WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 11:25 PM GMT

PDB ID : 1O5A

Title : Dissecting and Designing Inhibitor Selectivity Determinants at the S1 site Using an Artificial Ala190 Protease (Ala190 uPA)

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Deposited on : 2003-09-09

Resolution : 1.68 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.68 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	Percentile Ranks	Value
Rfree		0.216
Clashscore		6
Ramachandran outliers		0.8%
Sidechain outliers		4.1%
RSRZ outliers		3.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
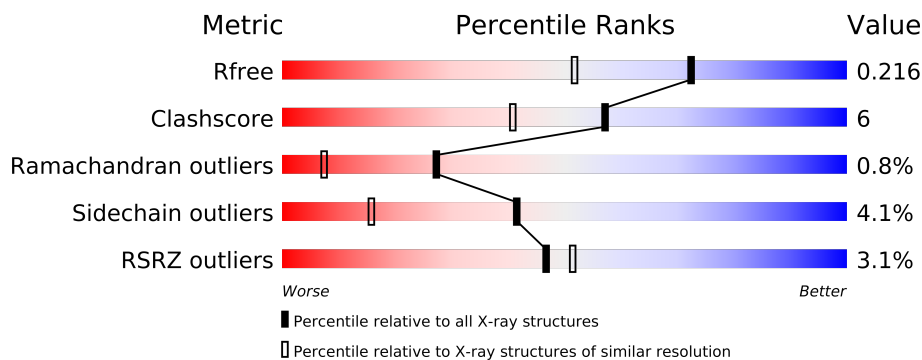
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3587 (1.70-1.66)
Clashscore	79885	4225 (1.70-1.66)
Ramachandran outliers	78287	4144 (1.70-1.66)
Sidechain outliers	78261	4143 (1.70-1.66)
RSRZ outliers	66119	3587 (1.70-1.66)

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	23	
2	B	253	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4624 atoms, of which 2381 are hydrogens 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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	9	Total	C	H	N	O	S	0	0	0
			147	46	75	13	12	1			

- Molecule 2 is a protein called Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	246	Total	C	H	N	O	S	0	4	0
			3871	1233	1920	339	361	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	145	ALA	ASN	ENGINEERED	UNP P00749
B	190	ALA	SER	ENGINEERED	UNP P00749

- Molecule 3 is 3-{5-[AMINO(IMINIO)METHYL]-1H-INDOL-2-YL}-1,1'-BIPHENYL-2-OLATE (three-letter code: 696) (formula: $C_{21}H_{17}N_3O$).
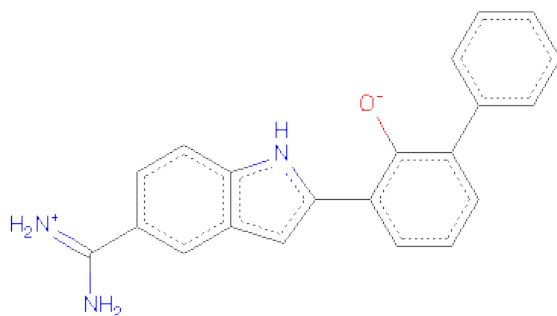
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			42	21	17	3	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
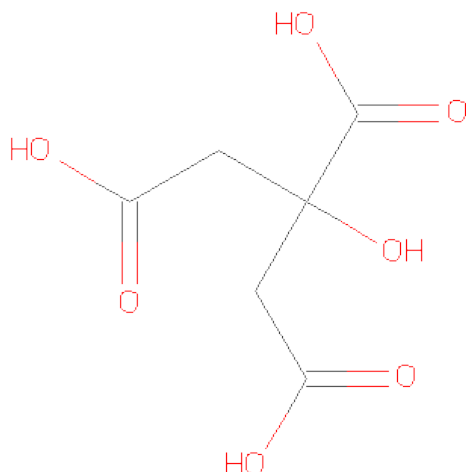
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	6	Total	H	O	0	0
			18	12	6		
5	B	176	Total	H	O	0	0
			528	352	176		

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: Urokinase-type plasminogen activator

Chain A:
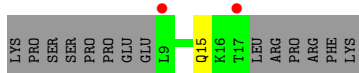
• Molecule 2: Urokinase-type plasminogen activator

Chain B:

