



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:57 am BST

PDB ID : 1EFM
Title : STRUCTURE OF THE GDP DOMAIN OF EF-TU AND LOCATION OF
THE AMINO ACIDS HOMOLOGOUS TO RAS ONCOGENE PROTEINS
Authors : Jurnak, F.
Deposited on : 1987-05-29
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

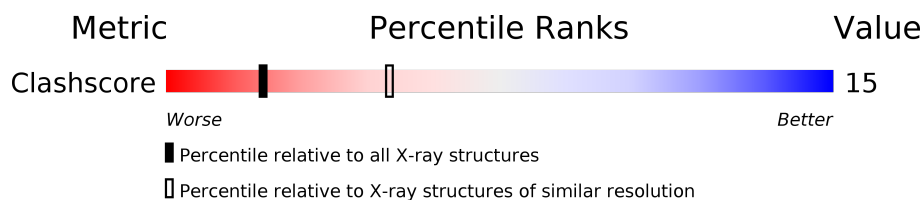
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	141614	3122 (2.70-2.70)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	379	 41% 58%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 187 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 ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	158	Total C 158 158	0	0	158

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	DELETION	UNP P02990
A	?	-	ARG	DELETION	UNP P02990
A	?	-	ALA	DELETION	UNP P02990
A	?	-	PHE	DELETION	UNP P02990
A	?	-	ASP	DELETION	UNP P02990
A	?	-	GLN	DELETION	UNP P02990
A	?	-	ILE	DELETION	UNP P02990
A	?	-	ASP	DELETION	UNP P02990
A	?	-	ASN	DELETION	UNP P02990
A	?	-	ALA	DELETION	UNP P02990
A	?	-	PRO	DELETION	UNP P02990
A	?	-	GLU	DELETION	UNP P02990
A	?	-	GLU	DELETION	UNP P02990
A	?	-	LYS	DELETION	UNP P02990

- 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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

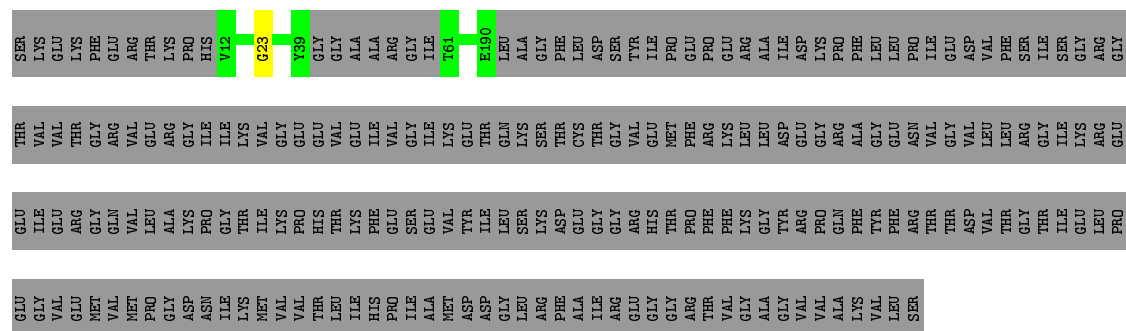


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

i

Note EDS was not executed.

Chain A: 41% 58%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.61Å 100.81Å 162.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	187	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	158	0	0	3	0
2	A	1	0	0	0	0
3	A	28	0	8	3	0
All	All	187	0	8	3	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 15.

All (3) 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:23:GLY:CA	3:A:395:GDP:O1A	2.58	0.52
1:A:23:GLY:CA	3:A:395:GDP:PA	3.01	0.49
1:A:23:GLY:CA	3:A:395:GDP:O3A	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	GDP	A	395	-	24,30,30	2.99	10 (41%)	31,47,47	3.95	17 (54%)

