



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 11:05 pm BST

PDB ID : 3EUA
Title : CRYSTAL STRUCTURE OF A PUTATIVE PHOSPHOSUGAR ISOMERASE (BSU32610) FROM BACILLUS SUBTILIS AT 1.90 Å RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-10-09
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

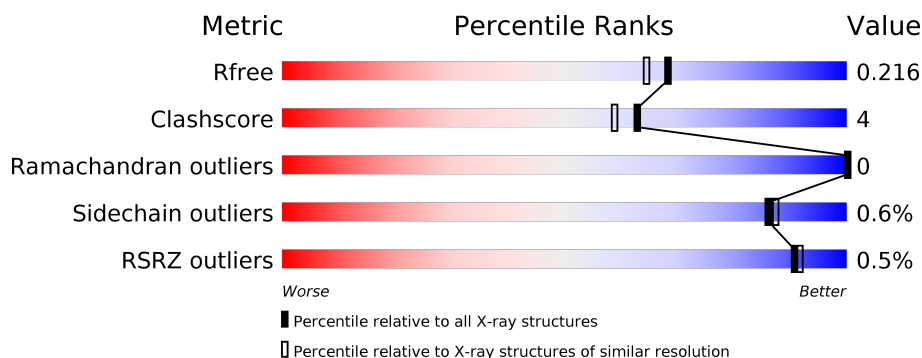
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 $\leq 5\%$. 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	329	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	329	<div> <div>%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	C	329	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	D	329	<div> <div>%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	E	329	<div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	F	329	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	329	<div><div></div><div>91%</div><div>8%</div></div>
1	H	329	<div>%<div><div></div><div>92%</div><div>7%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22425 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 PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	Se	0	2	0
			2574	1648	425	491	3	7			
1	B	324	Total	C	N	O	S	Se	0	3	0
			2560	1642	421	486	3	8			
1	C	324	Total	C	N	O	S	Se	0	3	0
			2578	1652	425	490	3	8			
1	D	324	Total	C	N	O	S	Se	0	4	0
			2579	1656	427	485	3	8			
1	E	324	Total	C	N	O	S	Se	0	3	0
			2567	1648	424	485	3	7			
1	F	329	Total	C	N	O	S	Se	0	4	0
			2619	1677	431	499	3	9			
1	G	328	Total	C	N	O	S	Se	0	3	0
			2608	1670	432	495	3	8			
1	H	327	Total	C	N	O	S	Se	0	3	0
			2594	1663	428	493	3	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP O32157
B	0	GLY	-	leader sequence	UNP O32157
C	0	GLY	-	leader sequence	UNP O32157
D	0	GLY	-	leader sequence	UNP O32157
E	0	GLY	-	leader sequence	UNP O32157
F	0	GLY	-	leader sequence	UNP O32157
G	0	GLY	-	leader sequence	UNP O32157
H	0	GLY	-	leader sequence	UNP O32157