4 Data and refinement statistics ⓘ

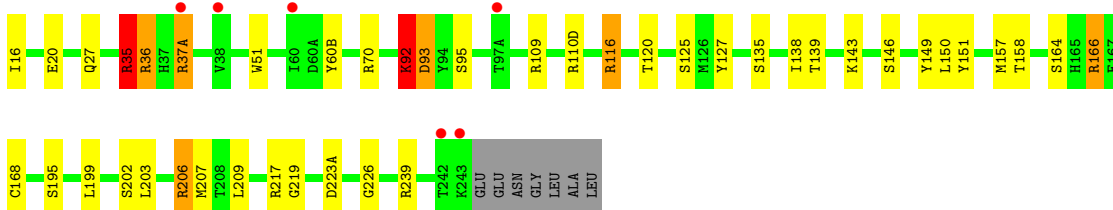| Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.78Å　49.87Å　66.74Å 90.00°　113.41°　90.00°	Depositor
Resolution (Å)	7.00　–　1.68 6.98　–　1.68	Depositor EDS
% Data completeness (in resolution range)	86.2 (7.00-1.68) 86.1 (6.98-1.68)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.58 (at 1.68Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.209　,　0.245 0.212　,　0.216	Depositor DCC
R_{free} test set	2384 reflections (9.93%)	DCC
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.2	EDS
Estimated twinning fraction	0.023 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
L-test for twinning	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Outliers	0 of 24014 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4624	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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: 696, CIT

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	1.17	0/72	1.32	0/93
2	B	1.33	1/2012 (0.0%)	1.40	15/2725 (0.6%)
All	All	1.32	1/2084 (0.0%)	1.40	15/2818 (0.5%)

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	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	51	TRP	NE1-CE2	-5.01	1.31	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	109	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	B	199	LEU	N-CA-C	-6.98	92.16	111.00
2	B	207	MET	N-CA-C	-6.65	93.03	111.00
2	B	37(A)	ARG	N-CA-C	-5.95	94.94	111.00
2	B	166	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	B	206	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	151	TYR	CB-CG-CD2	-5.63	117.62	121.00
2	B	37(A)	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	B	150	LEU	CB-CA-C	-5.58	99.60	110.20
2	B	36	ARG	NE-CZ-NH2	-5.53	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	226	GLY	N-CA-C	-5.44	99.50	113.10
2	B	92	LYS	N-CA-C	-5.32	96.63	111.00
2	B	217	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	B	35	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	B	223(A)	ASP	CB-CG-OD2	-5.12	113.69	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	110(D)	ARG	Sidechain
2	B	116	ARG	Sidechain
2	B	166	ARG	Sidechain
2	B	206	ARG	Sidechain
2	B	239	ARG	Sidechain
2	B	35	ARG	Sidechain
2	B	36	ARG	Sidechain
2	B	37(A)	ARG	Sidechain
2	B	70	ARG	Sidechain

5.2 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 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	72	75	0	0	0
2	B	1951	1920	0	22	0
3	B	25	17	0	8	0
4	B	13	5	0	0	0
5	A	6	12	0	0	0
5	B	176	352	0	12	0
All	All	2243	2381	0	26	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 6.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:146:SER:HG	5:B:330:HOH:H1	0.86	0.86
2:B:149:TYR:HH	5:B:384:HOH:H2	1.26	0.84
2:B:143:LYS:HZ2	5:B:358:HOH:H2	1.37	0.70
2:B:120:THR:HG1	5:B:382:HOH:H1	1.42	0.65
2:B:164:SER:HG	5:B:409:HOH:H2	1.46	0.64
2:B:95:SER:HG	5:B:361:HOH:H2	1.43	0.64
2:B:135:SER:HG	5:B:398:HOH:H1	1.48	0.59
3:B:251:696:HN3	5:B:343:HOH:H1	1.51	0.56
2:B:195:SER:OG	3:B:251:696:N3	2.37	0.56
2:B:92:LYS:H	2:B:92:LYS:CD	2.20	0.54
3:B:251:696:C6'	5:B:343:HOH:H2	2.12	0.54
2:B:195:SER:HG	3:B:251:696:HN3	1.53	0.52
3:B:251:696:O6'	5:B:343:HOH:O	2.24	0.50
2:B:27:GLN:HG3	2:B:139:THR:HG23	1.94	0.50
2:B:195:SER:OG	3:B:251:696:O6'	2.21	0.47
2:B:92:LYS:O	2:B:93:ASP:CB	2.62	0.47
2:B:92:LYS:H	2:B:92:LYS:HD2	1.79	0.47
2:B:195:SER:CB	5:B:343:HOH:H1	2.23	0.47
2:B:35:ARG:HD2	2:B:60(B):TYR:CD1	2.51	0.46
3:B:251:696:N3	5:B:343:HOH:O	2.49	0.44
2:B:157:MET:HG2	2:B:158:THR:N	2.33	0.43
2:B:27:GLN:CD	2:B:139:THR:HG23	2.38	0.43
2:B:138:ILE:C	2:B:139:THR:HG21	2.40	0.42
2:B:16:ILE:N	2:B:143:LYS:O	2.54	0.41
2:B:27:GLN:CG	2:B:139:THR:HG23	2.50	0.40
2:B:219:GLY:O	3:B:251:696:N1	2.55	0.40

