



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:17 AM UTC

PDB ID : 1BRC / pdb_00001brc
Title : RELOCATING A NEGATIVE CHARGE IN THE BINDING POCKET OF TRYPSIN
Authors : Perona, J.J.; Fletterick, R.J.
Deposited on : 1992-12-17
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

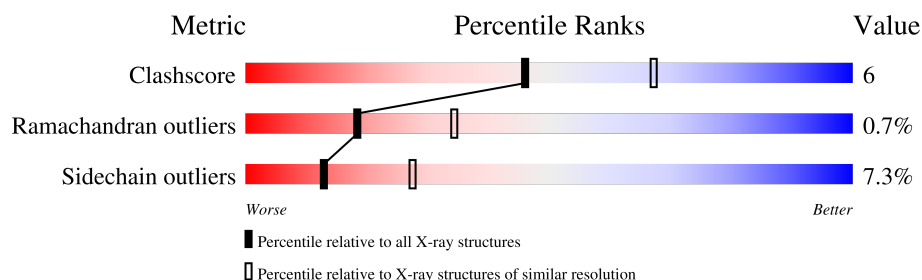
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	E	223	 77% 17% . .
2	I	56	 79% 20% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2195 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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	223	Total	C	N	O	S	0	0	0
			1643	1029	279	321	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	189	GLY	ASP	conflict	UNP P00763
E	226	ASP	GLY	conflict	UNP P00763

- Molecule 2 is a protein called AMYLOID BETA-PROTEIN PRECURSOR INHIBITOR DOMAIN (APPI).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	56	Total	C	N	O	S	0	0	0
			411	256	70	77	8			

- Molecule 3 is water.

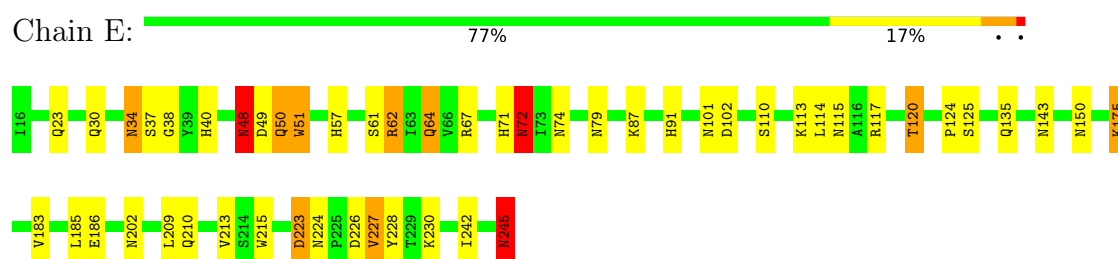
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	122	Total	O	0	0
			122	122		
3	I	19	Total	O	0	0
			19	19		

3 Residue-property plots

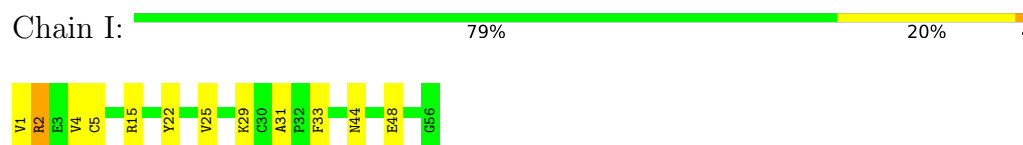
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: TRYPSIN



