



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:39 AM GMT

PDB ID : 2GWC
Title : Crystal structure of plant glutamate cysteine ligase in complex with a transition state analogue
Authors : Hothorn, M.; Wachter, A.; Gromes, R.; Stuwe, T.; Rausch, T.; Scheffzek, K.
Deposited on : 2006-05-04
Resolution : 2.18 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>

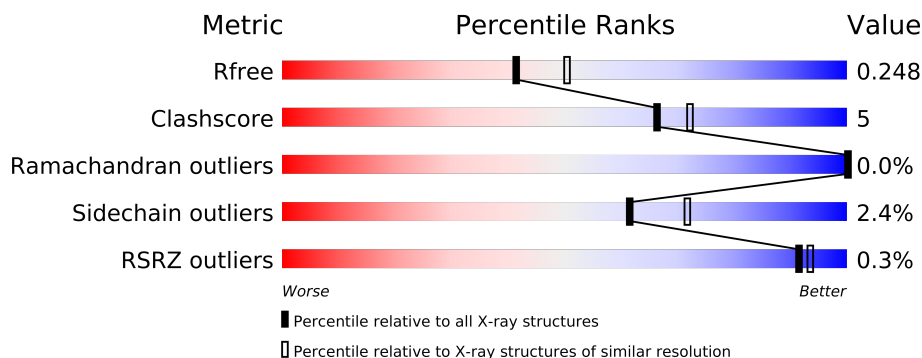
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.18 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	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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	449	
1	B	449	
1	C	449	
1	D	449	
1	E	449	
1	F	449	
1	G	449	
1	H	449	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	BSC	A	2	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
3	BSC	B	2	-	X
3	BSC	G	2	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29207 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 Glutamate cysteine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	1	0
			3509	2248	591	646	6	18			
1	B	436	Total	C	N	O	S	Se	0	1	0
			3500	2242	589	645	6	18			
1	C	436	Total	C	N	O	S	Se	0	1	0
			3500	2242	589	645	6	18			
1	D	438	Total	C	N	O	S	Se	0	3	0
			3526	2258	595	649	6	18			
1	E	436	Total	C	N	O	S	Se	0	2	0
			3506	2247	590	645	6	18			
1	F	439	Total	C	N	O	S	Se	0	1	0
			3517	2252	592	649	6	18			
1	G	438	Total	C	N	O	S	Se	0	1	0
			3512	2249	591	648	6	18			
1	H	436	Total	C	N	O	S	Se	0	1	0
			3500	2242	589	645	6	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	228	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	329	MSE	MET	MODIFIED RESIDUE	UNP O23736

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
A	496	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	119	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	228	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	329	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
B	496	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	119	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	228	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	329	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
C	496	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	119	MSE	MET	MODIFIED RESIDUE	UNP O23736

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	228	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	329	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
D	496	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	119	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	228	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	329	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
E	496	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	119	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	228	MSE	MET	MODIFIED RESIDUE	UNP O23736

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	329	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
F	496	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	119	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	228	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	329	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
G	496	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	119	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	141	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	195	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	202	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	216	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	224	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	228	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	238	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	239	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	257	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	291	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	306	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	329	MSE	MET	MODIFIED RESIDUE	UNP O23736

Continued on next page...

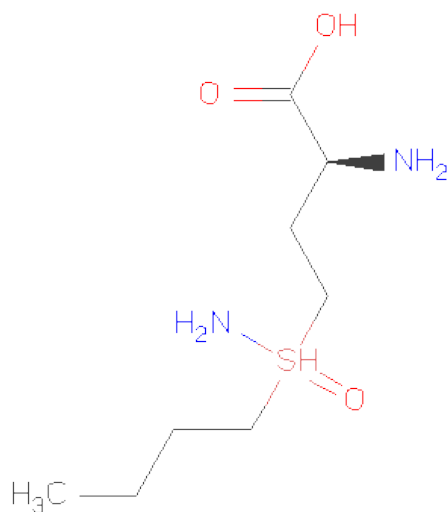
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	496	MSE	MET	MODIFIED RESIDUE	UNP O23736

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is (S)-2-AMINO-4-(AMINO-BUTYLHYDROSULFINYL)BUTANOICACID (three-letter code: BSC) (formula: C₈H₂₀N₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	B	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	C	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	D	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	E	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	F	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	G	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	H	1	Total	C	N	O	S	0	0
			14	8	2	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	128	Total	O	0	0
			128	128		
4	C	124	Total	O	0	0
			124	124		
4	D	120	Total	O	0	0
			120	120		

Continued on next page...

Continued from previous page...

