wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 08:06 AM EDT

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 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:

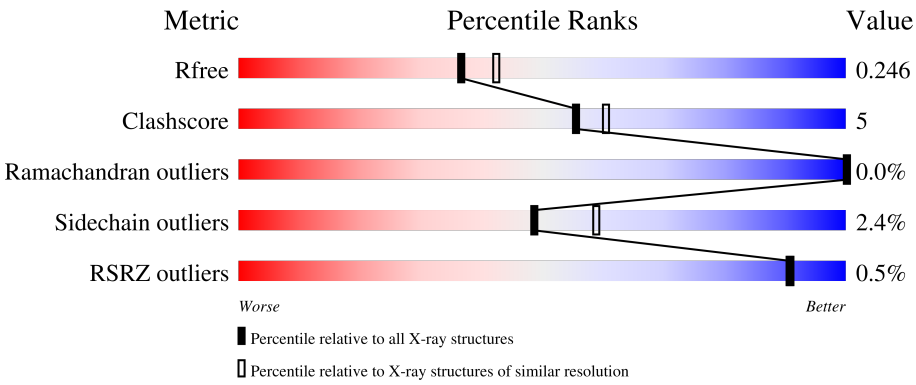
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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 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	449	88% 10% •
1	B	449	85% 12% •
1	C	449	88% 8% • •
1	D	449	% 86% 11% •
1	E	449	87% 10% • •

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Mol	Chain	Length	Quality of chain
1	F	449	87% 10% • •
1	G	449	% 86% 10% • •
1	H	449	86% 11% •

2 Entry composition (i)

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

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

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

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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

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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

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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

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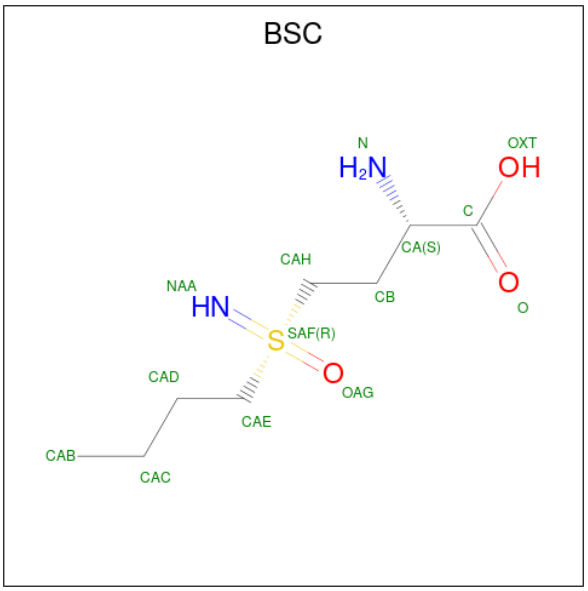
Chain	Residue	Modelled	Actual	Comment	Reference
H	344	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	384	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	386	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	431	MSE	MET	MODIFIED RESIDUE	UNP O23736
H	496	MSE	MET	MODIFIED RESIDUE	UNP O23736

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

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

- Molecule 3 is (2S)-2-amino-4-(S-butylsulfonimidoyl)butanoic acid (three-letter code: BSC) (formula: $C_8H_{18}N_2O_3S$).



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

- Molecule 4 is water.

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

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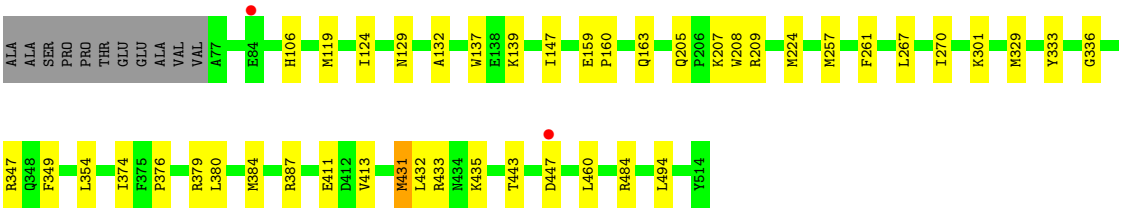
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	138	138	138	0	0
			Total	O		
4	F	119	119	119	0	0
			Total	O		
4	G	130	130	130	0	0
			Total	O		
4	H	107	107	107	0	0

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.

