

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 10:38 pm BST

PDB ID	:	1FV9
Title	:	Crystal structure of human microurokinase in complex with 2-amino-5-hydro
		xy-benzimidazole
Authors	:	Nienaber, V.
Deposited on	:	2000-09-19
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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

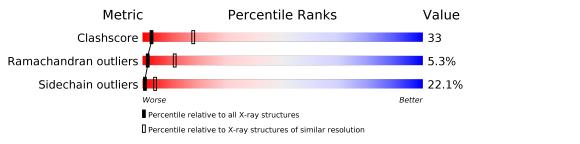
$\operatorname{MolProbity}$:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	Similar resolution
Metric	$(\# {\it Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 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	А	245	32%	43%	21%	• •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1949 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.

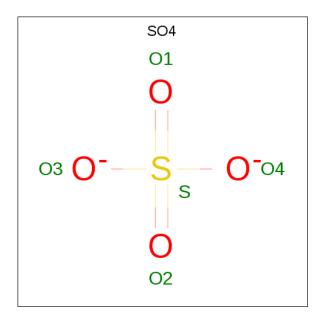
• Molecule 1 is a protein called UROKINASE.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Δ	245	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	А	240	1933	1218	338	361	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	120	ALA	CYS	CONFLICT	UNP P00749

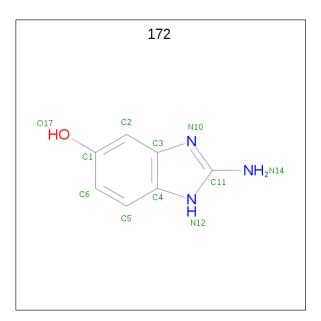
• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	А	1	Total 5	0 4	S 1	0	0

• Molecule 3 is 2-AMINO-5-HYDROXY-BENZIMIDAZOLE (three-letter code: 172) (formula: $C_7H_7N_3O$).





Μ	ol	Chain	Residues	Atoms				ZeroOcc	AltConf
3		А	1	Total 11	С 7	N 3	0 1	0	0

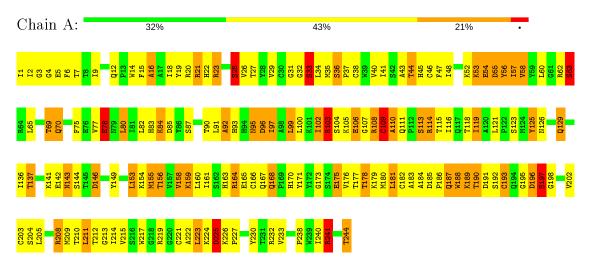


3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 colorcoded 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: UROKINASE





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	55.16Å 53.00 Å 82.30 Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	10.00 - 3.00	Depositor	
% Data completeness	(Not available) (10.00-3.00)	Depositor	
(in resolution range)		Depositor	
R_{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	X-PLOR 98.0	Depositor	
R, R_{free}	0.248 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1949	wwPDB-VP	
Average B, all atoms $(Å^2)$	11.0	wwPDB-VP	



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, $172\,$

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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
Mol	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	1.20	8/1982~(0.4%)	1.69	57/2684~(2.1%)

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	А	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	33	SER	CB-OG	6.73	1.50	1.42
1	А	197	SER	CB-OG	-6.67	1.33	1.42
1	А	241	ARG	NE-CZ	6.61	1.41	1.33
1	А	78	GLU	CG-CD	6.08	1.61	1.51
1	А	5	GLU	CG-CD	5.14	1.59	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Type Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	91	LEU	CA-CB-CG	12.51	144.07	115.30
1	А	62	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	А	96	ASP	CB-CG-OD1	11.44	128.59	118.30
1	А	225	ASP	CB-CG-OD2	-11.28	108.14	118.30
1	А	208	ARG	NE-CZ-NH2	-10.72	114.94	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	186	PRO	Peptide
1	А	25	SER	Peptide
1	А	53	LYS	Mainchain
1	А	56	TYR	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	А	1933	0	1881	128	0
2	А	5	0	0	0	0
3	А	11	0	6	1	0
All	All	1949	0	1887	128	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 33.

The worst 5 of 128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic}\\ {\rm distance}~({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:63:SER:HB2	1:A:69:THR:HG21	1.49	0.91
1:A:181:LEU:HG	1:A:232:ARG:HE	1.44	0.83
1:A:75:PHE:CD2	1:A:102:ILE:HB	2.18	0.78
1:A:103:ARG:HD3	1:A:107:GLY:HA2	1.71	0.72
1:A:37:PRO:C	1:A:109:CYS:HB3	2.09	0.72

There are no symmetry-related clashes.

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 re	esidues.
--------------------------------------	----------

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	А	243/245~(99%)	190~(78%)	40 (16%)	13~(5%)	2 11	

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	187	GLN
1	А	4	GLY
1	А	65	LEU
1	А	70	GLN
1	А	84	LYS

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	А	213/213~(100%)	166~(78%)	47 (22%)	1 4		

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	121	LEU
1	А	137	THR
1	А	205	LEU
1	А	125	TYR
1	А	144	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	94	HIS
1	А	243	HIS
1	А	95	ASN
1	А	79	ASN
1	А	111	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)

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 B		Type	Chain	nin Ros	Dog	Bos	Bos	Dog	Dog	Dog	Bos	Bos	Res	n Dog	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2												
2	SO4	А	245	-	$4,\!4,\!4$	0.38	0	$6,\!6,\!6$	0.75	0												
3	172	А	246	-	12,12,12	<mark>3.14</mark>	6 (50%)	$10,\!17,\!17$	2.96	<mark>6 (60%)</mark>												

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
3	172	А	246	-	-	-	0/2/2/2

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

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	А	246	172	C11-N12	5.61	1.42	1.34
3	А	246	172	C4-C3	-4.78	1.26	1.42
3	А	246	172	C11-N10	4.57	1.41	1.34

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	А	246	172	C2-C3	-4.22	1.35	1.41
3	А	246	172	C5-C4	-3.87	1.35	1.41

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

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	246	172	C11-N10-C3	-5.22	99.51	106.73
3	А	246	172	C11-N12-C4	-4.75	100.16	106.73
3	А	246	172	C2-C3-N10	-3.48	120.87	130.83
3	А	246	172	C6-C5-C4	-3.38	116.58	120.84
3	А	246	172	C5-C4-N12	-2.54	123.41	130.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	246	172	1	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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

