



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:52 AM GMT

PDB ID : 2XSS
Title : CRYSTAL STRUCTURE OF GAFB FROM THE HUMAN PHOSPHODI-
ESTERASE 5
Authors : Schlicker, C.; Russwurm, M.; Steegborn, C.
Deposited on : 2010-09-30
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

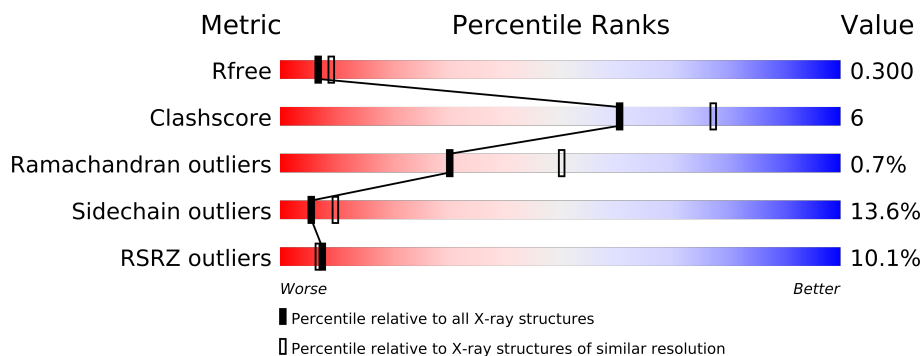
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	181	
1	B	181	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2377 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CGMP-SPECIFIC 3', 5'-CYCLIC PHOSPHODIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1215	768	205	230	12			
1	B	150	Total	C	N	O	S	0	0	0
			1162	738	196	216	12			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	MET	-	EXPRESSION TAG	UNP O76074
A	331	ALA	-	EXPRESSION TAG	UNP O76074
A	332	SER	-	EXPRESSION TAG	UNP O76074
A	333	TRP	-	EXPRESSION TAG	UNP O76074
A	334	SER	-	EXPRESSION TAG	UNP O76074
A	335	HIS	-	EXPRESSION TAG	UNP O76074
A	336	PRO	-	EXPRESSION TAG	UNP O76074
A	337	GLN	-	EXPRESSION TAG	UNP O76074
A	338	PHE	-	EXPRESSION TAG	UNP O76074
A	339	GLU	-	EXPRESSION TAG	UNP O76074
A	340	LYS	-	EXPRESSION TAG	UNP O76074
A	341	GLY	-	EXPRESSION TAG	UNP O76074
A	342	ALA	-	EXPRESSION TAG	UNP O76074
A	343	GLU	-	EXPRESSION TAG	UNP O76074
A	344	THR	-	EXPRESSION TAG	UNP O76074
A	345	ALA	-	EXPRESSION TAG	UNP O76074
A	510	ALA	-	EXPRESSION TAG	UNP O76074
B	330	MET	-	EXPRESSION TAG	UNP O76074
B	331	ALA	-	EXPRESSION TAG	UNP O76074
B	332	SER	-	EXPRESSION TAG	UNP O76074
B	333	TRP	-	EXPRESSION TAG	UNP O76074
B	334	SER	-	EXPRESSION TAG	UNP O76074
B	335	HIS	-	EXPRESSION TAG	UNP O76074
B	336	PRO	-	EXPRESSION TAG	UNP O76074
B	337	GLN	-	EXPRESSION TAG	UNP O76074

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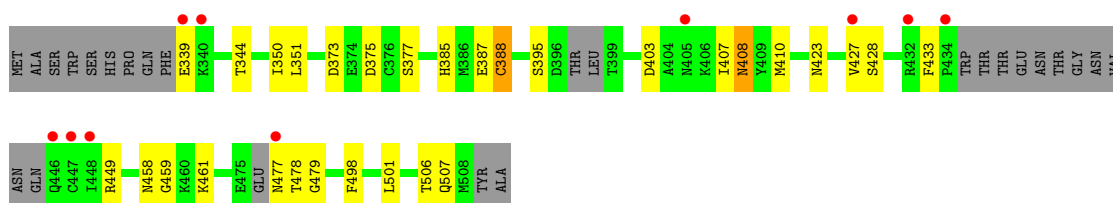
Chain	Residue	Modelled	Actual	Comment	Reference
B	338	PHE	-	EXPRESSION TAG	UNP O76074
B	339	GLU	-	EXPRESSION TAG	UNP O76074
B	340	LYS	-	EXPRESSION TAG	UNP O76074
B	341	GLY	-	EXPRESSION TAG	UNP O76074
B	342	ALA	-	EXPRESSION TAG	UNP O76074
B	343	GLU	-	EXPRESSION TAG	UNP O76074
B	344	THR	-	EXPRESSION TAG	UNP O76074
B	345	ALA	-	EXPRESSION TAG	UNP O76074
B	510	ALA	-	EXPRESSION TAG	UNP O76074

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 errors 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.

