Full wwPDB Geometry-Only Validation Report ⓘ

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PDB ID	:	2ZYE
Title	:	Structure of HIV-1 Protease in Complex with Potent Inhibitor KNI-272 Determined by Neutron Crystallography
Authors	:	Adachi, M.; Ohhara, T.; Tamada, T.; Okazaki, N.; Kuroki, R.
Deposited on	:	2009-01-20
Resolution	:	1.90 Å(reported)

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
NEUTRON DIFFRACTION

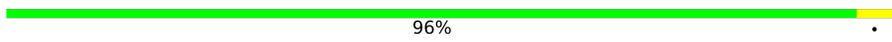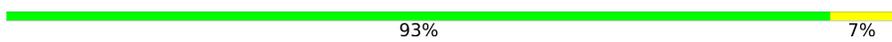The reported resolution of this entry is 1.90 Å.

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.
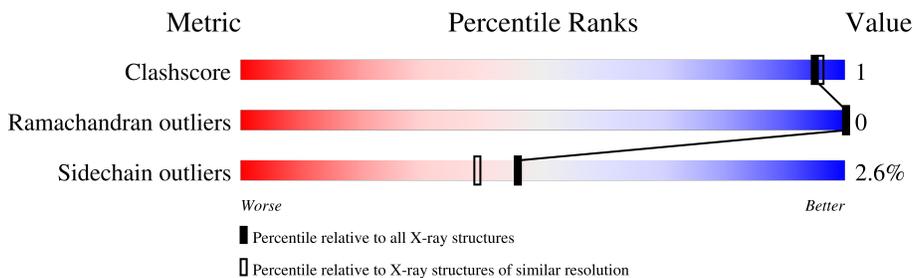
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	99	96% •
1	B	99	93% 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3843 atoms, of which 1591 are hydrogens and 520 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 protease.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	99	Total	C	D	H	N	O	S	30	93	0
			1711	501	167	776	130	134	3			
1	B	99	Total	C	D	H	N	O	S	37	93	0
			1718	502	168	775	131	140	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	GLN	engineered mutation	UNP Q9EKL4
A	33	ILE	VAL	engineered mutation	UNP Q9EKL4
A	63	ILE	LEU	engineered mutation	UNP Q9EKL4
A	67	ALA	CYS	engineered mutation	UNP Q9EKL4
A	95	ALA	CYS	engineered mutation	UNP Q9EKL4
B	107	LYS	GLN	engineered mutation	UNP Q9EKL4
B	133	ILE	VAL	engineered mutation	UNP Q9EKL4
B	163	ILE	LEU	engineered mutation	UNP Q9EKL4
B	167	ALA	CYS	engineered mutation	UNP Q9EKL4
B	195	ALA	CYS	engineered mutation	UNP Q9EKL4

- Molecule 2 is (4R)-N-tert-butyl-3-[(2S,3S)-2-hydroxy-3-({N-[(isoquinolin-5-yloxy)acetyl]-S-methyl-L-cysteinyl}amino)-4-phenylbutanoyl]-1,3-thiazolidine-4-carboxamide (three-letter code: KNI) (formula: $C_{33}H_{41}N_5O_6S_2$).
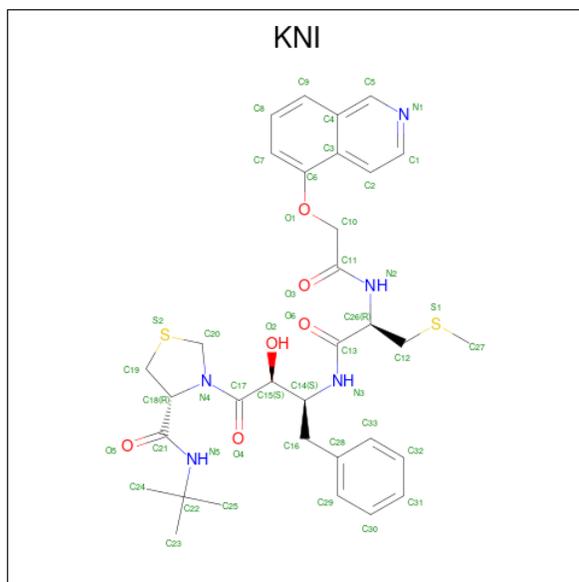
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	D	H	N	O	S		
2	B	1	90	33	4	40	5	6	2	3	1

• Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	57	Total	D	O	0	0
			134	77	57		
3	B	86	Total	D	O	0	0
			190	104	86		

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS was not executed.

- Molecule 1: protease

Chain A:

- Molecule 1: protease

Chain B:

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

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	1.23	2/1548 (0.1%)	1.11	4/2102 (0.2%)
1	B	1.14	2/1558 (0.1%)	1.14	6/2116 (0.3%)
All	All	1.19	4/3106 (0.1%)	1.12	10/4218 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59[A]	TYR	CE1-CZ	5.95	1.46	1.38
1	A	59[B]	TYR	CE1-CZ	5.95	1.46	1.38
1	B	142[A]	TRP	CB-CG	5.04	1.59	1.50
1	B	142[B]	TRP	CB-CG	5.04	1.59	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129[A]	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	B	129[B]	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	B	187[A]	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	B	187[B]	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	B	130[A]	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	B	130[B]	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	A	29[A]	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	29[B]	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	41[A]	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	41[B]	ARG	NE-CZ-NH2	-5.85	117.38	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	935	776	112	0	0
1	B	943	775	112	0	0
2	B	50	40	0	0	0
3	A	134	0	0	1	0
3	B	190	0	0	0	0
All	All	2252	1591	224	1	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 1.

All (1) 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)

There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 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	203/99 (205%)	202 (100%)	1 (0%)	0	100	100
1	B	207/99 (209%)	207 (100%)	0	0	100	100
All	All	410/198 (207%)	409 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	154/81 (190%)	152 (99%)	2 (1%)	69	68
1	B	150/81 (185%)	144 (96%)	6 (4%)	31	22
All	All	304/162 (188%)	296 (97%)	8 (3%)	46	39

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

Mol	Chain	Res	Type
1	A	43[A]	LYS
1	A	43[B]	LYS
1	B	107[A]	LYS
1	B	107[B]	LYS
1	B	123[A]	LEU
1	B	123[B]	LEU
1	B	155[A]	LYS
1	B	155[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.