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wwPDB X-ray Structure Validation Summary Report (i)

Oct 29, 2024 – 06:25 AM EDT

PDB ID	:	3TBF
Title	:	C-terminal domain of glucosamine-fructose-6-phosphate aminotransferase 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)

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

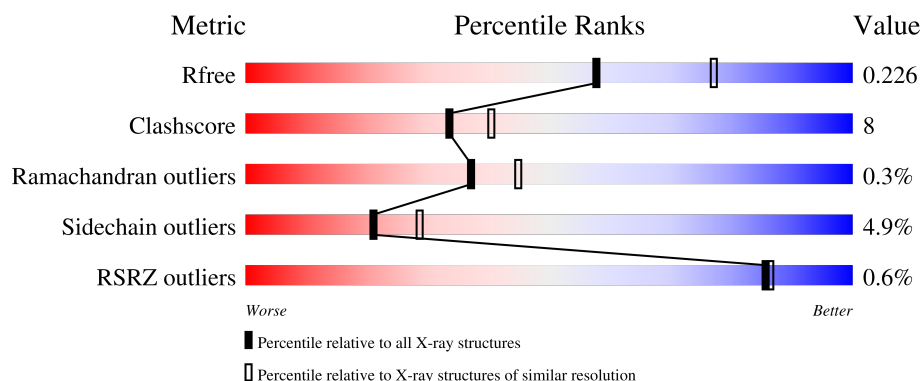|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.28 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		4.9%
RSRZ outliers		0.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	372	77% 18% · ·
1	B	372	% 76% 17% · 5%
1	C	372	78% 17% · ·
1	D	372	79% 16% · ·

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Mol	Chain	Length	Quality of chain
1	E	372	81% 15%
1	F	372	% 80% 15%
1	G	372	% 73% 21%
1	H	372	2% 73% 21%

2 Entry composition (i)

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

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

- Molecule 2 is water.

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

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

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain A:

- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain B:

- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain C:

F574 S575 I582 A592 P602 ARG ASN LEU ALA LYS SER VAL THR VAL GLU

• Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain D:

79%   16%

SER SER SER A245 S246 K256 E257 S266 L270 I278 S279 L280 D284 K285 L290 C302 P323 I332 R333 Y334 G342 S349 G352 V370 C374 I375 C376 N377 L383 I389 A390 F391 M392 T393 K394 A395 I399 S403 T404 K405

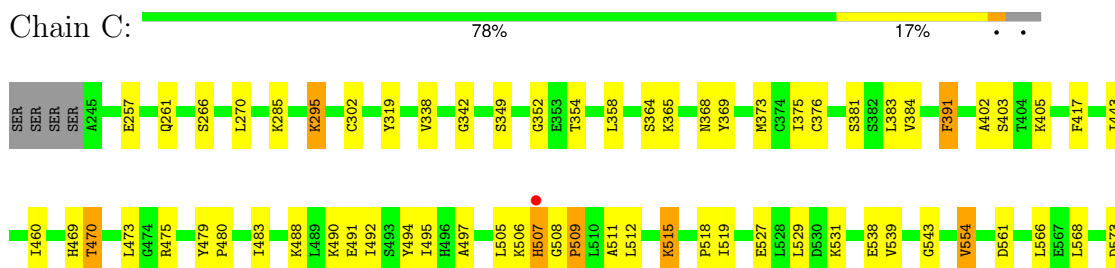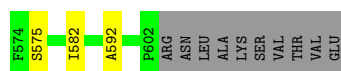T437 E438 E439 H469 T470 R475 Y479 P480 I483 E484 K488 L489 K490 Y494 A497 Y500 P501 S502 K506 H507 G508 P509 L510 A511 K515 V523 E527 D530 G543 V550 V554 K555 E556 R557 N562 L568 Q601 PRO ARG ASN LEU

ALA LYS SER VAL THR VAL GLU

• Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain E:

81%   15%

SER SER SER A245 S246 K256 V265 S266 A274 D275 D284 K285 R286 A287 K288 E292 C302 G303 T304 S305 Y306 Y334 M373 C374 I375 C376 N377 I389 A390 F391 G400 V401 A402 S403 V412 F417 L424 M448 I460 H469 T470 Y479

P480 E484 K488 A497 K506 H507 G508 P509 L510 K515 E527 K531 G543 K552 N562 S563 I564 E567 L568 D573 A576 P577 I582 L587 V591 Q601 P602 ARG ASN LEU ALA LYS SER VAL THR VAL GLU

• Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain F:

80%   15%

SER SER SER A245 E257 V265 L270 K285 K295 C302 G303 T304 M310 T311 A312 A329 R333 D341 S349 Q350 S351 G352 D356 N368 C376 N377 L383 F391 A395 S403 T404 K405 V412 A413 L414 T429 I433

L446 D454 S465 H469 I483 E484 K488 L489 K490 E491 I492 S502 L505 K506 H507 G508 P509 L510 P518 I519 V523 K531 N535 V539 R642 V550 D561 L568 V579 V580 T581 I582 P583 L586 L587 S588 A592 I593 I594 P602

ARG ASN LEU ALA LYS SER VAL THR VAL GLU

• Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain G:

73%   21%

SER SER SER SER ALA S246 K256 E257 L270 L273 G276 L280 K288 F291 E292 K295 H296 I297 C298 T304 V322 P323 V338 D341 G342 L344 F345 S349 G352 A355 E359 R362 N368 S372 M373 C376 N377 N380

L383 V384 R385 E386 I389 A390 F391 A395 G396 V397 E398 A402 S403 T404 K405 A406 L424 K425 E456 I460 Y463 F464 S465 H469 T470 I471 F472 R475 E484 L487 K488 L489 K490 E491 H496 Y500 P501 S502 G503 E504 L505 K506 H507 G508 P509 L510

