



# wwPDB X-ray Structure Validation Summary Report i

Jun 20, 2014 – 08:24 AM EDT

PDB ID : 4CEC  
Title : Interrogating HIV integrase for compounds that bind- a SAMPL challenge  
Authors : Peat, T.S.  
Deposited on : 2013-11-11  
Resolution : 1.75 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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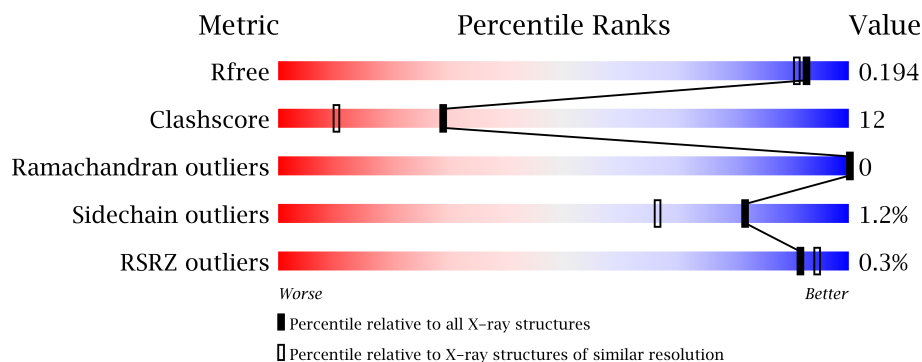
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	<b>FAILED</b>
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
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)	:	stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 1.75 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	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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  $\geq 3$ , 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	183	
1	B	183	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1212	-	X
2	SO4	B	1212	-	X
3	ACT	B	1213	-	X
4	CL	A	1214	-	X
4	CL	B	1214	-	X
5	GOL	A	1215	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 2793 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.

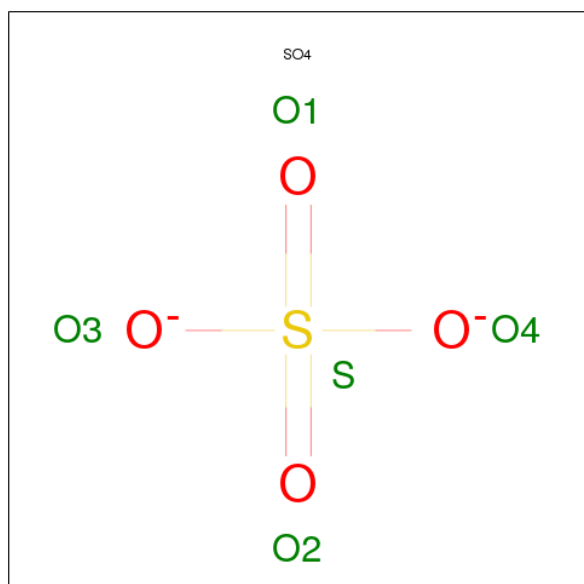
- Molecule 1 is a protein called INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	11	0
			1229	788	209	228	4			
1	B	149	Total	C	N	O	S	0	15	0
			1257	808	213	232	4			

There are 4 discrepancies between the modelled and reference sequences:

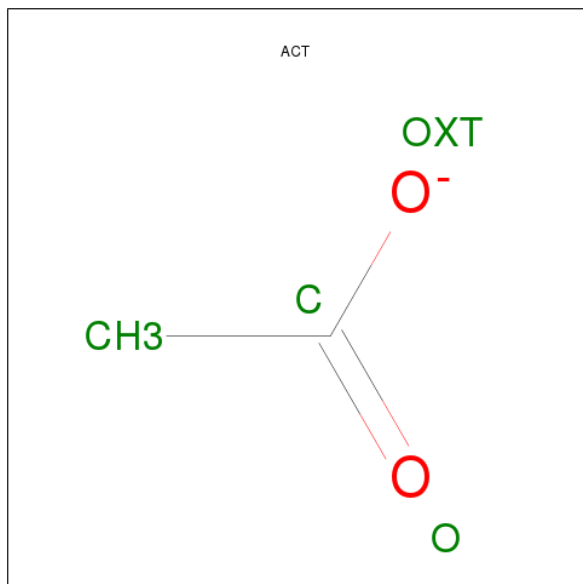
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ASP	PHE	ENGINEERED MUTATION	UNP Q76353
A	185	HIS	PHE	ENGINEERED MUTATION	UNP Q76353
B	139	ASP	PHE	ENGINEERED MUTATION	UNP Q76353
B	185	HIS	PHE	ENGINEERED MUTATION	UNP Q76353

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).

