



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:12 PM UTC

PDB ID : 5PTP / pdb_00005ptp
Title : STRUCTURE OF HYDROLASE (SERINE PROTEINASE)
Authors : Stroud, R.M.; Finer-Moore, J.
Deposited on : 1997-03-31
Resolution : 1.34 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
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

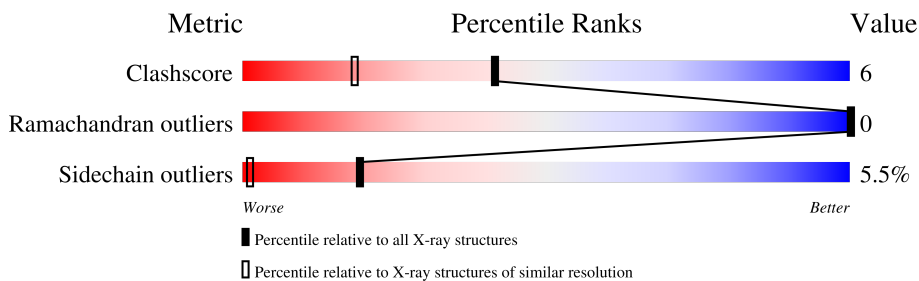
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 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	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)

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	A	223	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1867 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 BETA TRYPSIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	P	S	0	4	0
			1655	1026	281	333	1	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	MIS	SER	modified residue	UNP P00760

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.84Å 58.61Å 67.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.34	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-1.34)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1867	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: MIS, CA

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	1.24	1/1688 (0.1%)	2.33	100/2286 (4.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLY	N-CA	5.20	1.51	1.45

