



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1XFH
Title : Structure of glutamate transporter homolog from *Pyrococcus horikoshii*
Authors : Yernool, D.; Boudker, O.; Jin, Y.; Gouaux, E.
Deposited on : 2004-09-14
Resolution : 3.50 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
<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

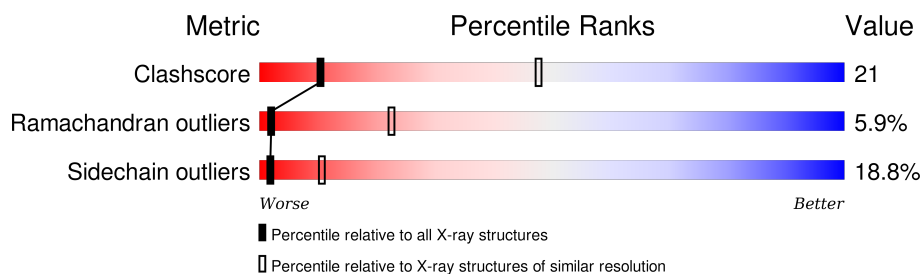
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	422	 49% 36% 10% . .
1	B	422	 48% 40% 8% .
1	C	422	 54% 34% 9% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8652 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 proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			
1	B	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			
1	C	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	ENGINEERED	UNP O59010
A	40	HIS	LYS	ENGINEERED	UNP O59010
A	125	HIS	LYS	ENGINEERED	UNP O59010
A	132	HIS	LYS	ENGINEERED	UNP O59010
A	223	HIS	LYS	ENGINEERED	UNP O59010
A	264	HIS	LYS	ENGINEERED	UNP O59010
A	368	HIS	GLU	ENGINEERED	UNP O59010
A	418	THR	-	CLONING ARTIFACT	UNP O59010
A	419	LEU	-	CLONING ARTIFACT	UNP O59010
A	420	VAL	-	CLONING ARTIFACT	UNP O59010
A	421	PRO	-	CLONING ARTIFACT	UNP O59010
A	422	ARG	-	CLONING ARTIFACT	UNP O59010
B	37	HIS	ASP	ENGINEERED	UNP O59010
B	40	HIS	LYS	ENGINEERED	UNP O59010
B	125	HIS	LYS	ENGINEERED	UNP O59010
B	132	HIS	LYS	ENGINEERED	UNP O59010
B	223	HIS	LYS	ENGINEERED	UNP O59010
B	264	HIS	LYS	ENGINEERED	UNP O59010
B	368	HIS	GLU	ENGINEERED	UNP O59010
B	418	THR	-	CLONING ARTIFACT	UNP O59010
B	419	LEU	-	CLONING ARTIFACT	UNP O59010
B	420	VAL	-	CLONING ARTIFACT	UNP O59010
B	421	PRO	-	CLONING ARTIFACT	UNP O59010