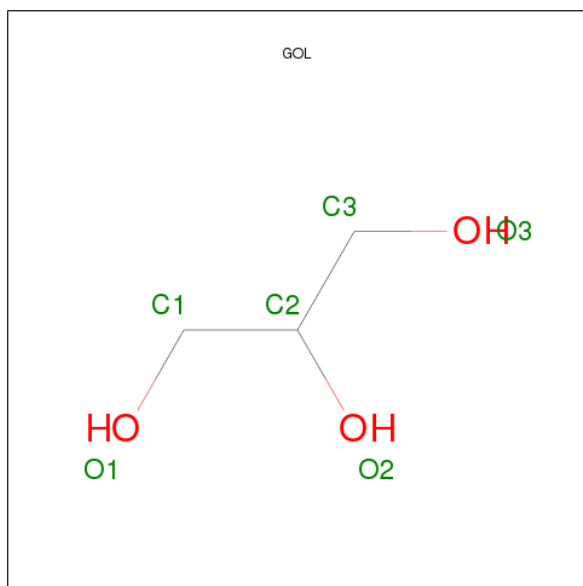


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

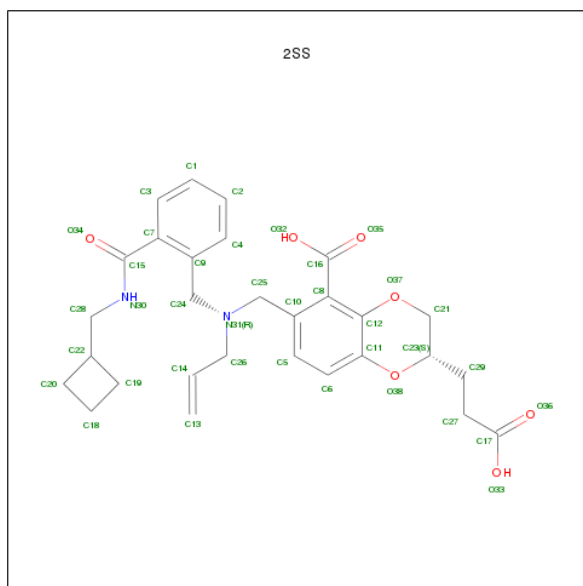
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is (2S)-6-[[[2-(CYCLOBUTYLMETHYLCARBAMOYL)PHENYL]METHYL-PROP-2-ENYL-AMINO]METHYL]-2-(3-HYDROXY-3-OXOPROPYL)-2,3-DIHYDRO-1,4-BENZODIOXINE-5-CARBOXYLICACID (three-letter code: 2SS) (formula:  $C_{29}H_{34}N_2O_7$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			38	29	2	7		
6	B	1	Total	C	N	O	0	0
			38	29	2	7		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	98	Total	O	0	0
			98	98		
7	B	81	Total	O	0	0
			81	81		

### 3 Residue-property plots

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.

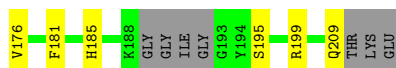
#### • Molecule 1: INTEGRASE

Chain A: 



#### • Molecule 1: INTEGRASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.58Å 70.58Å 66.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.08 – 1.75 35.29 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.08-1.75) 100.0 (35.29-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.166 , 0.195 0.165 , 0.194	Depositor DCC
$R_{free}$ test set	1902 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.8	EDS
Estimated twinning fraction	0.016 for -h,-k,l 0.487 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37527 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: GOL, 2SS, ACT, SO4, 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	0.60	0/1274	0.59	0/1727
1	B	0.61	0/1305	0.59	0/1769
All	All	0.60	0/2579	0.59	0/3496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1229	0	1252	16	0
1	B	1257	0	1290	34	0
2	A	15	0	0	2	0
2	B	15	0	0	3	0
3	A	4	0	3	10	0
3	B	4	0	3	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	6	0	8	7	0
5	B	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	38	0	32	2	0
6	B	38	0	32	1	0
7	A	98	0	0	8	1
7	B	81	0	0	5	1
All	All	2793	0	2628	65	1

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 12.

The worst 5 of 65 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:1213:ACT:H3	7:B:2026:HOH:O	1.36	1.25
3:B:1213:ACT:CH3	7:B:2026:HOH:O	1.89	1.09
1:B:139:ASP:OD1	1:B:141[B]:ILE:HG22	1.53	1.08
1:B:141[B]:ILE:HG23	1:B:143:TYR:CE2	1.91	1.06
1:B:141[B]:ILE:HD12	1:B:142:PRO:HD2	1.41	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:2029:HOH:O	7:B:2070:HOH:O[2_555]	2.19	0.01

## 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	156/183 (85%)	155 (99%)	1 (1%)	0	100	100
1	B	160/183 (87%)	160 (100%)	0	0	100	100
All	All	316/366 (86%)	315 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	134/150 (89%)	133 (99%)	1 (1%)	91	82
1	B	138/150 (92%)	136 (99%)	2 (1%)	78	62
All	All	272/300 (91%)	269 (99%)	3 (1%)	82	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	B	57	SER
1	B	152	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
1	B	209	GLN
1	B	171	HIS
1	A	171	HIS
1	B	148	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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<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	149/183 (81%)	-0.32	1 (0%) 84 91	11, 17, 33, 41	21 (14%)
1	B	149/183 (81%)	-0.33	0 100 100	10, 17, 34, 41	19 (12%)
All	All	298/366 (81%)	-0.32	1 (0%) 91 94	10, 17, 34, 41	40 (13%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	LYS	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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	1215	6/6	0.13	6.66	31,35,36,38	0
2	SO4	B	1212	5/5	0.14	4.19	31,32,34,35	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	1214	1/1	0.10	3.31	57,57,57,57	0
2	SO4	A	1212	5/5	0.12	2.62	29,31,32,33	5
4	CL	A	1214	1/1	0.10	2.13	62,62,62,62	0
3	ACT	B	1213	4/4	0.11	2.02	30,31,31,31	0
5	GOL	B	1215	6/6	0.10	1.62	32,34,36,38	0
2	SO4	B	1210	5/5	0.11	1.10	36,37,39,40	5
2	SO4	A	1211	5/5	0.09	0.93	19,22,23,24	5
3	ACT	A	1213	4/4	0.09	0.85	29,30,31,31	0
2	SO4	A	1210	5/5	0.10	0.56	36,37,39,39	5
6	2SS	A	1216	38/38	0.08	0.34	16,22,26,28	0
6	2SS	B	1216	38/38	0.08	0.13	15,22,26,28	0
2	SO4	B	1211	5/5	0.08	-0.40	20,24,25,26	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.