Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 06:33 am GMT

PDB ID	:	4BHH
Title	:	Crystal structure of tetramer of La Crosse virus nucleoprotein in complex with ssRNA
Authors	:	Reguera, J.; Malet, H.; Weber, F.; Cusack, S.
Deposited on	:	2013-04-03
Resolution	:	3.40 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:

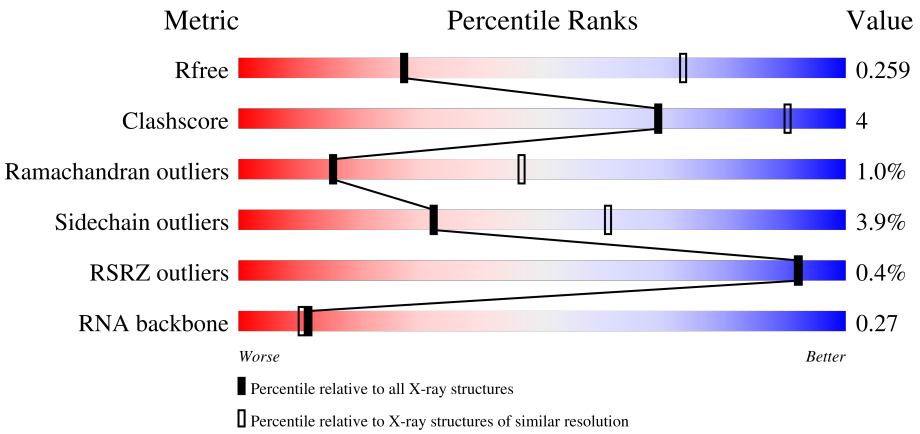
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	B	236	86% 11% • •
1	D	236	86% 8% 6%
1	F	236	91% 6% • •
1	Z	236	87% 7% 6%

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Mol	Chain	Length	Quality of chain
2	R	45	22% 31% 44%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8159 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 NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	231	1844	1180	320	338	6	0	0	0
1	D	223	1794	1152	311	325	6	0	0	0
1	F	232	1850	1183	321	340	6	0	0	0
1	Z	223	1794	1152	311	325	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P04873
D	0	GLY	-	expression tag	UNP P04873
F	0	GLY	-	expression tag	UNP P04873
Z	0	GLY	-	expression tag	UNP P04873

- Molecule 2 is a RNA chain called POLY-URIDINE 45-MER.

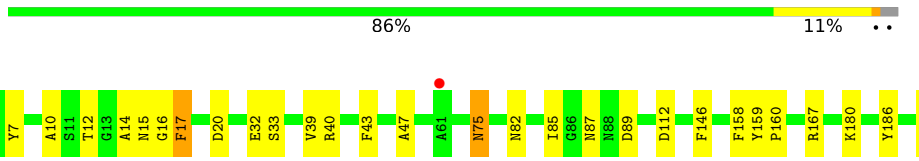
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	R	44	877	396	88	350	43	0	0	0

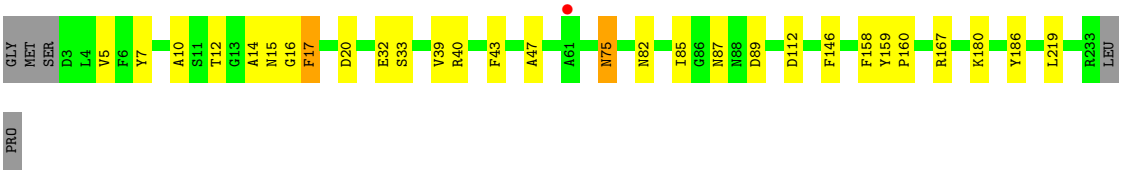
3 Residue-property plots (i)

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 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: NUCLEOPROTEIN

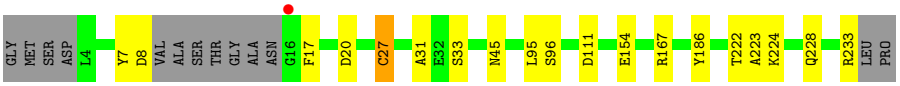
Chain B:





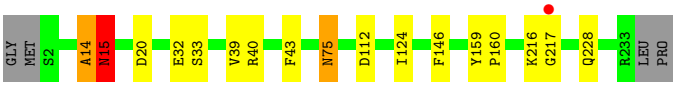
- Molecule 1: NUCLEOPROTEIN

Chain D:



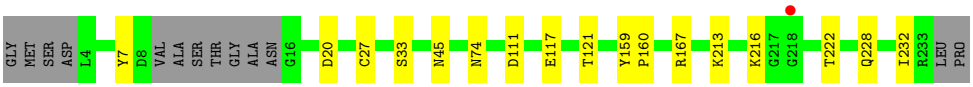
- Molecule 1: NUCLEOPROTEIN

Chain F:



