

# Full wwPDB X-ray Structure Validation Report (i)

#### May 28, 2020 – 10:08 pm BST

PDB ID : 2I2O

> Title : Crystal Structure of an eIF4G-like Protein from Danio rerio

Authors Bitto, E.; Wesenberg, G.E.; Phillips Jr., G.N.; Mccoy, J.G.; Bingman, C.A.;

Center for Eukaryotic Structural Genomics (CESG)

Deposited on 2006-08-16

1.92 Å(reported) Resolution

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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

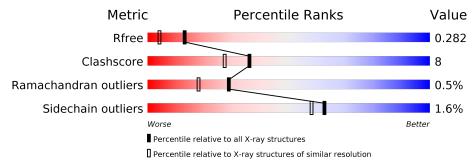
Validation Pipeline (wwPDB-VP) 2.11

## 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 1.92 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
Metric	$(\#\mathrm{Entries})$	$\mid \; (\#  ext{Entries},   ext{resolution range}( ext{Å})) \; \mid \;$
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)

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 <=5%

Mol	Chain	Length	Quality of chain				
1	A	224	80%	13%	6%		
1	В	224	81%	11%	• 6%		



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3896 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 eIF4G-like protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	211	Total 1739	C 1106				0	2	0
1	В	210	Total 1737	C 1106	N 295			0	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	_	CLONING ARTIFACT	UNP Q5EAQ1
A	0	ILE	-	CLONING ARTIFACT	UNP Q5EAQ1
A	1	ALA	-	CLONING ARTIFACT	UNP Q5EAQ1
В	-1	ALA	-	CLONING ARTIFACT	UNP Q5EAQ1
В	0	ILE	_	CLONING ARTIFACT	UNP Q5EAQ1
В	1	ALA	-	CLONING ARTIFACT	UNP Q5EAQ1

• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0

• Molecule 3 is water.

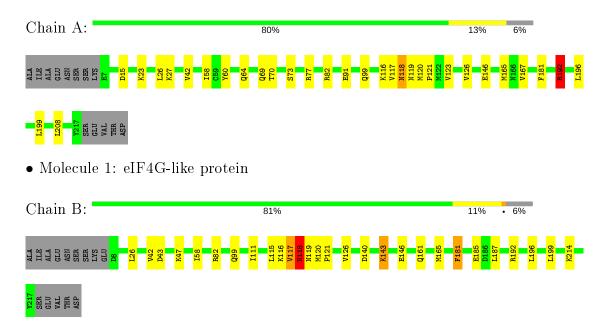
Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	202	Total O 202 202	0	0
3	В	216	Total O 216 216	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

• Molecule 1: eIF4G-like protein





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	$317.80\text{\AA}  40.95\text{Å}  40.92\text{Å}$	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.26^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	40.61 - 1.92	Depositor
rtesolution (A)	40.61 - 1.92	EDS
% Data completeness	97.4 (40.61-1.92)	Depositor
(in resolution range)	97.4 (40.61-1.92)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.52~({ m at}~1.92{ m \AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
$R, R_{free}$	0.190 , $0.235$	Depositor
$\Pi, \Pi free$	0.252 , $0.282$	DCC
$R_{free}$ test set	1998 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.35 \;, 35.5$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.032  for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.16% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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:

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.65	0/1763	0.73	3/2364 (0.1%)	
1	В	0.69	0/1761	0.68	0/2362	
All	All	0.67	0/3524	0.71	3/4726 (0.1%)	

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	В	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	192	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	192	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	192	ARG	CD-NE-CZ	5.06	130.68	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	${f Res}$	Type	Group
1	В	118	ASN	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	Α	1739	0	1753	32	0
1	В	1737	0	1755	29	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	202	0	0	4	0
3	В	216	0	0	3	0
All	All	3896	0	3508	56	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 8.

All (56) 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:181[B]:PHE:CZ	1:B:181[B]:PHE:HE2	1.70	1.08
1:B:117:VAL:O	1:B:120:MSE:HB3	1.63	0.98
1:B:26:LEU:HD21	1:B:58:ILE:HG13	1.47	0.96
1:A:181[B]:PHE:CZ	1:B:181[B]:PHE:CE2	2.61	0.88
1:A:208:LEU:HD22	3:A:650:HOH:O	1.80	0.81
1:A:117:VAL:O	1:A:120:MSE:HB3	1.82	0.79
1:B:99:GLN:NE2	1:B:146:GLU:OE2	2.19	0.75
1:A:181[B]:PHE:CE1	1:B:181[B]:PHE:HE2	2.09	0.71
1:B:119:ASN:O	1:B:121:PRO:HD3	1.95	0.67
1:B:43:ASP:OD1	1:B:82:ARG:NH2	2.22	0.66
1:A:181[B]:PHE:CE1	1:B:181[B]:PHE:CE2	2.82	0.66
1:A:167:VAL:HB	3:A:531:HOH:O	1.96	0.66
1:A:91:GLU:HG2	3:A:540:HOH:O	1.96	0.65
1:A:99:GLN:NE2	1:A:146:GLU:OE2	2.31	0.64
1:A:119:ASN:O	1:A:121:PRO:HD3	2.00	0.62
1:B:111:ILE:HG23	1:B:115:LEU:HD22	1.82	0.60
1:A:118:ASN:CG	1:A:119:ASN:H	2.04	0.60
1:B:140:ASP:HA	1:B:143:LYS:HD3	1.84	0.59
1:A:123:VAL:HG13	3:A:534:HOH:O	2.02	0.59
1:A:117:VAL:HB	1:A:120:MSE:HE2	1.86	0.57
1:A:42:VAL:HG11	1:A:82:ARG:HG3	1.89	0.55

