wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 11:52 AM EST

PDB ID	:	4OYE
Title	:	Crystal structure of GltPh R397A in apo
Authors	:	Boudker, O.; Oh, S.
Deposited on	:	2014-02-11
Resolution	:	4.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

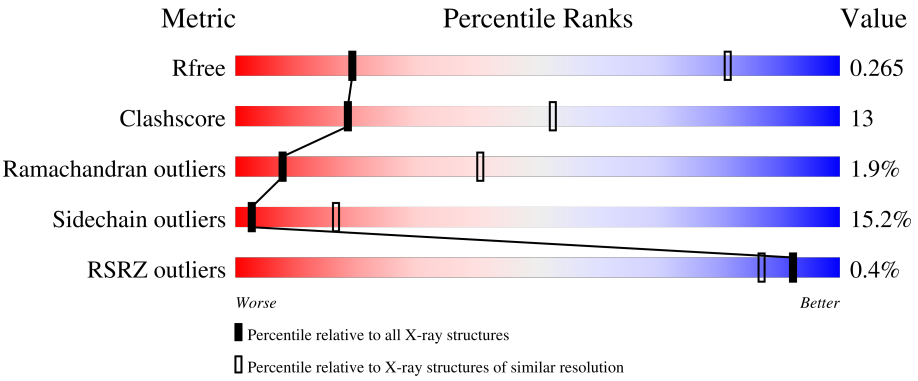
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	409	65% 28% 5%
1	B	409	% 69% 24% 5%
1	C	409	66% 28%
1	D	409	68% 25% 5%
1	E	409	69% 24% 6%

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Mol	Chain	Length	Quality of chain
1	F	409	68% 25% 5%
1	G	409	68% 25% 5%
1	H	409	68% 25% 5%
1	I	409	65% 28% 5%
1	J	409	67% 26% 5%
1	K	409	68% 24% 6%
1	L	409	68% 25% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 35277 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			2925	1930	465	513	17			
1	B	404	Total	C	N	O	S	0	0	0
			2939	1938	468	516	17			
1	C	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	D	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	E	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	F	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	G	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	H	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	I	403	Total	C	N	O	S	0	0	0
			2934	1935	467	515	17			
1	J	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	K	404	Total	C	N	O	S	0	0	0
			2939	1937	468	517	17			
1	L	404	Total	C	N	O	S	0	0	0
			2939	1938	469	515	17			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
A	368	HIS	GLU	engineered mutation	UNP O59010
A	397	ALA	ARG	engineered mutation	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	397	ALA	ARG	engineered mutation	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	397	ALA	ARG	engineered mutation	UNP O59010
D	37	HIS	ASP	engineered mutation	UNP O59010
D	40	HIS	LYS	engineered mutation	UNP O59010
D	132	HIS	LYS	engineered mutation	UNP O59010
D	223	HIS	LYS	engineered mutation	UNP O59010
D	264	HIS	LYS	engineered mutation	UNP O59010
D	368	HIS	GLU	engineered mutation	UNP O59010
D	397	ALA	ARG	engineered mutation	UNP O59010
E	37	HIS	ASP	engineered mutation	UNP O59010
E	40	HIS	LYS	engineered mutation	UNP O59010
E	132	HIS	LYS	engineered mutation	UNP O59010
E	223	HIS	LYS	engineered mutation	UNP O59010
E	264	HIS	LYS	engineered mutation	UNP O59010
E	368	HIS	GLU	engineered mutation	UNP O59010
E	397	ALA	ARG	engineered mutation	UNP O59010
F	37	HIS	ASP	engineered mutation	UNP O59010
F	40	HIS	LYS	engineered mutation	UNP O59010
F	132	HIS	LYS	engineered mutation	UNP O59010
F	223	HIS	LYS	engineered mutation	UNP O59010
F	264	HIS	LYS	engineered mutation	UNP O59010
F	368	HIS	GLU	engineered mutation	UNP O59010
F	397	ALA	ARG	engineered mutation	UNP O59010
G	37	HIS	ASP	engineered mutation	UNP O59010
G	40	HIS	LYS	engineered mutation	UNP O59010
G	132	HIS	LYS	engineered mutation	UNP O59010
G	223	HIS	LYS	engineered mutation	UNP O59010
G	264	HIS	LYS	engineered mutation	UNP O59010

