wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:58 AM GMT

PDB ID	:	3GPQ
Title	:	Crystal structure of macro domain of Chikungunya virus in complex with RNA
Authors	:	Malet, H.; Jamal, S.; Coutard, B.; Canard, B.
Deposited on	:	2009-03-23
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

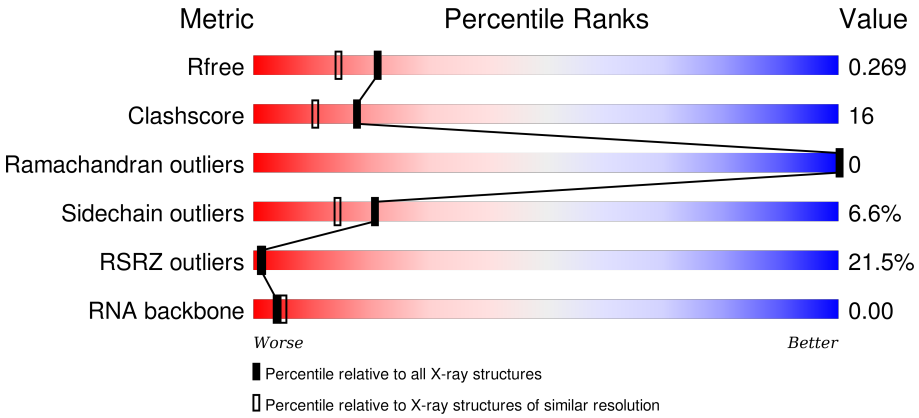
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)
RNA backbone	2183	1002 (2.72-1.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	168	11% 80% 15% • 5%
1	B	168	13% 81% 14% • 5%
1	C	168	26% 60% 28% • 11%
1	D	168	31% 60% 23% 5% 12%

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Mol	Chain	Length	Quality of chain
2	E	3	33% 33% 33%
2	F	3	33% 33% 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5084 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	15	1	0
			1232	768	215	241	8			
1	B	160	Total	C	N	O	S	17	1	0
			1232	768	215	241	8			
1	C	150	Total	C	N	O	S	79	0	0
			1156	722	201	225	8			
1	D	148	Total	C	N	O	S	43	0	0
			1134	709	199	219	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q8JUX6
A	-6	LYS	-	EXPRESSION TAG	UNP Q8JUX6
A	-5	HIS	-	EXPRESSION TAG	UNP Q8JUX6
A	-4	HIS	-	EXPRESSION TAG	UNP Q8JUX6
A	-3	HIS	-	EXPRESSION TAG	UNP Q8JUX6
A	-2	HIS	-	EXPRESSION TAG	UNP Q8JUX6
A	-1	HIS	-	EXPRESSION TAG	UNP Q8JUX6
A	0	HIS	-	EXPRESSION TAG	UNP Q8JUX6
B	-7	MET	-	EXPRESSION TAG	UNP Q8JUX6
B	-6	LYS	-	EXPRESSION TAG	UNP Q8JUX6
B	-5	HIS	-	EXPRESSION TAG	UNP Q8JUX6
B	-4	HIS	-	EXPRESSION TAG	UNP Q8JUX6
B	-3	HIS	-	EXPRESSION TAG	UNP Q8JUX6
B	-2	HIS	-	EXPRESSION TAG	UNP Q8JUX6
B	-1	HIS	-	EXPRESSION TAG	UNP Q8JUX6
B	0	HIS	-	EXPRESSION TAG	UNP Q8JUX6
C	-7	MET	-	EXPRESSION TAG	UNP Q8JUX6
C	-6	LYS	-	EXPRESSION TAG	UNP Q8JUX6
C	-5	HIS	-	EXPRESSION TAG	UNP Q8JUX6
C	-4	HIS	-	EXPRESSION TAG	UNP Q8JUX6
C	-3	HIS	-	EXPRESSION TAG	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	EXPRESSION TAG	UNP Q8JUX6
C	-1	HIS	-	EXPRESSION TAG	UNP Q8JUX6
C	0	HIS	-	EXPRESSION TAG	UNP Q8JUX6
D	-7	MET	-	EXPRESSION TAG	UNP Q8JUX6
D	-6	LYS	-	EXPRESSION TAG	UNP Q8JUX6
D	-5	HIS	-	EXPRESSION TAG	UNP Q8JUX6
D	-4	HIS	-	EXPRESSION TAG	UNP Q8JUX6
D	-3	HIS	-	EXPRESSION TAG	UNP Q8JUX6
D	-2	HIS	-	EXPRESSION TAG	UNP Q8JUX6
D	-1	HIS	-	EXPRESSION TAG	UNP Q8JUX6
D	0	HIS	-	EXPRESSION TAG	UNP Q8JUX6

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	P	0	0	0
			35	15	5	13	2			
2	F	2	Total	C	N	O	P	0	0	0
			45	20	10	13	2			

- Molecule 3 is water.

