Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 06:10 PM JST

PDB ID	:	8WQQ
Title	:	Proteomics study reveals that ASFV g5Rp protein interacts with eukaryotic translation initiation factor 5A and may regulate host translation
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Deposited on	:	2023-10-12
Resolution	:	2.30 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 ⓘ 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 ⓘ) were used in the production of this report:

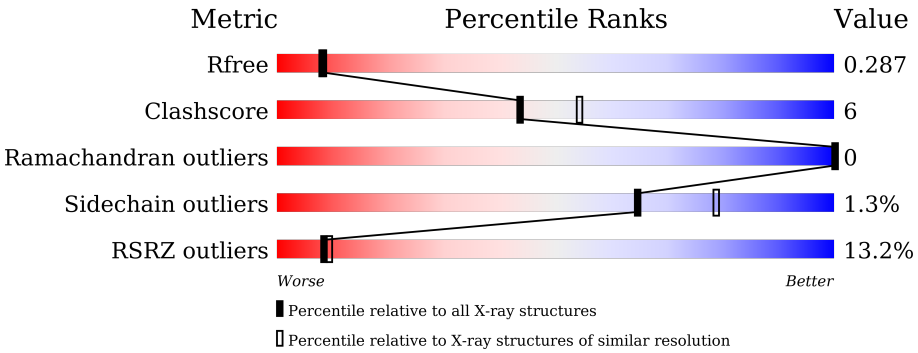
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	13% 79% 20%
1	B	243	13% 85% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4283 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 mRNA-decapping protein g5R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			2046	1322	344	367	13			
1	B	243	Total	C	N	O	S	0	0	0
			2046	1322	344	367	13			

- Molecule 2 is water.

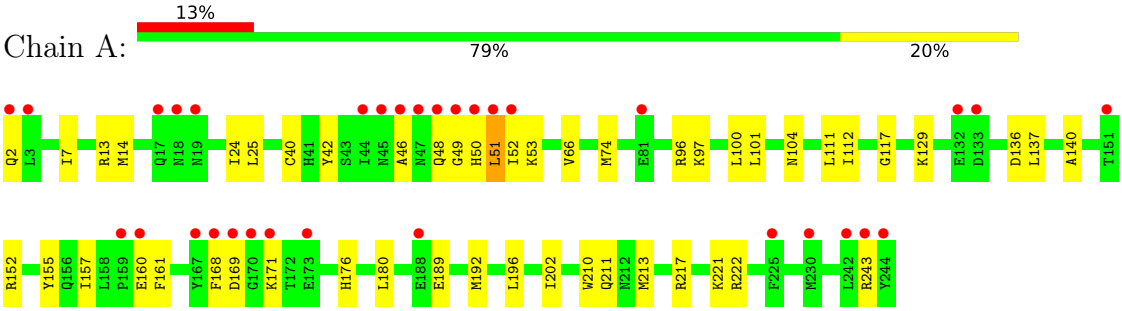
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total	O	0	0
			99	99		
2	B	92	Total	O	0	0
			92	92		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

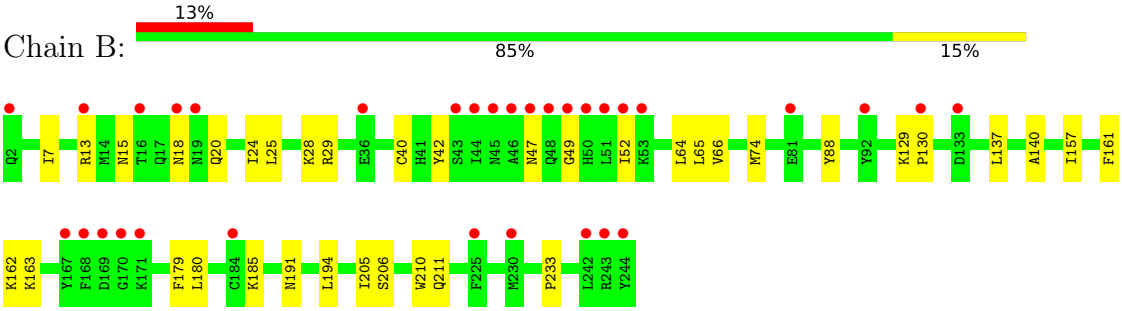
• Molecule 1: mRNA-decapping protein g5R

