL
S830	D716	G607	E505	G260	G260
ASP	D717	K506	K506	V266	V266
LEU	D722	Y613	N507	V389	N270
LYS	Y732	K617	G508	R398	I274
ILE	Y736	P618	E509	R399	N275
SER	P736	I619	V512	L400	L275
LEU	E737	L622	K513	E401	S276
SER	L738	A627	D514	I402	R277
ASN	K739	V636	L515	I403	V278
GLU	L740	K641	S516	Y404	L291
SER	V741	V642	L521	E405	R292
ASN	P752	K639	D528	I406	Q295
LYS	K753	L640	R532	H410	E296
VAL	I761	V646	S546	L411	V300
GLY	L765	N647	I547	I414	L304
ASN	D769	Y648	T551	V415	L304
	R770	L852	Y559	D421	R310
	K772	I657	N558	R424	F311
	V773	P658	N558	I431	K312
	F774	A659	N558	E433	S314
	A775	T660	S561	E434	LYS
	D776	S663	D564	G435	PHE
	Y777	E664	Y565	S436	GLY
	C783	Q665	Q566	R437	SER
	Q784			R438	THR
				I439	ARG
					GLY

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.82Å 123.82Å 123.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.18 – 2.45	Depositor
% Data completeness (in resolution range)	99.4 (49.18-2.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.37	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.261 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13413	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: A46, MPD, GLC, MES, 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	0.54	0/6611	0.61	0/8940
1	B	0.52	0/6553	0.61	0/8865
All	All	0.53	0/13164	0.61	0/17805

There are no bond length outliers.

There are no bond angle outliers.

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	6466	0	6451	160	0
1	B	6410	0	6394	153	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	12	0	12	3	0
3	B	12	0	13	3	0
4	A	15	0	7	0	0
4	B	15	0	7	0	0
5	A	23	0	15	0	0
5	B	23	0	15	1	0
6	B	16	0	28	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	199	0	0	8	0
7	B	198	0	0	13	0
All	All	13413	0	12966	312	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 12.

The worst 5 of 312 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:204:GLY:O	1:A:205:LYS:HD2	1.79	0.83
1:B:204:GLY:O	1:B:205:LYS:HD2	1.80	0.80
1:B:678:ASN:HD22	1:B:679:MET:H	1.29	0.77
1:A:678:ASN:HD22	1:A:679:MET:H	1.32	0.76
1:A:310:ARG:HE	3:A:848:MES:H72	1.50	0.76

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	792/849 (93%)	739 (93%)	45 (6%)	8 (1%)	18	19
1	B	785/849 (92%)	734 (94%)	43 (6%)	8 (1%)	18	19
All	All	1577/1698 (93%)	1473 (93%)	88 (6%)	16 (1%)	18	19

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ASP
1	A	435	GLY

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Mol	Chain	Res	Type
1	A	555	VAL
1	A	715	ILE
1	B	23	ASN

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	696/741 (94%)	663 (95%)	33 (5%)	30	41
1	B	691/741 (93%)	661 (96%)	30 (4%)	33	46
All	All	1387/1482 (94%)	1324 (96%)	63 (4%)	32	43

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	LEU
1	B	29	LYS
1	B	683	LEU
1	A	722	ASP
1	A	793	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	822	GLN
1	B	167	ASN
1	B	789	GLN
1	A	826	ASN
1	B	34	HIS

5.3.3 RNA ⓘ

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	GLC	A	847	-	12,12,12	0.45	0	17,17,17	0.67	0
3	MES	A	848	-	12,12,12	1.68	2 (16%)	14,16,16	3.23	5 (35%)
4	PLP	A	849	1	15,15,16	1.88	4 (26%)	20,22,23	1.17	1 (5%)
5	A46	A	850	-	22,25,25	1.48	3 (13%)	27,35,35	1.92	6 (22%)
2	GLC	B	847	-	12,12,12	0.39	0	17,17,17	0.49	0
3	MES	B	848	-	12,12,12	1.10	1 (8%)	14,16,16	2.39	5 (35%)
4	PLP	B	849	1	15,15,16	1.43	4 (26%)	20,22,23	1.10	0
5	A46	B	850	-	22,25,25	2.05	7 (31%)	27,35,35	2.12	9 (33%)
6	MPD	B	851	-	7,7,7	1.20	0	9,10,10	1.13	0
6	MPD	B	852	-	7,7,7	0.68	0	9,10,10	1.12	1 (11%)

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	A	847	-	-	0/2/22/22	0/1/1/1
3	MES	A	848	-	-	0/6/14/14	0/1/1/1
4	PLP	A	849	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A46	A	850	-	-	0/11/14/14	0/3/3/3
2	GLC	B	847	-	-	0/2/22/22	0/1/1/1
3	MES	B	848	-	-	0/6/14/14	0/1/1/1
4	PLP	B	849	1	-	0/6/6/8	0/1/1/1
5	A46	B	850	-	-	0/11/14/14	0/3/3/3
6	MPD	B	851	-	-	0/5/5/5	0/0/0/0
6	MPD	B	852	-	1/1/2/2	0/5/5/5	0/0/0/0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	850	A46	C16-CL1	-5.43	1.62	1.74
5	B	850	A46	C4-N1	-3.96	1.33	1.41
4	B	849	PLP	C4A-C4	-3.15	1.45	1.51
5	B	850	A46	C5-C3	-2.70	1.46	1.51
4	B	849	PLP	C5-C4	2.03	1.42	1.40

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	848	MES	O2S-S-C8	-6.16	101.50	106.79
5	B	850	A46	C7-C8-C12	-4.32	101.17	106.55
5	B	850	A46	C10-C9-C5	-3.36	117.79	121.20
3	B	848	MES	O3S-S-O2S	-2.80	104.96	111.37
5	A	850	A46	C15-C16-C14	-2.72	118.45	121.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	852	MPD	C4

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	848	MES	3	0
3	B	848	MES	3	0
5	B	850	A46	1	0
6	B	851	MPD	2	0
6	B	852	MPD	4	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 ⓘ

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.