



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:04 AM GMT

PDB ID : 3D8H
Title : Crystal structure of phosphoglycerate mutase from *Cryptosporidium parvum*, cgd7_4270
Authors : Wernimont, A.K.; Lew, J.; Wasney, G.; Alam, Z.; Kozieradzki, I.; Cossar, D.; Schapiro, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Wilkstrom, M.; Edwards, A.M.; Hui, R.; Artz, J.D.; Hills, T.; Structural Genomics Consortium (SGC)
Deposited on : 2008-05-23
Resolution : 2.01 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

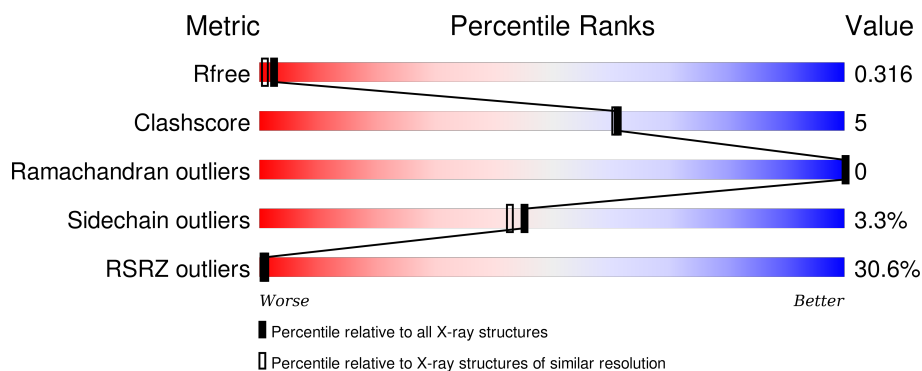
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 $\leq 5\%$. 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	267	
1	B	267	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3871 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 Glycolytic phosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	1	0
			1811	1167	296	339	9			
1	B	235	Total	C	N	O	S	0	3	0
			1854	1193	304	348	9			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q5CXZ9
A	2	GLY	-	EXPRESSION TAG	UNP Q5CXZ9
A	3	SER	-	EXPRESSION TAG	UNP Q5CXZ9
A	4	SER	-	EXPRESSION TAG	UNP Q5CXZ9
A	5	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
A	6	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
A	7	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
A	8	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
A	9	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
A	10	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
A	11	SER	-	EXPRESSION TAG	UNP Q5CXZ9
A	12	SER	-	EXPRESSION TAG	UNP Q5CXZ9
A	13	GLY	-	EXPRESSION TAG	UNP Q5CXZ9
A	14	LEU	-	EXPRESSION TAG	UNP Q5CXZ9
A	15	VAL	-	EXPRESSION TAG	UNP Q5CXZ9
A	16	PRO	-	EXPRESSION TAG	UNP Q5CXZ9
A	17	ARG	-	EXPRESSION TAG	UNP Q5CXZ9
A	18	GLY	-	EXPRESSION TAG	UNP Q5CXZ9
A	19	SER	-	EXPRESSION TAG	UNP Q5CXZ9
B	1	MET	-	EXPRESSION TAG	UNP Q5CXZ9
B	2	GLY	-	EXPRESSION TAG	UNP Q5CXZ9
B	3	SER	-	EXPRESSION TAG	UNP Q5CXZ9
B	4	SER	-	EXPRESSION TAG	UNP Q5CXZ9
B	5	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
B	6	HIS	-	EXPRESSION TAG	UNP Q5CXZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
B	8	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
B	9	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
B	10	HIS	-	EXPRESSION TAG	UNP Q5CXZ9
B	11	SER	-	EXPRESSION TAG	UNP Q5CXZ9
B	12	SER	-	EXPRESSION TAG	UNP Q5CXZ9
B	13	GLY	-	EXPRESSION TAG	UNP Q5CXZ9
B	14	LEU	-	EXPRESSION TAG	UNP Q5CXZ9
B	15	VAL	-	EXPRESSION TAG	UNP Q5CXZ9
B	16	PRO	-	EXPRESSION TAG	UNP Q5CXZ9
B	17	ARG	-	EXPRESSION TAG	UNP Q5CXZ9
B	18	GLY	-	EXPRESSION TAG	UNP Q5CXZ9
B	19	SER	-	EXPRESSION TAG	UNP Q5CXZ9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	114	Total O 114 114	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	52.25Å 158.37Å 140.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.50 – 2.01 40.50 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.50-2.01) 99.7 (40.50-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.256 0.300 , 0.316	Depositor DCC
R_{free} test set	1956 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 39074 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3871	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.1092e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.55	1/1857 (0.1%)	0.57	0/2526
1	B	0.45	0/1906	0.58	0/2590
All	All	0.50	1/3763 (0.0%)	0.58	0/5116

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLN	CD-OE1	10.65	1.47	1.24

There are no bond angle outliers.