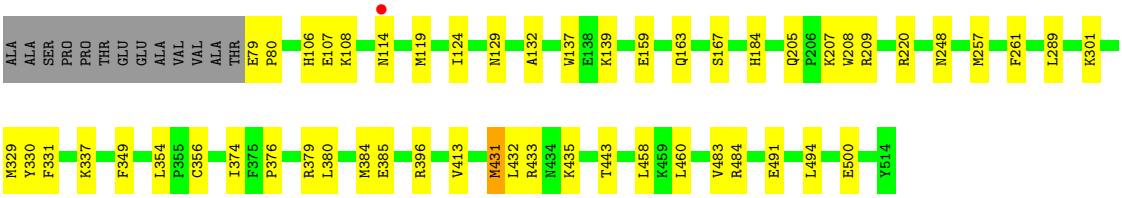
• Molecule 1: Glutamate cysteine ligase

Chain A:



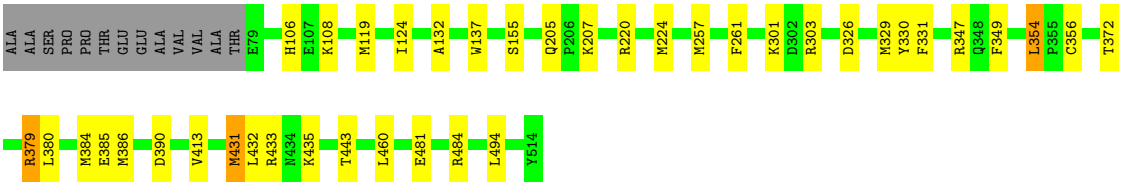
• Molecule 1: Glutamate cysteine ligase

Chain B:



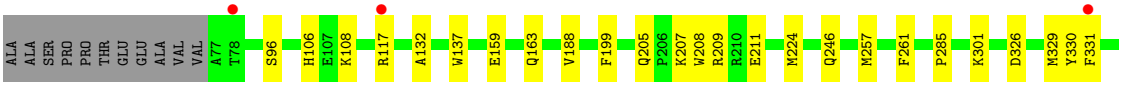
• Molecule 1: Glutamate cysteine ligase

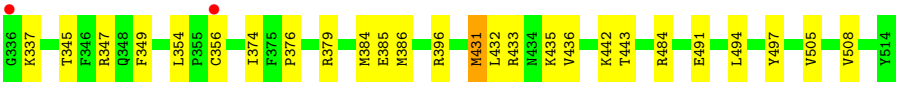
Chain C:



• Molecule 1: Glutamate cysteine ligase

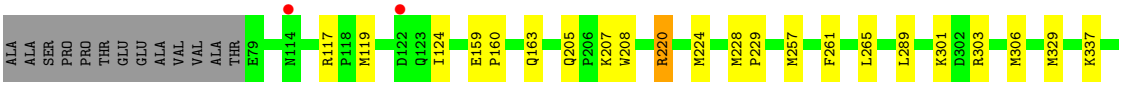
Chain D:

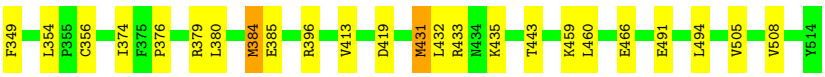




• Molecule 1: Glutamate cysteine ligase

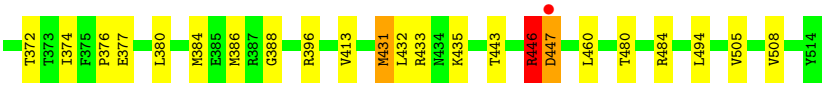
Chain E:





• Molecule 1: Glutamate cysteine ligase

Chain F:

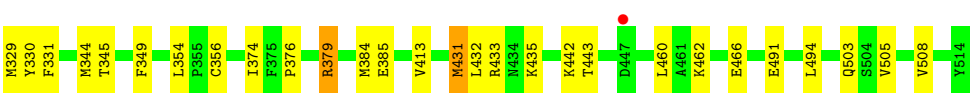


• Molecule 1: Glutamate cysteine ligase

Chain G:

• Molecule 1: Glutamate cysteine ligase

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	146.93 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.241 0.205 , 0.246	Depositor DCC
R_{free} test set	9951 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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 (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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 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	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
4	G	130	0	0	7	0
4	H	107	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29207	0	27818	283	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 5.

The worst 5 of 283 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: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 (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	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%)	47	52
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 (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	374/364 (103%)	364 (97%)	10 (3%)	44	54
1	B	374/364 (103%)	365 (98%)	9 (2%)	49	59
1	C	374/364 (103%)	365 (98%)	9 (2%)	49	59
1	D	377/364 (104%)	366 (97%)	11 (3%)	42	51
1	E	375/364 (103%)	365 (97%)	10 (3%)	44	54
1	F	375/364 (103%)	368 (98%)	7 (2%)	57	68
1	G	375/364 (103%)	365 (97%)	10 (3%)	44	54
1	H	374/364 (103%)	367 (98%)	7 (2%)	57	68
All	All	2998/2912 (103%)	2925 (98%)	73 (2%)	49	59