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

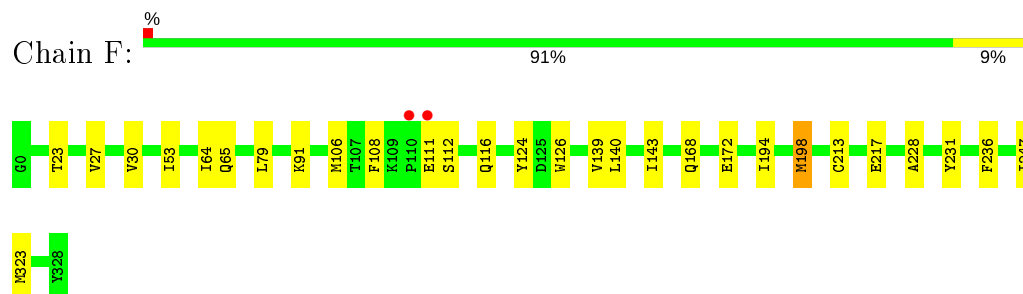


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

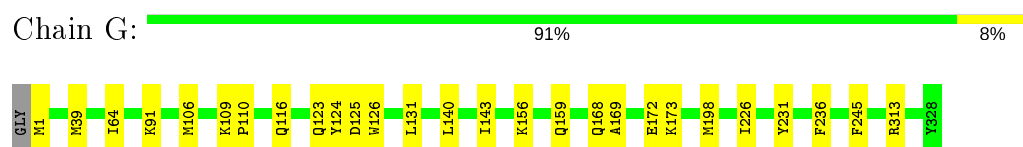
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total 167	O 167	0	2
4	B	176	Total 177	O 177	0	1
4	C	175	Total 175	O 175	0	0
4	D	157	Total 158	O 158	0	1
4	E	179	Total 180	O 180	0	1
4	F	193	Total 194	O 194	0	1
4	G	180	Total 180	O 180	0	0
4	H	477	Total 477	O 477	0	0

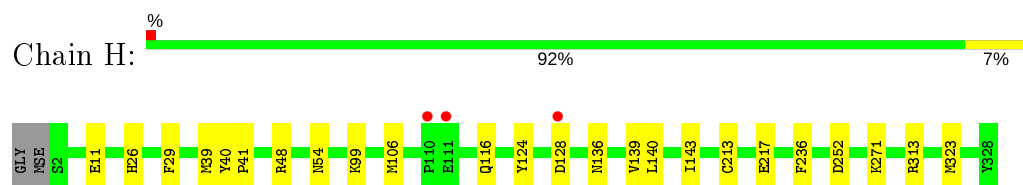
- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE



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- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.86Å 91.82Å 119.04Å 109.30° 100.45° 96.55°	Depositor
Resolution (Å)	29.98 – 1.90 29.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.98-1.90) 97.1 (29.97-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.168 , 0.212 0.175 , 0.216	Depositor DCC
R_{free} test set	8990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22425	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 52.31 % 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 4.9555e-05. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FLC

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	0.71	1/2626 (0.0%)	0.81	4/3549 (0.1%)
1	B	0.70	0/2612	0.80	2/3531 (0.1%)
1	C	0.74	1/2630 (0.0%)	0.81	2/3552 (0.1%)
1	D	0.75	1/2631 (0.0%)	0.80	0/3553
1	E	0.77	0/2619	0.83	2/3539 (0.1%)
1	F	0.83	3/2670 (0.1%)	0.83	1/3602 (0.0%)
1	G	0.79	1/2660 (0.0%)	0.85	2/3591 (0.1%)
1	H	0.77	1/2646 (0.0%)	0.85	3/3575 (0.1%)
All	All	0.76	8/21094 (0.0%)	0.82	16/28492 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	111	GLU	CG-CD	6.79	1.62	1.51
1	H	11	GLU	CD-OE1	6.62	1.32	1.25
1	C	198	MSE	SE-CE	-6.08	1.59	1.95
1	A	111	GLU	CG-CD	5.84	1.60	1.51
1	F	198[A]	MSE	SE-CE	-5.78	1.61	1.95

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	252	ASP	CB-CG-OD1	7.71	125.24	118.30
1	E	313	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	F	313	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	G	1	MSE	N-CA-C	6.19	127.72	111.00
1	E	313	ARG	NE-CZ-NH2	-6.15	117.23	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	2574	0	2490	26	0
1	B	2560	0	2470	24	0
1	C	2578	0	2500	29	0
1	D	2579	0	2505	18	0
1	E	2567	0	2494	19	0
1	F	2619	0	2544	31	0
1	G	2608	0	2538	22	0
1	H	2594	0	2513	17	0
2	C	13	0	5	0	0
2	H	13	0	5	0	0
3	C	6	0	8	0	0
3	H	6	0	8	0	0
4	A	167	0	0	0	0
4	B	177	0	0	1	0
4	C	175	0	0	0	0
4	D	158	0	0	0	0
4	E	180	0	0	0	0
4	F	194	0	0	1	0
4	G	180	0	0	4	0
4	H	477	0	0	2	0
All	All	22425	0	20080	174	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 4.

