



## wwPDB EM Map/Model Validation Report ⓘ

May 5, 2016 – 05:30 PM EDT

PDB ID : 4CRN  
EMDB ID: : EMD-2597  
Title : Cryo-EM of a pretermination complex with eRF1 and eRF3  
Authors : Preis, A.; Heuer, A.; Barrio-Garcia, C.; Hauser, A.; Eyler, D.; Berninghausen, O.; Green, R.; Becker, T.; Beckmann, R.  
Deposited on : 2014-02-28  
Resolution : 9.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

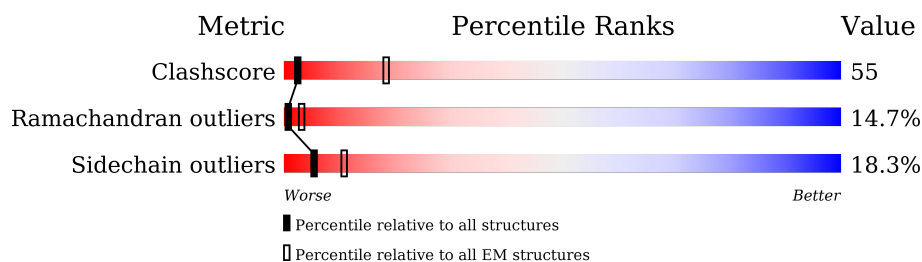
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.10 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	P	430	
2	X	437	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GNP	P	1685	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6693 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ERF3 IN RIBOSOME BOUND ERF1-ERF3-GDPNP COMPLEX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	430	Total	C	N	O	S	0	0
			3351	2119	577	634	21		

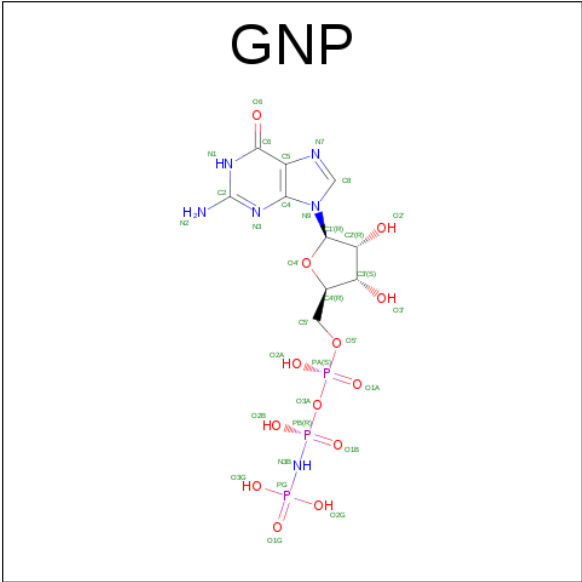
- Molecule 2 is a protein called ERF1 IN RIBOSOME-BOUND ERF1-ERF3-GDPNP COMPLEX.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	422	Total	C	N	O	S	0	1
			3310	2110	548	642	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	41	LEU	GLN	CONFLICT	UNP P12385
X	300	PHE	TYR	CONFLICT	UNP P12385

