

Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 03:12 PM EST

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 (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 (1)) 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)

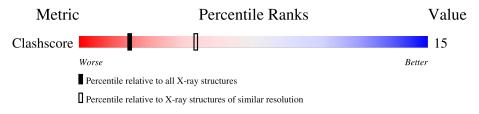
Validation Pipeline (wwPDB-VP) : 2.36

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 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	Similar resolution				
Wictife	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$				
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 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%

Note EDS was not executed.

\mathbf{M}	ol	Chain	Length	Q	uality of chain
1		A	379	41%	58%



2 Entry composition (i)

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:

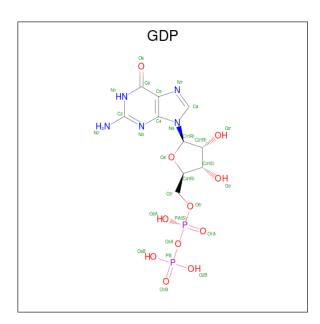
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P02990
A	?	-	ARG	deletion	UNP P02990
A	?	-	ALA	deletion	UNP P02990
A	?	-	PHE	deletion	UNP P02990
A	?	-	ASP	deletion	UNP P02990
A	?	-	GLN	deletion	UNP P02990
A	?	-	ILE	deletion	UNP P02990
A	?	-	ASP	deletion	UNP P02990
A	?	-	ASN	deletion	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: $C_{10}H_{15}N_5O_{11}P_2$).





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

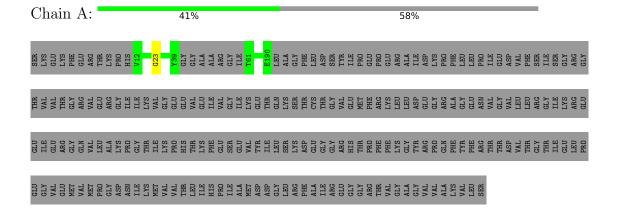


3 Residue-property plots (i)

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. 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. 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: ELONGATION FACTOR TU





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	98.61Å 100.81Å 162.47Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness	(Not available) ((Not available)-2.70)	Depositor
(in resolution range)	, , ,	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 (i)

5.1 Standard geometry (i)

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

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 (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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	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 monosaccharides 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	Chain	Chain	Dec	Link	B	ond leng	gths	В	ond ang	gles
				nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
	3	GDP	A	395	-	24,30,30	3.05	12 (50%)	30,47,47	3.08	14 (46%)		

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
3	A	395	GDP	O3'-C3'	-6.45	1.27	1.43
3	A	395	GDP	C5'-C4'	-5.64	1.34	1.51
3	A	395	GDP	C2-N2	-5.11	1.22	1.34
3	A	395	GDP	O4'-C1'	-4.77	1.34	1.41
3	A	395	GDP	C6-N1	-4.27	1.31	1.37
3	A	395	GDP	C4-N3	-3.98	1.27	1.37
3	A	395	GDP	PA-O5'	-3.81	1.43	1.59
3	A	395	GDP	C5-C4	-3.48	1.34	1.43
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	C5-C6	-2.28	1.42	1.47
3	A	395	GDP	PA-O1A	-2.05	1.43	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
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	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	C5-C6-N1	-3.56	107.67	113.95
3	A	395	GDP	O6-C6-C5	3.53	131.26	124.37
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	O2B-PB-O3A	2.30	112.35	104.64

There are no chirality outliers.

All (6) torsion outliers are listed below:



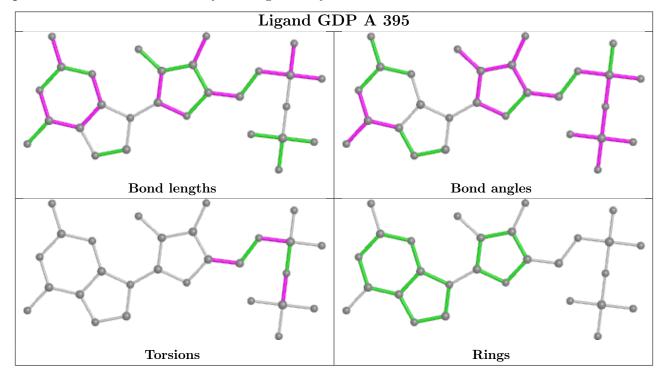
Mol	Chain	Res	Type	Atoms
3	A	395	GDP	C5'-O5'-PA-O3A
3	A	395	GDP	O4'-C4'-C5'-O5'
3	A	395	GDP	C5'-O5'-PA-O2A
3	A	395	GDP	C3'-C4'-C5'-O5'
3	A	395	GDP	C5'-O5'-PA-O1A
3	A	395	GDP	PA-O3A-PB-O1B

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 then 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 (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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