Chain A:



• Molecule 1: mRNA-decapping protein g5R

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.20Å 77.30Å 96.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.20 – 2.30 30.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.20-2.30) 99.2 (30.20-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.237 , 0.287 0.237 , 0.287	Depositor DCC
R_{free} test set	23373 reflections (7.86%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4283	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2164e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	1/2096 (0.0%)	0.56	3/2822 (0.1%)
1	B	0.35	0/2096	0.56	2/2822 (0.1%)
All	All	0.34	1/4192 (0.0%)	0.56	5/5644 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	LYS	CD-CE	5.17	1.64	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	LEU	CB-CG-CD2	-7.60	98.08	111.00
1	B	185	LYS	CD-CE-NZ	-7.07	95.44	111.70
1	A	160	GLU	CA-CB-CG	-6.54	99.00	113.40
1	B	185	LYS	CA-CB-CG	6.13	126.89	113.40
1	A	51	LEU	CB-CG-CD1	5.61	120.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	47	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	A	2046	0	2045	26	1
1	B	2046	0	2045	25	1
2	A	99	0	0	2	0
2	B	92	0	0	2	0
All	All	4283	0	4090	49	1

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 6.

All (49) 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:B:18:ASN:HD22	1:B:20:GLN:HB2	1.14	1.06
1:A:104:ASN:OD1	2:A:301:HOH:O	1.82	0.95
1:B:18:ASN:ND2	1:B:20:GLN:HB2	1.85	0.91
1:B:15:ASN:CG	1:B:18:ASN:OD1	2.33	0.67
1:A:46:ALA:HB1	1:A:50:HIS:HB2	1.75	0.66
1:B:52:ILE:O	2:B:301:HOH:O	2.15	0.64
1:B:7:ILE:HG22	1:B:140:ALA:HB2	1.79	0.63
1:A:221:LYS:HE2	1:A:222:ARG:HH12	1.66	0.60
1:B:18:ASN:OD1	1:B:18:ASN:N	2.35	0.59
1:B:194:LEU:HD11	1:B:205:ILE:HG22	1.85	0.59
1:A:25:LEU:HD12	1:A:211:GLN:HG3	1.88	0.56
1:B:129:LYS:HD3	1:B:130:PRO:O	2.07	0.55
1:A:50:HIS:HA	1:A:53:LYS:NZ	2.22	0.55
1:A:213:MET:HG3	1:A:217:ARG:HH11	1.72	0.54
1:A:7:ILE:HG22	1:A:140:ALA:HB2	1.91	0.53
1:A:202:ILE:HD12	1:B:64:LEU:HD21	1.89	0.53
1:A:51:LEU:HD23	1:A:111:LEU:HD13	1.90	0.53
1:A:97:LYS:HA	1:A:101:LEU:HD12	1.89	0.53
1:A:96:ARG:HG2	1:A:100:LEU:HD12	1.90	0.52
1:A:152:ARG:NH1	1:A:155:TYR:O	2.43	0.51
1:B:137:LEU:HD11	1:B:157:ILE:HD12	1.93	0.51
1:B:40:CYS:HA	1:B:42:TYR:CE2	2.47	0.50
1:B:25:LEU:HD12	1:B:211:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:O	1:A:52:ILE:HG12	2.13	0.48
1:B:66:VAL:HG22	1:B:74:MET:HE2	1.97	0.47
1:A:40:CYS:HA	1:A:42:TYR:CE2	2.49	0.47
1:B:129:LYS:HG2	1:B:130:PRO:HD2	1.96	0.47
1:A:24:ILE:HG12	1:A:210:TRP:CZ3	2.50	0.47
1:A:176:HIS:HD2	2:A:322:HOH:O	1.98	0.46
1:B:28:LYS:NZ	2:B:309:HOH:O	2.38	0.46
1:B:15:ASN:ND2	1:B:18:ASN:OD1	2.48	0.46
1:A:189:GLU:HB3	1:A:192:MET:HG2	1.99	0.45
1:B:162:LYS:HD2	1:B:179:PHE:CE2	2.51	0.45
1:A:49:GLY:HA2	1:A:52:ILE:HB	1.99	0.45
1:B:13:ARG:HB3	1:B:210:TRP:CH2	2.52	0.45
1:A:66:VAL:HG13	1:A:74:MET:HE3	1.99	0.45
1:A:196:LEU:HA	1:A:202:ILE:HD13	1.99	0.44
1:A:7:ILE:HD13	1:A:136:ASP:HA	1.99	0.44
1:A:112:ILE:HD13	1:A:112:ILE:HA	1.91	0.44
1:A:161:PHE:CD1	1:A:180:LEU:HB2	2.52	0.43
1:A:137:LEU:HD11	1:A:157:ILE:HD12	2.01	0.43
1:B:65:LEU:HD12	1:B:65:LEU:HA	1.89	0.42
1:B:24:ILE:HG12	1:B:210:TRP:CZ3	2.54	0.42
1:B:29:ARG:HA	1:B:206:SER:HB3	2.02	0.42
1:B:163:LYS:HE3	1:B:233:PRO:HG2	2.02	0.41
1:B:49:GLY:HA2	1:B:52:ILE:HB	2.03	0.41
1:A:117:GLY:HA2	1:B:191:ASN:O	2.21	0.41
1:B:161:PHE:CD1	1:B:180:LEU:HB2	2.56	0.41
1:A:2:GLN:HA	1:A:2:GLN:OE1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH2	1:B:88:TYR:OH[2_455]	2.10	0.10