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	1811	0	1798	19	0
1	B	1854	0	1826	21	0
2	A	92	0	0	1	0
2	B	114	0	0	0	0
All	All	3871	0	3624	40	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 5.

All (40) 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:95:ASN:H	1:A:95:ASN:HD22	1.46	0.64
1:B:236:ASP:HB3	1:B:238:TYR:H	1.61	0.64
1:A:95:ASN:H	1:A:95:ASN:ND2	1.97	0.62
1:A:142:VAL:HG13	1:A:167:THR:HB	1.85	0.58
1:B:115:LEU:HB3	1:B:120:THR:HG23	1.86	0.58
1:A:236:ASP:HB3	1:A:238:TYR:H	1.71	0.54
1:A:106:GLU:OE1	1:A:203:ASN:HB2	2.09	0.52
1:A:236:ASP:HB2	1:A:240:LYS:H	1.73	0.52
1:A:102:TRP:CD1	1:A:160:ILE:HD13	2.46	0.50
1:B:33:TRP:CZ3	1:B:114:GLY:HA2	2.47	0.49
1:B:105:ASN:O	1:B:204:SER:OG	2.30	0.49
1:B:106:GLU:OE1	1:B:203:ASN:HB2	2.15	0.47
1:B:142:VAL:HG13	1:B:167:THR:HB	1.96	0.47
1:A:108:HIS:HB3	1:A:169[A]:GLU:HB2	1.97	0.47
1:B:31:SER:HA	1:B:47:LEU:HA	1.97	0.47
1:B:102:TRP:CZ2	1:B:164:CYS:HB3	2.50	0.46
1:A:140:PRO:HD3	2:A:300:HOH:O	2.14	0.46
1:A:142:VAL:HG13	1:A:167:THR:CB	2.46	0.46
1:A:147:ASP:HA	1:A:148:PRO:HD2	1.80	0.45
1:A:32:GLU:HA	1:A:35:LYS:HD3	1.98	0.45
1:B:150:TRP:HA	1:B:151:PRO:HD3	1.89	0.45
1:A:216:THR:OG1	1:A:219:GLN:HB2	2.17	0.45
1:A:182:PHE:CZ	1:A:212:LEU:HD21	2.52	0.44
1:B:39:PHE:HE2	1:B:120:THR:HG21	1.81	0.44
1:A:21:TYR:HB2	1:A:235:LEU:HB2	2.00	0.44
1:B:107:ARG:NH1	1:B:132:TRP:O	2.51	0.44
1:B:39:PHE:CE2	1:B:120:THR:HG21	2.53	0.43
1:B:187:ALA:HB3	1:B:188:PRO:HD3	2.01	0.43
1:B:134:ARG:O	1:B:221:LEU:HD22	2.19	0.43
1:A:25:LEU:HD11	1:A:233:LEU:HD11	2.02	0.42
1:B:157:TYR:HA	1:B:160:ILE:HD12	2.01	0.42
1:B:44:ASP:O	1:B:78:LYS:HE2	2.20	0.42
1:B:217:PRO:O	1:B:221:LEU:HG	2.19	0.42
1:B:33:TRP:CH2	1:B:43:THR:HG21	2.56	0.41
1:A:108:HIS:HB3	1:A:169[B]:GLU:HB2	2.03	0.41
1:B:72:VAL:HG11	1:B:84:THR:HG23	2.01	0.41
1:A:165:LEU:HA	1:A:166:PRO:HD3	1.91	0.41
1:B:30:GLU:HG3	1:B:48:SER:OG	2.21	0.41
1:B:75:SER:HB2	1:B:105:ASN:OD1	2.22	0.40
1:A:75:SER:HB2	1:A:105:ASN:OD1	2.21	0.40

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	228/267 (85%)	225 (99%)	3 (1%)	0	100	100
1	B	234/267 (88%)	227 (97%)	7 (3%)	0	100	100
All	All	462/534 (86%)	452 (98%)	10 (2%)	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	198/236 (84%)	189 (96%)	9 (4%)	34	29
1	B	200/236 (85%)	196 (98%)	4 (2%)	63	65
All	All	398/472 (84%)	385 (97%)	13 (3%)	45	43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	35	LYS
1	A	45	VAL
1	A	93	ASN
1	A	94	ILE
1	A	95	ASN
1	A	171	LEU
1	A	204	SER

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Mol	Chain	Res	Type
1	A	218	GLU
1	B	19	SER
1	B	61	MET
1	B	93	ASN
1	B	95	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	116	ASN
1	A	128	GLN

