

Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2021 – 02:20 PM EST

PDB ID : 1LJ2

Title : Recognition of eIF4G by Rotavirus NSP3 reveals a basis for mRNA circular-

ization

Authors: Groft, C.M.; Burley, S.K.

Deposited on : 2002-04-18

Resolution : 2.38 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

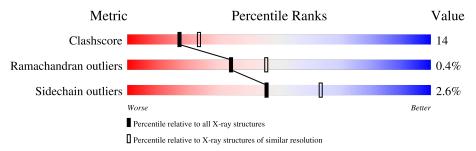
Validation Pipeline (wwPDB-VP) : 2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 2.38 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	$(\# \mathrm{Entries})$	$(\# \text{Entries, resolution range}(\mathring{A}))$		
Clashscore	141614	6082 (2.40-2.36)		
Ramachandran outliers	138981	5973 (2.40-2.36)		
Sidechain outliers	138945	5975 (2.40-2.36)		

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.

Mol	Chain	Length	Quality of chain						
1	A	110	67%	28%					
1	В	110	76%	22%					
2	С	28	36% 39%	• 21%)				
2	D	28	68%	21%	7% •				



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2327 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 NONSTRUCTURAL RNA-BINDING PROTEIN 34.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	106	Total 866	C 551	11	O 169	S 2	0	0	0
1	D	110		C		O	S	0	0	0
1	Б	110	893	566	149	175	3	U	0	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	SER	CYS	cloning artifact	UNP P03536
A	314	SER	CYS	cloning artifact	UNP P03536
В	306	SER	CYS	cloning artifact	UNP P03536
В	314	SER	CYS	cloning artifact	UNP P03536

• Molecule 2 is a protein called eukaryotic protein synthesis initiation factor.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	22	Total	С	N	О	S	0	0	0
2	2 C	22	159	94	30	34	1	U		U
2	D	27	Total	С	N	О	S	0	0	0
	ש	21	210	124	43	42	1			

• Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	2	Total Au 2 2	0	0
3	D	1	Total Au 1 1	0	0

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	В	85	Total O 85 85	0	0
4	С	14	Total O 14 14	0	0
4	D	14	Total O 14 14	0	0

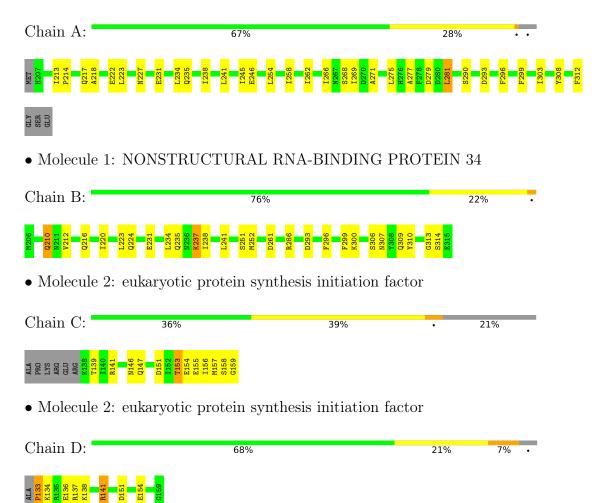


3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: NONSTRUCTURAL RNA-BINDING PROTEIN 34





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	59.69Å 74.04Å 77.46Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	20.00 - 2.38	Depositor	
% Data completeness	(Not available) (20.00-2.38)	Depositor	
(in resolution range)	(1100 available) (20.00 2.90)		
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	CNS	Depositor	
R, R_{free}	0.221 , 0.272	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2327	wwPDB-VP	
Average B, all atoms (Å ²)	29.0	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: AU

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	0.34	0/882	0.50	0/1194	
1	В	0.34	0/909	0.49	0/1228	
2	С	0.33	0/159	0.52	0/212	
2	D	0.34	0/210	0.76	1/276~(0.4%)	
All	All	0.34	0/2160	0.53	1/2910 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	D	133	PRO	N-CA-CB	6.28	110.83	103.30

