

Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 04:11 PM EDT

PDB ID : 3AO1

Title: Fragment-based approach to the design of ligands targeting a novel site in

HIV-1 integrase

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Deposited on : 2010-09-17

Resolution : 1.90 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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

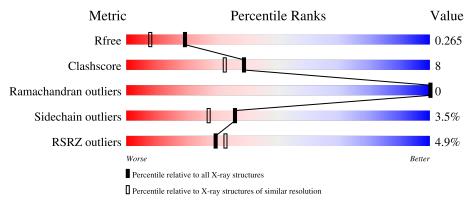
Validation Pipeline (wwPDB-VP) : 2.36

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 1.90 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 >=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 <=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	163	71%	14%	•	13%
1	В	163	74%	11%	•	13%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2270 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 POL polyprotein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	141	Total 1073	C 680		O 201	S 4	0	0	0
1	В	142	Total 1086	C 689	N 190	O 203	S 4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

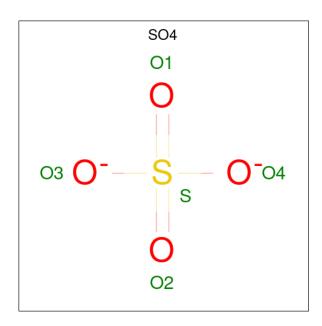
Chain	Residue	Modelled	Actual	Comment	Reference
A	56	SER	CYS	engineered mutation	UNP Q72498
A	131	ASP	TRP	engineered mutation	UNP Q72498
A	139	ASP	PHE	engineered mutation	UNP Q72498
A	185	HIS	PHE	engineered mutation	UNP Q72498
В	56	SER	CYS	engineered mutation	UNP Q72498
В	131	ASP	TRP	engineered mutation	UNP Q72498
В	139	ASP	PHE	engineered mutation	UNP Q72498
В	185	HIS	PHE	engineered mutation	UNP Q72498

• Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cd 2 2	0	0
2	В	2	Total Cd 2 2	0	0

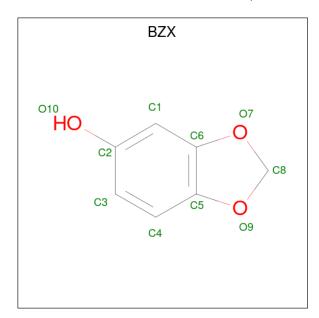
• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





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

 \bullet Molecule 4 is 1,3-benzodioxol-5-ol (three-letter code: BZX) (formula: $\mathrm{C_7H_6O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 7 3	0	0
4	A	1	Total C O 10 7 3	0	0
4	В	1	Total C O 10 7 3	0	0



• Molecule 5 is water.

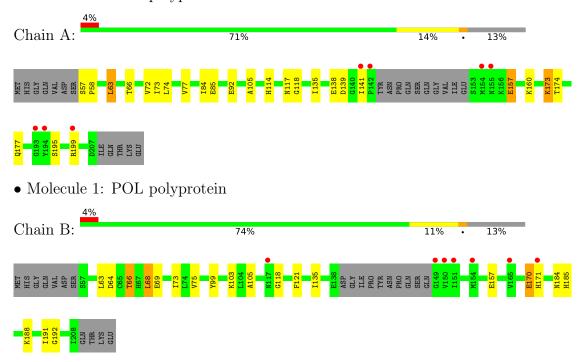
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0
5	В	38	Total O 38 38	0	0



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: POL polyprotein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	60.59Å 62.00Å 81.77Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 - 1.90	Depositor
rtesolution (A)	49.40 - 1.90	EDS
% Data completeness	99.7 (49.40-1.90)	Depositor
(in resolution range)	99.7 (49.40-1.90)	EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	2.69 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.268	Depositor
it, it free	0.213 , 0.265	DCC
R_{free} test set	1234 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 49.6	EDS
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2270	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: SO4, BZX, CD

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	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.43	0/1093	0.53	0/1479	
1	В	0.43	0/1105	0.54	0/1494	
All	All	0.43	0/2198	0.53	0/2973	

