



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:33 PM GMT

PDB ID : 1XOI
Title : Human Liver Glycogen Phosphorylase A complexed with Chloroindoloyl glycine amide
Authors : Wright, S.W.; Rath, V.L.; Gibbs, E.M.; Treadway, J.L.
Deposited on : 2004-10-06
Resolution : 2.10 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 (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

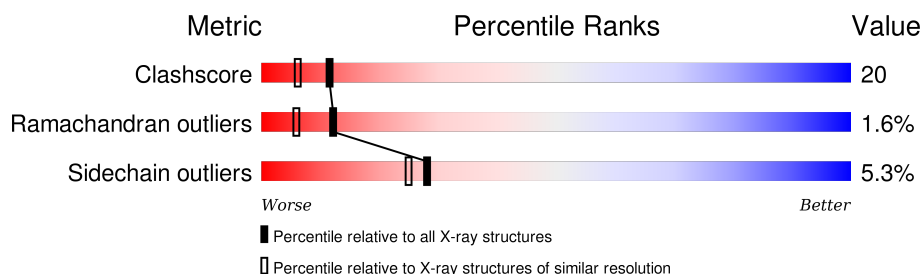
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	
1	B	846	

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
4	288	A	862	X	-	-	-
4	288	B	1862	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13762 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.

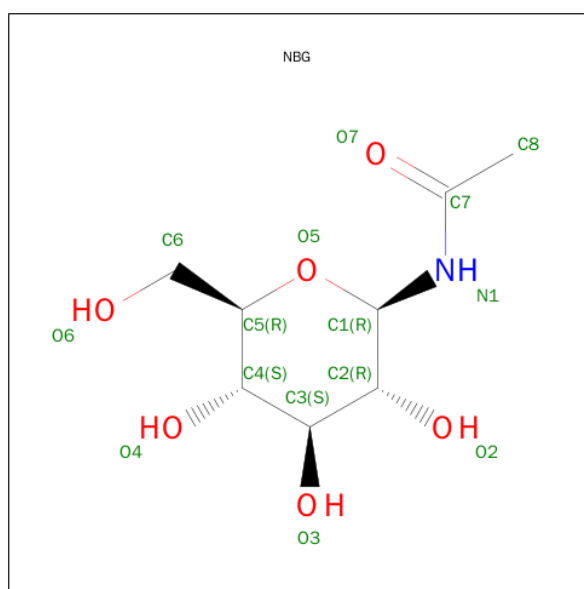
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			
1	B	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ALA	GLY	CONFLICT	UNP P06737
B	1323	ALA	GLY	CONFLICT	UNP P06737

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: C₈H₁₅NO₆).