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	GLN	OE1-CD-NE2	-12.07	110.53	122.60
1	A	192	GLN	CA-CB-CG	-11.80	90.50	114.10
1	A	50	GLN	OE1-CD-NE2	11.54	134.14	122.60
1	A	117	ARG	NE-CZ-NH2	-11.29	109.03	119.20
1	A	48	ASN	CA-C-O	-10.37	110.21	121.31
1	A	242	ILE	CA-CB-CG1	9.90	127.24	110.40
1	A	78	GLY	CA-C-O	-9.82	109.55	119.37
1	A	149	THR	CA-CB-CG2	8.71	125.31	110.50
1	A	241	THR	CA-C-O	-8.58	111.81	120.82
1	A	173	PRO	CB-CA-C	8.46	122.38	111.46
1	A	118	VAL	CA-C-O	-8.32	112.15	120.31
1	A	223	ASN	CA-CB-CG	-8.24	104.36	112.60
1	A	148	GLY	O-C-N	8.20	130.69	122.90
1	A	122	SER	CB-CA-C	8.19	123.36	109.53
1	A	79	ASN	CA-CB-CG	-7.92	104.68	112.60
1	A	192	GLN	OE1-CD-NE2	7.92	130.52	122.60
1	A	167	SER	CB-CA-C	-7.74	97.69	110.85
1	A	236	SER	O-C-N	7.70	130.00	122.07
1	A	97	ASN	CA-CB-CG	-7.65	104.95	112.60
1	A	149	THR	N-CA-CB	-7.49	98.23	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	PHE	CA-CB-CG	7.41	121.21	113.80
1	A	127	SER	CA-CB-OG	7.40	125.89	111.10
1	A	127	SER	O-C-N	7.35	131.80	123.27
1	A	125	THR	N-CA-C	-7.33	104.48	113.50
1	A	149	THR	N-CA-C	7.15	121.34	108.69
1	A	30	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	A	236	SER	CA-C-O	-7.07	113.40	120.82
1	A	86	SER	N-CA-CB	-7.05	100.18	110.47
1	A	37	SER	N-CA-C	-7.00	102.04	110.44
1	A	217	SER	CA-C-O	-7.00	111.75	120.57
1	A	71	ASP	N-CA-CB	6.89	122.14	110.49
1	A	127	SER	CA-C-O	-6.86	113.10	121.06
1	A	175	GLN	CA-C-O	-6.85	111.36	118.90
1	A	48	ASN	N-CA-CB	6.79	121.97	111.24
1	A	188	GLY	CA-C-O	-6.76	112.51	119.20
1	A	242	ILE	CB-CA-C	6.72	121.22	112.14
1	A	109	LYS	CG-CD-CE	6.71	126.73	111.30
1	A	34	ASN	OD1-CG-ND2	6.64	129.24	122.60
1	A	201	CYS	O-C-N	6.62	131.01	123.27
1	A	88	SER	CA-CB-OG	-6.61	97.89	111.10
1	A	145	LYS	CB-CG-CD	6.58	126.43	111.30
1	A	50	GLN	CG-CD-NE2	-6.55	106.58	116.40
1	A	216	GLY	CA-C-O	-6.55	115.19	121.41
1	A	125	THR	CA-CB-OG1	-6.53	99.80	109.60
1	A	199	VAL	N-CA-CB	6.46	120.04	111.90
1	A	150	SER	CA-CB-OG	-6.38	98.34	111.10
1	A	146	SER	CA-C-O	6.33	126.72	119.18
1	A	70	GLU	CG-CD-OE2	6.26	132.80	118.40
1	A	145	LYS	CD-CE-NZ	6.23	131.82	111.90
1	A	210	GLN	CG-CD-NE2	6.20	125.70	116.40
1	A	143	ASN	CA-C-O	-6.19	114.34	121.15
1	A	64	GLN	N-CA-CB	6.14	120.18	110.55
1	A	190	SER	CA-CB-OG	-6.10	98.90	111.10
1	A	41	PHE	CA-C-O	-6.08	111.69	118.69
1	A	38	GLY	CA-C-O	6.07	125.86	119.07
1	A	92	PRO	O-C-N	5.96	129.91	122.22
1	A	221	ALA	CA-C-O	-5.96	113.42	120.81
1	A	97	ASN	CB-CG-ND2	-5.93	107.50	116.40
1	A	157	CYS	CA-C-O	-5.92	114.18	121.11
1	A	122	SER	N-CA-CB	-5.90	101.16	110.06
1	A	92	PRO	CA-C-O	-5.88	110.61	119.55
1	A	66	LEU	CD1-CG-CD2	-5.87	97.88	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	SER	CA-CB-OG	-5.83	99.44	111.10
1	A	175	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	77	GLU	CB-CG-CD	5.69	122.27	112.60
1	A	193	GLY	N-CA-C	-5.69	107.52	114.92
1	A	149	THR	CA-CB-OG1	-5.62	101.17	109.60
1	A	125	THR	N-CA-CB	5.59	118.75	110.53
1	A	216	GLY	N-CA-C	-5.47	103.26	111.19
1	A	74	ASN	CA-C-O	-5.45	112.84	119.32
1	A	175	GLN	CG-CD-NE2	5.45	124.57	116.40
1	A	48	ASN	O-C-N	5.41	128.78	122.99
1	A	244	SER	CB-CA-C	-5.35	101.44	110.64
1	A	107	LYS	CA-C-O	-5.29	114.56	120.54
1	A	53	VAL	CB-CA-C	5.28	118.84	110.81
1	A	19	GLY	CA-C-O	-5.25	116.55	121.90
1	A	71	ASP	N-CA-C	-5.24	99.65	110.80
1	A	165[A]	ASP	CA-C-N	5.23	127.29	120.28
1	A	165[A]	ASP	C-N-CA	5.23	127.29	120.28
1	A	165[B]	ASP	CA-C-N	5.23	127.29	120.28
1	A	165[B]	ASP	C-N-CA	5.23	127.29	120.28
1	A	21	THR	CA-CB-OG1	-5.19	101.81	109.60
1	A	100	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	167	SER	CA-C-O	5.17	125.90	120.42
1	A	186[A]	GLU	N-CA-C	-5.17	106.92	113.18
1	A	186[B]	GLU	N-CA-C	-5.17	106.92	113.18
1	A	45	SER	O-C-N	5.17	129.36	123.31
1	A	74	ASN	OD1-CG-ND2	5.14	127.75	122.60
1	A	132	ALA	CA-C-N	5.14	130.37	122.20
1	A	132	ALA	C-N-CA	5.14	130.37	122.20
1	A	221(A)	GLN	CG-CD-NE2	5.12	124.09	116.40
1	A	170	SER	CA-C-O	-5.12	114.08	119.97
1	A	201	CYS	CA-C-O	-5.08	114.86	120.24
1	A	137	LEU	O-C-N	5.07	129.27	123.29
1	A	76	VAL	CB-CA-C	5.05	116.69	111.23
1	A	221(A)	GLN	CG-CD-OE1	-5.04	110.71	120.80
1	A	190	SER	N-CA-C	-5.03	104.04	110.53
1	A	141	TRP	CA-C-O	-5.03	113.79	119.78
1	A	47	ILE	CA-C-O	-5.02	114.49	118.90
1	A	80	GLU	N-CA-C	5.01	117.57	110.50