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	H(model)	H(added)	Clashes	Symm-Clashes
1	A	866	0	842	28	0
1	В	893	0	864	25	0
2	С	159	0	147	11	0
2	D	210	0	204	9	0
3	В	2	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	83	0	0	1	0
4	В	85	0	0	2	0
4	С	14	0	0	1	0
4	D	14	0	0	2	0
All	All	2327	0	2057	58	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 14.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 1 1	A. 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:B:210:GLN:HE21	1:B:210:GLN:H	1.09	0.98
2:C:146:ASN:O	2:C:147:GLN:HG3	1.88	0.72
1:A:279:ASP:OD1	1:B:237:LYS:HE2	1.91	0.71
2:C:141:ARG:HB3	2:C:151:ASP:OD1	1.92	0.69
1:A:271:ALA:HB1	4:A:1105:HOH:O	1.92	0.68
1:A:218:ALA:O	1:A:222:GLU:HG3	1.98	0.63
1:B:210:GLN:HE21	1:B:210:GLN:N	1.88	0.63
1:A:213:ILE:HB	1:A:214:PRO:HD3	1.82	0.61
1:B:231:GLU:O	1:B:235:GLN:HG3	2.03	0.59
1:B:309:GLN:HE21	1:B:310:TYR:H	1.49	0.59
1:A:290:SER:HA	1:B:252:MET:CE	2.34	0.58
2:C:155:GLU:O	2:C:158:SER:HB3	2.04	0.58
1:A:275:LEU:HD22	1:B:237:LYS:HG3	1.89	0.54
1:A:213:ILE:O	1:A:217:GLN:HG3	2.08	0.53
1:A:290:SER:HA	1:B:252:MET:HE2	1.90	0.53
1:B:220:ILE:O	1:B:224:GLN:HG3	2.09	0.52
1:A:217:GLN:HG2	1:B:216:GLN:HE22	1.75	0.52
2:D:137:ARG:HA	2:D:137:ARG:HH11	1.75	0.52
1:A:269:ILE:HD13	1:A:281:LEU:HD13	1.93	0.51
1:A:266:ILE:C	1:A:268:SER:H	2.15	0.50
2:D:141:ARG:HG3	2:D:151:ASP:OD2	2.12	0.50
1:A:312:PHE:HA	2:C:139:THR:O	2.11	0.50
1:A:254:LEU:HD21	1:B:293:ASP:HA	1.94	0.49
1:B:241:LEU:C	1:B:241:LEU:HD23	2.33	0.49
2:C:153:THR:HG22	2:C:157:MET:HE2	1.94	0.49
1:A:231:GLU:O	1:A:235:GLN:HG3	2.14	0.48
1:A:308:TYR:HE1	2:C:156:ILE:HD11	1.78	0.48
1:A:299:PHE:O	1:A:303:ILE:HG12	2.13	0.48
2:D:137:ARG:NH1	2:D:138:LYS:H	2.10	0.48

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A J		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:154:GLU:HA	2:C:157:MET:HE2	1.95	0.48
2:D:134:LYS:O	2:D:136:GLU:HG2	2.14	0.48
1:B:296:PHE:O	1:B:299:PHE:HB3	2.14	0.47
1:B:234:LEU:O	1:B:238:ILE:HG13	2.15	0.47
1:B:210:GLN:HG3	4:B:1223:HOH:O	2.15	0.47
1:A:296:PHE:O	1:A:299:PHE:HB3	2.16	0.46
1:A:293:ASP:CG	1:B:252:MET:HE3	2.36	0.46
2:C:156:ILE:C	2:C:158:SER:H	2.19	0.46
1:A:223:LEU:O	1:A:227:ASN:HB3	2.16	0.45
1:A:223:LEU:HD13	1:B:223:LEU:HB2	1.98	0.45
1:A:308:TYR:CE1	2:C:156:ILE:HD11	2.52	0.45
2:D:141:ARG:CG	2:D:151:ASP:OD2	2.65	0.45
1:A:241:LEU:O	1:A:245:ILE:HG13	2.16	0.45
1:A:246:GLU:HG3	1:A:266:ILE:HG21	1.98	0.45
1:B:212:VAL:O	1:B:216:GLN:HG3	2.17	0.45
1:A:293:ASP:OD2	1:B:252:MET:HE3	2.17	0.44
1:A:258:ILE:O	1:A:262:ILE:HG13	2.17	0.44
2:C:159:GLY:HA2	4:C:1194:HOH:O	2.17	0.43
2:C:141:ARG:NH2	2:C:151:ASP:OD2	2.46	0.43
2:D:133:PRO:N	4:D:1166:HOH:O	2.51	0.43
1:A:234:LEU:O	1:A:238:ILE:HG13	2.20	0.42
1:B:313:GLY:O	2:D:138:LYS:HA	2.19	0.41
1:B:306:SER:O	1:B:307:ASN:HB2	2.20	0.41
1:A:290:SER:HA	1:B:252:MET:HE1	2.00	0.41
1:B:286:ARG:NE	4:B:1295:HOH:O	2.44	0.41
2:D:154:GLU:HB3	4:D:1182:HOH:O	2.21	0.41
1:B:296:PHE:CE2	1:B:300:LYS:HD2	2.56	0.40
1:B:314:SER:HA	2:D:137:ARG:O	2.21	0.40
1:A:238:ILE:HD13	1:A:277:ALA:CB	2.51	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	Perce	ntiles
1	A	104/110 (94%)	103 (99%)	1 (1%)	0	100	100
1	В	108/110 (98%)	108 (100%)	0	0	100	100
2	C	20/28 (71%)	16 (80%)	3 (15%)	1 (5%)	2	1
2	D	25/28~(89%)	22~(88%)	3 (12%)	0	100	100
All	All	257/276~(93%)	249 (97%)	7 (3%)	1 (0%)	34	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	153	THR

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	97/102 (95%)	96 (99%)	1 (1%)	76 87
1	В	99/102 (97%)	95 (96%)	4 (4%)	31 47
2	С	16/24 (67%)	16 (100%)	0	100 100
2	D	21/24 (88%)	20 (95%)	1 (5%)	25 39
All	All	233/252 (92%)	227 (97%)	6 (3%)	46 64

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	LEU
1	В	210	GLN
1	В	237	LYS
1	В	251	SER
1	В	261	ASP
2	D	141	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:



Mol	Chain	Res	Type
1	В	207	HIS
1	В	210	GLN
1	В	211	ASN
1	В	216	GLN
1	В	276	HIS
1	В	309	GLN
2	С	147	GLN
2	D	147	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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)

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.