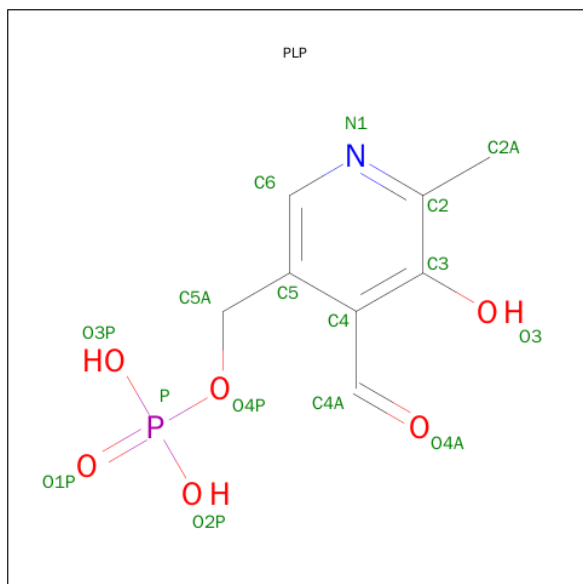
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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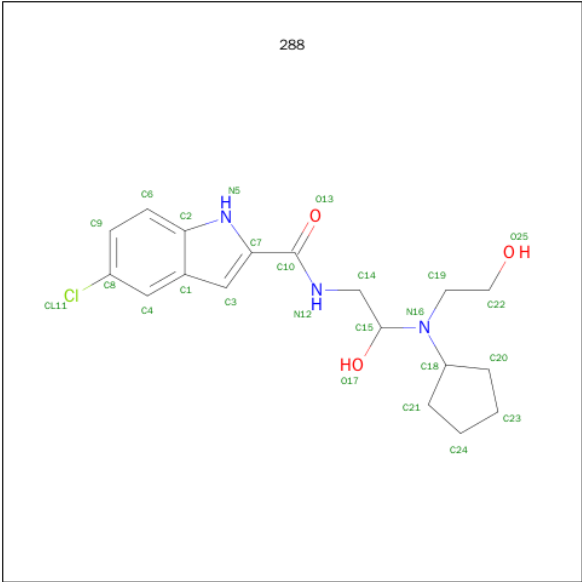
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is 5-CHLORO-1H-INDOLE-2-CARBOXYLIC ACID{[CYCLOPENTYL-(2-HYDROXY-ETHYL)-CARBAMOYL]-METHYL}-AMIDE (three-letter code: 288) (formula: $C_{18}H_{24}ClN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		
4	B	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	323	Total	O	0	0
			323	323		
5	B	313	Total	O	0	0
			313	313		

K1759	L1640	L1543	K1437	P1342	R1247
D1760	K1641	L1543	A1442	A1345	A1248
M1763	V1642	S1546	H1443	I1346	P1249
M1764	F1644	Q1547	I1446	P1347	ASN
R1770	L1645	E1550	V1447	E1348	ASP
F1771	E1646	T1551	G1448	PHE	ASN
K1772	M1647	T1551	S1449	I1352	LEU
		V1555	A1451	M1361	ASP
A1775	S1651	I1557	H1450	M1365	ARG
D1776	L1652	N1558	V1452		PHE
	I1657	P1559	V1455	Q1369	ASN
C1783	P1658	S1560	A1456	K1370	VAL
K1786	I1666	S1561	K1457		GLY
	S1674	M1562	I1458	Y1374	ASP
Q1789			H1459		Y1262
M1792	K1680	Q1566		H1377	M1274
R1793		V1567	I1462	T1378	I1275
P1794	L1683	K1568	V1463	V1379	S1276
		H1571	K1466	L1380	R1277
L1802	I1689		V1467	P1381	V1278
K1810	G1690	K1574	F1468		
	T1691	R1575	K1469	E1382	F1286
D1814	M1692	Q1576		E1385	
R1815	V1697	L1577	E1473	R1386	Q1295
	E1698	N1579	L1474	V1389	V1299
K1818			E1475	D1390	V1300
	E1701	K1592	P1476		
P1829	E1702	D1593	D1477	P1397	L1304
S1830	F1709	P1594	P1488		I1308
D1831	I1710	K1595	W1491	I1402	
K1833		L1597	L1492	E1405	K1312
I1834	I1715	F1598	L1493	I1406	A1313
S1835		V1599	L1494		S1314
L1836	E1727	P1600	L1499	K1409	K1315
S1837	A1728	R1601		R1413	F1316
R1838	K1729		L1502	I1414	G1317
GLU	E1730	G1607		V1415	S1318
SER			K1506		T1319
ASN	E1733	Y1613		P1419	R1320
LYS	A1734	H1614		K1420	G1321
VAL	L1735	M1615	E1509	D1421	A1322
ASN	P1736			V1422	A1323
GLY		I1619	V1512	D1423	T1324
ASN	L1740	T1620		R1424	V1325
		K1621	D1528	L1425	F1326
	Q1744	L1622	V1529	L1426	D1327
			F1530		A1328
	P1752	N1632	L1531	L1430	F1329
K1753	K1753	D1633	R1532	I1431	P1330
Q1754	Q1754	P1634		E1432	
P1755	P1755	M1635	K1536	E1433	A1334
D1756	D1756	V1636		E1434	
L1757	L1757		Q1539	G1435	L1337
F1758	F1758	K1639	E1540	S1436	H1341

