wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:32 PM GMT

PDB ID	:	1BA8
Title	:	THROMBIN INHIBITOR WITH A RIGID TRIPEPTIDYL ALDEHYDES
Authors	:	Krishnan, R.; Zhang, E.; Hakansson, K.; Arni, R.K.; Tulinsky, A.; Lim-Wilby, M.S.L.; Levy, O.E.; Semple, J.E.; Brunck, T.K.
Deposited on	:	1998-04-23
Resolution	:	1.80 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:

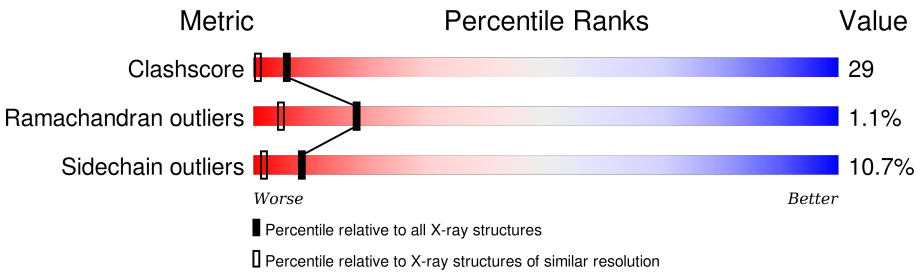
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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	A	36	31% 39% 11% • 17%
2	B	259	56% 29% 11% • •
3	C	13	31% 23% 8% 38%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2551 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 THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	30	240	150	39	50	1	0	0	0

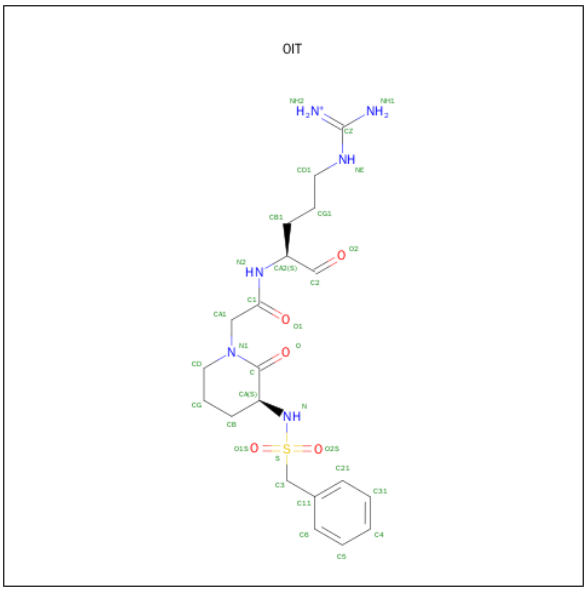
- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	2039	1299	360	366	14	0	0	0

- Molecule 3 is a protein called HIRUGEN.

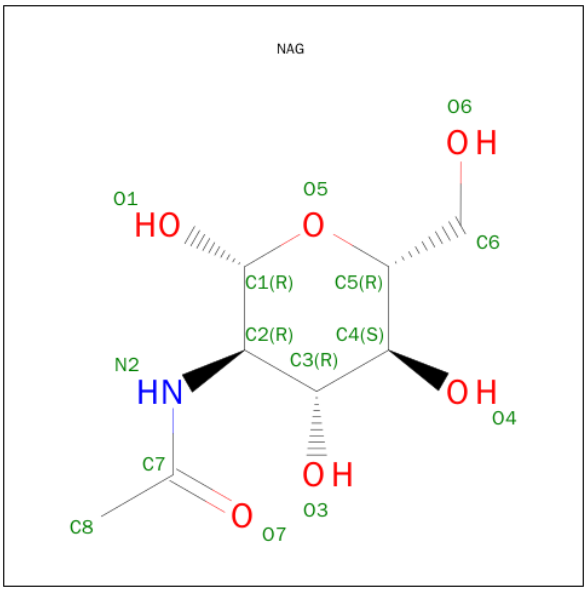
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	8	68	43	8	16	1	0	0	0

- Molecule 4 is AMINO({(4S)-4-[({(3S)-3-[(BENZYLSULFONYL)AMINO]-2-OXOPIPERIDIN-1-YL}ACETYL)AMINO]-5-OXOPENTYL}AMINO)METHANIMINIUM (three-letter code: 0IT) (formula: $C_{20}H_{31}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	32	20	6	5	1	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	16	16	16	0	0
			Total	O		
6	B	140	140	140	0	0
			Total	O		
6	C	2	2	2	0	0

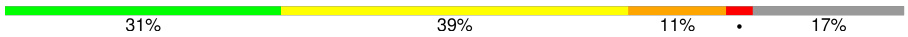
3 Residue-property plots (i)

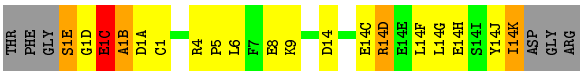
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