- Molecule 1: NUCLEOPROTEIN

Chain Z:



- Molecule 2: POLY-URIDINE 45-MER

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.95Å 86.46Å 90.19Å 90.00° 106.63° 90.00°	Depositor
Resolution (Å)	44.35 – 3.40 44.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.35-3.40) 99.7 (44.31-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.198 , 0.252 0.202 , 0.259	Depositor DCC
R_{free} test set	944 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.810	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8159	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	B	0.38	0/1889	0.56	0/2553
1	D	0.40	0/1838	0.57	0/2481
1	F	0.36	0/1895	0.55	0/2561
1	Z	0.41	0/1838	0.58	0/2481
2	R	0.35	0/964	0.83	0/1488
All	All	0.38	0/8424	0.61	0/11564

There are no bond length outliers.

There are no bond angle outliers.

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	B	1844	0	1816	14	0
1	D	1794	0	1771	7	0
1	F	1850	0	1821	6	0
1	Z	1794	0	1771	5	0
2	R	877	0	442	33	0
All	All	8159	0	7621	58	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 4.

All (58) 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)
2:R:42:U:H6	2:R:42:U:H5"	1.30	0.93
1:B:14:ALA:O	1:B:16:GLY:N	2.16	0.78
2:R:42:U:H5"	2:R:42:U:C6	2.22	0.67
2:R:4:U:C4	2:R:5:U:C5	2.85	0.65
2:R:3:U:O2'	2:R:4:U:OP1	2.18	0.62
1:F:43:PHE:CD1	1:F:146:PHE:CE1	2.88	0.62
2:R:30:U:O2	2:R:30:U:H5'	2.01	0.59
2:R:27:U:H2'	2:R:28:U:C6	2.39	0.58
1:B:43:PHE:CD1	1:B:146:PHE:CE1	2.92	0.58
1:B:167:ARG:NH2	2:R:20:U:O2	2.37	0.57
1:Z:117:GLU:O	1:Z:121:THR:OG1	2.14	0.57
2:R:4:U:H2'	2:R:4:U:O2	2.06	0.56
2:R:9:U:H5"	2:R:9:U:H6	1.71	0.55
1:B:47:ALA:HB2	2:R:21:U:C4	2.43	0.54
2:R:27:U:H2'	2:R:28:U:H6	1.73	0.54
2:R:30:U:O2	2:R:30:U:C5'	2.56	0.54
1:F:75:ASN:N	1:F:75:ASN:OD1	2.42	0.53
1:B:5:VAL:O	1:B:7:TYR:CE1	2.61	0.53
1:B:75:ASN:N	1:B:75:ASN:OD1	2.42	0.52
2:R:23:U:C6	2:R:23:U:C5'	2.93	0.51
2:R:36:U:O2'	2:R:37:U:OP1	2.26	0.49
2:R:26:U:H2'	2:R:26:U:O2	2.11	0.49
1:B:180:LYS:HE3	2:R:18:U:O4	2.13	0.49
2:R:42:U:H6	2:R:42:U:C5'	2.14	0.49
2:R:23:U:H2'	2:R:23:U:O2	2.14	0.48
2:R:15:U:H2'	2:R:15:U:O2	2.16	0.46
2:R:19:U:O2	2:R:19:U:O4'	2.30	0.46
1:B:10:ALA:N	1:B:82:ASN:OD1	2.49	0.45
1:Z:45:ASN:N	1:Z:45:ASN:OD1	2.49	0.45
1:F:159:TYR:N	1:F:160:PRO:CD	2.80	0.45
2:R:31:U:O2	1:Z:167:ARG:NH1	2.50	0.45
1:B:159:TYR:N	1:B:160:PRO:CD	2.79	0.44
1:D:45:ASN:OD1	1:D:45:ASN:N	2.49	0.44
1:B:158:PHE:CZ	1:B:186:TYR:CD1	3.06	0.44
1:B:39:VAL:O	1:B:40:ARG:C	2.56	0.44
1:D:167:ARG:CZ	2:R:9:U:O2	2.66	0.43
2:R:22:U:H2'	2:R:23:U:H5"	2.01	0.43
1:B:158:PHE:CE2	1:B:186:TYR:CE1	3.07	0.43
2:R:30:U:H2'	2:R:31:U:H5"	2.00	0.43
1:D:154:GLU:HA	1:D:186:TYR:CE1	2.54	0.42
1:D:223:ALA:O	1:D:224:LYS:C	2.57	0.42
1:D:17:PHE:O	2:R:3:U:H2'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:CYS:O	1:D:31:ALA:N	2.41	0.42
2:R:41:U:O2	2:R:41:U:O4'	2.36	0.42
2:R:5:U:H2'	2:R:6:U:H6	1.85	0.42
2:R:12:U:H6	2:R:12:U:H5"	1.84	0.42
2:R:25:U:O2'	2:R:26:U:OP1	2.30	0.42
1:F:39:VAL:O	1:F:40:ARG:C	2.59	0.41
1:Z:159:TYR:N	1:Z:160:PRO:CD	2.83	0.41
1:Z:74:ASN:C	1:Z:74:ASN:OD1	2.58	0.41
1:B:17:PHE:HA	1:B:87:ASN:CG	2.41	0.41
1:D:95:LEU:O	1:D:96:SER:C	2.60	0.41
2:R:6:U:H2'	2:R:7:U:C6	2.56	0.41
2:R:26:U:O2	2:R:26:U:C2'	2.68	0.41
1:B:85:ILE:HG23	1:B:89:ASP:HB2	2.03	0.40
2:R:23:U:C6	2:R:23:U:H5"	2.56	0.40
1:F:124:ILE:HD11	2:R:44:U:O2	2.21	0.40
1:F:14:ALA:O	1:F:15:ASN:ND2	2.50	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	B	229/236 (97%)	199 (87%)	27 (12%)	3 (1%)	12 39
1	D	219/236 (93%)	199 (91%)	20 (9%)	0	100 100
1	F	230/236 (98%)	200 (87%)	25 (11%)	5 (2%)	6 29
1	Z	219/236 (93%)	193 (88%)	25 (11%)	1 (0%)	29 61
All	All	897/944 (95%)	791 (88%)	97 (11%)	9 (1%)	15 46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	ASN
1	F	14	ALA
1	F	216	LYS
1	B	17	PHE
1	Z	216	LYS
1	F	217	GLY
1	B	32	GLU
1	F	15	ASN
1	F	32	GLU