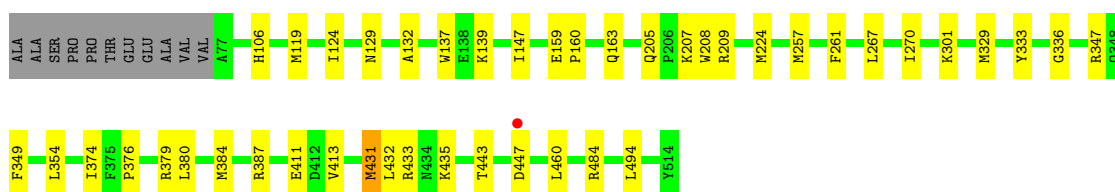
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	138	Total 138	O 138	0	0
4	F	119	Total 119	O 119	0	0
4	G	130	Total 130	O 130	0	0
4	H	107	Total 107	O 107	0	0

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.

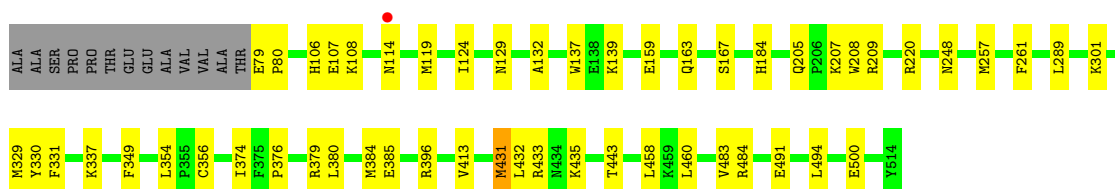
- Molecule 1: Glutamate cysteine ligase

Chain A:



- Molecule 1: Glutamate cysteine ligase

Chain B:



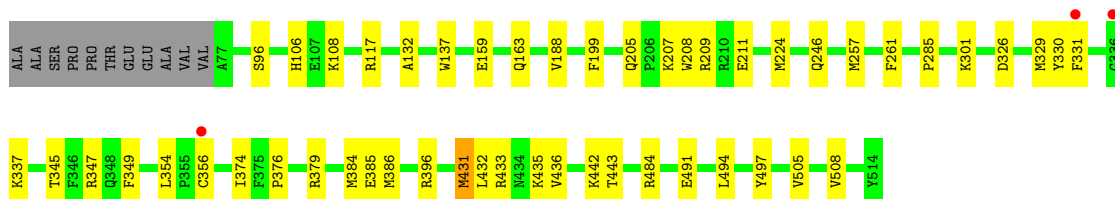
- Molecule 1: Glutamate cysteine ligase

Chain C:



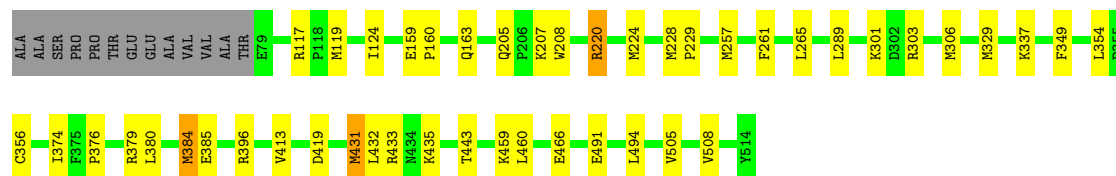
- Molecule 1: Glutamate cysteine ligase

Chain D:



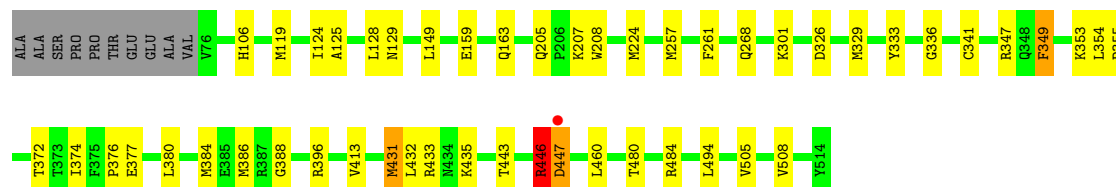
- Molecule 1: Glutamate cysteine ligase

Chain E:



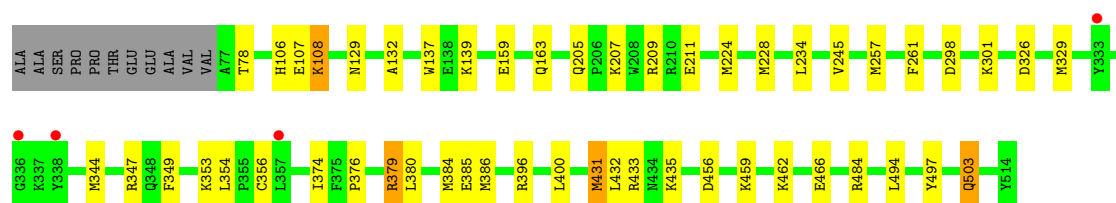
- Molecule 1: Glutamate cysteine ligase

Chain F:



