



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:45 AM GMT

PDB ID : 3DMJ
Title : CRYSTAL STRUCTURE OF HIV-1 V106A and Y181C MUTANT REVERSE
TRANSCRIPTASE IN COMPLEX WITH GW564511.
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Deposited on : 2008-07-01
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

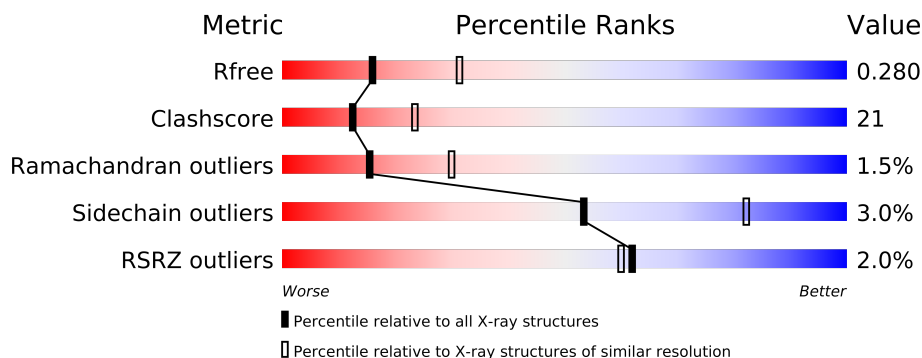
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7765 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Reverse transcriptase/ribonucleaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4347	2814	723	801	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	ALA	VAL	ENGINEERED	UNP P04585
A	181	CYS	TYR	ENGINEERED	UNP P04585

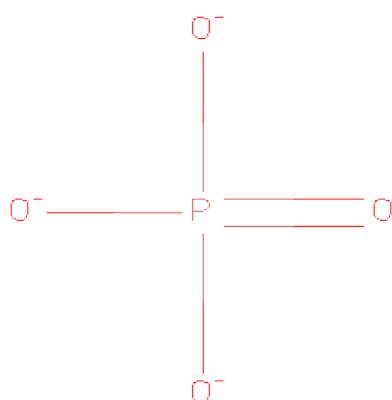
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3309	2151	552	598	8			

There are 2 discrepancies between the modelled and reference sequences:

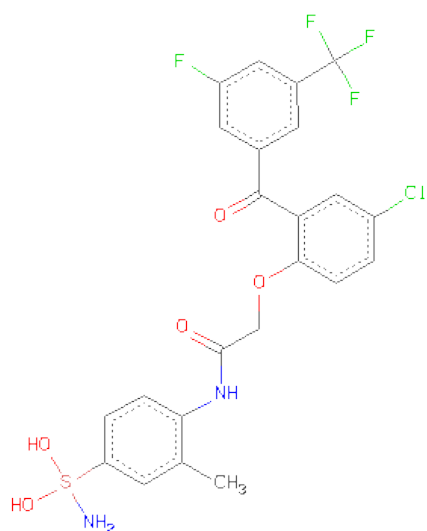
Chain	Residue	Modelled	Actual	Comment	Reference
B	106	ALA	VAL	ENGINEERED	UNP P04585
B	181	CYS	TYR	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is N-{4-[AMINO(DIHYDROXY)-LAMBDA 4 -SULFANYL]-2-METHYLPHENYL}-2-(4-CHLORO-2-{[3-FLUORO-5-(TRIFLUOROMETHYL)PHENYL]CARBONYL}PHENOXY)ACETAMIDE (three-letter code: GWE) (formula: C₂₃H₁₉ClF₄N₂O₅S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	S	0	0
			36	23	1	4	2	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total 32	O 32	0	0
5	B	31	Total 31	O 31	0	0

G359	A360	H361	T362	N363	D364	V365	K366	Q367	L368	T369	E370	Q373	K374	I375	T376	T377	E378	S379	I380	V381	I382	W383	G384	K385	T386	P387	K388	F389	I393	Q394	W398	W402	F416	P420	V423	K424	L425	W426	L429	E430	K431	E432	P433	I434	V435	G436	A437	GLU	THR	PHE
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.19Å 108.99Å 71.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.60 29.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.78-2.60) 99.9 (29.78-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.284 0.199 , 0.280	Depositor DCC
R_{free} test set	1679 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 33834 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7765	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GWE, CSD, PO4

