



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2016 – 08:53 PM EDT

PDB ID : 5FH2
Title : The structure of rat cytosolic PEPCK variant E89Q in complex with GTP
Authors : Johnson, T.A.; Holyoak, T.
Deposited on : 2015-12-21
Resolution : 1.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

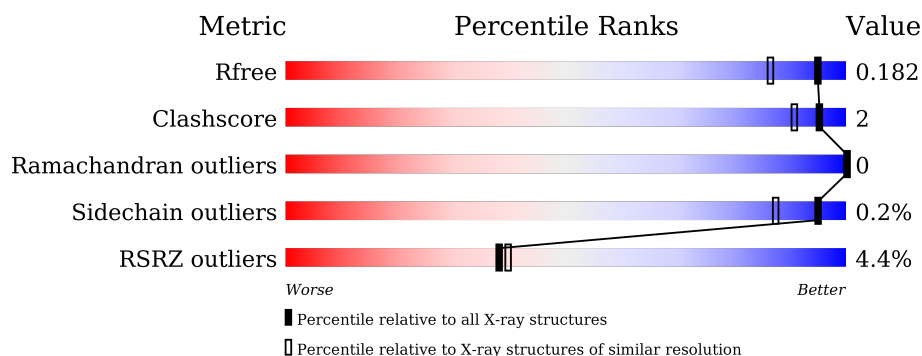
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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.

Mol	Chain	Length	Quality of chain
1	A	622	<div> <div>4%</div> <div>95%</div> <div>...</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5659 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 Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4867	3117	829	889	32	0	9	0

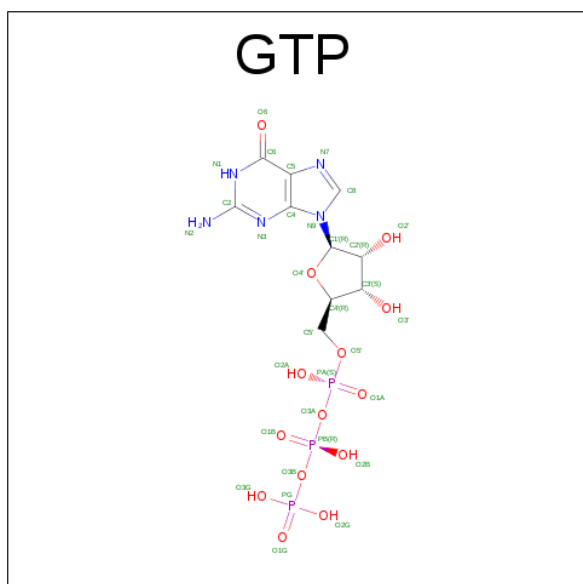
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	GLN	GLU	engineered mutation	UNP P07379

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

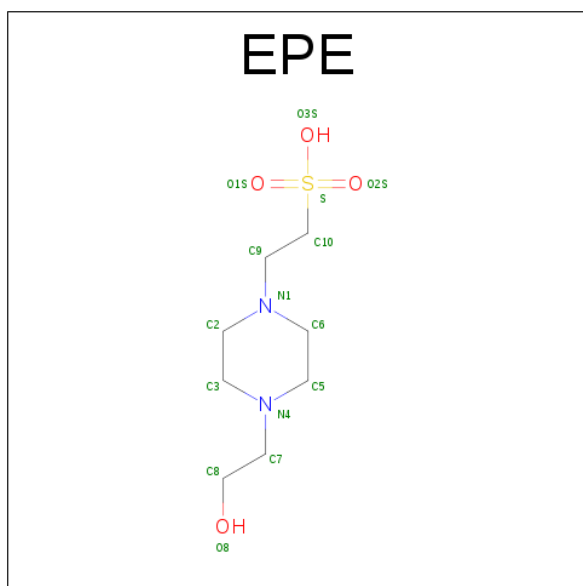
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

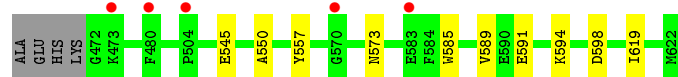
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	742	Total	O	0	0
			742	742		

- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.72Å 118.80Å 60.53Å 90.00° 109.53° 90.00°	Depositor
Resolution (Å)	59.40 – 1.49 38.83 – 1.49	Depositor EDS
% Data completeness (in resolution range)	95.8 (59.40-1.49) 95.8 (38.83-1.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.49Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.147 , 0.172 0.157 , 0.182	Depositor DCC
R_{free} test set	4756 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5659	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GTP, NA, EPE, MN

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	0.62	0/5021	0.80	5/6793 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	461	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	139	MET	CG-SD-CE	-6.16	90.34	100.20
1	A	598	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	A	253	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	4867	0	4840	16	0
2	A	2	0	0	0	0
3	A	32	0	12	0	0
4	A	15	0	18	0	0
5	A	1	0	0	0	0
6	A	742	0	0	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5659	0	4870	16	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 2.