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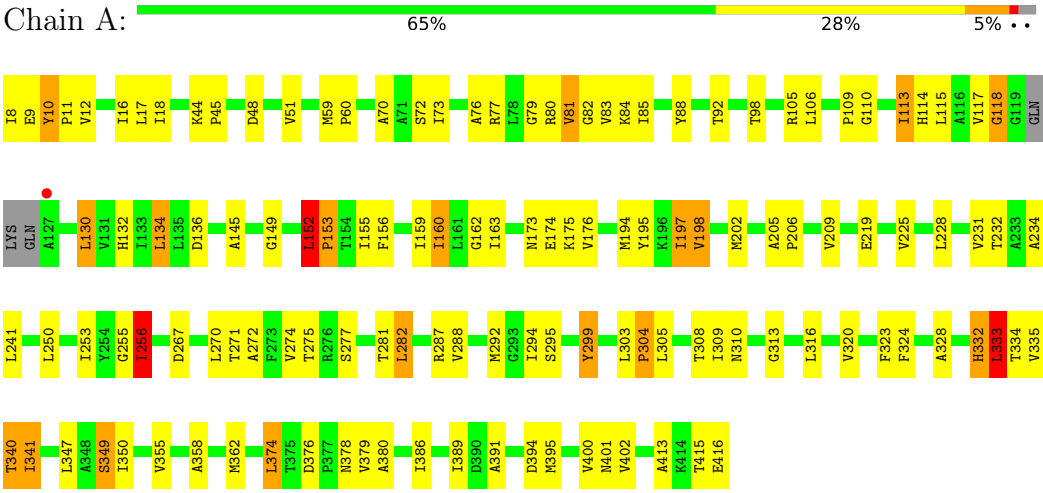
Chain	Residue	Modelled	Actual	Comment	Reference
G	368	HIS	GLU	engineered mutation	UNP O59010
G	397	ALA	ARG	engineered mutation	UNP O59010
H	37	HIS	ASP	engineered mutation	UNP O59010
H	40	HIS	LYS	engineered mutation	UNP O59010
H	132	HIS	LYS	engineered mutation	UNP O59010
H	223	HIS	LYS	engineered mutation	UNP O59010
H	264	HIS	LYS	engineered mutation	UNP O59010
H	368	HIS	GLU	engineered mutation	UNP O59010
H	397	ALA	ARG	engineered mutation	UNP O59010
I	37	HIS	ASP	engineered mutation	UNP O59010
I	40	HIS	LYS	engineered mutation	UNP O59010
I	132	HIS	LYS	engineered mutation	UNP O59010
I	223	HIS	LYS	engineered mutation	UNP O59010
I	264	HIS	LYS	engineered mutation	UNP O59010
I	368	HIS	GLU	engineered mutation	UNP O59010
I	397	ALA	ARG	engineered mutation	UNP O59010
J	37	HIS	ASP	engineered mutation	UNP O59010
J	40	HIS	LYS	engineered mutation	UNP O59010
J	132	HIS	LYS	engineered mutation	UNP O59010
J	223	HIS	LYS	engineered mutation	UNP O59010
J	264	HIS	LYS	engineered mutation	UNP O59010
J	368	HIS	GLU	engineered mutation	UNP O59010
J	397	ALA	ARG	engineered mutation	UNP O59010
K	37	HIS	ASP	engineered mutation	UNP O59010
K	40	HIS	LYS	engineered mutation	UNP O59010
K	132	HIS	LYS	engineered mutation	UNP O59010
K	223	HIS	LYS	engineered mutation	UNP O59010
K	264	HIS	LYS	engineered mutation	UNP O59010
K	368	HIS	GLU	engineered mutation	UNP O59010
K	397	ALA	ARG	engineered mutation	UNP O59010
L	37	HIS	ASP	engineered mutation	UNP O59010
L	40	HIS	LYS	engineered mutation	UNP O59010
L	132	HIS	LYS	engineered mutation	UNP O59010
L	223	HIS	LYS	engineered mutation	UNP O59010
L	264	HIS	LYS	engineered mutation	UNP O59010
L	368	HIS	GLU	engineered mutation	UNP O59010
L	397	ALA	ARG	engineered mutation	UNP O59010

3 Residue-property plots (i)

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.