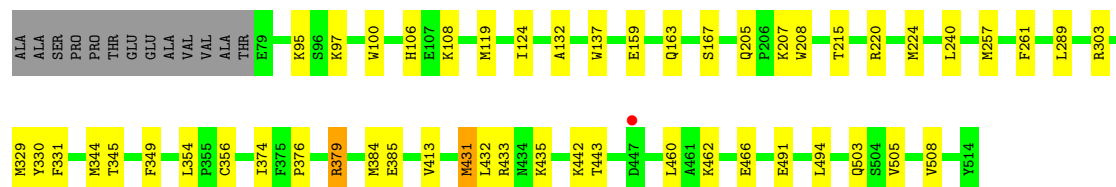
- Molecule 1: Glutamate cysteine ligase

Chain G:



- Molecule 1: Glutamate cysteine ligase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.04Å 198.92Å 114.97Å 90.00° 99.66° 90.00°	Depositor
Resolution (Å)	99.50 – 2.18 99.46 – 2.18	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.50-2.18) 97.5 (99.46-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	146.93 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.241 0.207 , 0.248	Depositor DCC
R_{free} test set	9951 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 197261 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29207	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 62.30 % 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 1.1499e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.73	0/3580	0.76	2/4812 (0.0%)
1	B	0.68	0/3571	0.76	2/4799 (0.0%)
1	C	0.68	0/3571	0.75	3/4799 (0.1%)
1	D	0.73	0/3603	0.77	1/4843 (0.0%)
1	E	0.72	0/3580	0.77	3/4810 (0.1%)
1	F	0.68	0/3588	0.72	1/4823 (0.0%)
1	G	0.72	0/3583	0.78	2/4816 (0.0%)
1	H	0.70	0/3571	0.76	3/4799 (0.1%)
All	All	0.71	0/28647	0.76	17/38501 (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	F	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	303	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	396	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	A	379	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	303	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	E	396	ARG	NE-CZ-NH2	-6.72	116.94	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	388	GLY	Peptide
1	F	447	ASP	Peptide

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	3509	0	3461	31	0
1	B	3500	0	3451	38	0
1	C	3500	0	3451	27	0
1	D	3526	0	3484	38	0
1	E	3506	0	3464	37	0
1	F	3517	0	3465	35	0
1	G	3512	0	3463	40	0
1	H	3500	0	3451	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	14	0	16	1	0
3	B	14	0	16	1	0
3	C	14	0	16	1	0
3	D	14	0	16	1	0
3	E	14	0	16	1	0
3	F	14	0	16	1	0
3	G	14	0	16	3	0
3	H	14	0	16	3	0
4	A	151	0	0	2	0
4	B	128	0	0	3	0
4	C	124	0	0	1	0
4	D	120	0	0	1	0
4	E	138	0	0	6	0
4	F	119	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	130	0	0	7	0
4	H	107	0	0	5	0
All	All	29207	0	27818	283	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 5.

The worst 5 of 283 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:329:MSE:HE1	1:C:354:LEU:HD21	1.18	1.18
1:E:329:MSE:HE1	1:E:354:LEU:HD21	1.19	1.12
1:B:329:MSE:HE1	1:B:354:LEU:HD21	1.26	1.09
1:H:329:MSE:HE1	1:H:354:LEU:HD21	1.27	1.09
1:B:329:MSE:CE	1:B:354:LEU:HD21	1.89	1.02

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	437/449 (97%)	430 (98%)	7 (2%)	0	100	100
1	B	435/449 (97%)	426 (98%)	9 (2%)	0	100	100
1	C	435/449 (97%)	428 (98%)	7 (2%)	0	100	100
1	D	439/449 (98%)	433 (99%)	6 (1%)	0	100	100
1	E	436/449 (97%)	427 (98%)	9 (2%)	0	100	100
1	F	438/449 (98%)	429 (98%)	8 (2%)	1 (0%)	56	60
1	G	437/449 (97%)	427 (98%)	10 (2%)	0	100	100
1	H	435/449 (97%)	428 (98%)	7 (2%)	0	100	100
All	All	3492/3592 (97%)	3428 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	446	ARG

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	374/364 (103%)	364 (97%)	10 (3%)	57	66
1	B	374/364 (103%)	365 (98%)	9 (2%)	61	72
1	C	374/364 (103%)	365 (98%)	9 (2%)	61	72
1	D	377/364 (104%)	366 (97%)	11 (3%)	55	64
1	E	375/364 (103%)	365 (97%)	10 (3%)	57	66
1	F	375/364 (103%)	368 (98%)	7 (2%)	69	80
1	G	375/364 (103%)	365 (97%)	10 (3%)	57	66
1	H	374/364 (103%)	367 (98%)	7 (2%)	69	80
All	All	2998/2912 (103%)	2925 (98%)	73 (2%)	61	72