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 (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	1073	0	1073	20	0
1	В	1086	0	1094	16	0
2	A	2	0	0	0	1
2	В	2	0	0	0	0
3	A	5	0	0	0	0
4	A	20	0	10	0	0
4	В	10	0	5	2	0
5	A	34	0	0	1	0
5	В	38	0	0	4	1
All	All	2270	0	2182	33	1

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 8.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1 D 101 H D H A	* D 01 / HOH 0	distance (Å)	overlap (Å)
1:B:191:ILE:HA	5:B:214:HOH:O	1.72	0.89
1:A:138:GLU:HB3	1:A:141:ILE:HD13	1.58	0.83
1:A:66:THR:HG22	1:A:73:ILE:HB	1.76	0.67
1:B:66:THR:HG23	1:B:73:ILE:HB	1.78	0.65
1:B:118:GLY:HA3	5:B:3:HOH:O	1.99	0.63
1:B:68:LEU:HD23	1:B:69:GLU:HG3	1.86	0.58
1:B:170:GLU:HG2	1:B:171:HIS:ND1	2.19	0.57
1:B:184:ASN:HB3	4:B:1:BZX:H8A	1.86	0.57
1:A:118:GLY:HA3	5:A:30:HOH:O	2.05	0.56
1:A:63:LEU:HD21	1:A:74:LEU:CD1	2.36	0.55
1:A:105:ALA:O	1:B:185:HIS:HE1	1.91	0.54
1:A:173:LYS:HG3	1:A:174:THR:N	2.24	0.53
1:A:72:VAL:HG11	1:A:92:GLU:HG3	1.92	0.52
1:A:105:ALA:HB2	1:A:135:ILE:HD11	1.92	0.52
1:A:85:GLU:HG3	5:B:218:HOH:O	2.09	0.52
1:A:195:SER:O	1:A:199:ARG:HG3	2.11	0.49
1:B:170:GLU:HG2	1:B:171:HIS:CE1	2.48	0.49
1:A:63:LEU:HD21	1:A:74:LEU:HD11	1.96	0.48
1:B:63:LEU:HD12	1:B:75:VAL:O	2.14	0.47
1:B:188:LYS:HA	1:B:188:LYS:HD2	1.71	0.47
1:A:77:VAL:HG22	1:A:84:ILE:HG22	1.98	0.46
1:A:114:HIS:HD2	1:A:138:GLU:HB2	1.81	0.46
1:A:117:ASN:HD22	1:A:139:ASP:HB3	1.81	0.45
1:A:157:GLU:O	1:A:160:LYS:HB3	2.15	0.45
1:B:192:GLY:N	5:B:214:HOH:O	2.41	0.44
1:B:63:LEU:HD23	1:B:121:PHE:CE1	2.53	0.44
1:A:173:LYS:HD3	1:B:99:TYR:CE1	2.53	0.43
1:A:177:GLN:HG3	1:B:103:LYS:HG2	2.01	0.43
1:B:184:ASN:CB	4:B:1:BZX:H8A	2.49	0.43
1:A:173:LYS:CB	1:A:173:LYS:NZ	2.82	0.42
1:B:105:ALA:HB2	1:B:135:ILE:HD11	2.01	0.42
1:A:57:SER:N	1:A:58:PRO:HD2	2.35	0.41
1:A:63:LEU:CD2	1:A:74:LEU:HD11	2.51	0.40

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-1 Atom-2		Clash overlap (Å)
2:A:1003:CD:CD	5:B:223:HOH:O[4_455]	1.95	0.25

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	Perce	ntiles
1	A	137/163 (84%)	134 (98%)	3 (2%)	0	100	100
1	В	138/163 (85%)	135 (98%)	3 (2%)	0	100	100
All	All	275/326~(84%)	269 (98%)	6 (2%)	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	112/133 (84%)	109 (97%)	3 (3%)	44 38		
1	В	114/133 (86%)	109 (96%)	5 (4%)	28 19		
All	All	226/266 (85%)	218 (96%)	8 (4%)	36 27		