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({f \AA})$	overlap (Å)
1:B:181[A]:PHE:HE1	1:B:196:LEU:CA	2.22	0.53
1:A:126:VAL:HG21	1:A:165[B]:MSE:SE	2.60	0.51
1:A:181[B]:PHE:HD2	1:A:199:LEU:HD12	1.75	0.51
1:B:214:LYS:HG3	3:B:658:HOH:O	2.11	0.51
1:B:126:VAL:HG21	1:B:165[A]:MSE:HG2	1.93	0.50
1:A:26:LEU:HD21	1:A:58:ILE:HG13	1.93	0.49
1:A:116:LYS:HE2	1:A:121:PRO:HG3	1.95	0.49
1:A:117:VAL:O	1:A:118:ASN:HB3	2.12	0.49
1:A:181[A]:PHE:HE1	1:B:181[A]:PHE:CZ	2.31	0.48
1:A:117:VAL:HB	1:A:120:MSE:CE	2.44	0.48
1:A:23:LYS:HA	1:A:26:LEU:HD12	1.94	0.48
1:B:118:ASN:HB3	1:B:120:MSE:H	1.77	0.48
1:A:126:VAL:CG2	1:A:165[B]:MSE:HG2	2.44	0.47
1:B:126:VAL:CG1	1:B:165[A]:MSE:HG2	2.44	0.47
1:B:126:VAL:HG11	1:B:165[A]:MSE:HG2	1.96	0.47
1:B:126:VAL:CG2	1:B:165[A]:MSE:HG2	2.44	0.47
1:B:42:VAL:HG11	1:B:82:ARG:HG3	1.98	0.46
1:A:126:VAL:HG21	1:A:165[B]:MSE:HG2	1.98	0.46
1:B:185:GLU:CD	3:B:614:HOH:O	2.54	0.46
1:A:181[B]:PHE:CE1	1:A:192:ARG:HG3	2.51	0.45
1:A:73:SER:OG	1:A:77:ARG:NH1	2.49	0.45
1:B:126:VAL:HG21	1:B:165[A]:MSE:SE	2.67	0.44
1:A:118:ASN:CG	1:A:119:ASN:N	2.71	0.43
1:A:181[B]:PHE:HE2	1:A:196:LEU:CA	2.33	0.42
1:B:117:VAL:CG2	1:B:120:MSE:HE3	2.50	0.41
1:B:161:GLN:O	1:B:165[B]:MSE:HG2	2.20	0.41
1:A:60:TYR:O	1:A:64:GLN:HG2	2.20	0.41
1:B:165[B]:MSE:HE3	3:B:521:HOH:O	2.19	0.41
1:B:181[A]:PHE:HD1	1:B:199:LEU:HD12	1.85	0.41
1:A:181[B]:PHE:CE2	1:A:196:LEU:HB2	2.55	0.41
1:A:69:GLN:HG2	1:A:70:THR:HG23	2.04	0.40
1:B:116:LYS:HE2	1:B:121:PRO:HG3	2.04	0.40
1:B:187:LEU:HB2	1:B:192:ARG:NH1	2.36	0.40
1:B:47:LYS:HA	1:B:47:LYS:HD3	1.93	0.40

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	$211/224 \ (94\%)$	204 (97%)	6 (3%)	1 (0%)	29 18
1	В	211/224~(94%)	206 (98%)	4 (2%)	1 (0%)	29 18
All	All	422/448 (94%)	410 (97%)	10 (2%)	2 (0%)	29 18

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	A	118	ASN
1	В	118	ASN

#### 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	195/199 (98%)	192 (98%)	3 (2%)	65 61
1	В	195/199 (98%)	191 (98%)	4 (2%)	53 46
All	All	390/398 (98%)	383 (98%)	7 (2%)	62 53

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	27	LYS
1	A	192	ARG
1	В	117	VAL

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	В	143	LYS
1	В	181[A]	PHE
1	В	181[B]	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