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	337	LYS
1	E	220	ARG
1	H	220	ARG
1	D	484	ARG
1	E	301	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	335	ASN
1	E	205	GLN
1	H	205	GLN
1	D	369	ASN
1	D	510	GLN

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 ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
3	BSC	A	2	2	9,13,13	0.62	0	9,17,17	1.77	2 (22%)
3	BSC	B	2	2	9,13,13	0.59	0	9,17,17	1.82	2 (22%)
3	BSC	C	2	2	9,13,13	0.72	0	9,17,17	1.51	1 (11%)
3	BSC	D	2	2	9,13,13	0.84	0	9,17,17	1.45	1 (11%)
3	BSC	E	2	2	9,13,13	0.78	1 (11%)	9,17,17	0.75	0
3	BSC	F	2	2	9,13,13	0.61	0	9,17,17	0.77	0
3	BSC	G	2	2	9,13,13	0.55	0	9,17,17	1.18	2 (22%)
3	BSC	H	2	2	9,13,13	0.71	0	9,17,17	1.81	2 (22%)

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
3	BSC	A	2	2	-	0/9/15/15	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BSC	B	2	2	-	0/9/15/15	0/0/0/0
3	BSC	C	2	2	-	0/9/15/15	0/0/0/0
3	BSC	D	2	2	-	0/9/15/15	0/0/0/0
3	BSC	E	2	2	-	0/9/15/15	0/0/0/0
3	BSC	F	2	2	-	0/9/15/15	0/0/0/0
3	BSC	G	2	2	-	0/9/15/15	0/0/0/0
3	BSC	H	2	2	-	0/9/15/15	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	BSC	OXT-C	-2.24	1.22	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	BSC	CAH-CB-CA	-4.19	106.57	112.56
3	A	2	BSC	CAH-CB-CA	-4.07	106.74	112.56
3	C	2	BSC	C-CA-N	3.65	115.41	109.36
3	B	2	BSC	CAH-CB-CA	-3.56	107.47	112.56
3	B	2	BSC	C-CA-N	3.49	115.15	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	438/449 (97%)	-0.10	1 (0%) 93 94	20, 23, 28, 37	0
1	B	436/449 (97%)	-0.10	1 (0%) 93 94	20, 23, 28, 35	0
1	C	436/449 (97%)	-0.13	0 100 100	19, 23, 28, 36	0
1	D	438/449 (97%)	-0.06	3 (0%) 84 87	19, 23, 28, 37	0
1	E	436/449 (97%)	-0.11	0 100 100	20, 23, 28, 34	0
1	F	439/449 (97%)	-0.05	1 (0%) 93 94	20, 23, 28, 39	0
1	G	438/449 (97%)	-0.04	4 (0%) 81 83	20, 23, 28, 38	0
1	H	436/449 (97%)	-0.12	1 (0%) 93 94	19, 23, 28, 36	0
All	All	3497/3592 (97%)	-0.09	11 (0%) 91 93	19, 23, 28, 39	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ASP	4.4
1	F	447	ASP	4.3
1	B	114	ASN	3.2
1	H	447	ASP	2.7
1	D	356	CYS	2.5

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BSC	B	2	14/14	0.18	4.64	29,33,35,35	0
3	BSC	G	2	14/14	0.17	3.24	30,33,34,35	0
3	BSC	A	2	14/14	0.15	2.99	25,27,32,33	0
3	BSC	D	2	14/14	0.13	1.87	28,29,31,31	0
3	BSC	F	2	14/14	0.14	1.74	24,26,30,30	0
3	BSC	C	2	14/14	0.13	1.55	30,31,32,32	0
2	MG	F	1	1/1	0.15	1.42	27,27,27,27	0
3	BSC	H	2	14/14	0.13	1.26	26,29,33,33	0
3	BSC	E	2	14/14	0.12	1.19	29,31,32,34	0
2	MG	C	1	1/1	0.14	0.94	28,28,28,28	0
2	MG	H	1	1/1	0.13	0.50	38,38,38,38	0
2	MG	B	1	1/1	0.12	0.29	27,27,27,27	0
2	MG	A	1	1/1	0.12	-0.53	28,28,28,28	0
2	MG	D	1	1/1	0.10	-1.01	36,36,36,36	0
2	MG	E	1	1/1	0.09	-1.40	34,34,34,34	0
2	MG	G	1	1/1	0.10	-2.01	37,37,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.