All (16) 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:573:ASN:ND2	6:A:803:HOH:O	2.28	0.65
1:A:318:ASP:OD2	6:A:801:HOH:O	2.15	0.60
1:A:115:ARG:NH2	6:A:807:HOH:O	2.37	0.57
1:A:115:ARG:NH1	6:A:806:HOH:O	2.37	0.57
1:A:585:TRP:O	1:A:589[B]:VAL:HG23	2.06	0.55
1:A:591[B]:GLU:CD	1:A:594[B]:LYS:NZ	2.62	0.53
1:A:589[B]:VAL:HG21	1:A:619:ILE:HD12	1.90	0.52
1:A:591[B]:GLU:OE1	1:A:594[B]:LYS:NZ	2.43	0.50
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.96	0.48
1:A:256[B]:LYS:HE2	6:A:952:HOH:O	2.15	0.46
1:A:550:ALA:HB1	1:A:557:TYR:HB3	1.99	0.44
1:A:391:TRP:CD2	1:A:399:CYS:HB3	2.53	0.44
1:A:3:PRO:HG3	6:A:1491:HOH:O	2.17	0.44
1:A:7:ASN:HB2	6:A:812:HOH:O	2.19	0.43
1:A:545[B]:GLU:OE2	6:A:802:HOH:O	2.20	0.43
1:A:278:LYS:HG2	6:A:957:HOH:O	2.19	0.41

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)
6:A:808:HOH:O	6:A:815:HOH:O[1_655]	1.73	0.47

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	618/622 (99%)	601 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	522/519 (101%)	521 (100%)	1 (0%)	95	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	GTP	A	703	2	26,34,34	1.14	2 (7%)	29,54,54	2.22	4 (13%)
4	EPE	A	704	-	15,15,15	1.85	2 (13%)	19,20,20	1.90	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
3	GTP	A	703	2	-	0/18/38/38	0/3/3/3
4	EPE	A	704	-	-	0/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	704	EPE	C10-S	-6.30	1.68	1.77
3	A	703	GTP	C2'-C1'	-2.13	1.50	1.53
3	A	703	GTP	C5-C4	2.06	1.45	1.40
4	A	704	EPE	O2S-S	2.71	1.53	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	GTP	C5-C6-N1	-6.59	114.90	123.52
3	A	703	GTP	C6-C5-C4	-3.43	116.94	120.86
3	A	703	GTP	N3-C2-N1	-2.83	123.71	127.56
4	A	704	EPE	O2S-S-C10	7.87	112.43	106.87
3	A	703	GTP	C6-N1-C2	7.96	125.21	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	613/622 (98%)	0.10	27 (4%) 38 40	15, 21, 39, 76	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	PRO	8.3
1	A	394	GLN	5.7
1	A	87	ARG	5.5
1	A	393	PRO	3.6
1	A	396	GLU	3.6
1	A	205	PRO	3.3
1	A	397	GLU	3.2
1	A	8	GLY	3.1
1	A	395	ASP	3.1
1	A	392	ARG	3.0
1	A	389	LYS	2.9
1	A	90	SER	2.9
1	A	7	ASN	2.9
1	A	473	LYS	2.9
1	A	391	TRP	2.8
1	A	3	PRO	2.6
1	A	570	GLY	2.4
1	A	21	ASP	2.4
1	A	88	ILE	2.4
1	A	480	PHE	2.3
1	A	432	ILE	2.2
1	A	390	GLU	2.2
1	A	583	GLU	2.1
1	A	85	VAL	2.1
1	A	86	ALA	2.1
1	A	149	LEU	2.1
1	A	388	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EPE	A	704	15/15	0.89	0.21	0.83	23,24,38,45	15
3	GTP	A	703	32/32	0.99	0.06	-0.85	15,17,19,21	0
5	NA	A	705	1/1	0.97	0.05	-1.27	24,24,24,24	0
2	MN	A	701	1/1	1.00	0.07	-1.49	15,15,15,15	0
2	MN	A	702	1/1	1.00	0.07	-	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.