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	123.91Å 123.91Å 123.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.10	Depositor
% Data completeness (in resolution range)	92.6 (99.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.206 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13762	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: 288, NBG, 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	0.36	0/6653	0.61	0/8998
1	B	0.37	0/6653	0.62	1/8998 (0.0%)
All	All	0.36	0/13306	0.61	1/17996 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1323	ALA	N-CA-C	-5.38	96.46	111.00

There are no chirality outliers.

There are no planarity outliers.

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	6508	0	6518	278	0
1	B	6508	0	6518	264	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	1	0
3	B	15	0	7	0	0
4	A	25	0	22	0	0
4	B	25	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	323	0	0	51	0
5	B	313	0	0	35	0
All	All	13762	0	13124	536	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 20.

The worst 5 of 536 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:1434:GLU:H	1:B:1434:GLU:CD	1.62	0.98
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.10	0.98
1:A:236:ASN:HB3	1:A:834:ILE:HB	1.46	0.97
1:A:434:GLU:CD	1:A:434:GLU:H	1.65	0.96
1:B:1168:GLN:HE21	1:B:1647:ASN:H	1.03	0.96

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	800/846 (95%)	748 (94%)	39 (5%)	13 (2%)	12	6
1	B	800/846 (95%)	749 (94%)	38 (5%)	13 (2%)	12	6
All	All	1600/1692 (95%)	1497 (94%)	77 (5%)	26 (2%)	12	6

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	PHE
1	A	318	SER

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Mol	Chain	Res	Type
1	B	1317	GLY
1	B	1320	ARG
1	B	1322	ALA

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	702/739 (95%)	663 (94%)	39 (6%)	26	22
1	B	702/739 (95%)	666 (95%)	36 (5%)	29	26
All	All	1404/1478 (95%)	1329 (95%)	75 (5%)	28	25

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	692	MET
1	B	1078	CYS
1	B	1730	GLU
1	A	730	GLU
1	A	833	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	614	HIS
1	B	1073	HIS
1	B	1576	GLN
1	A	754	GLN
1	B	1032	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$
3	PLP	A	860	-	15,15,16	2.63	6 (40%)	21,22,23	1.29	2 (9%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.32	2 (9%)
4	288	A	862	-	22,27,27	2.65	3 (13%)	27,37,37	1.84	6 (22%)
3	PLP	B	1860	-	15,15,16	2.58	3 (20%)	21,22,23	1.29	2 (9%)
2	NBG	B	1861	-	15,15,15	1.76	3 (20%)	21,21,21	1.26	1 (4%)
4	288	B	1862	-	22,27,27	2.73	2 (9%)	27,37,37	1.73	5 (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
3	PLP	A	860	-	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	288	A	862	-	1/1/4/5	0/14/27/27	0/3/3/3
3	PLP	B	1860	-	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1
4	288	B	1862	-	1/1/4/5	0/14/27/27	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	288	O17-C15	-11.59	1.21	1.41
4	A	862	288	O17-C15	-10.97	1.22	1.41
3	B	1860	PLP	C4A-C4	-7.36	1.36	1.51
3	A	860	PLP	C4A-C4	-7.18	1.37	1.51
3	B	1860	PLP	C3-C2	-5.11	1.37	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	860	PLP	O2P-P-O4P	-2.95	98.08	106.56
2	A	861	NBG	C2-C1-N1	-2.68	108.44	111.44
4	A	862	288	C14-N12-C10	-2.44	117.47	121.85
3	B	1860	PLP	O3P-P-O2P	2.06	115.21	107.38
3	B	1860	PLP	O3P-P-O1P	2.30	117.97	110.58

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	862	288	C15
4	B	1862	288	C15

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	860	PLP	1	0
4	B	1862	288	3	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 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.