



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:16 PM GMT

PDB ID : 1SUQ
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN
COMPLEX WITH JANSSEN-R185545
Authors : Das, K.; Arnold, E.
Deposited on : 2004-03-26
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

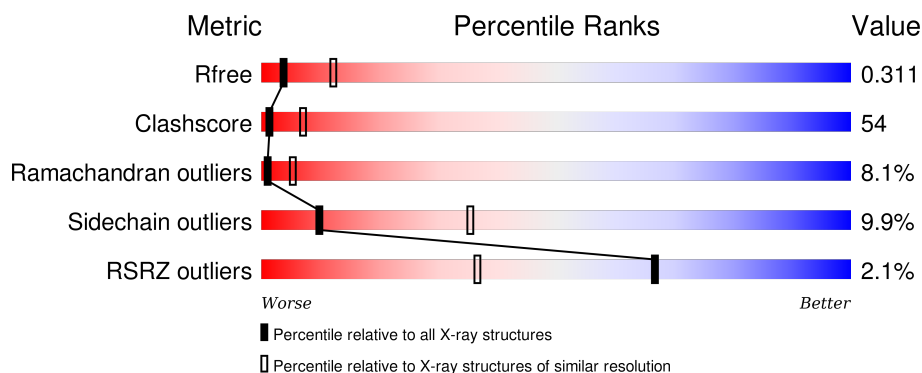
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	560	<div> <div></div> <div>32% 55% 10% ..</div> </div>
2	B	430	<div> <div>4%</div> <div>30% 56% 12% ..</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8053 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	121	0	0
			4497	2912	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	60	0	0
			3526	2297	584	638	7			

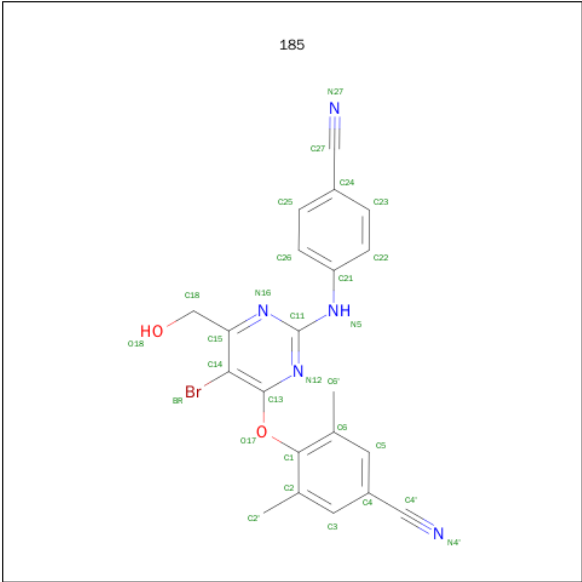
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (6-[4-(AMINOMETHYL)-2,6-DIMETHYLPHENOXY]-2-{[4-(AMINOMETHYL)PHENYL]AMINO}-5-BROMOPYRIMIDIN-4-YL)METHANOL (three-letter code: 185) (formula: C₂₁H₁₆BrN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
4	A	1	29	1	21	5	2	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.11Å 69.47Å 104.26Å 90.00° 106.82° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 34.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (19.99-3.00) 93.0 (34.75-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.325 0.255 , 0.311	Depositor DCC
R_{free} test set	1430 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 71.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 29227 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8053	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 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 185

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	0.49	0/4615	0.79	5/6270 (0.1%)
2	B	0.57	1/3631 (0.0%)	0.85	0/4936
All	All	0.53	1/8246 (0.0%)	0.82	5/11206 (0.0%)

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	1	0
2	B	0	1
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	383	TRP	CB-CG	-5.36	1.40	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	PRO	C-N-CD	-9.69	99.29	120.60
1	A	225	PRO	C-N-CA	6.90	150.99	122.00
1	A	226	PRO	N-CA-C	5.41	126.16	112.10
1	A	228	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	224	GLU	C-N-CD	-5.29	108.95	120.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	31	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	Sidechain

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	4497	0	4555	494	0
2	B	3526	0	3559	375	0
3	A	1	0	0	0	0
4	A	29	0	15	8	0
All	All	8053	0	8129	849	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 54.

The worst 5 of 849 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:226:PRO:HG3	1:A:235:HIS:CE1	1.72	1.25
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.16	1.11
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.21	1.10
2:B:314:VAL:HG22	2:B:315:HIS:H	1.16	1.10
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.27	1.09

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	550/560 (98%)	400 (73%)	110 (20%)	40 (7%)	1	6
2	B	425/430 (99%)	319 (75%)	67 (16%)	39 (9%)	1	4
All	All	975/990 (98%)	719 (74%)	177 (18%)	79 (8%)	1	5

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	54	ASN
1	A	114	ALA
1	A	122	GLU
1	A	195	ILE

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	493/500 (99%)	445 (90%)	48 (10%)	10	37
2	B	388/392 (99%)	349 (90%)	39 (10%)	9	34
All	All	881/892 (99%)	794 (90%)	87 (10%)	10	35

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	473	THR

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Mol	Chain	Res	Type
2	B	12	LEU
2	B	363	ASN
1	A	496	VAL
1	A	514	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	ASN
1	A	500	GLN
2	B	363	ASN
1	A	475	GLN
1	A	487	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
4	185	A	600	-	30,31,31	1.67	5 (16%)	37,43,43	1.87	6 (16%)

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
4	185	A	600	-	-	0/14/14/14	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	185	BR-C14	-3.66	1.80	1.89
4	A	600	185	O18-C18	-3.23	1.27	1.41
4	A	600	185	C23-C22	2.82	1.43	1.38
4	A	600	185	C13-N12	3.40	1.37	1.32
4	A	600	185	C22-C21	3.80	1.45	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	185	N16-C11-N12	-4.83	118.80	126.22
4	A	600	185	C14-C13-N12	-4.19	119.52	124.00
4	A	600	185	BR-C14-C13	-2.45	117.36	121.48
4	A	600	185	C11-N16-C15	2.19	121.80	116.00
4	A	600	185	C11-N12-C13	4.32	121.60	115.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	185	8	0

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 [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	A	545/560 (97%)	-0.25	4 (0%)	89 70	38, 92, 113, 121	18 (3%)
2	B	427/430 (99%)	-0.18	16 (3%)	45 19	22, 75, 115, 121	15 (3%)
All	All	972/990 (98%)	-0.22	20 (2%)	67 36	22, 86, 114, 121	33 (3%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	PRO	4.4
2	B	225	PRO	3.9
2	B	5	ILE	3.9
2	B	2	ILE	3.6
2	B	3	SER	3.5

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	185	A	600	29/29	0.91	0.35	1.97	80,94,97,119	0
3	MG	A	601	1/1	0.81	0.09	-2.76	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.