

Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 08:19 pm GMT

PDB ID : 4B44

Title: Bacterial translation initiation factor IF2 (1-363), complex with GDP at pH8.0

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Deposited on : 2012-07-27

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 : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

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)

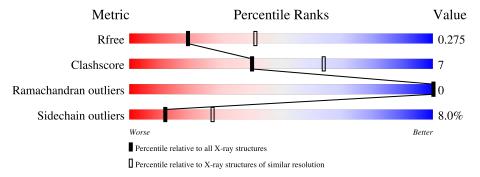
Validation Pipeline (wwPDB-VP) : 2.36

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
TVIOUTE	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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%

Mol	Chain	Length	Quality of chain				
1	A	363	73%	20%			



2 Entry composition (i)

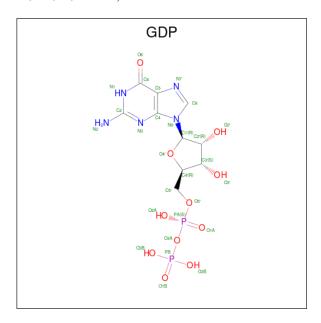
There are 3 unique types of molecules in this entry. The entry contains 2741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSLATION INITIATION FACTOR IF-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	347	Total 2688	C 1681	N 477	O 521	S 9	0	1	0

• Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	٨	1	Total	С	N	О	Р	0	0
	A	1	28	10	5	11	2	U	0

• Molecule 3 is water.

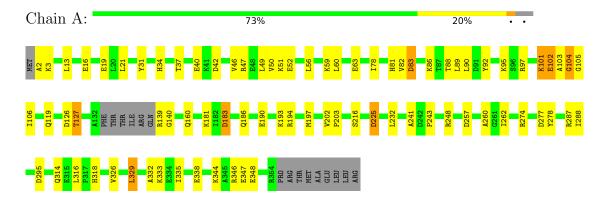
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O 25 25	0	0



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. 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: TRANSLATION INITIATION FACTOR IF-2





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	45.15Å 62.20Å 159.96Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	43.45 - 2.70	Depositor	
resolution (A)	40.48 - 2.29	EDS	
% Data completeness	98.8 (43.45-2.70)	Depositor	
(in resolution range)	75.4 (40.48-2.29)	EDS	
R_{merge}	0.16	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.06 (at 2.29Å)	Xtriage	
Refinement program	PHENIX (PHENIX.REFINE: DEV_1269)	Depositor	
R, R_{free}	0.212 , 0.271	Depositor	
it, it free	0.256 , 0.275	DCC	
R_{free} test set	791 reflections (5.00%)	wwPDB-VP	
Wilson B-factor (A^2)	40.1	Xtriage	
Anisotropy	1.041	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29, 43.8	EDS	
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.92	EDS	
Total number of atoms	2741	wwPDB-VP	
Average B, all atoms (Å ²)	69.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.54% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: 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).

Mal	Chain	Bond	lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ $\# Z > 5$		
1	A	0.67	0/2726	0.61	3/3670 (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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	104	GLY	N-CA-C	6.42	129.15	113.10
1	A	103	ALA	CB-CA-C	5.61	118.51	110.10
1	A	127	THR	C-N-CD	5.40	139.74	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	LYS	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	2688	0	2724	39	0
2	A	28	0	12	2	0
3	A	25	0	0	1	0
All	All	2741	0	2736	39	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 7.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A4 a 2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:A:257:ASP:HB3	1:A:260:ALA:HB3	1.59	0.82
1:A:105:GLY:N	1:A:106:ILE:HA	2.12	0.62
1:A:101:LYS:O	1:A:102:GLU:HB3	1.98	0.62
1:A:86:LYS:NZ	2:A:1355:GDP:O3B	2.33	0.62
1:A:88:THR:OG1	2:A:1355:GDP:O2A	2.21	0.58
1:A:193:LYS:O	1:A:197:MET:HG3	2.04	0.57
1:A:139:ARG:HG3	1:A:140:GLY:H	1.71	0.55
1:A:181:LYS:NZ	3:A:2011:HOH:O	2.40	0.55
1:A:105:GLY:H	1:A:106:ILE:HA	1.71	0.54
1:A:102:GLU:HG2	1:A:102:GLU:O	2.08	0.51
1:A:78:ILE:HD12	1:A:90:LEU:HG	1.93	0.51
1:A:183:ASP:OD1	1:A:216:SER:OG	2.17	0.51
1:A:82:VAL:O	1:A:83:ASP:HB2	2.12	0.50
1:A:127:THR:O	1:A:127:THR:OG1	2.27	0.49
1:A:262:ILE:HG23	1:A:316:LEU:HD23	1.95	0.48
1:A:16:GLU:HB2	1:A:19:GLU:HB2	1.96	0.47
1:A:225:ASP:N	1:A:225:ASP:OD1	2.46	0.47
1:A:186:GLN:OE1	1:A:186:GLN:N	2.39	0.47
1:A:102:GLU:O	1:A:104:GLY:HA2	2.16	0.46
1:A:278:TYR:CE1	1:A:287:ARG:HB2	2.51	0.46
1:A:335:ILE:O	1:A:338:GLU:HG2	2.16	0.46
1:A:344:LYS:O	1:A:347:GLU:HB2	2.17	0.44
1:A:106:ILE:N	1:A:295:ASP:O	2.50	0.44
1:A:278:TYR:CZ	1:A:329:LEU:HB2	2.53	0.44
1:A:190:GLU:O	1:A:194:ARG:HG3	2.19	0.43
1:A:241:ALA:O	1:A:243:PRO:HD3	2.19	0.43
1:A:13:LEU:HD13	1:A:50:VAL:HG21	2.00	0.42
1:A:21:LEU:HD22	1:A:31:TYR:CZ	2.55	0.42
1:A:81:HIS:HD2	1:A:160:GLN:HB2	1.85	0.42

