



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1NRP / pdb_00001nrp
Title : CRYSTALLOGRAPHIC STRUCTURES OF THROMBIN COMPLEXED
WITH THROMBIN RECEPTOR PEPTIDES: EXISTENCE OF EX-
PECTED AND NOVEL BINDING MODES
Authors : Tulinsky, A.; Mathews, I.I.
Deposited on : 1994-01-18
Resolution : 3.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

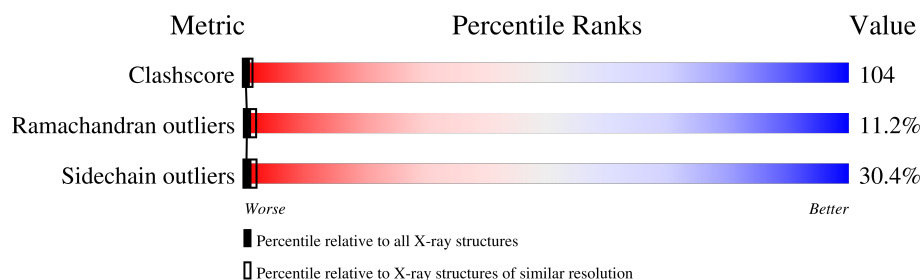
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	R	23	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HMR	R	41	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2445 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 (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	29	Total	C	N	O	S	0	0	0
			240	149	41	49	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	257	Total	C	N	O	S	0	0	0
			2049	1306	362	367	14			

- Molecule 3 is a protein called RECEPTOR BASED PEPTIDE NR'S.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	10	Total	C	N	O	0	0	0
			83	56	11	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	41	HMR	ARG	conflict	UNP P25116

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	11	Total	O	0	0
			11	11		
4	H	61	Total	O	0	0
			61	61		
4	R	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

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	128.30Å 51.10Å 63.00Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2445	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: HMR

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	1.33	1/242 (0.4%)	1.93	5/321 (1.6%)
2	H	1.32	12/2101 (0.6%)	2.49	164/2839 (5.8%)
3	R	0.92	0/78	2.79	8/102 (7.8%)
All	All	1.31	13/2421 (0.5%)	2.45	177/3262 (5.4%)

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	2
2	H	0	4
All	All	0	6

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	220	CYS	CA-C	-7.72	1.44	1.52
2	H	118	ILE	N-CA	7.52	1.55	1.46
2	H	151	GLN	N-CA	-7.04	1.38	1.46
2	H	149(A)	ALA	N-CA	6.86	1.59	1.46
2	H	94	TYR	N-CA	6.37	1.53	1.46

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	178	ASP	CA-CB-CG	17.03	129.63	112.60
3	R	39	ASP	CA-CB-CG	13.52	126.12	112.60
2	H	67	ARG	CA-C-N	11.91	141.50	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	67	ARG	C-N-CA	11.91	141.50	122.68
2	H	50	ARG	CA-C-O	-10.87	111.24	121.02

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	137	ARG	Sidechain
2	H	75	ARG	Sidechain
2	H	97	ARG	Sidechain
1	L	14(D)	ARG	Sidechain
1	L	15	ARG	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	240	0	240	39	0
2	H	2049	0	2000	448	1
3	R	83	0	69	16	1
4	H	61	0	0	0	0
4	L	11	0	0	0	0
4	R	1	0	0	0	0
All	All	2445	0	2309	487	1

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 104.

The worst 5 of 487 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:96:TRP:HA	2:H:99:LEU:HD23	1.20	1.17
2:H:36(A):SER:HA	2:H:38:GLN:N	1.60	1.16
1:L:7:PHE:HA	1:L:12:LEU:HB2	1.28	1.15
2:H:86:GLU:CB	2:H:109:LYS:HA	1.81	1.11
2:H:26:MET:HE2	2:H:157:VAL:HG21	1.26	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ARG:CG	3:R:53:GLU:OE1[4_645]	2.13	0.07

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	27/36 (75%)	13 (48%)	6 (22%)	8 (30%)	0	0
2	H	253/259 (98%)	175 (69%)	55 (22%)	23 (9%)	0	2
3	R	5/23 (22%)	2 (40%)	2 (40%)	1 (20%)	0	0
All	All	285/318 (90%)	190 (67%)	63 (22%)	32 (11%)	0	1

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1	CYS
1	L	10	LYS
1	L	14(A)	LYS
1	L	14(L)	ASP
2	H	22	ALA

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	27/31 (87%)	10 (37%)	17 (63%)	0	0
2	H	217/225 (96%)	157 (72%)	60 (28%)	0	2
3	R	9/22 (41%)	9 (100%)	0	100	100
All	All	253/278 (91%)	176 (70%)	77 (30%)	0	1

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	145	LYS
2	H	229	THR
2	H	157	VAL
2	H	174	ILE
2	H	240	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	159	ASN
2	H	204(B)	ASN
2	H	244	GLN
2	H	205	ASN
2	H	95	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	HMR	R	41	3	5,5,12	1.50	1 (20%)	5,5,14	2.48	3 (60%)

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	HMR	R	41	3	-	3/3/3/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	41	HMR	CA-CB	-2.26	1.50	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	41	HMR	O-C-CA	-3.78	114.39	125.38
3	R	41	HMR	CA-CB-N	2.69	117.89	110.61
3	R	41	HMR	CC-CB-CA	-2.48	108.68	111.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	41	HMR	C-CA-CB-N
3	R	41	HMR	C-CA-CB-CC
3	R	41	HMR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides 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

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.