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	GDP	A	395	-	-	6/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	395	GDP	O3'-C3'	-6.45	1.27	1.43
3	A	395	GDP	C2-N2	-5.90	1.22	1.33
3	A	395	GDP	C5'-C4'	-5.64	1.34	1.51
3	A	395	GDP	C4-N3	-5.10	1.27	1.35
3	A	395	GDP	O4'-C1'	-4.77	1.34	1.41
3	A	395	GDP	PA-O5'	-3.81	1.43	1.59
3	A	395	GDP	C5-C4	-2.54	1.34	1.40
3	A	395	GDP	C2'-C1'	-2.46	1.50	1.53
3	A	395	GDP	PA-O2A	-2.39	1.44	1.55
3	A	395	GDP	PA-O1A	-2.05	1.43	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	395	GDP	C5-C6-N1	-11.52	107.67	123.43
3	A	395	GDP	C6-N1-C2	7.34	127.59	115.93
3	A	395	GDP	C2'-C3'-C4'	-6.78	89.47	102.64
3	A	395	GDP	O3B-PB-O1B	-6.61	84.81	110.68
3	A	395	GDP	C5'-C4'-C3'	6.46	139.38	115.18
3	A	395	GDP	C2-N3-C4	-5.70	108.85	115.36
3	A	395	GDP	O3A-PB-O1B	5.27	140.39	111.19
3	A	395	GDP	O4'-C1'-C2'	-4.03	101.04	106.93
3	A	395	GDP	O2'-C2'-C3'	-3.56	100.30	111.82
3	A	395	GDP	O3'-C3'-C2'	3.40	122.82	111.82
3	A	395	GDP	C3'-C2'-C1'	3.33	106.00	100.98
3	A	395	GDP	O5'-PA-O1A	-3.23	96.46	109.07
3	A	395	GDP	PA-O3A-PB	-2.89	122.92	132.83
3	A	395	GDP	O2B-PB-O1B	-2.75	99.93	110.68
3	A	395	GDP	N3-C2-N1	-2.30	124.15	127.22
3	A	395	GDP	O2B-PB-O3A	2.30	112.35	104.64
3	A	395	GDP	C4-C5-N7	2.29	111.78	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

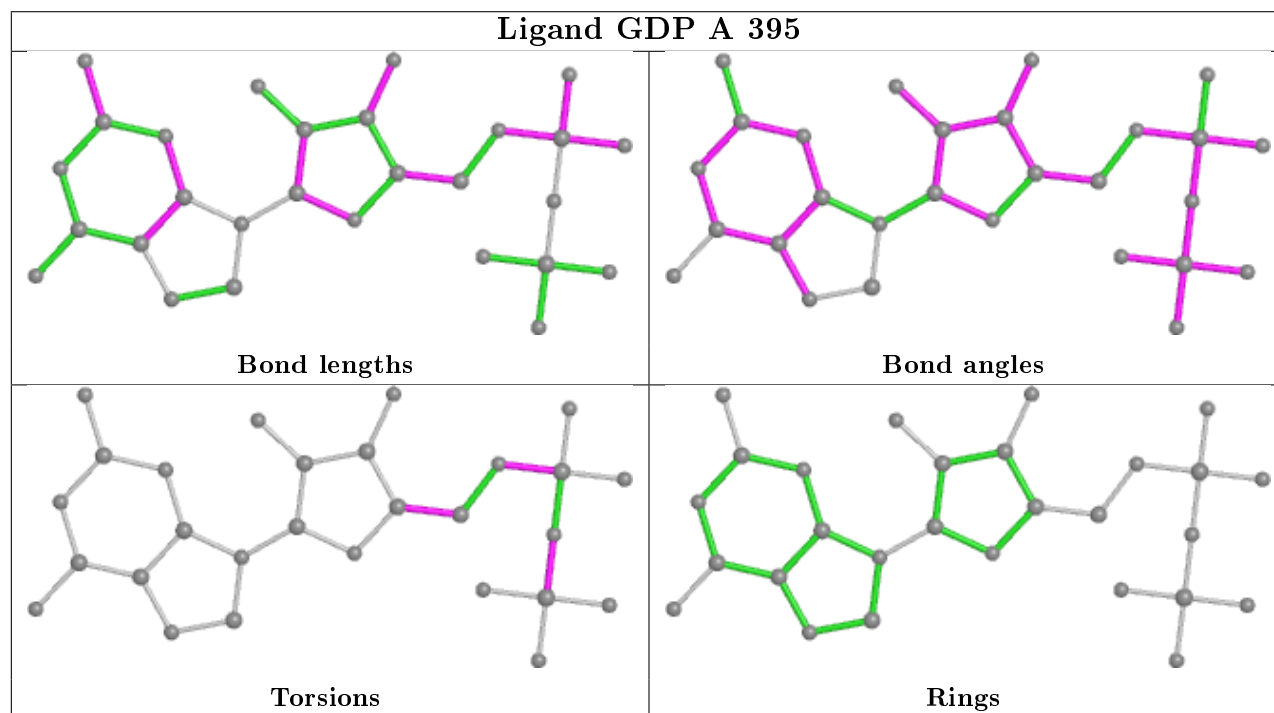
Mol	Chain	Res	Type	Atoms
3	A	395	GDP	C5'-O5'-PA-O3A
3	A	395	GDP	O4'-C4'-C5'-O5'
3	A	395	GDP	C5'-O5'-PA-O2A
3	A	395	GDP	C3'-C4'-C5'-O5'
3	A	395	GDP	C5'-O5'-PA-O1A
3	A	395	GDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	395	GDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.