



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 06:17 PM EDT

PDB ID : 3IR2  
Title : Crystal structure of the APOBEC3G catalytic domain  
Authors : Shandilya, S.M.D.; Schiffer, C.A.  
Deposited on : 2009-08-21  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)

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<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>.

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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 : 2.35  
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) : 2.35

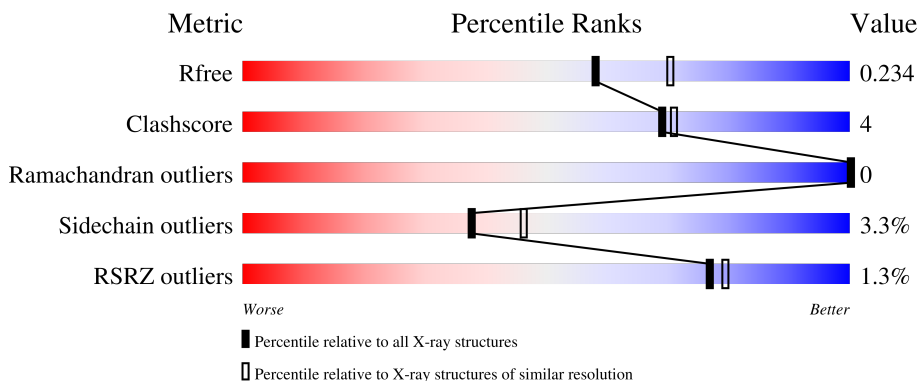
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	207	 84% 6% • 9%
1	B	207	 83% 6% • 10%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3371 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-3G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	188	1500	953	263	273	11	0	0	0
1	B	187	1486	944	261	270	11	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	GLY	-	expression tag	UNP Q9HC16
A	179	PRO	-	expression tag	UNP Q9HC16
A	180	LEU	-	expression tag	UNP Q9HC16
A	181	GLY	-	expression tag	UNP Q9HC16
A	182	SER	-	expression tag	UNP Q9HC16
A	183	PRO	-	expression tag	UNP Q9HC16
A	184	GLU	-	expression tag	UNP Q9HC16
A	185	PHE	-	expression tag	UNP Q9HC16
A	186	GLU	-	expression tag	UNP Q9HC16
A	187	LEU	-	expression tag	UNP Q9HC16
A	188	GLY	-	expression tag	UNP Q9HC16
A	189	THR	-	expression tag	UNP Q9HC16
A	190	THR	-	expression tag	UNP Q9HC16
A	234	LYS	LEU	engineered mutation	UNP Q9HC16
A	243	ALA	CYS	engineered mutation	UNP Q9HC16
A	310	LYS	PHE	engineered mutation	UNP Q9HC16
A	321	ALA	CYS	engineered mutation	UNP Q9HC16
A	356	ALA	CYS	engineered mutation	UNP Q9HC16
B	178	GLY	-	expression tag	UNP Q9HC16
B	179	PRO	-	expression tag	UNP Q9HC16
B	180	LEU	-	expression tag	UNP Q9HC16
B	181	GLY	-	expression tag	UNP Q9HC16
B	182	SER	-	expression tag	UNP Q9HC16
B	183	PRO	-	expression tag	UNP Q9HC16
B	184	GLU	-	expression tag	UNP Q9HC16

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Chain	Residue	Modelled	Actual	Comment	Reference
B	185	PHE	-	expression tag	UNP Q9HC16
B	186	GLU	-	expression tag	UNP Q9HC16
B	187	LEU	-	expression tag	UNP Q9HC16
B	188	GLY	-	expression tag	UNP Q9HC16
B	189	THR	-	expression tag	UNP Q9HC16
B	190	THR	-	expression tag	UNP Q9HC16
B	234	LYS	LEU	engineered mutation	UNP Q9HC16
B	243	ALA	CYS	engineered mutation	UNP Q9HC16
B	310	LYS	PHE	engineered mutation	UNP Q9HC16
B	321	ALA	CYS	engineered mutation	UNP Q9HC16
B	356	ALA	CYS	engineered mutation	UNP Q9HC16

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

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	200	Total O 200 200	0	0

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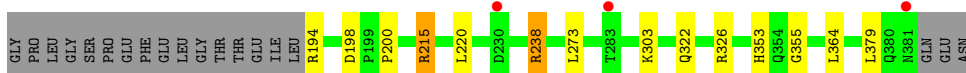
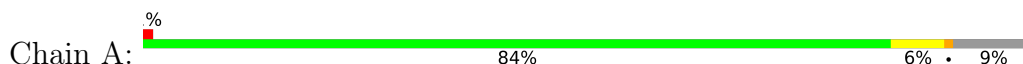
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	177	Total 177	O 177	0	0