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	241/243 (99%)	233 (97%)	8 (3%)	0	100	100
1	B	241/243 (99%)	232 (96%)	9 (4%)	0	100	100
All	All	482/486 (99%)	465 (96%)	17 (4%)	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	Rotameric	Outliers	Percentiles	
1	A	226/226 (100%)	220 (97%)	6 (3%)	40	57
1	B	226/226 (100%)	226 (100%)	0	100	100
All	All	452/452 (100%)	446 (99%)	6 (1%)	65	79

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

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	MET
1	A	129	LYS
1	A	168	PHE
1	A	169	ASP
1	A	243	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	B	200	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	243/243 (100%)	0.91	32 (13%)	8	9	24, 41, 75, 89	0
1	B	243/243 (100%)	0.90	32 (13%)	8	9	23, 40, 76, 96	0
All	All	486/486 (100%)	0.90	64 (13%)	8	9	23, 41, 77, 96	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	TYR	8.1
1	B	49	GLY	7.1
1	B	46	ALA	6.5
1	B	170	GLY	6.4
1	A	244	TYR	5.6
1	B	48	GLN	5.5
1	A	48	GLN	5.2
1	B	52	ILE	5.0
1	B	45	ASN	4.6
1	A	51	LEU	4.4
1	A	170	GLY	4.3
1	A	49	GLY	3.8
1	B	50	HIS	3.7
1	A	52	ILE	3.7
1	B	167	TYR	3.6
1	A	168	PHE	3.6
1	A	2	GLN	3.5
1	B	16	THR	3.5
1	A	230	MET	3.4
1	A	18	ASN	3.2
1	B	225	PHE	3.1
1	B	44	ILE	3.1
1	A	243	ARG	3.1
1	A	171	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	3	LEU	3.0
1	B	243	ARG	3.0
1	B	36	GLU	2.9
1	A	50	HIS	2.9
1	B	168	PHE	2.9
1	B	53	LYS	2.9
1	B	51	LEU	2.9
1	A	44	ILE	2.8
1	B	92	TYR	2.8
1	B	47	ASN	2.8
1	B	81	GLU	2.8
1	A	46	ALA	2.8
1	A	17	GLN	2.8
1	A	169	ASP	2.7
1	B	18	ASN	2.7
1	A	47	ASN	2.7
1	B	2	GLN	2.7
1	A	133	ASP	2.6
1	A	160	GLU	2.6
1	A	173	GLU	2.6
1	A	225	PHE	2.6
1	A	159	PRO	2.6
1	B	171	LYS	2.5
1	A	19	ASN	2.4
1	B	13	ARG	2.4
1	A	167	TYR	2.4
1	A	132	GLU	2.4
1	B	133	ASP	2.4
1	B	19	ASN	2.3
1	A	81	GLU	2.3
1	A	151	THR	2.3
1	B	184	CYS	2.3
1	A	242	LEU	2.2
1	B	130	PRO	2.2
1	A	45	ASN	2.2
1	A	188	GLU	2.2
1	B	230	MET	2.2
1	B	242	LEU	2.1
1	B	43	SER	2.1
1	B	169	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.