Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:47 PM GMT

PDB ID	:	3WUS
Title	:	Crystal Structure of the Vif-Binding Domain of Human APOBEC3F
Authors	:	Nakashima, M.; Kawamura, T.; Ode, H.; Watanabe, N.; Iwatani, Y.
Deposited on	:	2014-05-02
Resolution	:	2.54 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
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:

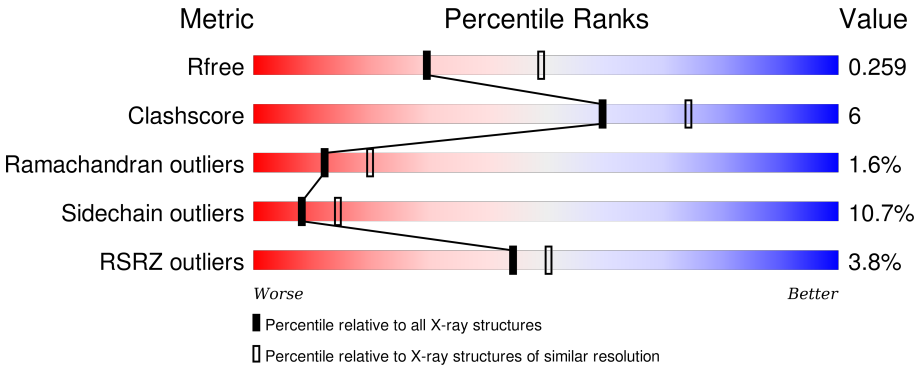
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.54 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	190	5% 78% 16%
1	B	190	3% 76% 15% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3139 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 DNA dC->dU-editing enzyme APOBEC-3F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			
1	B	184	Total	C	N	O	S	0	0	0
			1565	1017	255	282	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	MET	-	EXPRESSION TAG	UNP Q8IUX4
A	185	ASN	-	EXPRESSION TAG	UNP Q8IUX4
A	186	PRO	-	EXPRESSION TAG	UNP Q8IUX4
B	184	MET	-	EXPRESSION TAG	UNP Q8IUX4
B	185	ASN	-	EXPRESSION TAG	UNP Q8IUX4
B	186	PRO	-	EXPRESSION TAG	UNP Q8IUX4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

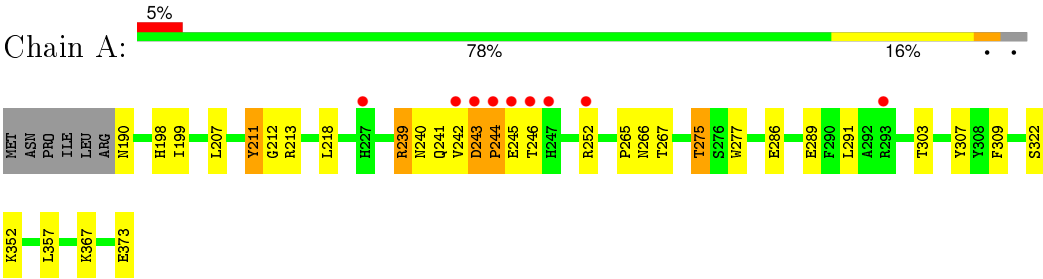
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		

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.

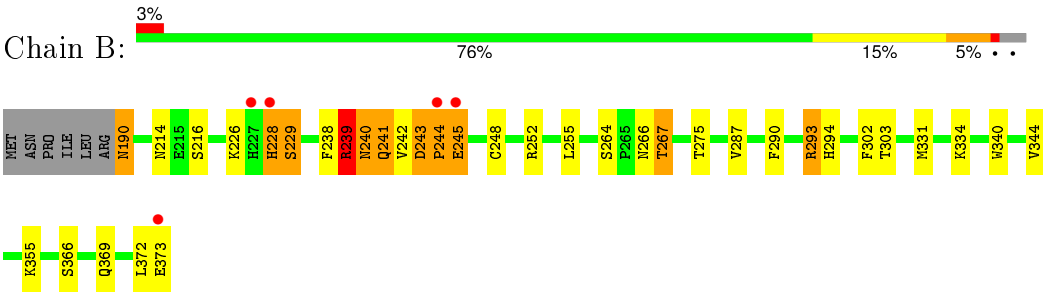
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain A:



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3F

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.29Å 117.29Å 78.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.54 47.08 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.54) 99.8 (47.08-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.200 , 0.256 0.205 , 0.259	Depositor DCC
R_{free} test set	1069 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 27.7	EDS
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 20881 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3139	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.82	0/1623	0.92	2/2204 (0.1%)
1	B	0.85	0/1623	0.89	1/2204 (0.0%)
All	All	0.83	0/3246	0.91	3/4408 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	GLY	N-CA-C	-6.70	96.34	113.10
1	A	239	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	B	239	ARG	NE-CZ-NH2	5.11	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	TYR	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	1565	0	1441	12	0
1	B	1565	0	1441	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
All	All	3139	0	2882	34	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 6.

