



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:37 am BST

PDB ID : 1MKX
Title : THE CO-CRYSTAL STRUCTURE OF UNLIGANDED BOVINE ALPHA-THROMBIN AND PRETHROMBIN-2: MOVEMENT OF THE YPPW SEGMENT AND ACTIVE SITE RESIDUES UPON LIGAND BINDING
Authors : Malkowski, M.G.; Edwards, B.F.P.
Deposited on : 1997-03-13
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 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) : 2.11

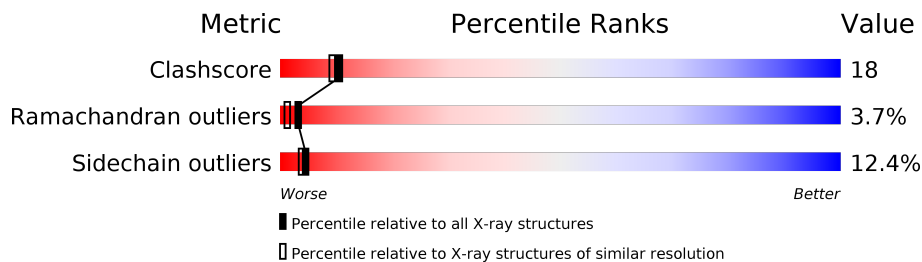
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	L	49	 35% 22% • 41%
2	H	259	 61% 33% ••• 6%
3	K	308	 54% 33% 6% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5012 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 ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	29	243	153	38	51	1	0	0	0

- Molecule 2 is a protein called ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	255	2064	1320	369	363	12	0	0	0

- Molecule 3 is a protein called PRETHROMBIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	K	287	2326	1483	413	417	13	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	32	Total 32	O 32	0	0
4	H	205	Total 205	O 205	0	0
4	K	142	Total 142	O 142	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.52Å 87.99Å 101.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 18.76 – 1.92	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.20) 78.0 (18.76-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 1.93Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , 0.255 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 107.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.054 for k,h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5012	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	L	0.96	0/246	0.96	0/328
2	H	0.86	1/2118 (0.0%)	1.02	3/2867 (0.1%)
3	K	0.80	0/2384	0.97	4/3222 (0.1%)
All	All	0.84	1/4748 (0.0%)	0.99	7/6417 (0.1%)

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
3	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	192	GLU	CG-CD	5.73	1.60	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	K	17	VAL	N-CA-C	8.99	135.28	111.00
2	H	157	VAL	CB-CA-C	-7.40	97.33	111.40
3	K	16	ILE	N-CA-C	6.83	129.44	111.00
2	H	147	THR	N-CA-C	6.75	129.23	111.00
3	K	101	ARG	NE-CZ-NH1	-5.36	117.62	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	225	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	L	243	0	233	6	0
2	H	2064	0	2065	76	0
3	K	2326	0	2318	75	0
4	H	205	0	0	7	0
4	K	142	0	0	7	0
4	L	32	0	0	0	0
All	All	5012	0	4616	152	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 18.

The worst 5 of 152 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)
3:K:129(B):LYS:NZ	3:K:204(A):TYR:HB2	1.75	1.02
3:K:1(C):GLU:HG3	3:K:1:CYS:HB3	1.42	1.01
3:K:14(B):THR:HG22	3:K:137:ARG:NH2	1.78	0.99
2:H:145:ARG:NH1	2:H:150:VAL:HG13	1.81	0.95
3:K:129(B):LYS:HZ3	3:K:204(A):TYR:HB2	1.43	0.84

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 residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	27/49 (55%)	23 (85%)	4 (15%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	253/259 (98%)	233 (92%)	14 (6%)	6 (2%)	6	3
3	K	285/308 (92%)	237 (83%)	33 (12%)	15 (5%)	2	0
All	All	565/616 (92%)	493 (87%)	51 (9%)	21 (4%)	3	1

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	77(A)	ARG
2	H	149	THR
3	K	14(L)	GLU
3	K	17	VAL
3	K	149(C)	VAL

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	L	27/43 (63%)	22 (82%)	5 (18%)	1	1
2	H	223/226 (99%)	200 (90%)	23 (10%)	7	6
3	K	251/269 (93%)	217 (86%)	34 (14%)	4	3
All	All	501/538 (93%)	439 (88%)	62 (12%)	4	4

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	1(A)	ASP
3	K	29	TRP
3	K	221	ASP
3	K	12	VAL
3	K	41	LEU

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

Mol	Chain	Res	Type
3	K	11	GLN
3	K	204(B)	ASN
3	K	14(A)	GLN
2	H	127	GLN
3	K	127	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](#)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.