



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:35 PM GMT

PDB ID : 7KME
Title : CRYSTAL STRUCTURE OF HUMAN ALPHA-THROMBIN INHIBITED
WITH SEL2711.
Authors : Mochalkin, I.; Tulinsky, A.
Deposited on : 1999-02-26
Resolution : 2.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

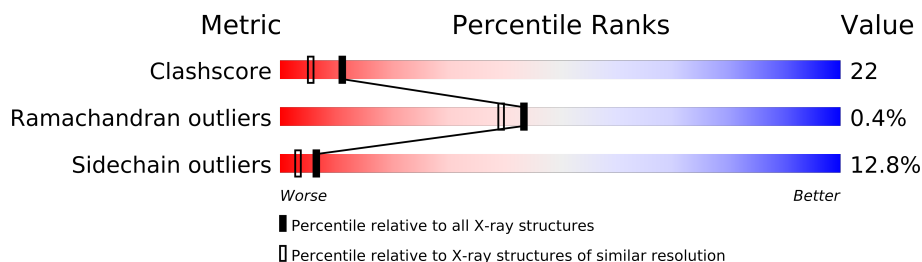
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	10	
4	J	7	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2465 atoms, of which 0 are hydrogen 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 THROMBIN L-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	25	Total	C	N	O	S	0	0	0
			201	127	30	43	1			

- Molecule 2 is a protein called THROMBIN H-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2014	1286	353	361	14			

- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			79	50	10	18	1			

- Molecule 4 is a protein called SEL2711.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			39	29	6	4			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	17	Total	O	0	0
			17	17		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	106	Total 106	O 106	0	0
6	I	5	Total 5	O 5	0	0
6	J	2	Total 2	O 2	0	0

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.

Note EDS was not executed.

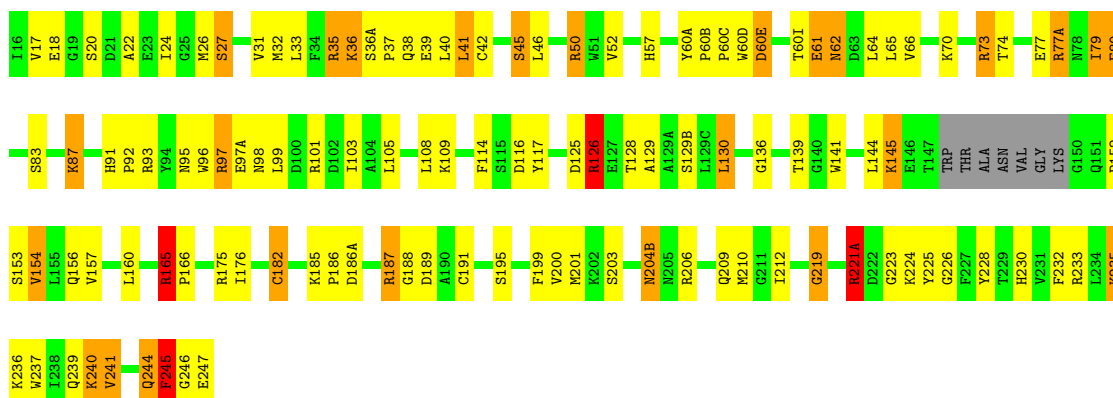
• Molecule 1: THROMBIN L-CHAIN

Chain L: 



• Molecule 2: THROMBIN H-CHAIN

Chain H: 



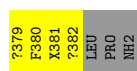
• Molecule 3: HIRUGEN

Chain I: 



• Molecule 4: SEL2711

Chain J: 



4 Data and refinement statistics

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	71.05Å 71.82Å 73.45Å 90.00° 101.20° 90.00°	Depositor
Resolution (Å)	9.00 – 2.10	Depositor
% Data completeness (in resolution range)	78.0 (9.00-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2465	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, CHG, NA, PRR, OBN, 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	L	0.96	0/203	1.33	0/271
2	H	0.98	4/2066 (0.2%)	1.83	28/2791 (1.0%)
3	I	0.75	0/63	1.45	0/82
All	All	0.97	4/2332 (0.2%)	1.78	28/3144 (0.9%)