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	B	193/197 (98%)	187 (97%)	6 (3%)	40	68
1	D	188/197 (95%)	179 (95%)	9 (5%)	25	56
1	F	194/197 (98%)	188 (97%)	6 (3%)	40	68
1	Z	188/197 (95%)	179 (95%)	9 (5%)	25	56
All	All	763/788 (97%)	733 (96%)	30 (4%)	32	61

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	THR
1	B	20	ASP
1	B	33	SER
1	B	75	ASN
1	B	112	ASP
1	B	219	LEU
1	D	7	TYR
1	D	8	ASP
1	D	20	ASP
1	D	27	CYS
1	D	33	SER
1	D	111	ASP
1	D	222	THR

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Mol	Chain	Res	Type
1	D	228	GLN
1	D	233	ARG
1	F	15	ASN
1	F	20	ASP
1	F	33	SER
1	F	75	ASN
1	F	112	ASP
1	F	228	GLN
1	Z	7	TYR
1	Z	20	ASP
1	Z	27	CYS
1	Z	33	SER
1	Z	111	ASP
1	Z	213	LYS
1	Z	222	THR
1	Z	228	GLN
1	Z	232	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	176	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	43/45 (95%)	27 (62%)	12 (27%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	4	U
2	R	8	U
2	R	9	U
2	R	10	U
2	R	11	U
2	R	12	U
2	R	13	U
2	R	14	U
2	R	15	U

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Mol	Chain	Res	Type
2	R	16	U
2	R	19	U
2	R	20	U
2	R	21	U
2	R	22	U
2	R	23	U
2	R	24	U
2	R	25	U
2	R	26	U
2	R	27	U
2	R	30	U
2	R	31	U
2	R	36	U
2	R	37	U
2	R	41	U
2	R	42	U
2	R	43	U
2	R	44	U

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	3	U
2	R	9	U
2	R	13	U
2	R	14	U
2	R	20	U
2	R	21	U
2	R	23	U
2	R	24	U
2	R	25	U
2	R	35	U
2	R	36	U
2	R	42	U

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)

There are no ligands in this entry.

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)

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, 95th 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	B	231/236 (97%)	-0.15	1 (0%)	92	92	55, 82, 112, 139	0
1	D	223/236 (94%)	-0.18	1 (0%)	92	92	42, 83, 122, 148	0
1	F	232/236 (98%)	-0.04	1 (0%)	92	92	57, 89, 126, 151	0
1	Z	223/236 (94%)	-0.26	1 (0%)	92	92	39, 73, 111, 138	0
2	R	44/45 (97%)	-0.34	0	100	100	55, 88, 117, 146	0
All	All	953/989 (96%)	-0.17	4 (0%)	92	92	39, 82, 117, 151	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	2.8
1	Z	218	GLY	2.8
1	D	16	GLY	2.7
1	F	217	GLY	2.1

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.