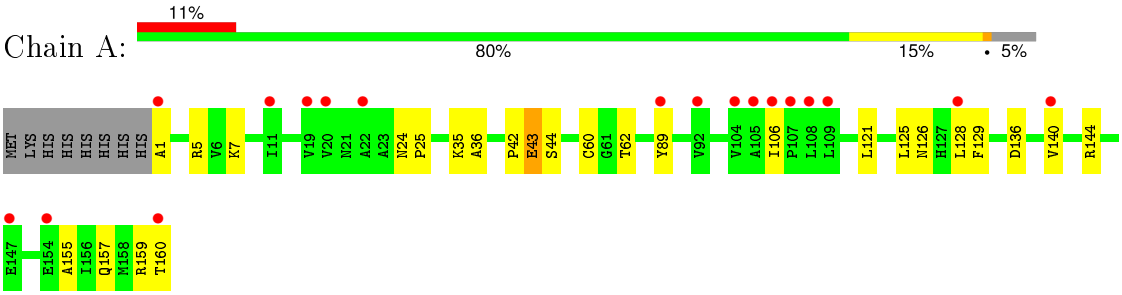
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		
3	B	96	Total	O	0	0
			96	96		
3	C	35	Total	O	0	0
			35	35		
3	D	28	Total	O	0	0
			28	28		
3	E	3	Total	O	0	0
			3	3		
3	F	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

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 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.

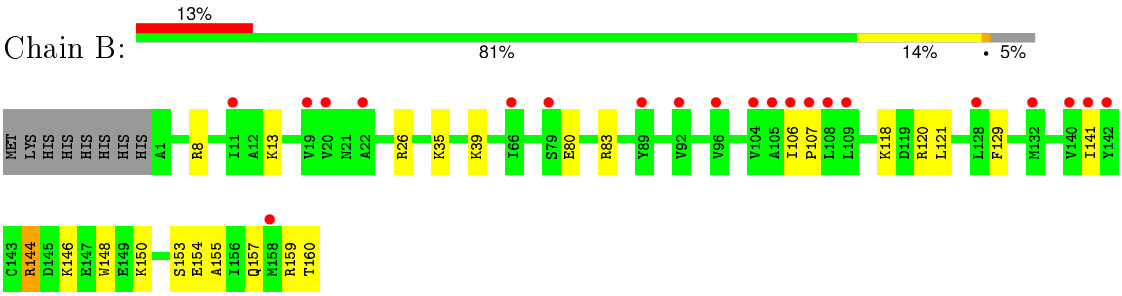
- Molecule 1: Non-structural protein 3

Chain A:



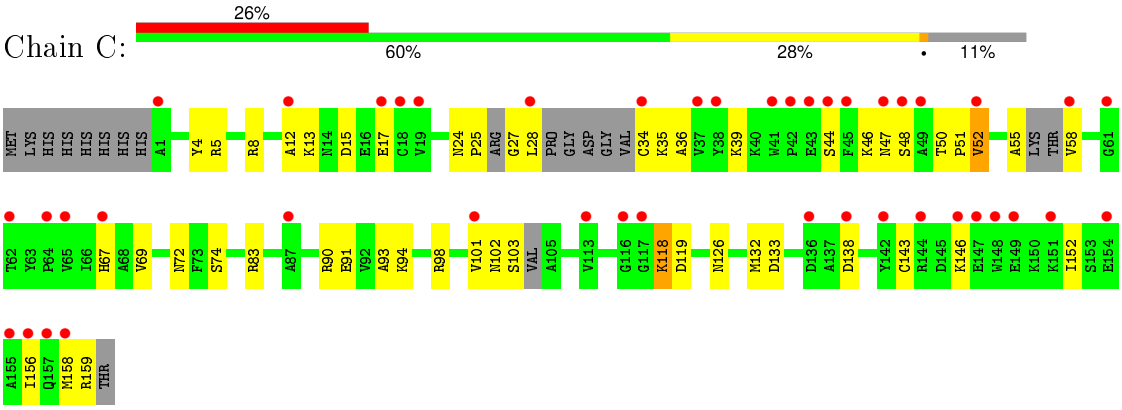
- Molecule 1: Non-structural protein 3

Chain B:



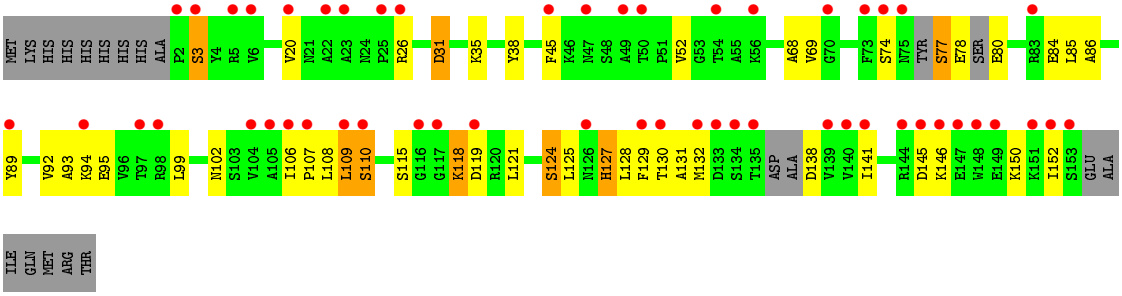
- Molecule 1: Non-structural protein 3

Chain C:



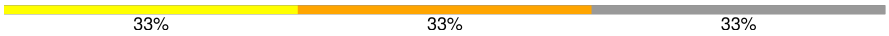
- Molecule 1: Non-structural protein 3

Chain D:



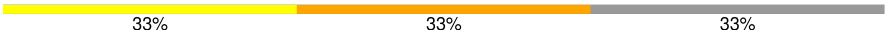
- Molecule 2: RNA (5'-R(*AP*AP*A)-3')

Chain E:



- Molecule 2: RNA (5'-R(*AP*AP*A)-3')

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	86.82Å 86.82Å 81.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.42 – 2.00 28.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.42-2.00) 99.6 (28.42-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.215 , 0.260 0.230 , 0.269	Depositor DCC
R_{free} test set	2379 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.6	EDS
Estimated twinning fraction	0.006 for -h,-k,l 0.032 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 46174 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5084	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.85	0/1258	0.73	0/1704
1	B	0.88	0/1258	0.73	0/1704
1	C	0.76	0/1174	0.71	0/1583
1	D	0.75	0/1153	0.72	0/1556
2	E	1.62	1/38 (2.6%)	1.70	1/55 (1.8%)
2	F	1.91	1/50 (2.0%)	1.67	2/74 (2.7%)
All	All	0.84	2/4931 (0.0%)	0.75	3/6676 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	A	OP3-P	-11.07	1.47	1.61
2	E	1	A	OP3-P	-8.97	1.50	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	A	OP1-P-OP2	-6.99	109.12	119.60
2	E	2	A	C1'-O4'-C4'	-6.96	104.33	109.90
2	F	1	A	O4'-C1'-N9	5.04	112.23	108.20

There are no chirality outliers.

There are no planarity outliers.

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	A	1232	0	1222	22	0
1	B	1232	0	1222	19	0
1	C	1156	0	1139	46	0
1	D	1134	0	1126	59	0
2	E	35	0	18	0	0
2	F	45	0	23	1	0
3	A	83	0	0	5	0
3	B	96	0	0	3	0
3	C	35	0	0	6	0
3	D	28	0	0	8	0
3	E	3	0	0	0	0
3	F	5	0	0	1	0
All	All	5084	0	4750	146	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 16.

The worst 5 of 146 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:A:126:ASN:HB3	3:A:163:HOH:O	1.36	1.21
1:D:106:ILE:HA	3:D:175:HOH:O	1.38	1.18
1:D:86:ALA:HB2	1:D:127:HIS:CE1	1.81	1.14
1:D:20:VAL:HB	3:D:175:HOH:O	1.54	1.08
1:D:132:MET:HE1	3:D:163:HOH:O	1.51	1.06

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	159/168 (95%)	157 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	159/168 (95%)	158 (99%)	1 (1%)	0	100	100
1	C	140/168 (83%)	130 (93%)	10 (7%)	0	100	100
1	D	140/168 (83%)	130 (93%)	10 (7%)	0	100	100
All	All	598/672 (89%)	575 (96%)	23 (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	134/141 (95%)	130 (97%)	4 (3%)	48	47
1	B	134/141 (95%)	130 (97%)	4 (3%)	48	47
1	C	125/141 (89%)	113 (90%)	12 (10%)	10	6
1	D	124/141 (88%)	110 (89%)	14 (11%)	7	4
All	All	517/564 (92%)	483 (93%)	34 (7%)	21	14

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	94	LYS
1	C	158	MET
1	D	124	SER
1	C	118	LYS
1	B	144	ARG

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

Mol	Chain	Res	Type
1	D	127	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	1/3 (33%)	1 (100%)	0
2	F	1/3 (33%)	1 (100%)	0
All	All	2/6 (33%)	2 (100%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	A
2	F	2	A

There are no RNA pucker outliers to report.

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 carbohydrates 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	160/168 (95%)	0.49	18 (11%) 7 7	14, 21, 30, 39	5 (3%)
1	B	160/168 (95%)	0.55	21 (13%) 5 5	13, 18, 29, 41	7 (4%)
1	C	150/168 (89%)	1.59	43 (28%) 1 1	13, 32, 47, 84	19 (12%)
1	D	148/168 (88%)	1.58	52 (35%) 0 1	20, 35, 50, 54	12 (8%)
2	E	2/3 (66%)	0.72	0 100 100	49, 49, 49, 67	0
2	F	2/3 (66%)	0.63	0 100 100	39, 39, 39, 66	0
All	All	622/678 (91%)	1.03	134 (21%) 1 1	13, 26, 46, 84	43 (6%)

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	SER	7.0
1	C	44	SER	6.1
1	D	148	TRP	6.1
1	C	38	TYR	6.0
1	D	130	THR	5.5

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.