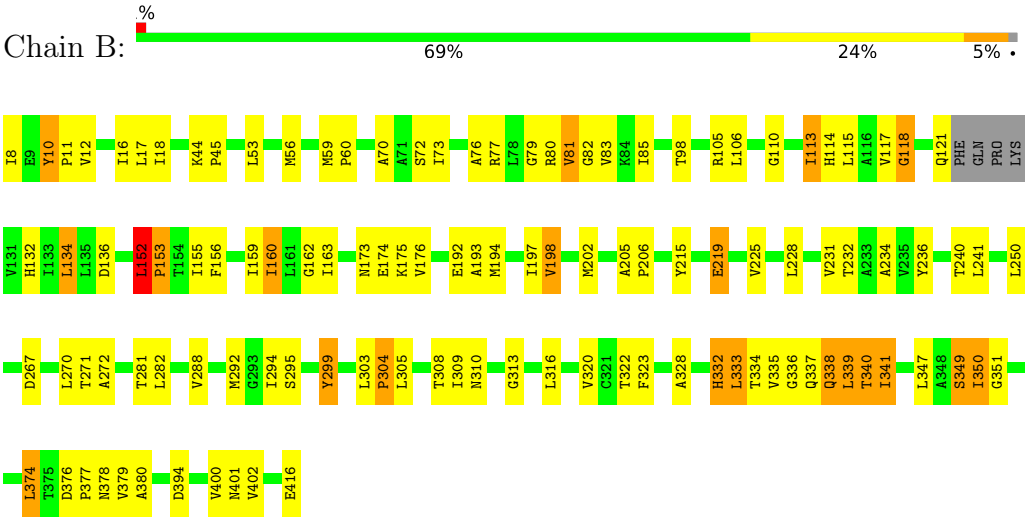
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain A:



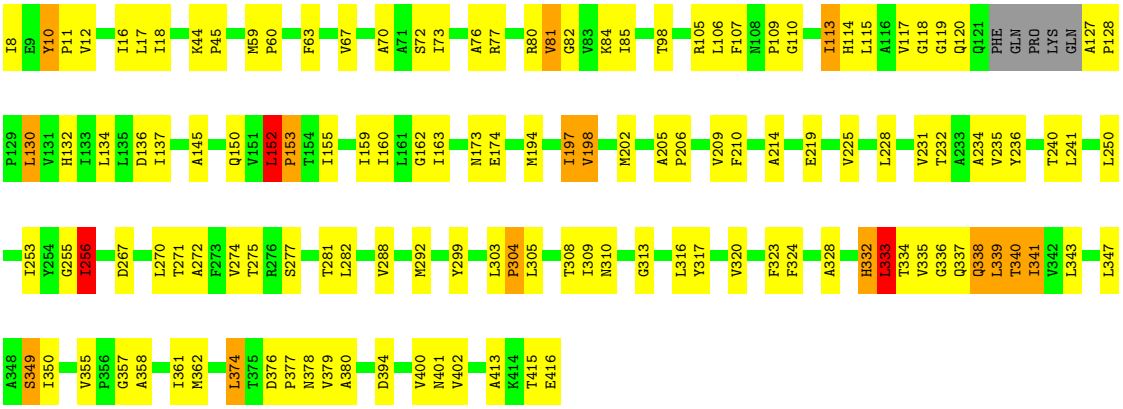
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain B:



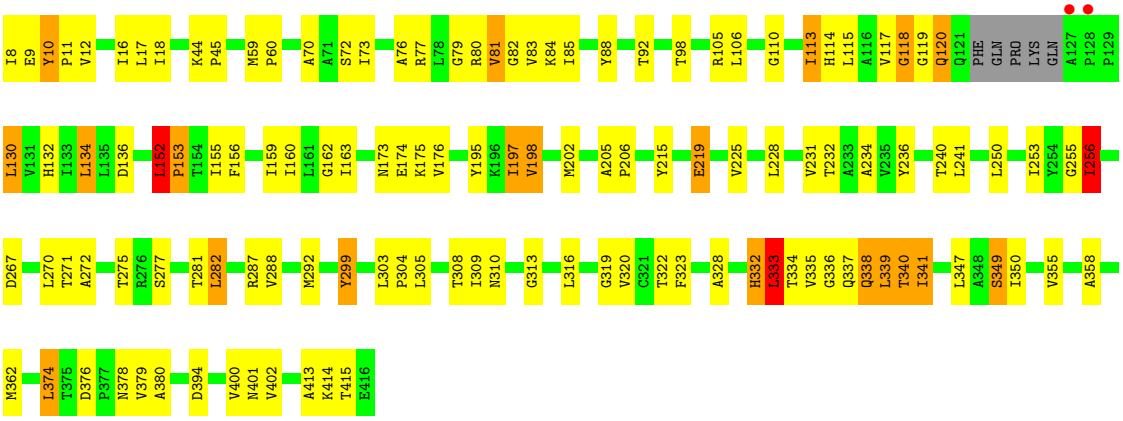
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain C:



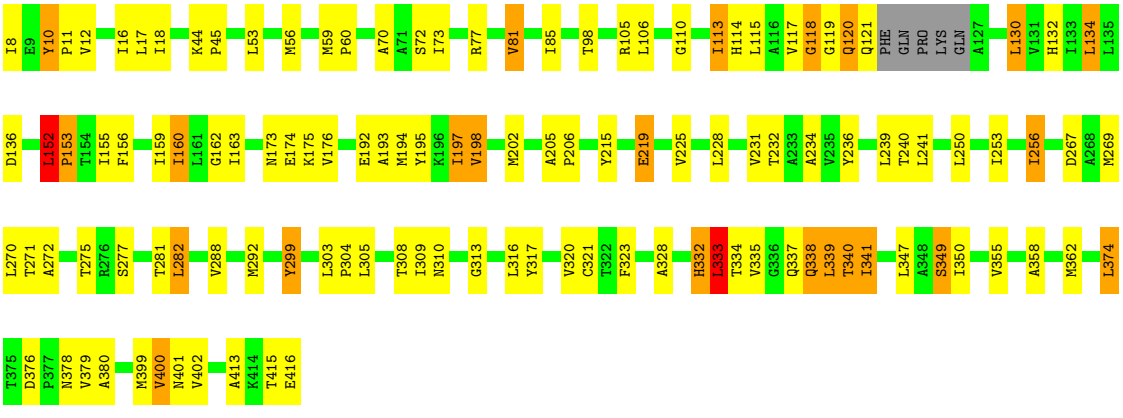
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain D:



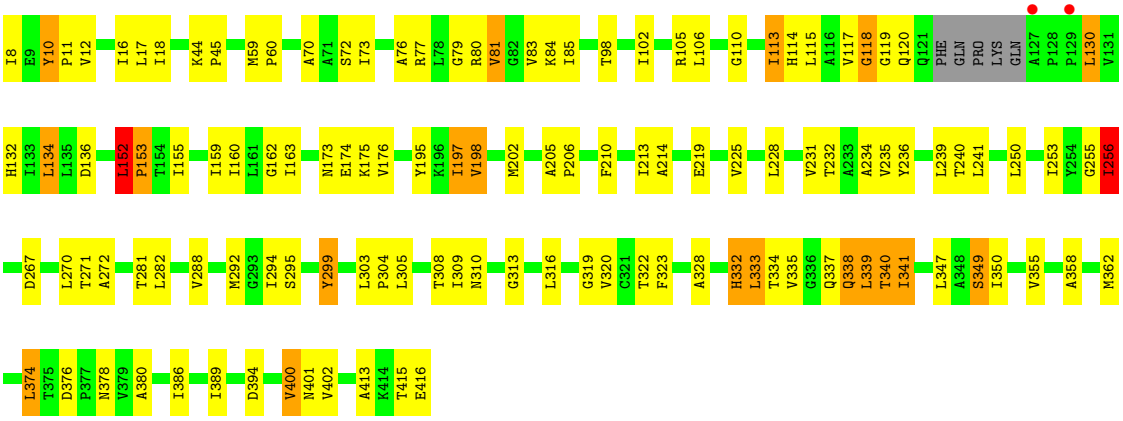
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain E:



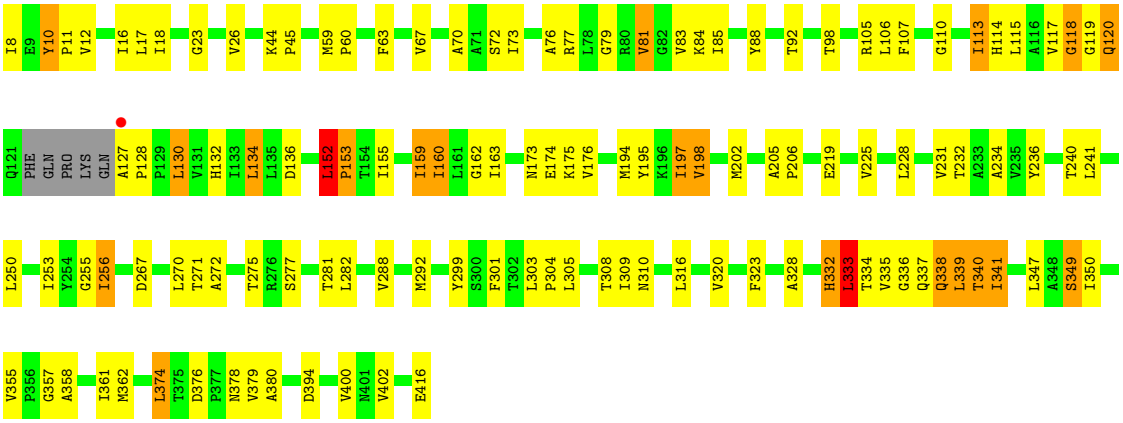
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain F:



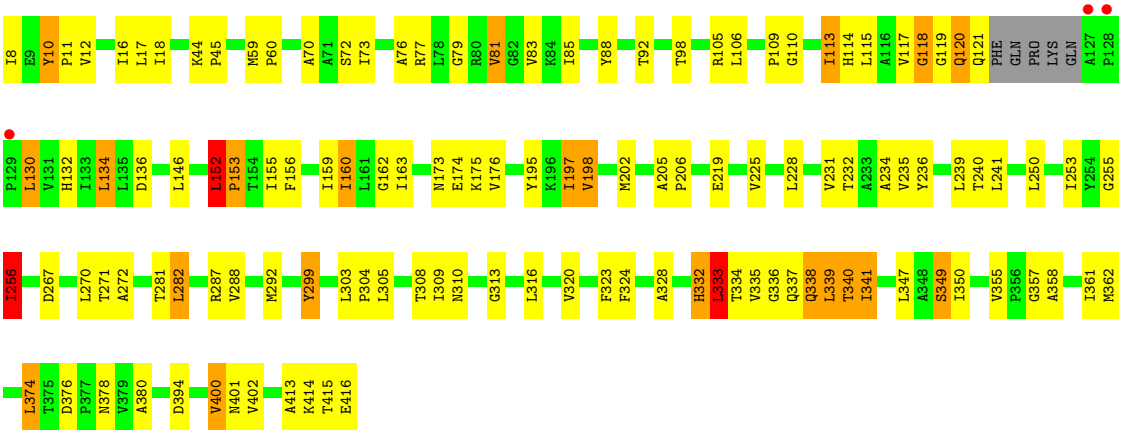
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain G:



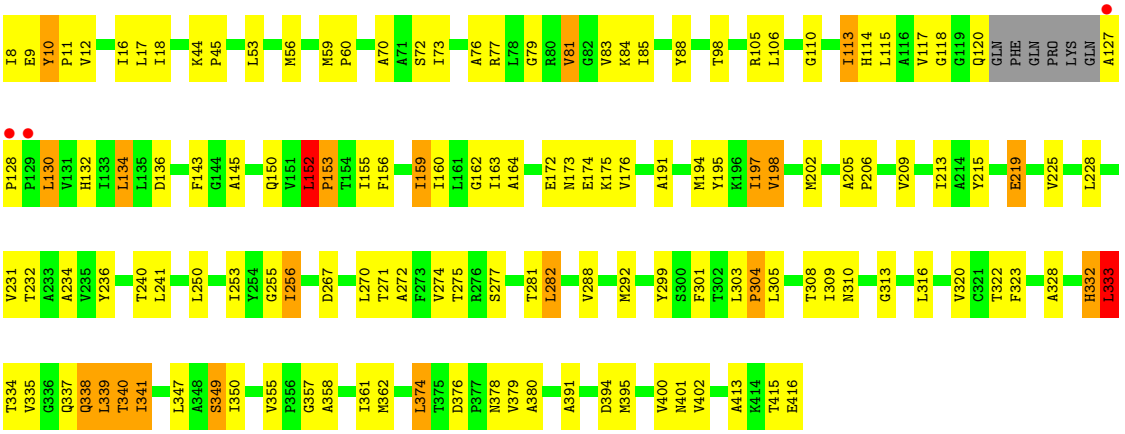
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain H:



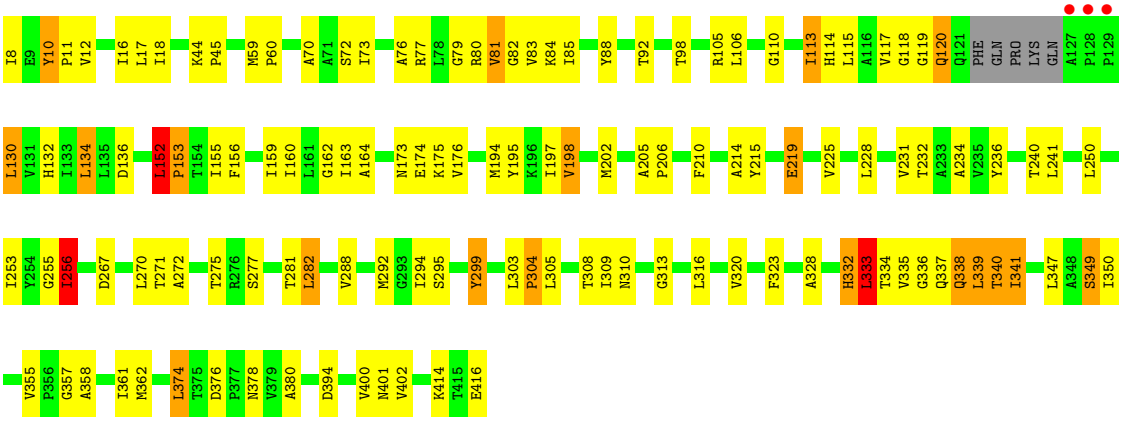
• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain I:



• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain J:

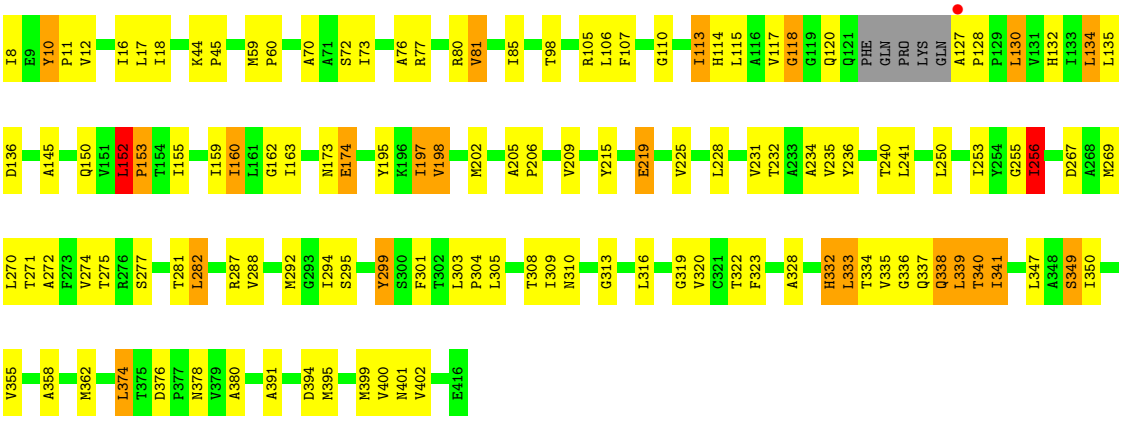


• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain K:

• Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain L:


I8 E9 Y10 P11 V12 I16 L17 I18 K44 P45 M59 P60 A70 A71 S72 I73 A76 R77 R80 V81 I85 T98 R105 L106 F107 G110 I113 H114 L115 A116 V117 G118 G119 Q120 Q121 PHE GLN PRO LYS GLN A127 P128 P129 L130 V131 H132 I133 L134 L135
D136 A145 Q150 V151 L152 P153 T154 I155 I159 I160 L161 G162 I163 N173 E174 Y195 K196 I197 V198 M202 A205 P206 V209 Y215 E219 V225 L228 V231 T232 A233 A234 V235 Y236 T240 L241 L250 I253 Y254 G255 I256 D267 A268 M269
L270 T271 A272 F273 V274 T275 R276 S277 T281 L282 R287 V288 M292 G293 I294 S295 Y299 S300 F301 T302 L303 P304 L305 T308 I309 N310 G313 L316 G319 V320 C321 T322 F323 A328 H332 L333 T334 V335 G336 Q337 Q338 L339 T340 I341 L347 A348 S349 I350
V355 A358 M362 L374 T375 D376 P377 N378 V379 A380 A391 D394 M395 M399 V400 N401 V402 E416

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.36Å 424.42Å 113.98Å 90.00° 119.38° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 19.98 – 4.00	Depositor EDS
% Data completeness (in resolution range)	70.3 (20.00-4.00) 70.4 (19.98-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.249 , 0.266 0.250 , 0.265	Depositor DCC
R_{free} test set	2728 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	1.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.068 for -h-l,k,h 0.068 for l,k,-h-l 0.208 for h,-k,-h-l 0.078 for -h-l,-k,l 0.076 for l,-k,h	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	35277	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.49	0/2980	0.65	1/4074 (0.0%)
1	B	0.56	0/2994	0.69	0/4093
1	C	0.55	0/2998	0.68	1/4098 (0.0%)
1	D	0.50	0/2998	0.65	1/4098 (0.0%)
1	E	0.52	0/2998	0.67	1/4098 (0.0%)
1	F	0.56	0/2998	0.69	0/4098
1	G	0.51	0/2998	0.66	1/4098 (0.0%)
1	H	0.49	0/2998	0.67	1/4098 (0.0%)
1	I	0.52	0/2989	0.68	1/4086 (0.0%)
1	J	0.46	0/2998	0.65	1/4098 (0.0%)
1	K	0.51	0/2994	0.66	0/4094
1	L	0.55	0/2994	0.68	0/4093
All	All	0.52	0/35937	0.67	8/49126 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	333	LEU	CA-CB-CG	5.46	127.85	115.30
1	I	333	LEU	CA-CB-CG	5.34	127.58	115.30
1	J	333	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	333	LEU	CA-CB-CG	5.24	127.34	115.30
1	G	333	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	174	GLU	Peptide

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	2925	0	3069	85	0
1	B	2939	0	3079	78	0
1	C	2943	0	3085	92	0
1	D	2943	0	3085	79	0
1	E	2943	0	3085	75	0
1	F	2943	0	3085	77	0
1	G	2943	0	3085	80	0
1	H	2943	0	3085	79	0
1	I	2934	0	3077	90	0
1	J	2943	0	3085	76	0
1	K	2939	0	3074	79	0
1	L	2939	0	3081	83	0
All	All	35277	0	36975	956	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 13.