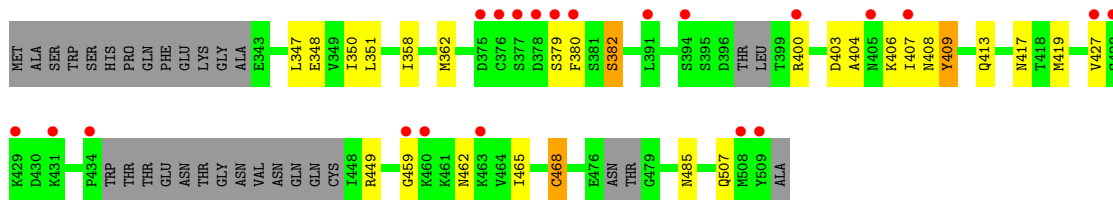
- Molecule 1: CGMP-SPECIFIC 3', 5'-CYCLIC PHOSPHODIESTERASE

Chain A: 



- Molecule 1: CGMP-SPECIFIC 3', 5'-CYCLIC PHOSPHODIESTERASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.75Å 64.75Å 145.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.39 – 2.50 44.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.39-2.50) 99.0 (44.39-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.248 , 0.317 0.242 , 0.300	Depositor DCC
R_{free} test set	631 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.3	EDS
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 12657 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2377	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.72	1/1230 (0.1%)	0.72	0/1647
1	B	0.78	2/1177 (0.2%)	0.75	0/1580
All	All	0.75	3/2407 (0.1%)	0.73	0/3227

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	468	CYS	CB-SG	-8.62	1.67	1.82
1	A	388	CYS	CB-SG	-7.55	1.69	1.82
1	B	409	TYR	CG-CD1	5.17	1.45	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1215	0	0	7	0
1	B	1162	0	0	7	0
All	All	2377	0	0	14	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (14) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:413:GLN:O	1:B:417:ASN:CB	2.38	0.72
1:B:404:ALA:O	1:B:413:GLN:NE2	2.23	0.71
1:B:413:GLN:O	1:B:417:ASN:CG	2.47	0.52
1:A:373:ASP:OD1	1:A:375:ASP:N	2.43	0.52
1:A:410:MET:CE	1:A:433:PHE:CD1	2.93	0.52
1:B:413:GLN:O	1:B:417:ASN:N	2.43	0.51
1:A:408:ASN:OD1	1:A:408:ASN:N	2.44	0.50
1:B:348:GLU:OE2	1:B:382:SER:OG	2.30	0.49
1:A:477:ASN:O	1:A:479:GLY:N	2.46	0.48
1:B:379:SER:OG	1:B:380:PHE:N	2.49	0.46
1:B:403:ASP:O	1:B:409:TYR:CD2	2.71	0.43
1:A:385:HIS:NE2	1:A:387:GLU:OE1	2.51	0.43
1:A:458:ASN:O	1:A:459:GLY:C	2.59	0.41
1:A:458:ASN:O	1:A:461:LYS:N	2.54	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	148/181 (82%)	134 (90%)	13 (9%)	1 (1%)	30	50
1	B	142/181 (78%)	130 (92%)	11 (8%)	1 (1%)	30	50
All	All	290/362 (80%)	264 (91%)	24 (8%)	2 (1%)	30	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	THR
1	B	459	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	135/165 (82%)	117 (87%)	18 (13%)	6	10
1	B	129/165 (78%)	111 (86%)	18 (14%)	5	9
All	All	264/330 (80%)	228 (86%)	36 (14%)	5	10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	GLU
1	A	344	THR
1	A	350	ILE
1	A	351	LEU
1	A	377	SER
1	A	388	CYS
1	A	395	SER
1	A	403	ASP
1	A	407	ILE
1	A	408	ASN
1	A	423	ASN
1	A	427	VAL
1	A	428	SER
1	A	449	ARG
1	A	498	PHE
1	A	501	LEU
1	A	506	THR
1	A	507	GLN
1	B	347	LEU
1	B	350	ILE
1	B	351	LEU
1	B	358	ILE
1	B	362	MET
1	B	382	SER
1	B	400	ARG
1	B	406	LYS
1	B	407	ILE
1	B	408	ASN
1	B	419	MET

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Mol	Chain	Res	Type
1	B	427	VAL
1	B	449	ARG
1	B	462	ASN
1	B	465	ILE
1	B	468	CYS
1	B	485	ASN
1	B	507	GLN

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 chains 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 ⓘ

There are no ligands in this entry.

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 ⓘ

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	156/181 (86%)	0.37	10 (6%)	19 19	27, 53, 103, 131	0
1	B	150/181 (82%)	0.85	21 (14%)	3 3	37, 72, 132, 148	0
All	All	306/362 (84%)	0.61	31 (10%)	7 7	27, 63, 125, 148	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	CYS	9.5
1	A	448	ILE	6.6
1	B	428	SER	6.0
1	B	376	CYS	5.2
1	B	407	ILE	4.9
1	A	340	LYS	4.4
1	A	446	GLN	4.1
1	B	508	MET	4.0
1	B	427	VAL	3.9
1	B	429	LYS	3.7
1	B	378	ASP	3.7
1	B	375	ASP	3.6
1	B	405	ASN	3.5
1	A	427	VAL	3.2
1	B	394	SER	3.0
1	B	377	SER	3.0
1	B	379	SER	3.0
1	B	380	PHE	3.0
1	B	509	TYR	2.8
1	B	460	LYS	2.7
1	A	434	PRO	2.7
1	A	477	ASN	2.6
1	B	400	ARG	2.5
1	B	463	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	339	GLU	2.4
1	B	459	GLY	2.4
1	A	405	ASN	2.2
1	B	391	LEU	2.2
1	B	434	PRO	2.2
1	A	432	ARG	2.1
1	B	431	LYS	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.