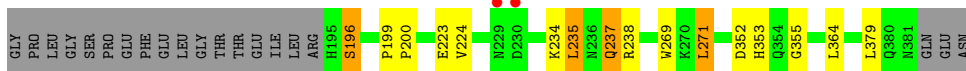
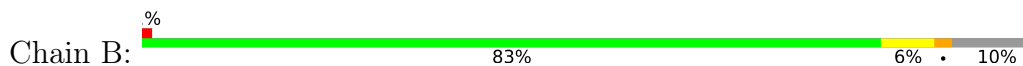
### 3 Residue-property plots [i](#)

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: DNA dC->dU-editing enzyme APOBEC-3G



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.34Å 72.53Å 97.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 30.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-2.25) 97.0 (30.91-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.53 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.5.0093	Depositor
R, $R_{free}$	0.166 , 0.208 0.191 , 0.234	Depositor DCC
$R_{free}$ test set	1171 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtrriage
Anisotropy	0.390	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.15 % 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 7.1388e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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

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	0.55	0/1547	0.60	0/2104
1	B	0.57	0/1532	0.60	0/2085
All	All	0.56	0/3079	0.60	0/4189

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

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	1500	0	1360	12	0
1	B	1486	0	1346	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	200	0	0	2	0
5	B	177	0	0	2	0
All	All	3371	0	2706	21	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 (21) 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:353:HIS:HD2	1:A:355:GLY:H	1.33	0.76
1:B:353:HIS:HD2	1:B:355:GLY:H	1.43	0.66
1:A:238:ARG:HA	1:A:238:ARG:HE	1.60	0.66
1:A:215:ARG:HD3	3:A:2:CL:CL	2.35	0.64
1:A:194:ARG:N	5:A:466:HOH:O	2.36	0.59
1:B:234:LYS:HE3	5:B:439:HOH:O	2.03	0.57
1:A:238:ARG:HA	1:A:238:ARG:NE	2.20	0.56
1:B:196:SER:HB3	1:B:352:ASP:HB2	1.90	0.54
1:B:199:PRO:HB2	1:B:200:PRO:HD3	1.90	0.54
1:A:322:GLN:HE21	1:A:326:ARG:HH12	1.59	0.51
1:A:364:LEU:HD23	1:A:364:LEU:C	2.31	0.51
1:A:353:HIS:HD2	1:A:355:GLY:N	2.07	0.50
1:B:237:GLN:HE21	1:B:237:GLN:HA	1.76	0.49
1:A:353:HIS:CD2	1:A:355:GLY:H	2.24	0.47
1:B:224:VAL:HG12	1:B:235:LEU:HD23	1.98	0.45
1:A:303:LYS:HE2	5:A:413:HOH:O	2.18	0.44
1:A:198:ASP:OD1	1:A:200:PRO:HD2	2.17	0.44
1:A:220:LEU:C	1:A:220:LEU:HD23	2.40	0.42
1:B:223:GLU:OE2	5:B:439:HOH:O	2.21	0.42
1:B:269:TRP:HB2	1:B:271:LEU:HD13	2.01	0.41
1:B:364:LEU:HD23	1:B:364:LEU:C	2.42	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	186/207 (90%)	181 (97%)	5 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	185/207 (89%)	180 (97%)	5 (3%)	0	100	100
All	All	371/414 (90%)	361 (97%)	10 (3%)	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	154/182 (85%)	150 (97%)	4 (3%)	46	55
1	B	152/182 (84%)	146 (96%)	6 (4%)	32	38
All	All	306/364 (84%)	296 (97%)	10 (3%)	38	46

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ARG
1	A	238	ARG
1	A	273	LEU
1	A	379	LEU
1	B	196	SER
1	B	235	LEU
1	B	237	GLN
1	B	238	ARG
1	B	271	LEU
1	B	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	245	GLN
1	A	322	GLN

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Mol	Chain	Res	Type
1	A	353	HIS
1	B	237	GLN
1	B	245	GLN
1	B	353	HIS

### 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 8 ligands modelled in this entry, 8 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	188/207 (90%)	-0.10	3 (1%) 72 74	12, 23, 29, 53	0
1	B	187/207 (90%)	-0.12	2 (1%) 80 82	16, 23, 30, 42	0
All	All	375/414 (90%)	-0.11	5 (1%) 77 79	12, 23, 30, 53	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	ASN	4.2
1	A	283	THR	2.3
1	B	229	ASN	2.1
1	A	230	ASP	2.0
1	B	230	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](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	385	1/1	0.88	0.07	40,40,40,40	0
4	MG	B	385	1/1	0.98	0.08	32,32,32,32	0
2	ZN	B	1001	1/1	0.99	0.09	35,35,35,35	0
2	ZN	B	1101	1/1	0.99	0.07	34,34,34,34	0
3	CL	A	2	1/1	0.99	0.11	33,33,33,33	0
3	CL	B	1	1/1	0.99	0.12	31,31,31,31	0
2	ZN	A	1001	1/1	0.99	0.09	37,37,37,37	0
2	ZN	A	1101	1/1	0.99	0.06	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.