All (34) 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:243:ASP:HB2	1:B:244:PRO:HD2	1.54	0.88
1:A:243:ASP:HB2	1:A:244:PRO:HD2	1.64	0.80
1:B:302:PHE:HB3	1:B:331:MET:HG2	1.81	0.62
1:A:275:THR:HG22	1:A:303:THR:HA	1.85	0.59
1:A:275:THR:HG23	1:A:277:TRP:O	2.03	0.58
1:A:265:PRO:O	1:A:266:ASN:HB2	2.03	0.57
1:A:309:PHE:CE1	1:A:367:LYS:HE2	2.42	0.55
1:B:245:GLU:HA	1:B:245:GLU:OE1	2.05	0.55
1:B:293:ARG:HG2	1:B:294:HIS:CD2	2.42	0.55
1:B:372:LEU:O	1:B:373:GLU:CB	2.55	0.54
1:A:211:TYR:O	1:A:213:ARG:NH2	2.38	0.52
1:A:243:ASP:CB	1:A:244:PRO:HD2	2.39	0.51
1:B:228:HIS:N	1:B:228:HIS:CD2	2.78	0.50
1:B:243:ASP:HB2	1:B:244:PRO:CD	2.31	0.49
1:B:248:CYS:HB2	1:B:252:ARG:HB2	1.94	0.48
1:B:239:ARG:HD3	1:B:240:ASN:O	2.12	0.48
1:A:243:ASP:O	1:A:244:PRO:O	2.31	0.47
1:A:252:ARG:NH1	1:A:286:GLU:OE1	2.47	0.47
1:B:190:ASN:HD21	1:B:239:ARG:H	1.61	0.47
1:B:340:TRP:CZ3	1:B:344:VAL:HG11	2.51	0.46
1:B:243:ASP:O	1:B:244:PRO:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASN:HD21	1:B:238:PHE:HA	1.80	0.46
1:B:242:VAL:O	1:B:242:VAL:HG12	2.16	0.45
1:B:290:PHE:CE1	1:B:294:HIS:CD2	3.05	0.45
1:A:357:LEU:HD23	1:A:357:LEU:C	2.38	0.44
1:B:255:LEU:HD11	1:B:287:VAL:HG22	1.99	0.44
1:A:198:HIS:CD2	1:A:199:ILE:HD12	2.54	0.43
1:B:303:THR:C	1:B:331:MET:HG3	2.39	0.42
1:B:241:GLN:HG3	1:B:248:CYS:SG	2.59	0.42
1:B:347:ASP:O	1:B:348:ASP:HB2	2.18	0.42
1:B:372:LEU:O	1:B:373:GLU:HB2	2.19	0.42
1:B:226:LYS:CA	1:B:267:THR:HG23	2.50	0.42
1:B:226:LYS:O	1:B:229:SER:HB2	2.21	0.41
1:A:243:ASP:O	1:A:244:PRO:C	2.59	0.41

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 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	182/190 (96%)	168 (92%)	11 (6%)	3 (2%)	12	20
1	B	182/190 (96%)	167 (92%)	12 (7%)	3 (2%)	12	20
All	All	364/380 (96%)	335 (92%)	23 (6%)	6 (2%)	12	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	PRO
1	B	243	ASP
1	B	244	PRO
1	B	345	TYR
1	A	289	GLU

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Mol	Chain	Res	Type
1	A	243	ASP

5.3.2 Protein sidechains

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	169/175 (97%)	151 (89%)	18 (11%)	8 14
1	B	169/175 (97%)	151 (89%)	18 (11%)	8 14
All	All	338/350 (97%)	302 (89%)	36 (11%)	8 14

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	207	LEU
1	A	218	LEU
1	A	239	ARG
1	A	240	ASN
1	A	241	GLN
1	A	242	VAL
1	A	245	GLU
1	A	246	THR
1	A	267	THR
1	A	275	THR
1	A	291	LEU
1	A	307	TYR
1	A	322	SER
1	A	323	GLN
1	A	329	GLU
1	A	352	LYS
1	A	373	GLU
1	B	190	ASN
1	B	214	ASN
1	B	216	SER
1	B	228	HIS

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Mol	Chain	Res	Type
1	B	229	SER
1	B	239	ARG
1	B	240	ASN
1	B	241	GLN
1	B	245	GLU
1	B	264	SER
1	B	266	ASN
1	B	267	THR
1	B	275	THR
1	B	293	ARG
1	B	334	LYS
1	B	355	LYS
1	B	366	SER
1	B	369	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	241	GLN
1	A	298	ASN
1	A	315	GLN
1	B	190	ASN
1	B	228	HIS
1	B	240	ASN
1	B	294	HIS
1	B	315	GLN
1	B	360	ASN
1	B	369	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

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	184/190 (96%)	0.18	9 (4%) 33 39	33, 53, 94, 147	0
1	B	184/190 (96%)	0.06	5 (2%) 58 63	31, 50, 89, 131	0
All	All	368/380 (96%)	0.12	14 (3%) 44 50	31, 51, 91, 147	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	PRO	6.5
1	A	245	GLU	5.1
1	B	244	PRO	4.0
1	A	247	HIS	3.4
1	A	252	ARG	3.3
1	B	228	HIS	3.2
1	A	227	HIS	2.7
1	A	243	ASP	2.6
1	A	293	ARG	2.6
1	A	242	VAL	2.4
1	A	246	THR	2.4
1	B	373	GLU	2.4
1	B	227	HIS	2.4
1	B	245	GLU	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	401	1/1	0.99	0.06	-	70,70,70,70	0
2	ZN	B	401	1/1	0.99	0.12	-	61,61,61,61	0

6.5 Other polymers

There are no such residues in this entry.