The worst 5 of 174 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:106[B]:MSE:CE	1:E:106[B]:MSE:SE	2.20	1.40
1:F:198[A]:MSE:HE3	1:F:228:ALA:HA	1.30	1.13
1:B:198:MSE:HE3	1:B:226:ILE:HB	1.32	1.09
1:A:198:MSE:HE3	1:A:228:ALA:HA	1.36	1.06
1:G:198:MSE:HE2	1:G:226:ILE:HB	1.47	0.94

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	325/329 (99%)	316 (97%)	9 (3%)	0	100	100
1	B	325/329 (99%)	318 (98%)	7 (2%)	0	100	100
1	C	325/329 (99%)	318 (98%)	7 (2%)	0	100	100
1	D	326/329 (99%)	319 (98%)	7 (2%)	0	100	100
1	E	325/329 (99%)	317 (98%)	8 (2%)	0	100	100
1	F	331/329 (101%)	323 (98%)	8 (2%)	0	100	100
1	G	329/329 (100%)	323 (98%)	6 (2%)	0	100	100
1	H	328/329 (100%)	323 (98%)	5 (2%)	0	100	100
All	All	2614/2632 (99%)	2557 (98%)	57 (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	266/267 (100%)	265 (100%)	1 (0%)	91	91
1	B	263/267 (98%)	261 (99%)	2 (1%)	81	82
1	C	267/267 (100%)	264 (99%)	3 (1%)	73	73
1	D	265/267 (99%)	263 (99%)	2 (1%)	81	82
1	E	265/267 (99%)	263 (99%)	2 (1%)	81	82
1	F	271/267 (102%)	270 (100%)	1 (0%)	91	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	270/267 (101%)	268 (99%)	2 (1%)	84	84
1	H	267/267 (100%)	266 (100%)	1 (0%)	91	91
All	All	2134/2136 (100%)	2120 (99%)	14 (1%)	86	84

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	79	LEU
1	D	236	PHE
1	G	159	GLN
1	C	323[B]	MSE
1	F	236	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 ⓘ

4 ligands are modelled in this entry.

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
2	FLC	H	329	-	3,12,12	0.55	0	3,17,17	1.87	1 (33%)
3	GOL	H	330	-	5,5,5	0.57	0	5,5,5	0.48	0
2	FLC	C	329	-	3,12,12	0.61	0	3,17,17	0.75	0
3	GOL	C	330	-	5,5,5	0.46	0	5,5,5	0.89	0

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
2	FLC	H	329	-	-	0/6/16/16	-
3	GOL	H	330	-	-	3/4/4/4	-
2	FLC	C	329	-	-	1/6/16/16	-
3	GOL	C	330	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	329	FLC	CB-CA-CAC	-2.99	110.20	114.98

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	330	GOL	C1-C2-C3-O3
3	C	330	GOL	C1-C2-C3-O3
3	H	330	GOL	O2-C2-C3-O3
3	C	330	GOL	O2-C2-C3-O3
2	C	329	FLC	OHB-CB-CG-CGC

There are no ring outliers.

No monomer is involved in short contacts.

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	319/329 (96%)	-0.31	1 (0%) 94 94	17, 22, 29, 36	0
1	B	318/329 (96%)	-0.23	2 (0%) 89 90	17, 22, 29, 36	0
1	C	318/329 (96%)	-0.29	2 (0%) 89 90	17, 22, 30, 38	0
1	D	318/329 (96%)	-0.20	2 (0%) 89 90	17, 22, 28, 37	0
1	E	318/329 (96%)	-0.36	1 (0%) 94 94	17, 22, 29, 37	0
1	F	322/329 (97%)	-0.36	2 (0%) 89 90	17, 22, 30, 38	0
1	G	321/329 (97%)	-0.29	0 100 100	17, 22, 30, 48	0
1	H	321/329 (97%)	-0.37	3 (0%) 84 85	17, 22, 30, 42	0
All	All	2555/2632 (97%)	-0.30	13 (0%) 91 92	17, 22, 30, 48	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	110	PRO	5.4
1	B	110	PRO	4.5
1	C	6	ALA	2.7
1	A	327	GLU	2.6
1	C	110	PRO	2.6

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 [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. 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	B-factors(\AA^2)	Q<0.9
3	GOL	C	330	6/6	0.80	0.19	41,46,47,49	0
2	FLC	C	329	13/13	0.81	0.16	38,42,44,47	0
2	FLC	H	329	13/13	0.81	0.17	35,40,44,46	0
3	GOL	H	330	6/6	0.86	0.28	37,37,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.