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

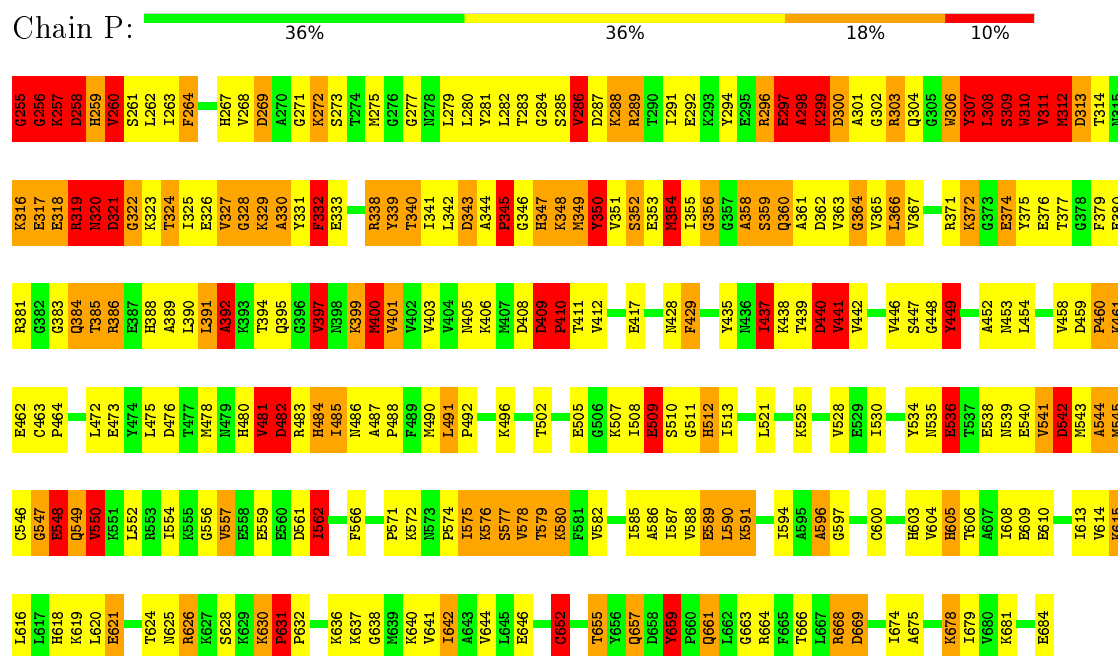


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	P	1	32	10	6	13	3	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ERF3 IN RIBOSOME BOUND ERF1-ERF3-GDPNP COMPLEX






## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	0.02	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	TEMCAM F416 CMOS TVIPS	Depositor

## 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: GNP

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  >2	RMSZ	# Z  >2
1	P	0.96	6/3412 (0.2%)	1.77	88/4600 (1.9%)
2	X	1.94	17/3363 (0.5%)	2.21	148/4532 (3.3%)
All	All	1.53	23/6775 (0.3%)	2.00	236/9132 (2.6%)

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	P	0	95
2	X	1	25
All	All	1	120

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	379	ASN	CG-ND2	81.72	3.37	1.32
2	X	183	SER	C-N	22.62	1.86	1.34
2	X	182	GLN	C-N	16.32	1.71	1.34
2	X	421	SER	C-N	-14.59	1.00	1.34
1	P	330	ALA	C-N	13.98	1.66	1.34

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	379	ASN	OD1-CG-ND2	-44.57	19.39	121.90
2	X	269	ALA	O-C-N	-24.66	83.25	122.70
2	X	183	SER	O-C-N	23.00	159.49	122.70
1	P	545	MET	CG-SD-CE	21.25	134.19	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	X	183	SER	CA-C-N	-17.73	78.19	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	142	LYS	CA

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	255	GLY	Mainchain
1	P	256	GLY	Peptide
1	P	257	LYS	Mainchain
1	P	260	VAL	Peptide
1	P	264	PHE	Mainchain

## 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	P	3351	0	3391	331	0
2	X	3310	0	3337	425	0
3	P	32	0	12	56	0
All	All	6693	0	6740	740	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 55.

The worst 5 of 740 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:P:331:TYR:CZ	1:P:536:GLU:HG3	1.34	1.59
1:P:304:GLN:NE2	3:P:1685:GNP:H3'	1.15	1.47
2:X:352:ALA:CB	2:X:361:MET:HG3	1.46	1.44
2:X:343:GLU:HB3	2:X:344:PRO:CD	1.45	1.43
2:X:161:ASN:ND2	2:X:390:LYS:HB2	1.18	1.41

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 PDB entries followed by that with respect to all EM entries.

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	P	428/430 (100%)	299 (70%)	69 (16%)	60 (14%)	0	6
2	X	420/437 (96%)	297 (71%)	58 (14%)	65 (16%)	0	5
All	All	848/867 (98%)	596 (70%)	127 (15%)	125 (15%)	1	6

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	258	ASP
1	P	260	VAL
1	P	285	SER
1	P	298	ALA
1	P	300	ASP

### 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 PDB entries followed by that with respect to all EM entries.

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	P	365/365 (100%)	304 (83%)	61 (17%)	3	19
2	X	362/377 (96%)	290 (80%)	72 (20%)	1	11
All	All	727/742 (98%)	594 (82%)	133 (18%)	5	14

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	681	LYS
2	X	96	ASP
2	X	334	GLU
2	X	13	LYS
2	X	58	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	161	ASN
2	X	396	GLN
2	X	177	HIS
1	P	605	HIS
2	X	279	GLN

### 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](#)

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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GNP	P	1685	-	29,34,34	2.48	11 (37%)	28,54,54	1.86	7 (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	GNP	P	1685	-	-	0/16/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1685	GNP	C4-N9	-6.42	1.39	1.47
3	P	1685	GNP	C5-C6	-5.75	1.42	1.53
3	P	1685	GNP	PB-O3A	-4.51	1.53	1.59
3	P	1685	GNP	PB-O2B	-3.15	1.48	1.56
3	P	1685	GNP	PG-O2G	-3.12	1.48	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1685	GNP	O3G-PG-O1G	-3.05	105.56	113.58
3	P	1685	GNP	O6-C6-N1	-2.27	119.82	122.80
3	P	1685	GNP	PA-O3A-PB	-2.14	124.94	132.71
3	P	1685	GNP	O3G-PG-O2G	3.12	116.73	107.67
3	P	1685	GNP	O2B-PB-O1B	3.69	117.29	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1685	GNP	56	0

## 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.