



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:52 PM GMT

PDB ID : 3TBF
Title : C-terminal domain of glucosamine-fructose-6-phosphateaminotransferase from *Francisella tularensis*.
Authors : Osipiuk, J.; Zhou, M.; Maltseva, N.; Kim, Y.; Papazisi, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2011-08-05
Resolution : 2.28 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

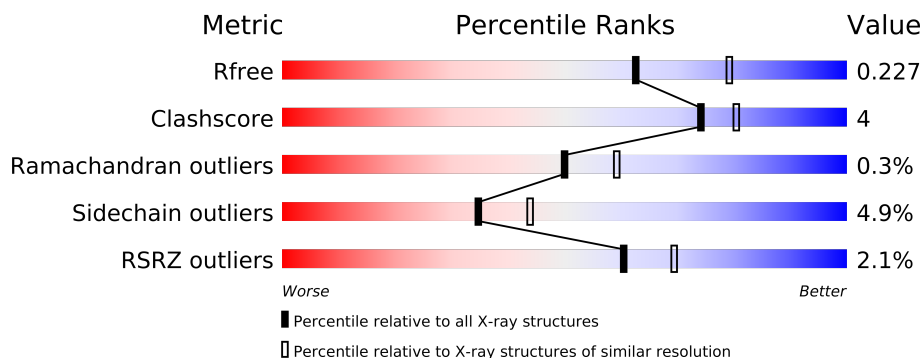
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.28 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	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (2.30-2.26)

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	372	
1	B	372	
1	C	372	
1	D	372	
1	E	372	
1	F	372	
1	G	372	
1	H	372	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22905 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 Glucosamine--fructose-6-phosphateaminotransferase [isomerizing].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	3	0
			2792	1786	456	539	5	6			
1	B	354	Total	C	N	O	S	Se	0	1	0
			2745	1755	447	532	5	6			
1	C	358	Total	C	N	O	S	Se	0	4	0
			2794	1787	455	539	7	6			
1	D	357	Total	C	N	O	S	Se	0	4	0
			2790	1785	455	537	7	6			
1	E	358	Total	C	N	O	S	Se	0	4	0
			2793	1786	455	538	8	6			
1	F	358	Total	C	N	O	S	Se	0	3	0
			2790	1786	455	536	7	6			
1	G	357	Total	C	N	O	S	Se	0	4	0
			2791	1785	454	539	7	6			
1	H	357	Total	C	N	O	S	Se	0	6	0
			2796	1786	456	541	7	6			

- Molecule 2 is water.

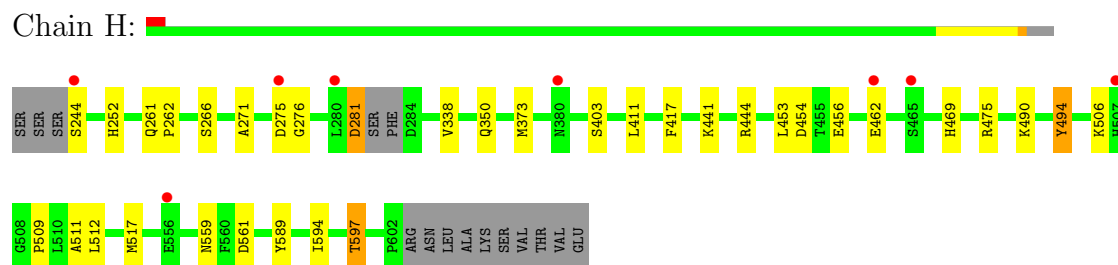
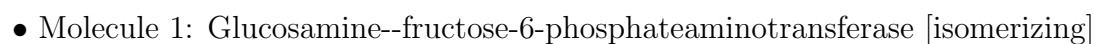
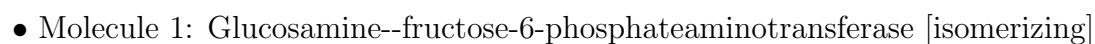
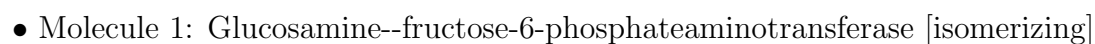
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	1
			68	68		
2	B	66	Total	O	0	0
			66	66		
2	C	97	Total	O	0	0
			97	97		
2	D	97	Total	O	0	0
			97	97		
2	E	93	Total	O	0	0
			93	93		
2	F	85	Total	O	0	0
			85	85		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	51	Total	O	0	0
			51	51		
2	H	57	Total	O	0	0
			57	57		

- Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 262.91Å 83.80Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	45.80 – 2.28 45.80 – 2.28	Depositor EDS
% Data completeness (in resolution range)	74.7 (45.80-2.28) 74.7 (45.80-2.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109 (and PHENIX)	Depositor
R, R_{free}	0.172 , 0.232 0.169 , 0.227	Depositor DCC
R_{free} test set	5212 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 15.7	EDS
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 104079 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22905	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.91	5/2843 (0.2%)	0.81	1/3837 (0.0%)
1	B	0.88	1/2787 (0.0%)	0.77	0/3762
1	C	0.88	1/2847 (0.0%)	0.80	2/3842 (0.1%)
1	D	0.88	2/2842 (0.1%)	0.78	0/3833
1	E	0.91	0/2846	0.77	1/3841 (0.0%)
1	F	0.87	0/2840	0.79	0/3833
1	G	0.81	0/2844	0.75	0/3838
1	H	0.84	0/2853	0.76	0/3849
All	All	0.87	9/22702 (0.0%)	0.78	4/30635 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	CYS	CB-SG	-7.25	1.70	1.82
1	D	302	CYS	CB-SG	-7.05	1.70	1.82
1	C	538	GLU	CG-CD	6.17	1.61	1.51
1	A	376	CYS	CB-SG	5.85	1.92	1.82
1	A	438	GLU	CG-CD	5.69	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	475	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	286	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	E	582	ILE	CG1-CB-CG2	-5.45	99.41	111.40
1	C	475	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	2792	0	0	7	0
1	B	2745	0	0	10	0
1	C	2794	0	0	6	0
1	D	2790	0	0	13	0
1	E	2793	0	0	16	0
1	F	2790	0	0	18	0
1	G	2791	0	0	17	0
1	H	2796	0	0	12	0
2	A	68	0	0	0	0
2	B	66	0	0	0	0
2	C	97	0	0	1	0
2	D	97	0	0	4	0
2	E	93	0	0	3	0
2	F	85	0	0	3	0
2	G	51	0	0	2	0
2	H	57	0	0	1	0
All	All	22905	0	0	92	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 4.

The worst 5 of 92 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:302[B]:CYS:SG	1:F:507:HIS:NE2	2.35	0.99
1:F:298:CYS:SG	2:F:634:HOH:O	2.37	0.82
1:G:484:GLU:OE2	1:G:488:LYS:NZ	2.16	0.79
1:F:395:ALA:O	1:F:405:LYS:NZ	2.20	0.74
1:F:341:ASP:OD1	1:F:368:ASN:ND2	2.22	0.72

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	358/372 (96%)	348 (97%)	10 (3%)	0	100	100
1	B	351/372 (94%)	339 (97%)	11 (3%)	1 (0%)	50	59
1	C	360/372 (97%)	349 (97%)	8 (2%)	3 (1%)	27	29
1	D	359/372 (96%)	348 (97%)	11 (3%)	0	100	100
1	E	360/372 (97%)	350 (97%)	9 (2%)	1 (0%)	50	59
1	F	359/372 (96%)	348 (97%)	9 (2%)	2 (1%)	33	38
1	G	359/372 (96%)	343 (96%)	16 (4%)	0	100	100
1	H	359/372 (96%)	338 (94%)	19 (5%)	2 (1%)	33	38
All	All	2865/2976 (96%)	2763 (96%)	93 (3%)	9 (0%)	50	59

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	508	GLY
1	B	506	LYS
1	C	368	ASN
1	H	271	ALA
1	H	275	ASP

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	310/314 (99%)	297 (96%)	13 (4%)	40	51
1	B	304/314 (97%)	285 (94%)	19 (6%)	25	31
1	C	311/314 (99%)	294 (94%)	17 (6%)	30	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	310/314 (99%)	292 (94%)	18 (6%)	28	34
1	E	311/314 (99%)	302 (97%)	9 (3%)	55	69
1	F	310/314 (99%)	300 (97%)	10 (3%)	51	66
1	G	311/314 (99%)	294 (94%)	17 (6%)	30	37
1	H	312/314 (99%)	295 (95%)	17 (5%)	31	38
All	All	2479/2512 (99%)	2359 (95%)	120 (5%)	35	45

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	290	LEU
1	E	266	SER
1	H	456	GLU
1	D	332	ILE
1	D	399	ILE

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	357/372 (95%)	-0.23	3 (0%) 83 89	9, 24, 48, 59	0
1	B	354/372 (95%)	-0.19	6 (1%) 67 75	12, 29, 52, 74	0
1	C	358/372 (96%)	-0.33	6 (1%) 67 75	13, 27, 48, 67	0
1	D	357/372 (95%)	-0.13	12 (3%) 43 52	14, 30, 52, 65	0
1	E	358/372 (96%)	-0.12	8 (2%) 59 68	13, 26, 50, 66	0
1	F	358/372 (96%)	-0.17	6 (1%) 67 75	13, 30, 51, 62	0
1	G	357/372 (95%)	0.00	12 (3%) 43 52	17, 35, 62, 77	0
1	H	357/372 (95%)	-0.13	8 (2%) 59 68	14, 33, 63, 76	0
All	All	2856/2976 (95%)	-0.16	61 (2%) 60 69	9, 29, 54, 77	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	LEU	6.1
1	G	289[A]	GLU	4.8
1	H	280	LEU	4.7
1	D	285	LYS	4.2
1	G	285	LYS	4.1

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.