A511 K515 P518 I519 V520 V523 L529 L533 V539 G543 V550 D551 V554 K555 E556 I564 E567 L668 I594 T597 D598 P602 ARG ASN LEU ALA LYS SER VAL THR VAL GLU

● Molecule 1: Glucosamine–fructose-6-phosphate aminotransferase [isomerizing]

Chain H:

2%

73% 21%

SER SER SER S244 K256 E257 I258 Y259 E260 Q261 P262 V265 S266 I269 L270 A271 S272 L273 A274 D275 G276 L280 D281 SER PHE D284 K285 R286 L290 F291 E292 T304 M310 Y314 P323 R333 V338 L344 Q350 E359 S360 L361 V370 G371 S372

M373 C374 I375 C376 L383 E398 A402 S403 T404 K405 L411 V412 I416 F417 L424 L451 K452 L453 D454 T455 E456 I460 S461 E462 H469 T470 R475 G476 L477 Y478 Y479 P480 I483 E484 L487 K488 L489 K490 E491 I492 S493 Y494 Y500 P501 S502 G503 E504

L505 K506 H507 G508 P509 L510 A511 L512 V513 M517 P518 I519 V539 D551 V554 N559 F560 D561 L566 E567 L568 I582 P583 A592 I593 I594 T597 P602 ARG ASN LEU ALA LYS SER VAL THR VAL GLU

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
$< I/\sigma(I) >$ [1]	4.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.172 , 0.232 0.169 , 0.226	Depositor DCC
R_{free} test set	5213 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.8	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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 Too-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 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	2792	0	2840	38	0
1	B	2745	0	2792	44	0
1	C	2794	0	2847	43	0
1	D	2790	0	2850	36	0
1	E	2793	0	2847	39	0
1	F	2790	0	2847	46	0
1	G	2791	0	2841	61	0
1	H	2796	0	2852	58	0
2	A	68	0	0	0	0
2	B	66	0	0	2	0
2	C	97	0	0	0	0
2	D	97	0	0	2	0
2	E	93	0	0	4	0
2	F	85	0	0	2	0
2	G	51	0	0	1	0
2	H	57	0	0	0	0
All	All	22905	0	22716	342	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 8.

The worst 5 of 342 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:E:302[B]:CYS:SG	1:F:507:HIS:NE2	2.35	0.99
1:E:302[B]:CYS:HG	1:F:507:HIS:HE2	0.88	0.88
1:H:257:GLU:HG2	1:H:405:LYS:HE2	1.63	0.81
1:D:374[A]:CYS:SG	1:D:376[A]:CYS:HB2	2.23	0.79
1:G:484:GLU:OE2	1:G:488:LYS:NZ	2.16	0.79

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%)	37	45
1	C	360/372 (97%)	349 (97%)	8 (2%)	3 (1%)	16	19
1	D	359/372 (96%)	348 (97%)	11 (3%)	0	100	100
1	E	360/372 (97%)	350 (97%)	9 (2%)	1 (0%)	37	45
1	F	359/372 (96%)	348 (97%)	9 (2%)	2 (1%)	22	25
1	G	359/372 (96%)	343 (96%)	16 (4%)	0	100	100
1	H	359/372 (96%)	338 (94%)	19 (5%)	2 (1%)	22	25
All	All	2865/2976 (96%)	2763 (96%)	93 (3%)	9 (0%)	37	45

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%)	25	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	304/314 (97%)	285 (94%)	19 (6%)	15	19
1	C	311/314 (99%)	294 (94%)	17 (6%)	18	24
1	D	310/314 (99%)	292 (94%)	18 (6%)	17	22
1	E	311/314 (99%)	302 (97%)	9 (3%)	37	51
1	F	310/314 (99%)	300 (97%)	10 (3%)	34	47
1	G	311/314 (99%)	294 (94%)	17 (6%)	18	24
1	H	312/314 (99%)	295 (95%)	17 (5%)	18	24
All	All	2479/2512 (99%)	2359 (95%)	120 (5%)	21	29

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

Mol	Chain	Res	Type
1	D	383	LEU
1	H	456	GLU
1	E	403	SER
1	H	411	LEU
1	H	561	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	377	ASN
1	H	261	GLN
1	H	585	GLN
1	H	469	HIS
1	D	410	GLN

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 oligosaccharides 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	351/372 (94%)	-0.56	0	100	100	9, 24, 48, 58	3 (0%)
1	B	348/372 (93%)	-0.45	5 (1%)	73	74	12, 29, 52, 74	1 (0%)
1	C	352/372 (94%)	-0.52	1 (0%)	90	91	13, 27, 48, 67	4 (1%)
1	D	351/372 (94%)	-0.45	1 (0%)	90	91	14, 30, 52, 65	4 (1%)
1	E	352/372 (94%)	-0.55	1 (0%)	90	91	13, 26, 50, 66	4 (1%)
1	F	352/372 (94%)	-0.44	2 (0%)	85	86	13, 29, 51, 62	3 (0%)
1	G	351/372 (94%)	-0.27	2 (0%)	85	86	17, 35, 62, 77	4 (1%)
1	H	351/372 (94%)	-0.26	6 (1%)	69	70	14, 33, 63, 76	6 (1%)
All	All	2808/2976 (94%)	-0.44	18 (0%)	85	86	9, 29, 54, 77	29 (1%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	280	LEU	4.2
1	B	280	LEU	3.4
1	H	281	ASP	2.9
1	C	507	HIS	2.9
1	H	507	HIS	2.9

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 monosaccharides in this entry.

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6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.