• Molecule 2: AMYLOID BETA-PROTEIN PRECURSOR INHIBITOR DOMAIN (APPI)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.10Å 93.10Å 62.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2195	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	E	0.90	5/1678 (0.3%)	1.73	35/2292 (1.5%)
2	I	0.77	0/421	1.60	7/569 (1.2%)
All	All	0.87	5/2099 (0.2%)	1.70	42/2861 (1.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	91	HIS	CD2-NE2	-6.31	1.30	1.37
1	E	227	VAL	CA-CB	6.23	1.63	1.54
1	E	71	HIS	CD2-NE2	-5.81	1.31	1.37
1	E	57	HIS	CD2-NE2	-5.77	1.31	1.37
1	E	40	HIS	CD2-NE2	-5.29	1.32	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	245	ASN	CA-CB-CG	12.47	125.07	112.60
1	E	48	ASN	CA-CB-CG	8.85	121.45	112.60
1	E	210	GLN	OE1-CD-NE2	-8.66	113.94	122.60
1	E	72	ASN	CB-CG-ND2	8.33	128.90	116.40
1	E	64	GLN	OE1-CD-NE2	-8.01	114.59	122.60
1	E	72	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	E	57	HIS	CA-CB-CG	7.59	121.39	113.80
1	E	245	ASN	CB-CG-ND2	7.46	127.59	116.40
1	E	223	ASP	CA-CB-CG	-7.28	105.32	112.60
1	E	226	ASP	CA-CB-CG	7.00	119.59	112.60
1	E	48	ASN	OD1-CG-ND2	-6.97	115.63	122.60
2	I	2	ARG	N-CA-C	6.81	125.30	110.80
2	I	2	ARG	CA-C-O	-6.49	111.24	120.51
1	E	242	ILE	N-CA-C	-6.31	104.36	110.42
1	E	202	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	E	101	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	E	150	ASN	OD1-CG-ND2	-6.23	116.37	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	44	ASN	CA-CB-CG	6.18	118.78	112.60
1	E	51	TRP	CG-CD2-CE3	6.17	140.07	133.90
1	E	91	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	E	48	ASN	CB-CG-ND2	6.13	125.60	116.40
1	E	120	THR	N-CA-CB	-6.12	101.02	110.56
1	E	30	GLN	OE1-CD-NE2	-5.95	116.65	122.60
2	I	25	VAL	N-CA-C	5.92	118.49	111.09
1	E	125	SER	N-CA-C	-5.88	105.20	112.90
1	E	23	GLN	OE1-CD-NE2	-5.81	116.79	122.60
1	E	245	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	E	71	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	E	102	ASP	CA-CB-CG	5.60	118.20	112.60
1	E	135	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	E	50	GLN	OE1-CD-NE2	-5.35	117.25	122.60
2	I	33	PHE	CA-CB-CG	5.30	119.10	113.80
2	I	15	ARG	N-CA-C	5.26	119.91	111.81
1	E	51	TRP	CB-CG-CD1	-5.19	119.11	126.90
1	E	224	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	E	143	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	E	175	LYS	CA-CB-CG	5.10	124.30	114.10
2	I	1	VAL	N-CA-CB	-5.08	102.86	111.50
1	E	215	TRP	CG-CD2-CE3	5.06	138.96	133.90
1	E	223	ASP	N-CA-C	5.05	118.70	112.24
1	E	61	SER	CA-CB-OG	-5.04	101.03	111.10
1	E	51	TRP	CE2-CD2-CG	-5.02	101.17	107.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	E	1643	0	1565	20	0
2	I	411	0	356	3	0
3	E	122	0	0	0	0
3	I	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2195	0	1921	23	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 6.

All (23) 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:E:87:LYS:NZ	1:E:245:ASN:HB2	2.02	0.75
1:E:115:ASN:HD22	1:E:117:ARG:H	1.49	0.60
1:E:48:ASN:HD21	1:E:51:TRP:HD1	1.51	0.58
1:E:183:VAL:HB	1:E:228:TYR:CE2	2.39	0.57
1:E:87:LYS:HZ3	1:E:245:ASN:HB2	1.71	0.55
1:E:72:ASN:HD22	1:E:74:ASN:H	1.52	0.55
1:E:124:PRO:HG3	1:E:209:LEU:O	2.08	0.54
1:E:183:VAL:HB	1:E:228:TYR:HE2	1.72	0.54
1:E:48:ASN:HD22	1:E:50:GLN:H	1.55	0.53
1:E:213:VAL:HA	1:E:228:TYR:CD1	2.44	0.53
1:E:34:ASN:ND2	1:E:38:GLY:H	2.07	0.51
1:E:113:LYS:NZ	1:E:114:LEU:O	2.45	0.49
1:E:213:VAL:HA	1:E:228:TYR:HD1	1.78	0.48
1:E:62:ARG:HG3	1:E:62:ARG:HH11	1.79	0.46
2:I:4:VAL:HG23	2:I:5:CYS:SG	2.55	0.46
1:E:72:ASN:ND2	1:E:74:ASN:H	2.14	0.46
2:I:22:TYR:CE1	2:I:31:ALA:HB3	2.51	0.46
1:E:183:VAL:CB	1:E:228:TYR:HE2	2.31	0.43
1:E:64:GLN:NE2	1:E:67:ARG:HE	2.17	0.42
2:I:4:VAL:HG23	2:I:5:CYS:N	2.34	0.42
1:E:62:ARG:HG3	1:E:62:ARG:NH1	2.36	0.41
1:E:79:ASN:CG	1:E:117:ARG:HD2	2.46	0.40
1:E:64:GLN:HE21	1:E:67:ARG:HE	1.69	0.40

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	E	221/223 (99%)	212 (96%)	8 (4%)	1 (0%)	24	43
2	I	54/56 (96%)	52 (96%)	1 (2%)	1 (2%)	6	11
All	All	275/279 (99%)	264 (96%)	9 (3%)	2 (1%)	18	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	2	ARG
1	E	49	ASP

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	E	180/185 (97%)	166 (92%)	14 (8%)	11	24
2	I	40/45 (89%)	38 (95%)	2 (5%)	22	44
All	All	220/230 (96%)	204 (93%)	16 (7%)	13	27

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	34	ASN
1	E	37	SER
1	E	48	ASN
1	E	62	ARG
1	E	72	ASN
1	E	110	SER
1	E	120	THR
1	E	175	LYS
1	E	185	LEU
1	E	186	GLU
1	E	223	ASP

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Mol	Chain	Res	Type
1	E	227	VAL
1	E	230	LYS
1	E	245	ASN
2	I	29	LYS
2	I	48	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	30	GLN
1	E	34	ASN
1	E	48	ASN
1	E	64	GLN
1	E	72	ASN
1	E	115	ASN
1	E	135	GLN
1	E	150	ASN
1	E	210	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 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.