The worst 5 of 956 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:C:73:ILE:CD1	1:I:172:GLU:CB	2.19	1.19
1:C:73:ILE:HD13	1:I:172:GLU:CB	1.79	1.12
1:C:73:ILE:HD11	1:I:172:GLU:CB	2.03	0.89
1:B:338:GLN:O	1:B:341:ILE:HD13	1.81	0.80
1:F:338:GLN:O	1:F:341:ILE:HD13	1.85	0.75

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	398/409 (97%)	356 (89%)	34 (8%)	8 (2%)	7	40
1	B	400/409 (98%)	355 (89%)	37 (9%)	8 (2%)	7	40
1	C	400/409 (98%)	354 (88%)	39 (10%)	7 (2%)	8	41
1	D	400/409 (98%)	354 (88%)	38 (10%)	8 (2%)	7	40
1	E	400/409 (98%)	359 (90%)	34 (8%)	7 (2%)	8	41
1	F	400/409 (98%)	356 (89%)	37 (9%)	7 (2%)	8	41
1	G	400/409 (98%)	352 (88%)	41 (10%)	7 (2%)	8	41
1	H	400/409 (98%)	352 (88%)	40 (10%)	8 (2%)	7	40
1	I	399/409 (98%)	356 (89%)	36 (9%)	7 (2%)	8	41
1	J	400/409 (98%)	359 (90%)	33 (8%)	8 (2%)	7	40
1	K	400/409 (98%)	355 (89%)	37 (9%)	8 (2%)	7	40
1	L	400/409 (98%)	355 (89%)	38 (10%)	7 (2%)	8	41
All	All	4797/4908 (98%)	4263 (89%)	444 (9%)	90 (2%)	8	40

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ILE
1	B	256	ILE
1	C	256	ILE
1	D	256	ILE
1	E	256	ILE

5.3.2 Protein sidechains (i)

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	302/318 (95%)	257 (85%)	45 (15%)	3	17
1	B	303/318 (95%)	256 (84%)	47 (16%)	2	16
1	C	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	D	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	E	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	F	304/318 (96%)	259 (85%)	45 (15%)	3	17
1	G	304/318 (96%)	259 (85%)	45 (15%)	3	17
1	H	304/318 (96%)	257 (84%)	47 (16%)	2	16
1	I	303/318 (95%)	257 (85%)	46 (15%)	3	16
1	J	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	K	303/318 (95%)	257 (85%)	46 (15%)	3	16
1	L	303/318 (95%)	256 (84%)	47 (16%)	2	16
All	All	3642/3816 (95%)	3090 (85%)	552 (15%)	3	16

5 of 552 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	81	VAL
1	K	197	ILE
1	K	72	SER
1	L	159	ILE
1	E	130	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	338	GLN
1	K	338	GLN
1	J	150	GLN
1	J	338	GLN
1	L	337	GLN

5.3.3 RNA

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 monosaccharides 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

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, 95^{th} 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	402/409 (98%)	-0.66	1 (0%) 95 93	92, 145, 192, 218	0
1	B	404/409 (98%)	-0.65	3 (0%) 87 82	80, 127, 179, 232	0
1	C	404/409 (98%)	-0.66	0 100 100	71, 127, 176, 212	0
1	D	404/409 (98%)	-0.65	2 (0%) 91 85	98, 146, 193, 249	0
1	E	404/409 (98%)	-0.66	0 100 100	88, 138, 184, 213	0
1	F	404/409 (98%)	-0.68	2 (0%) 91 85	84, 127, 179, 219	0
1	G	404/409 (98%)	-0.66	1 (0%) 95 93	90, 144, 184, 218	0
1	H	404/409 (98%)	-0.65	3 (0%) 87 82	87, 146, 199, 260	0
1	I	403/409 (98%)	-0.62	3 (0%) 87 82	92, 143, 187, 228	0
1	J	404/409 (98%)	-0.67	3 (0%) 87 82	100, 158, 199, 236	0
1	K	404/409 (98%)	-0.67	0 100 100	94, 136, 184, 240	0
1	L	404/409 (98%)	-0.72	1 (0%) 95 93	88, 128, 174, 210	0
All	All	4845/4908 (98%)	-0.66	19 (0%) 92 87	71, 138, 188, 260	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	ALA	6.8
1	A	127	ALA	5.6
1	B	127	ALA	5.3
1	I	127	ALA	5.0
1	H	127	ALA	4.8

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.