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	A	1655	0	1604	21	1
2	A	1	0	0	0	0
3	A	211	0	0	2	0
All	All	1867	0	1604	21	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 6.

All (21) 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:34:ASN:ND2	1:A:38:GLY:H	1.76	0.84
1:A:72:ASN:HD22	1:A:74:ASN:H	1.30	0.76
1:A:64:GLN:HE22	1:A:65(A):ARG:HH21	1.34	0.75
1:A:149:THR:HG23	1:A:151:TYR:HE1	1.52	0.73
1:A:64:GLN:HE21	1:A:65(A):ARG:HE	1.33	0.72
1:A:165[A]:ASP:OD1	3:A:389:HOH:O	2.08	0.72
1:A:149:THR:HG23	1:A:151:TYR:CE1	2.25	0.71
1:A:64:GLN:NE2	1:A:65(A):ARG:HE	1.89	0.69
1:A:72:ASN:ND2	1:A:74:ASN:H	1.96	0.63
1:A:25:ASN:HD22	1:A:117:ARG:HH11	1.50	0.59
1:A:236:SER:O	1:A:240[B]:GLN:HG3	2.04	0.57
1:A:72:ASN:HD22	1:A:72:ASN:C	2.15	0.55
1:A:144:THR:OG1	1:A:145:LYS:HE2	2.11	0.51
1:A:88:SER:HB3	1:A:104:MET:HE1	1.92	0.51
1:A:230:LYS:NZ	3:A:454:HOH:O	2.45	0.49
1:A:88:SER:HB3	1:A:104:MET:CE	2.47	0.45
1:A:29:TYR:CZ	1:A:200:VAL:HG21	2.54	0.43
1:A:64:GLN:NE2	1:A:65(A):ARG:HH21	2.11	0.42
1:A:242:ILE:HD13	1:A:242:ILE:HG21	1.70	0.42
1:A:121:ILE:HD12	1:A:121:ILE:HA	1.90	0.42
1:A:56:ALA:HB1	1:A:90:VAL:HG13	2.03	0.41

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)
1:A:59:TYR:OH	1:A:153:ASP:OD2[4_456]	1.96	0.24

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	224/223 (100%)	220 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/183 (102%)	176 (94%)	11 (6%)	18	1

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	72	ASN
1	A	109	LYS
1	A	122	SER
1	A	127	SER
1	A	147	SER
1	A	166	SER
1	A	167	SER

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Mol	Chain	Res	Type
1	A	240[A]	GLN
1	A	240[B]	GLN
1	A	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	30	GLN
1	A	34	ASN
1	A	64	GLN
1	A	72	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	$\# Z > 2$
1	MIS	A	195	1	11,12,13	1.54	2 (18%)	11,16,18	1.76	4 (36%)

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
1	MIS	A	195	1	-	3/11/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	MIS	P-O1P	-3.59	1.38	1.55
1	A	195	MIS	P-O3P	-2.98	1.50	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	MIS	O3P-C1-C3	3.17	118.65	107.72
1	A	195	MIS	P-O3P-C1	2.95	131.17	121.10
1	A	195	MIS	O1P-P-O3P	2.86	118.35	106.70
1	A	195	MIS	OG-P-O2P	-2.31	99.79	108.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	195	MIS	CB-OG-P-O2P
1	A	195	MIS	CA-CB-OG-P
1	A	195	MIS	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.