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	7/23 (30%)	7 (100%)	0	0	100	100
2	B	247/253 (98%)	232 (94%)	13 (5%)	2 (1%)	27	7
All	All	254/276 (92%)	239 (94%)	13 (5%)	2 (1%)	27	7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	93	ASP
2	B	127	TYR

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	8/22 (36%)	7 (88%)	1 (12%)	7	1
2	B	216/218 (99%)	208 (96%)	8 (4%)	45	19
All	All	224/240 (93%)	215 (96%)	9 (4%)	41	16

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
2	B	20	GLU
2	B	92	LYS
2	B	116	ARG
2	B	125	SER
2	B	168	CYS
2	B	202	SER
2	B	203	LEU
2	B	209	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	78	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	#$\|Z\| > 2$
4	CIT	B	2	-	12,12,12	2.32	6 (50%)	17,17,17	1.67	3 (17%)
3	696	B	251	-	28,28,28	2.26	7 (25%)	40,40,40	1.25	4 (10%)

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	CIT	B	2	-	-	0/16/16/16	0/0/0/0
3	696	B	251	-	-	0/11/12/12	0/2/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	251	696	C1-C7	-6.55	1.42	1.48
3	B	251	696	C5'-C1B	-5.18	1.40	1.49
4	B	2	CIT	O5-C6	4.86	1.38	1.22
3	B	251	696	C8-N3	-4.45	1.32	1.36
3	B	251	696	C1'-C8	-4.43	1.40	1.48
4	B	2	CIT	C4-C3	3.02	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	CIT	C2-C3	3.00	1.57	1.53
3	B	251	696	O6'-C6'	2.62	1.38	1.27
3	B	251	696	C3-C2	2.47	1.41	1.36
3	B	251	696	C2-C1	2.36	1.43	1.39
4	B	2	CIT	O4-C5	-2.36	1.22	1.30
4	B	2	CIT	O6-C6	-2.32	1.21	1.30
4	B	2	CIT	O2-C1	-2.18	1.22	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	251	696	C1B-C5'-C6'	4.47	125.31	120.90
4	B	2	CIT	O7-C3-C4	-4.11	100.94	109.22
4	B	2	CIT	O6-C6-C3	2.84	117.02	112.89
3	B	251	696	C2-C1-C7	2.82	122.53	120.39
3	B	251	696	C1'-C8-N3	2.82	125.25	121.45
4	B	2	CIT	O7-C3-C6	2.49	112.54	108.95
3	B	251	696	CN4-C5-C6	-2.04	129.18	136.53

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(Å²)	Q<0.9
1	A	9/23 (39%)	2.30	2 (22%)	1	2	23, 34, 48, 51	2 (22%)
2	B	246/253 (97%)	0.11	6 (2%)	56	60	11, 24, 40, 64	19 (7%)
All	All	255/276 (92%)	0.19	8 (3%)	47	51	11, 24, 41, 64	21 (8%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	LEU	12.7
2	B	243	LYS	10.0
1	A	17	THR	7.0
2	B	37(A)	ARG	5.0
2	B	97(A)	THR	4.1
2	B	242	THR	2.7
2	B	60	ILE	2.4
2	B	38	VAL	2.1

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, 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	696	B	251	25/25	0.09	-	14,18,21,24	0
4	CIT	B	2	13/13	0.22	-	33,43,52,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.