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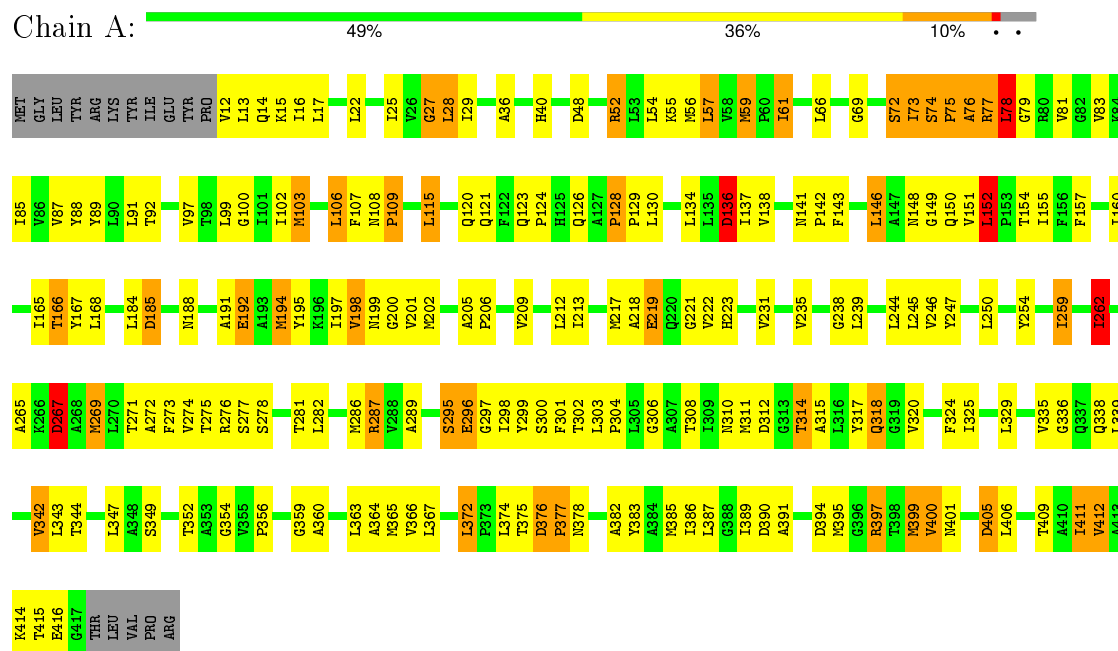
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ARG	-	CLONING ARTIFACT	UNP O59010
C	37	HIS	ASP	ENGINEERED	UNP O59010
C	40	HIS	LYS	ENGINEERED	UNP O59010
C	125	HIS	LYS	ENGINEERED	UNP O59010
C	132	HIS	LYS	ENGINEERED	UNP O59010
C	223	HIS	LYS	ENGINEERED	UNP O59010
C	264	HIS	LYS	ENGINEERED	UNP O59010
C	368	HIS	GLU	ENGINEERED	UNP O59010
C	418	THR	-	CLONING ARTIFACT	UNP O59010
C	419	LEU	-	CLONING ARTIFACT	UNP O59010
C	420	VAL	-	CLONING ARTIFACT	UNP O59010
C	421	PRO	-	CLONING ARTIFACT	UNP O59010
C	422	ARG	-	CLONING ARTIFACT	UNP O59010

3 Residue-property plots

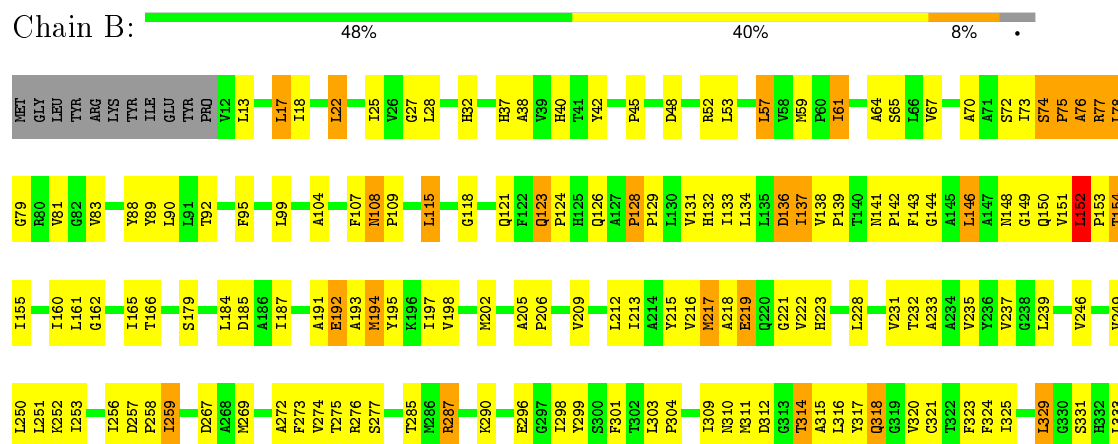
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

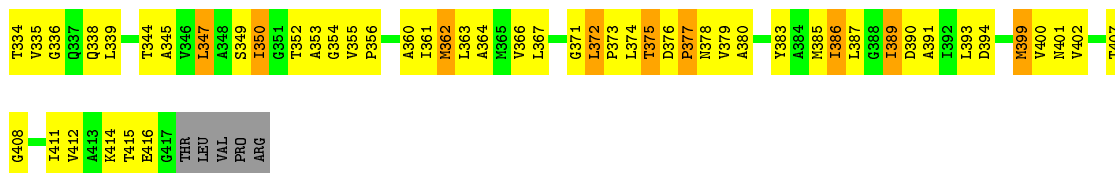
Note EDS was not executed.