All (8) residues with a non-rotameric sidechain are listed below:

\mathbf{Mol}	Chain	Res	Type
1	A	63	LEU
1	A	157	GLU
1	A	173	LYS

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Mol	Chain	Res	Type
1	В	64	ASP
1	В	66	THR
1	В	68	LEU
1	В	157	GLU
1	В	170	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	В	95	GLN
1	В	137	GLN
1	В	185	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, 4 are monoatomic - leaving 4 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	Tuno	Chain	Res	Res Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1	-	4,4,4	0.18	0	6,6,6	0.26	0
4	BZX	A	214	-	11,11,11	1.06	1 (9%)	15,15,15	1.66	4 (26%)
4	BZX	В	1	-	11,11,11	1.03	1 (9%)	15,15,15	1.89	5 (33%)
4	BZX	A	213	-	11,11,11	0.99	1 (9%)	15,15,15	1.86	6 (40%)

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	BZX	A	213	-	=	_	0/2/2/2
4	BZX	A	214	-	-	-	0/2/2/2
4	BZX	В	1	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
4	A	214	BZX	C6-C5	2.65	1.46	1.39
4	В	1	BZX	C6-C5	2.62	1.45	1.39
4	A	213	BZX	C6-C5	2.50	1.45	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	1	BZX	C8-O9-C5	3.49	109.88	105.34
4	A	213	BZX	C3-C2-C1	2.93	123.38	120.17
4	В	1	BZX	C8-O7-C6	2.92	109.13	105.34
4	A	213	BZX	O9-C5-C6	-2.72	106.68	109.78
4	В	1	BZX	O9-C5-C6	-2.45	106.99	109.78
4	A	213	BZX	C8-O9-C5	2.39	108.45	105.34
4	A	213	BZX	O9-C8-O7	-2.36	104.31	108.08
4	A	214	BZX	C8-O7-C6	2.35	108.40	105.34
4	A	214	BZX	C8-O9-C5	2.33	108.36	105.34
4	A	214	BZX	C4-C3-C2	2.29	122.39	119.88
4	A	213	BZX	C3-C4-C5	-2.18	115.90	120.06
4	A	214	BZX	C3-C4-C5	-2.14	115.99	120.06
4	A	213	BZX	O7-C6-C1	2.13	130.69	127.85
4	В	1	BZX	C3-C2-C1	2.10	122.47	120.17
4	В	1	BZX	C3-C4-C5	-2.05	116.14	120.06



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	1	BZX	2	0

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^{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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	141/163 (86%)	0.36	7 (4%) 28 32	25, 35, 53, 67	0
1	В	142/163 (87%)	0.55	7 (4%) 29 33	25, 35, 64, 85	0
All	All	283/326 (86%)	0.46	14 (4%) 29 33	25, 35, 60, 85	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	150	VAL	8.7	
1	В	151	ILE	6.7	
1	В	149	GLY	4.3	
1	A	154	MET	3.1	
1	A	194	TYR	2.7	
1	В	154	MET	2.7	
1	A	155	ASN	2.7	
1	В	117	ASN	2.5	
1	В	165	VAL	2.2	
1	В	171	HIS	2.1	
1	A	199	ARG	2.1	
1	A	141	ILE	2.1	
1	A	142	PRO	2.1	
1	A	193	GLY	2.1	

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^{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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	BZX	A	214	10/10	0.68	0.26	38,39,44,45	10
4	BZX	A	213	10/10	0.81	0.27	29,31,34,35	10
4	BZX	В	1	10/10	0.90	0.19	27,29,32,32	10
2	CD	В	1002	1/1	0.94	0.14	55,55,55,55	0
3	SO4	A	1	5/5	0.95	0.10	44,47,50,52	0
2	CD	В	1001	1/1	0.99	0.13	48,48,48,48	0
2	CD	A	1003	1/1	0.99	0.06	36,36,36,36	0
2	CD	A	1004	1/1	0.99	0.13	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.