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:2:ALA:HA	1:A:3:LYS:HA	1.80	0.41
1:A:326:VAL:HG21	1:A:332:ALA:HB2	2.01	0.41
1:A:47:ARG:O	1:A:51:LYS:HG3	2.21	0.41
1:A:56:LEU:O	1:A:60:LEU:HG	2.21	0.41
1:A:126:ASP:HB3	1:A:127:THR:H	1.64	0.41
1:A:78:ILE:HD13	1:A:89:LEU:HD23	2.02	0.41
1:A:42:ASP:O	1:A:46:VAL:HG23	2.21	0.41
1:A:92:TYR:HA	1:A:95:LYS:HE3	2.02	0.40
1:A:202:VAL:HA	1:A:203:PRO:HD3	1.95	0.40
1:A:277:ASP:HB2	1:A:288:ILE:HD12	2.04	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	344/363~(95%)	324 (94%)	20 (6%)	0	100 100

There are no Ramachandran outliers to report.

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	Analysed Rotameric		Percentiles	
1	A	$276/290 \ (95\%)$	254 (92%)	22 (8%)	12 27	



All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	37	THR
1	A	40	GLU
1	A	49	LEU
1	A	52	GLU
1	A	59	LYS
1	A	63	GLU
1	A	83	ASP
1	A	97	ARG
1	A	102	GLU
1	A	119	GLN
1	A	183	ASP
1	A	225	ASP
1	A	232	LEU
1	A	248	ARG
1	A	274	ARG
1	A	314	GLN
1	A	318	HIS
1	A	329	LEU
1	A	333	LYS
1	A	346	ARG
1	A	348	GLU

Sometimes 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 monosaccharides in this entry.



5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	Bo	ond leng	ths	В	ond ang	les
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	A	1355	-	24,30,30	1.04	1 (4%)	30,47,47	1.27	3 (10%)

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
2	GDP	A	1355	-	-	6/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	A	1355	GDP	C6-N1	-2.95	1.33	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
2	A	1355	GDP	PA-O3A-PB	-3.55	120.66	132.83
2	A	1355	GDP	C8-N7-C5	2.50	107.75	102.99
2	A	1355	GDP	C5-C6-N1	2.42	118.22	113.95

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1355	GDP	C5'-O5'-PA-O3A
2	A	1355	GDP	C5'-O5'-PA-O1A
2	A	1355	GDP	C5'-O5'-PA-O2A
2	A	1355	GDP	O4'-C4'-C5'-O5'

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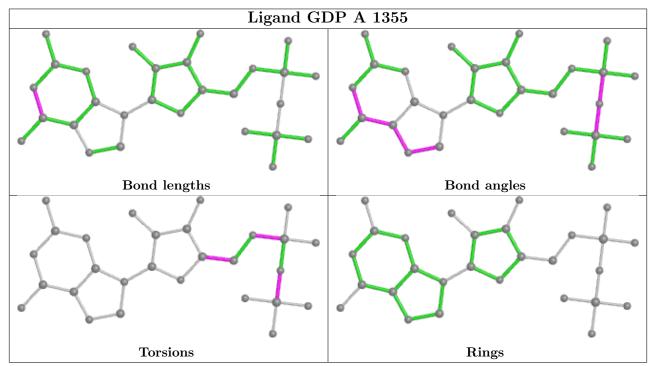
Mol	Chain	Res	Type	Atoms
2	A	1355	GDP	C3'-C4'-C5'-O5'
2	A	1355	GDP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1355	GDP	2	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)

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.

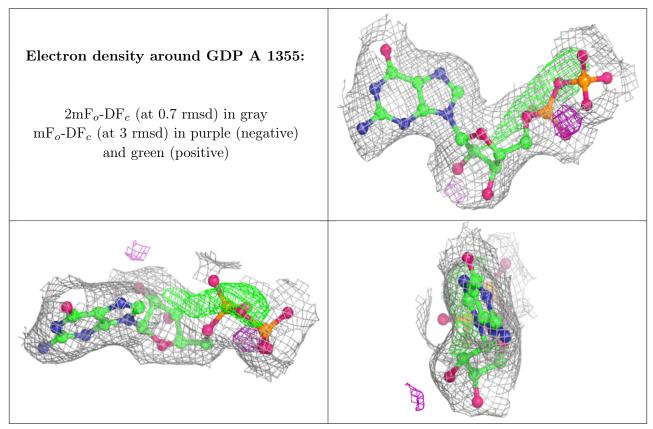
6.3 Carbohydrates (i)

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.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

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