- Molecule 1: proton glutamate symport protein



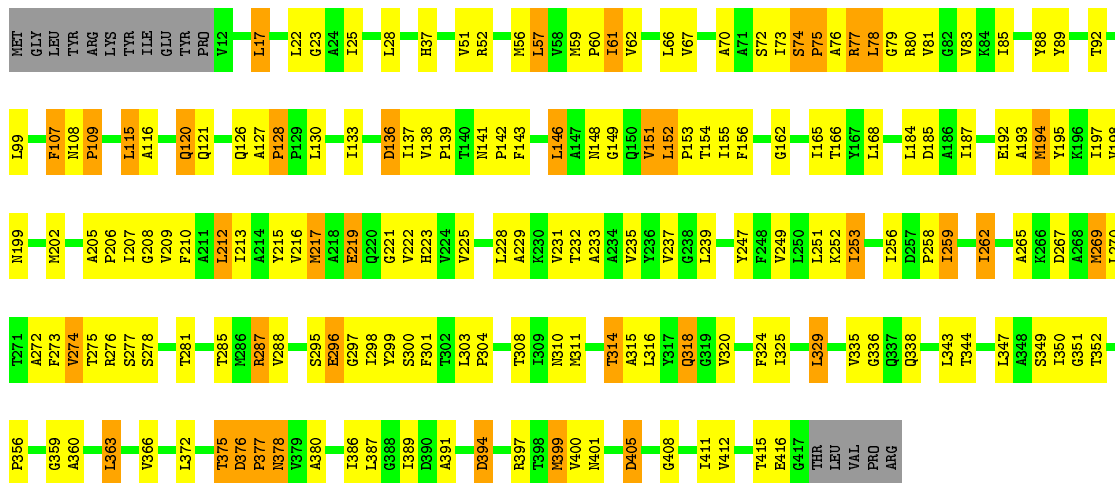
- Molecule 1: proton glutamate symport protein





- Molecule 1: proton glutamate symport protein

Chain C: 54% 34% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	116.00Å 116.00Å 322.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50	Depositor
% Data completeness (in resolution range)	97.1 (10.00-3.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.290 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8652	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

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	0.61	1/2937 (0.0%)	0.85	8/4019 (0.2%)
1	B	0.51	1/2937 (0.0%)	0.75	3/4019 (0.1%)
1	C	0.51	1/2937 (0.0%)	0.77	3/4019 (0.1%)
All	All	0.54	3/8811 (0.0%)	0.79	14/12057 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLU	C-N	-5.61	1.23	1.33
1	B	416	GLU	C-N	-5.29	1.23	1.33
1	C	416	GLU	C-N	-5.25	1.23	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	394	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	136	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	394	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	149	GLY	N-CA-C	-5.91	98.31	113.10
1	A	390	ASP	CB-CG-OD2	5.76	123.49	118.30

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	2884	0	2927	135	0
1	B	2884	0	2927	137	0
1	C	2884	0	2927	116	0
All	All	8652	0	8781	374	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 21.

The worst 5 of 374 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:155:ILE:HD11	1:A:304:PRO:HB2	1.40	1.02
1:C:81:VAL:HG21	1:C:298:ILE:HD12	1.42	1.01
1:A:81:VAL:HG21	1:A:298:ILE:HD12	1.46	0.96
1:A:109:PRO:HB3	1:A:324:PHE:HA	1.48	0.92
1:A:138:VAL:O	1:C:52:ARG:NH1	2.03	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	404/422 (96%)	301 (74%)	69 (17%)	34 (8%)	1	13
1	B	404/422 (96%)	316 (78%)	70 (17%)	18 (4%)	3	30
1	C	404/422 (96%)	311 (77%)	74 (18%)	19 (5%)	3	29
All	All	1212/1266 (96%)	928 (77%)	213 (18%)	71 (6%)	2	22

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LEU

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Mol	Chain	Res	Type
1	A	75	PRO
1	A	76	ALA
1	A	77	ARG
1	A	356	PRO

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	279/330 (84%)	226 (81%)	53 (19%)	2	10
1	B	279/330 (84%)	225 (81%)	54 (19%)	2	10
1	C	279/330 (84%)	229 (82%)	50 (18%)	2	13
All	All	837/990 (84%)	680 (81%)	157 (19%)	2	11

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	126	GLN
1	B	259	ILE
1	C	318	GLN
1	B	137	ILE
1	B	179	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	ASN
1	B	310	ASN
1	C	148	ASN
1	B	108	ASN
1	C	150	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.