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	L	0	1
2	H	0	9
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	246	GLY	CA-C	-12.50	1.31	1.51
2	H	247	GLU	C-O	5.73	1.34	1.23
2	H	247	GLU	CA-C	-5.18	1.39	1.52
2	H	97	ARG	CD-NE	-5.02	1.38	1.46

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	221(A)	ARG	NE-CZ-NH1	34.27	137.43	120.30
2	H	221(A)	ARG	NE-CZ-NH2	-23.41	108.59	120.30
2	H	126	ARG	NE-CZ-NH1	18.04	129.32	120.30
2	H	126	ARG	NE-CZ-NH2	-15.51	112.54	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	73	ARG	NE-CZ-NH1	11.11	125.86	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	117	TYR	Mainchain
2	H	126	ARG	Sidechain
2	H	24	ILE	Mainchain
2	H	97	ARG	Sidechain
1	L	14	ASP	Mainchain

5.2 Close contacts ⓘ

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	L	201	0	191	6	0
2	H	2014	0	1969	89	0
3	I	79	0	58	7	0
4	J	39	0	34	3	0
5	H	2	0	0	0	0
6	H	106	0	0	0	0
6	I	5	0	0	2	0
6	J	2	0	0	0	0
6	L	17	0	0	4	0
All	All	2465	0	2252	103	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 22.

The worst 5 of 103 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:35:ARG:HD3	2:H:39:GLU:OE2	1.76	0.86
2:H:33:LEU:HD22	2:H:64:LEU:HD22	1.61	0.82
3:I:359:ILE:CD1	3:I:363:TYS:HB3	2.09	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.64	0.80
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.23	0.74

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	L	23/36 (64%)	22 (96%)	1 (4%)	0	100	100
2	H	248/259 (96%)	228 (92%)	19 (8%)	1 (0%)	43	39
3	I	7/10 (70%)	6 (86%)	1 (14%)	0	100	100
All	All	278/305 (91%)	256 (92%)	21 (8%)	1 (0%)	43	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	245	PHE

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	L	22/31 (71%)	20 (91%)	2 (9%)	14	8
2	H	215/225 (96%)	186 (86%)	29 (14%)	6	3
3	I	6/9 (67%)	6 (100%)	0	100	100
All	All	243/265 (92%)	212 (87%)	31 (13%)	6	3

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	80	GLU
2	H	109	LYS
2	H	240	LYS
2	H	83	SER
2	H	129(B)	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
2	H	98	ASN
2	H	239	GLN
2	H	156	GLN
2	H	78	ASN
2	H	204(B)	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	TYS	I	363	3	16,16,17	5.13	3 (18%)	20,22,24	1.70	4 (20%)
4	0BN	J	380	4	14,14,15	9.12	8 (57%)	16,18,20	1.61	2 (12%)
4	CHG	J	381	4	10,10,11	7.00	4 (40%)	10,12,14	2.88	6 (60%)
4	PRR	J	382	4	12,12,13	16.62	5 (41%)	13,15,17	1.91	4 (30%)

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	I	363	3	-	0/9/11/13	0/1/1/1
4	0BN	J	380	4	-	0/8/10/12	0/1/1/1
4	CHG	J	381	4	-	0/4/14/16	0/1/1/1
4	PRR	J	382	4	-	0/4/6/8	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	382	PRR	O-C	57.11	1.51	1.11
4	J	380	0BN	O-C	25.64	1.29	1.11
4	J	381	CHG	O-C	21.16	1.26	1.11
4	J	380	0BN	C6-C10	-20.66	1.28	1.49
3	I	363	TYS	O-C	19.91	1.25	1.11

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	381	CHG	C6-C1-CA	-5.70	103.57	112.10
4	J	380	0BN	C-CA-N	-5.07	108.77	113.83
4	J	381	CHG	C2-C1-CA	-4.71	105.05	112.10
3	I	363	TYS	CG-CB-CA	-4.67	103.40	114.42
4	J	382	PRR	C8-C9-N1	-4.27	117.85	121.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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