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

Mol	Chain	Res	Type
1	G	108	LYS
1	H	433	ARG
1	G	301	LYS
1	G	503	GLN
1	C	354	LEU

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

Mol	Chain	Res	Type
1	E	129	ASN
1	F	205	GLN
1	H	369	ASN
1	E	205	GLN

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Mol	Chain	Res	Type
1	E	434	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	E	2	2	9,13,13	1.01	1 (11%)	8,17,17	0.80	0
3	BSC	A	2	2	9,13,13	1.37	1 (11%)	8,17,17	1.19	1 (12%)
3	BSC	D	2	2	9,13,13	1.46	1 (11%)	8,17,17	0.87	0
3	BSC	F	2	2	9,13,13	1.04	1 (11%)	8,17,17	0.80	0
3	BSC	C	2	2	9,13,13	0.83	0	8,17,17	1.32	1 (12%)
3	BSC	G	2	2	9,13,13	0.75	0	8,17,17	1.01	0
3	BSC	B	2	2	9,13,13	1.07	1 (11%)	8,17,17	1.23	1 (12%)
3	BSC	H	2	2	9,13,13	1.10	1 (11%)	8,17,17	1.44	2 (25%)

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	E	2	2	-	1/13/15/15	-
3	BSC	A	2	2	-	1/13/15/15	-
3	BSC	D	2	2	-	0/13/15/15	-
3	BSC	F	2	2	-	3/13/15/15	-
3	BSC	C	2	2	-	1/13/15/15	-
3	BSC	G	2	2	-	3/13/15/15	-
3	BSC	B	2	2	-	1/13/15/15	-
3	BSC	H	2	2	-	3/13/15/15	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	BSC	CB-CAH	-3.65	1.49	1.52
3	D	2	BSC	CB-CAH	-3.55	1.49	1.52
3	E	2	BSC	OXT-C	-2.63	1.22	1.30
3	H	2	BSC	CB-CAH	-2.38	1.50	1.52
3	B	2	BSC	CB-CAH	-2.29	1.50	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2	BSC	CAD-CAE-SAF	2.89	118.94	112.02
3	H	2	BSC	CAD-CAE-SAF	2.64	118.36	112.02
3	H	2	BSC	CB-CA-C	-2.18	104.67	110.45
3	C	2	BSC	CB-CAH-SAF	-2.18	109.25	114.10
3	A	2	BSC	CB-CA-C	-2.14	104.77	110.45

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	BSC	CAC-CAD-CAE-SAF
3	B	2	BSC	CAC-CAD-CAE-SAF
3	E	2	BSC	CAC-CAD-CAE-SAF
3	G	2	BSC	CAC-CAD-CAE-SAF
3	H	2	BSC	CAB-CAC-CAD-CAE

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	BSC	1	0
3	A	2	BSC	1	0
3	D	2	BSC	1	0
3	F	2	BSC	1	0
3	C	2	BSC	1	0
3	G	2	BSC	3	0
3	B	2	BSC	1	0
3	H	2	BSC	3	0

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)

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	420/449 (93%)	0.03	2 (0%)	91	91	20, 23, 28, 37	0
1	B	418/449 (93%)	0.04	1 (0%)	95	95	20, 23, 27, 35	0
1	C	418/449 (93%)	0.03	0	100	100	19, 23, 27, 36	0
1	D	420/449 (93%)	0.09	5 (1%)	79	79	19, 23, 27, 37	0
1	E	418/449 (93%)	0.02	2 (0%)	91	91	20, 23, 27, 33	0
1	F	421/449 (93%)	0.10	1 (0%)	95	95	20, 23, 28, 39	0
1	G	420/449 (93%)	0.11	5 (1%)	79	79	20, 23, 28, 38	0
1	H	418/449 (93%)	0.04	1 (0%)	95	95	19, 23, 28, 36	0
All	All	3353/3592 (93%)	0.06	17 (0%)	91	91	19, 23, 28, 39	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ASP	4.5
1	F	447	ASP	4.5
1	B	114	ASN	3.4
1	G	333	TYR	3.1
1	H	447	ASP	2.9

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

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)

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(Å^2)	Q<0.9
2	MG	D	1	1/1	0.85	0.07	36,36,36,36	0
2	MG	G	1	1/1	0.89	0.07	37,37,37,37	0
2	MG	A	1	1/1	0.91	0.07	28,28,28,28	0
2	MG	B	1	1/1	0.91	0.06	27,27,27,27	0
2	MG	E	1	1/1	0.93	0.05	34,34,34,34	0
2	MG	H	1	1/1	0.93	0.10	38,38,38,38	0
2	MG	C	1	1/1	0.94	0.09	28,28,28,28	0
3	BSC	B	2	14/14	0.94	0.20	29,33,35,35	0
3	BSC	G	2	14/14	0.94	0.18	30,33,34,35	0
3	BSC	C	2	14/14	0.95	0.16	30,31,32,32	0
3	BSC	H	2	14/14	0.96	0.15	26,29,33,33	0
3	BSC	D	2	14/14	0.97	0.13	28,29,31,31	0
3	BSC	E	2	14/14	0.97	0.12	29,31,32,34	0
3	BSC	F	2	14/14	0.97	0.16	24,26,30,30	0
2	MG	F	1	1/1	0.97	0.09	27,27,27,27	0
3	BSC	A	2	14/14	0.97	0.17	25,27,32,33	0

6.5 Other polymers (i)

There are no such residues in this entry.