5.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

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	229/267 (85%)	1.68	83 (36%) 0 1	24, 35, 43, 50	0
1	B	235/267 (88%)	1.32	59 (25%) 1 1	31, 36, 40, 51	1 (0%)
All	All	464/534 (86%)	1.50	142 (30%) 1 1	24, 35, 43, 51	1 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	VAL	7.6
1	A	120	THR	6.5
1	A	148	PRO	6.0
1	A	220	ILE	6.0
1	A	124	PHE	5.3
1	A	121	ALA	5.0
1	A	115	LEU	4.9
1	A	146	SER	4.9
1	A	132	TRP	4.9
1	A	111	ALA	4.9
1	A	128	GLN	4.8
1	B	99	ILE	4.8
1	B	131	ILE	4.7
1	B	181	TYR	4.5
1	A	114	GLY	4.5
1	A	155	LEU	4.5
1	B	155	LEU	4.4
1	A	241	VAL	4.3
1	A	244	LYS	4.3
1	A	223	VAL	4.2
1	A	181	TYR	4.2
1	A	116	ASN	4.1
1	A	134	ARG	4.0
1	A	242	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	76	VAL	3.9
1	B	74	THR	3.9
1	B	132	TRP	3.9
1	A	185	VAL	3.9
1	B	98	ILE	3.8
1	A	81	ILE	3.8
1	B	85	TRP	3.8
1	B	124	PHE	3.7
1	A	98	ILE	3.7
1	A	218	GLU	3.6
1	A	233	LEU	3.5
1	B	72	VAL	3.4
1	B	101	HIS	3.4
1	B	247	LEU	3.4
1	B	198	VAL	3.4
1	B	97	PRO	3.4
1	A	112	LEU	3.4
1	B	83	THR	3.3
1	B	185	VAL	3.3
1	A	131	ILE	3.3
1	A	74	THR	3.3
1	A	221	LEU	3.3
1	A	72	VAL	3.2
1	A	87	VAL	3.2
1	A	198	VAL	3.2
1	B	104	LEU	3.2
1	A	94	ILE	3.2
1	A	153	ASN	3.2
1	A	39	PHE	3.2
1	B	180	PRO	3.1
1	A	245	TYR	3.1
1	B	75	SER	3.1
1	B	81	ILE	3.1
1	B	73	TYR	3.1
1	B	129	VAL	3.1
1	A	127	ASP	3.0
1	A	235	LEU	3.0
1	A	247	LEU	3.0
1	B	186	ILE	3.0
1	A	186	ILE	2.9
1	A	22	LYS	2.9
1	B	182	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	220	ILE	2.9
1	A	99	ILE	2.8
1	B	223	VAL	2.8
1	A	187	ALA	2.8
1	B	96	CYS	2.8
1	A	167	THR	2.8
1	A	73	TYR	2.7
1	B	187	ALA	2.7
1	B	148	PRO	2.7
1	A	135	SER	2.7
1	B	153	ASN	2.7
1	A	109	TYR	2.7
1	A	97	PRO	2.7
1	A	165	LEU	2.7
1	A	35	LYS	2.7
1	B	52	VAL	2.7
1	B	178	VAL	2.7
1	B	127	ASP	2.7
1	A	145	LYS	2.7
1	A	85	TRP	2.7
1	B	71	VAL	2.6
1	A	236	ASP	2.6
1	A	71	VAL	2.6
1	B	146	SER	2.6
1	A	234	GLU	2.6
1	A	158	LYS	2.6
1	A	243	LYS	2.6
1	A	110	GLY	2.6
1	A	142	VAL	2.6
1	A	83	THR	2.5
1	A	67	PHE	2.5
1	B	134	ARG	2.5
1	A	102	TRP	2.5
1	B	170	CYS	2.5
1	B	243	LYS	2.5
1	B	156	ILE	2.4
1	B	250	GLU	2.4
1	A	101	HIS	2.4
1	A	180	PRO	2.4
1	B	197	LEU	2.4
1	A	37	ASN	2.4
1	A	215	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	135	SER	2.4
1	B	128	GLN	2.3
1	A	225	ILE	2.3
1	A	150	TRP	2.3
1	A	178	VAL	2.3
1	A	248	ILE	2.3
1	B	16	PRO	2.3
1	B	171	LEU	2.3
1	A	33	TRP	2.3
1	A	133	ARG	2.3
1	A	137	ASP	2.3
1	A	84	THR	2.2
1	B	248	ILE	2.2
1	A	75	SER	2.2
1	A	113	GLN	2.2
1	B	67	PHE	2.2
1	B	102	TRP	2.2
1	B	80	ALA	2.2
1	A	130	LYS	2.2
1	B	77	LEU	2.2
1	B	86	THR	2.2
1	B	82	MET	2.1
1	B	33	TRP	2.1
1	A	188	PRO	2.1
1	A	76	VAL	2.1
1	A	82	MET	2.1
1	B	136	PHE	2.1
1	A	216	THR	2.0
1	A	160	ILE	2.0
1	B	51	GLY	2.0
1	B	122	SER	2.0
1	B	199	SER	2.0
1	A	96	CYS	2.0
1	B	138	VAL	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.