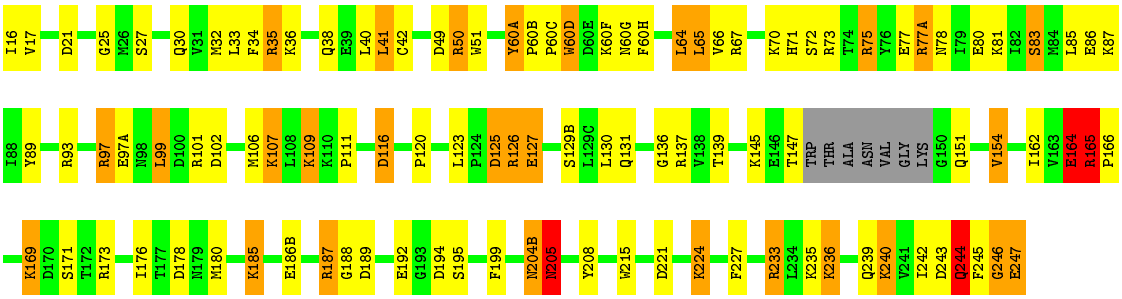
Chain A:





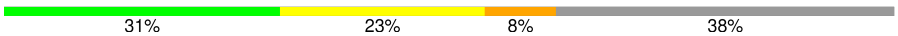
- Molecule 2: THROMBIN

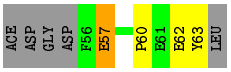
Chain B:



- Molecule 3: HIRUGEN

Chain C:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.26Å 72.29Å 72.99Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	7.00 – 1.80	Depositor
% Data completeness (in resolution range)	75.0 (7.00-1.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2551	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: 0IT, NAG, TYS

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	1.36	3/242 (1.2%)	2.08	10/322 (3.1%)
2	B	1.08	0/2091	2.06	64/2823 (2.3%)
3	C	0.93	0/53	1.80	1/70 (1.4%)
All	All	1.11	3/2386 (0.1%)	2.05	75/3215 (2.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14(K)	ILE	CB-CG2	7.73	1.76	1.52
1	A	14(K)	ILE	CB-CG1	6.64	1.72	1.54
1	A	8	GLU	CD-OE2	-5.26	1.19	1.25

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	233	ARG	NE-CZ-NH2	-16.44	112.08	120.30
2	B	101	ARG	NE-CZ-NH1	15.90	128.25	120.30
2	B	233	ARG	NE-CZ-NH1	14.20	127.40	120.30
2	B	77(A)	ARG	NE-CZ-NH2	-13.78	113.41	120.30
2	B	173	ARG	NE-CZ-NH1	13.36	126.98	120.30

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	A	240	0	239	35	0
2	B	2039	0	2007	114	0
3	C	68	0	49	6	0
4	B	32	0	31	8	0
5	B	14	0	13	1	0
6	A	16	0	0	1	0
6	B	140	0	0	6	0
6	C	2	0	0	0	0
All	All	2551	0	2339	138	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 29.

The worst 5 of 138 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)
1:A:14(K):ILE:CB	1:A:14(K):ILE:CG2	1.76	1.56
1:A:14(K):ILE:CG1	1:A:14(K):ILE:CD1	1.80	1.52
2:B:195:SER:OG	4:B:1:0IT:C2	1.67	1.40
2:B:86:GLU:HG3	2:B:109:LYS:NZ	1.39	1.33
2:B:75:ARG:NH2	3:C:57:GLU:HB2	1.58	1.17

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	A	28/36 (78%)	24 (86%)	2 (7%)	2 (7%)	1 0
2	B	248/259 (96%)	241 (97%)	6 (2%)	1 (0%)	39 23
3	C	6/13 (46%)	6 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	282/308 (92%)	271 (96%)	8 (3%)	3 (1%)	17 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(C)	GLU
1	A	1(B)	ALA
2	B	77(A)	ARG

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	A	27/31 (87%)	25 (93%)	2 (7%)	17 5
2	B	220/225 (98%)	195 (89%)	25 (11%)	7 1
3	C	5/10 (50%)	5 (100%)	0	100 100
All	All	252/266 (95%)	225 (89%)	27 (11%)	8 2

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	129(B)	SER
2	B	154	VAL
2	B	240	LYS
2	B	145	LYS
2	B	65	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	30	GLN
2	B	71	HIS
2	B	156	GLN
2	B	204(B)	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	TYS	C	63	3	15,16,17	0.89	0	16,22,24	1.80	4 (25%)

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	TYS	C	63	3	-	0/9/11/13	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	63	TYS	O-C-CA	-4.80	113.00	125.49
3	C	63	TYS	CG-CB-CA	-2.81	107.87	114.21
3	C	63	TYS	O2-S-O1	2.06	121.43	112.46
3	C	63	TYS	CE2-CZ-CE1	2.23	123.82	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	63	TYS	2	0

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	0IT	B	1	-	29,33,33	1.53	5 (17%)	30,44,44	2.26	11 (36%)
5	NAG	B	400	2	14,14,15	0.77	0	15,19,21	2.25	4 (26%)

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	0IT	B	1	-	-	0/23/41/41	0/2/2/2
5	NAG	B	400	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	0IT	CA-N	-3.02	1.41	1.46
4	B	1	0IT	CB-CA	-2.63	1.48	1.53
4	B	1	0IT	CA2-N2	2.11	1.49	1.46
4	B	1	0IT	CA-C	3.25	1.57	1.52
4	B	1	0IT	S-N	3.51	1.67	1.62

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	400	NAG	C2-N2-C7	-6.13	115.17	123.04
4	B	1	0IT	CA1-N1-C	-5.10	114.98	119.73
4	B	1	0IT	O2S-S-N	-4.03	101.58	107.03
4	B	1	0IT	C3-C11-C21	-2.72	116.81	120.52
4	B	1	0IT	O-C-CA	-2.12	115.94	120.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	0IT	8	0
5	B	400	NAG	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 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.