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	0.39	0/4453	0.64	0/6051
2	B	0.39	0/3401	0.63	0/4618
All	All	0.39	0/7854	0.63	0/10669

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	183	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4347	0	4390	189	0
2	B	3309	0	3340	148	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	36	0	17	0	0
5	A	32	0	0	1	0
5	B	31	0	0	3	0
All	All	7765	0	7747	326	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 326 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:353:LYS:HE3	2:B:430:GLU:HB3	1.31	1.12
2:B:235:HIS:HB2	2:B:238:LYS:HD2	1.47	0.94
1:A:448:ARG:NH2	1:A:475:GLN:H	1.67	0.93
1:A:115:TYR:HB2	1:A:151:GLN:HE21	1.37	0.89
1:A:217:PRO:HB2	1:A:222:GLN:HE21	1.42	0.84

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	525/560 (94%)	486 (93%)	28 (5%)	11 (2%)	11	19
2	B	393/440 (89%)	364 (93%)	26 (7%)	3 (1%)	27	53
All	All	918/1000 (92%)	850 (93%)	54 (6%)	14 (2%)	15	30

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	113	ASP

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Mol	Chain	Res	Type
2	B	195	ILE
1	A	91	GLN
1	A	133	PRO

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	475/498 (95%)	456 (96%)	19 (4%)	42	73
2	B	363/399 (91%)	357 (98%)	6 (2%)	73	92
All	All	838/897 (93%)	813 (97%)	25 (3%)	53	82

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	LYS
1	A	368	LEU
2	B	300	GLU
1	A	340	GLN
1	A	386	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	ASN
2	B	57	ASN
2	B	394	GLN
1	A	520	GLN
2	B	137	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	280	1	7,7,8	7.01	2 (28%)	6,8,10	5.97	4 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	0/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	18.21	1.23	1.11
1	A	280	CSD	CA-C	2.92	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	CA-CB-SG	10.91	126.39	110.82
1	A	280	CSD	C-CA-N	-6.29	107.55	113.83
1	A	280	CSD	OD2-SG-CB	5.58	119.87	97.42
1	A	280	CSD	OD2-SG-OD1	4.86	117.46	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PO4	A	1301	-	4,4,4	0.88	0	6,6,6	0.31	0
4	GWE	A	999	-	37,38,38	2.55	10 (27%)	57,57,57	4.88	12 (21%)
3	PO4	B	1300	-	4,4,4	0.85	0	6,6,6	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	GWE	A	999	-	-	0/29/29/29	0/3/3/3
3	PO4	B	1300	-	-	0/0/0/0	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	GWE	C17-C18	6.26	1.51	1.40
4	A	999	GWE	C2-C1	5.87	1.51	1.40
4	A	999	GWE	C3-C4	5.69	1.48	1.38
4	A	999	GWE	C5-C6	5.47	1.49	1.38
4	A	999	GWE	C21-C22	4.79	1.48	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	GWE	C20-S1-N2	-35.29	109.07	109.75
4	A	999	GWE	O4-S1-C20	3.90	109.33	106.91
4	A	999	GWE	C2-C7-C8	2.99	124.83	119.65
4	A	999	GWE	C1-C2-C7	-2.66	118.90	122.73
4	A	999	GWE	O5-S1-C20	2.49	108.45	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	A	532/560 (95%)	-0.31	7 (1%) 74 75	25, 56, 96, 137	0
2	B	401/440 (91%)	-0.19	12 (2%) 48 45	29, 53, 98, 123	0
All	All	933/1000 (93%)	-0.26	19 (2%) 62 60	25, 55, 98, 137	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	195	ILE	3.9
1	A	52	PRO	3.9
1	A	221	HIS	3.8
2	B	432	GLU	3.1
2	B	198	HIS	2.8

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

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.13	-0.22	45,53,58,72	0

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	B	1300	5/5	0.24	0.77	123,126,136,137	0
4	GWE	A	999	36/36	0.14	-0.23	26,44,59,81	0
3	PO4	A	1301	5/5	0.13	-0.24	116,123,130,134	0

6.5 Other polymers

There are no such residues in this entry.