wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:22 PM GMT

PDB ID	:	1TBQ
Title	:	CRYSTAL STRUCTURE OF INSECT DERIVED DOUBLE DOMAIN KAZAL INHIBITOR RHODNIIN IN COMPLEX WITH THROMBIN
Authors	:	Van De Locht, A.; Lamba, D.; Bode, W.
Deposited on	:	1995-03-02
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

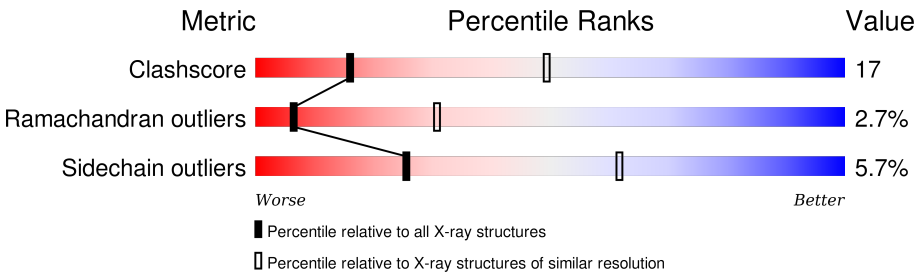
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	J	49	71% 27% •
1	L	49	69% 27% •
2	H	259	63% 35% •
2	K	259	64% 31% •
3	R	103	57% 39% •
3	S	103	61% 35% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6911 atoms, of which 308 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 THROMBIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	L	49	423	255	18	66	83	1	25	0	0
1	J	49	423	255	18	66	83	1	29	0	0

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	259	2206	1337	112	376	369	12	157	0	0
2	K	259	2206	1337	112	376	369	12	208	0	0

- Molecule 3 is a protein called RHODNIIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	R	103	790	455	24	131	168	12	46	0	0
3	S	103	790	455	24	131	168	12	63	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	H	29	29	29	0	0
4	J	2	2	2	0	0
4	K	23	23	23	0	0
4	L	5	5	5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	R	10	10	10	0	0
			Total	O		
4	S	4	4	4	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 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.

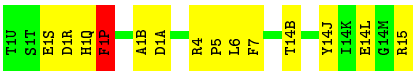
Note EDS was not executed.

- Molecule 1: THROMBIN

Chain L:

- Molecule 1: THROMBIN

Chain J:

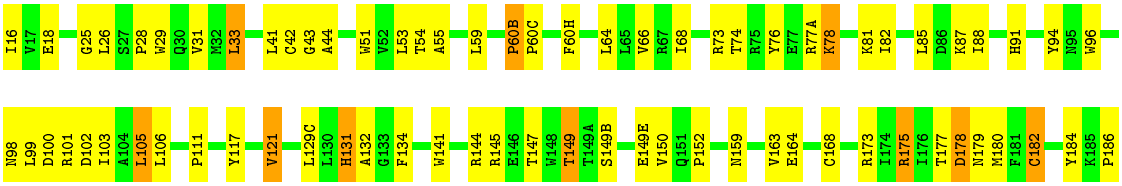


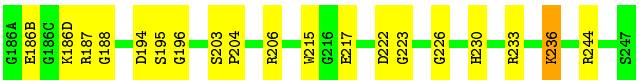
- Molecule 2: THROMBIN

Chain H:

- Molecule 2: THROMBIN

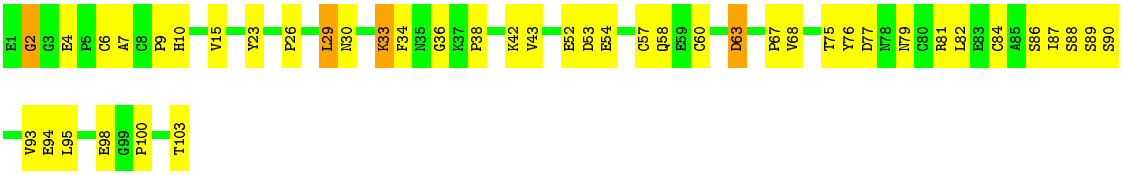
Chain K:





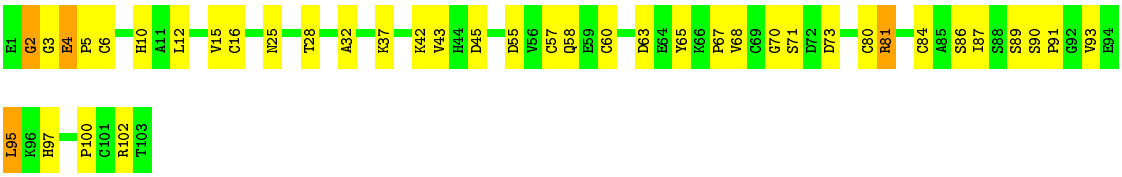
- Molecule 3: RHODNIIN

Chain R:



- Molecule 3: RHODNIIN

Chain S:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.31Å 111.60Å 112.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10	Depositor
% Data completeness (in resolution range)	75.1 (8.00-3.10)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6911	wwPDB-VP
Average B, all atoms ($Å^2$)	12.0	wwPDB-VP

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	J	0.49	0/414	0.72	0/552
1	L	0.50	0/414	0.62	0/552
2	H	0.48	0/2148	0.76	1/2905 (0.0%)
2	K	0.47	0/2148	0.73	0/2905
3	R	0.49	0/782	0.75	0/1060
3	S	0.48	0/782	0.73	0/1060
All	All	0.48	0/6688	0.73	1/9034 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	199	PHE	N-CA-C	-5.49	96.18	111.00

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	J	405	18	372	13	0
1	L	405	18	372	11	0
2	H	2094	112	2097	78	0
2	K	2094	112	2097	79	0
3	R	766	24	675	31	0
3	S	766	24	675	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	29	0	0	6	0
4	J	2	0	0	0	0
4	K	23	0	0	1	0
4	L	5	0	0	0	0
4	R	10	0	0	1	0
4	S	4	0	0	0	0
All	All	6603	308	6288	206	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 17.

The worst 5 of 206 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)
2:K:177:THR:HG22	2:K:179:ASN:H	1.40	0.83
2:H:76:TYR:HB2	3:R:87:ILE:HD11	1.63	0.81
2:K:173:ARG:NH1	3:S:2:GLY:HA3	1.98	0.79
2:H:93:ARG:HH11	2:H:93:ARG:HG2	1.50	0.78
2:K:145:ARG:HB2	2:K:150:VAL:HG12	1.65	0.76

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	J	47/49 (96%)	39 (83%)	5 (11%)	3 (6%)	2 10
1	L	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2 10
2	H	257/259 (99%)	222 (86%)	31 (12%)	4 (2%)	12 44
2	K	257/259 (99%)	232 (90%)	20 (8%)	5 (2%)	10 40
3	R	101/103 (98%)	83 (82%)	14 (14%)	4 (4%)	4 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	101/103 (98%)	86 (85%)	12 (12%)	3 (3%)	5	28
All	All	810/822 (98%)	699 (86%)	89 (11%)	22 (3%)	6	31

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(K)	ILE
1	J	1(P)	PHE
2	K	244	ARG
3	S	4	GLU
1	L	1(Q)	HIS

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	J	43/43 (100%)	42 (98%)	1 (2%)	58	84
1	L	43/43 (100%)	41 (95%)	2 (5%)	32	70
2	H	226/226 (100%)	216 (96%)	10 (4%)	35	71
2	K	226/226 (100%)	212 (94%)	14 (6%)	23	59
3	R	89/89 (100%)	81 (91%)	8 (9%)	12	41
3	S	89/89 (100%)	83 (93%)	6 (7%)	20	56
All	All	716/716 (100%)	675 (94%)	41 (6%)	25	62

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	105	LEU
2	K	147	THR
3	S	81	ARG
2	K	111	PRO
2	K	121	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	60(G)	ASN
3	R	58	GLN
2	K	205	ASN
2	H	71	HIS
2	K	151	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.