wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2023 – 02:11 PM EDT

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 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

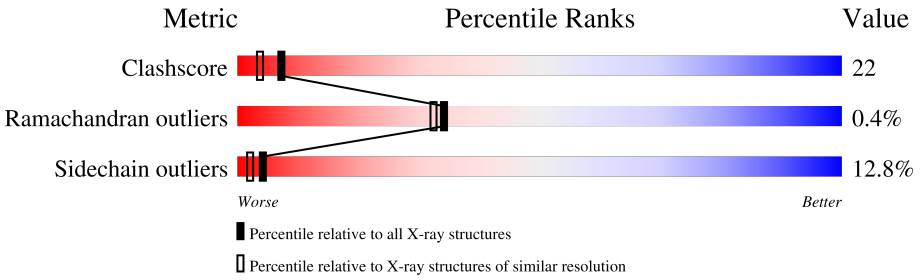
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 of 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	L	36	50% 17% • 31%
2	H	259	51% 35% 10% • •
3	I	10	60% 30% 10%
4	J	7	14% 43% 43%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2465 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 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		

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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. 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.

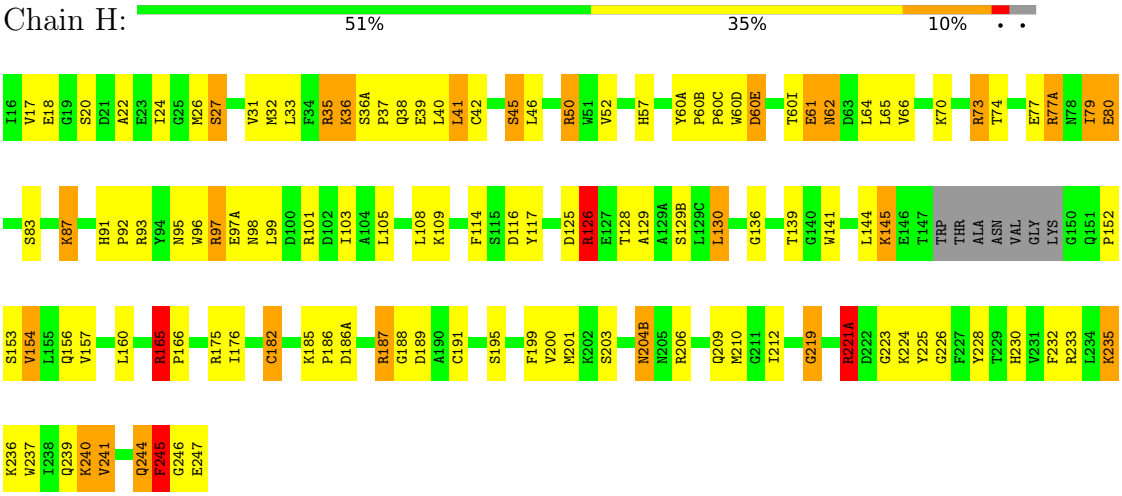
Note EDS was not executed.

• Molecule 1: THROMBIN L-CHAIN

Chain L:

• Molecule 2: THROMBIN H-CHAIN

Chain H:

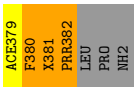


• Molecule 3: HIRUGEN

Chain I:

• Molecule 4: SEL2711

Chain J:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: PRR, CHG, 0BN, NA, TYS, ACE

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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 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	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

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 22.

The worst 5 of 103 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:359:ILE:CD1	3:I:363:TYS:HB3	2.09	0.81
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 (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	23/36 (64%)	22 (96%)	1 (4%)	0	100 100
2	H	248/259 (96%)	228 (92%)	19 (8%)	1 (0%)	34 32
3	I	7/10 (70%)	6 (86%)	1 (14%)	0	100 100
All	All	278/305 (91%)	256 (92%)	21 (8%)	1 (0%)	34 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	245	PHE

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	22/31 (71%)	20 (91%)	2 (9%)	9 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	215/225 (96%)	186 (86%)	29 (14%)	4 2
3	I	6/9 (67%)	6 (100%)	0	100 100
All	All	243/265 (92%)	212 (87%)	31 (13%)	4 2

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

Mol	Chain	Res	Type
2	H	80	GLU
2	H	239	GLN
2	H	109	LYS
2	H	241	VAL
2	H	195	SER

Sometimes 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	156	GLN
2	H	204(B)	ASN
2	H	239	GLN
2	H	78	ASN
2	H	62	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)

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	$\#\|Z\|>2$
4	CHG	J	381	4	9,10,11	1.84	2 (22%)	7,12,14	1.89	2 (28%)
4	PRR	J	382	4	11,12,13	3.28	5 (45%)	11,15,17	2.74	3 (27%)
3	TYS	I	363	3	15,16,17	1.61	2 (13%)	18,22,24	1.84	3 (16%)
4	0BN	J	380	4	13,14,15	4.08	7 (53%)	11,18,20	1.18	1 (9%)

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	CHG	J	381	4	-	0/5/14/16	0/1/1/1
4	PRR	J	382	4	-	2/5/6/8	0/1/1/1
3	TYS	I	363	3	-	0/10/11/13	0/1/1/1
4	0BN	J	380	4	-	4/9/10/12	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	380	0BN	C6-C10	-10.63	1.28	1.47
4	J	382	PRR	O-C	7.84	1.51	1.19
4	J	380	0BN	C9-CA	5.44	1.65	1.53
4	J	382	PRR	C10-N1	-5.38	1.33	1.48
3	I	363	TYS	OH-S	4.99	1.65	1.58

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	382	PRR	C5-CA-C	7.63	125.78	111.47
3	I	363	TYS	CG-CB-CA	-5.28	103.40	114.10
4	J	382	PRR	C8-C9-N1	-3.53	117.85	120.92
3	I	363	TYS	OH-S-O2	-3.43	97.71	107.71
4	J	381	CHG	C4-C5-C6	-2.64	106.03	111.42

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	382	PRR	C8-C5-CA-C
4	J	382	PRR	C8-C5-CA-N

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Mol	Chain	Res	Type	Atoms
4	J	380	0BN	N2-C10-C6-C5
4	J	380	0BN	N2-C10-C6-C7
4	J	380	0BN	N3-C10-C6-C5

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	381	CHG	1	0
4	J	382	PRR	1	0
3	I	363	TYS	3	0
4	J	380	0BN	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.