



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:36 PM UTC

PDB ID : 1APT / pdb_00001apt
Title : CRYSTALLOGRAPHIC ANALYSIS OF A PEPSTATIN ANALOGUE
BINDING TO THE ASPARTYL PROTEINASE PENICILLOPEPSIN AT 1.8
ANGSTROMS RESOLUTION
Authors : Sielecki, A.R.; James, M.N.G.
Deposited on : 1991-12-16
Resolution : 1.80 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

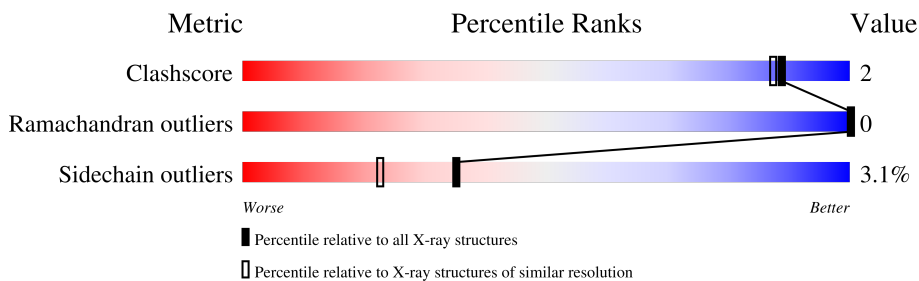
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	323	 77% 21% .
2	I	4	 75% 25%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2659 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.

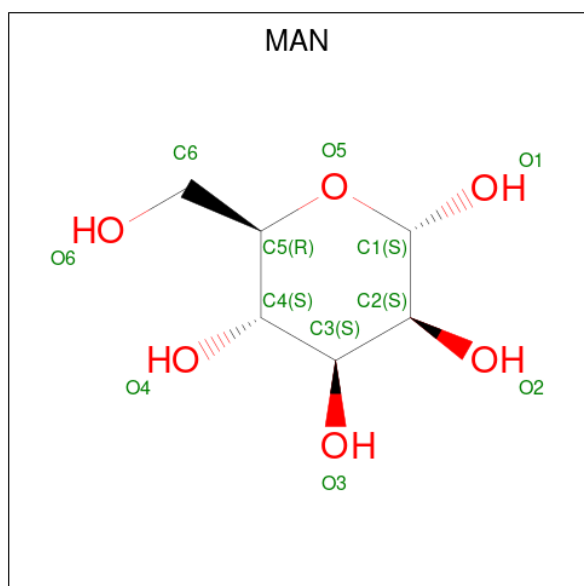
- Molecule 1 is a protein called PENICILLOPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	323	2366	1479	377	508	2	0	0	0

- Molecule 2 is a protein called INHIBITOR ISOVALERYL (IVA)-VAL-VAL-LYSTA-O-ET (LYSTA IS A LYSYL SIDE CHAIN ANALOGUE OF STATIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	4	35	25	4	6	0	0	0

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	E	1	11	6	5	0	0

- Molecule 4 is water.

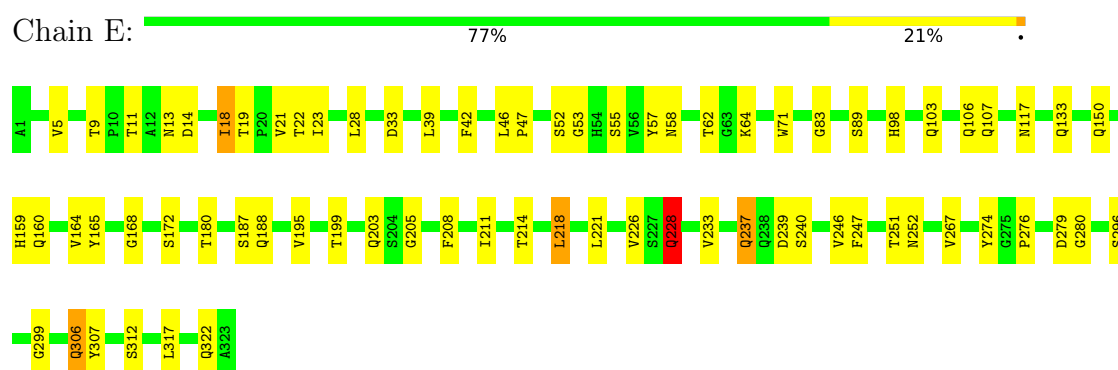
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	244	Total 244	O 244	0	0
4	I	3	Total 3	O 3	0	0

3 Residue-property plots

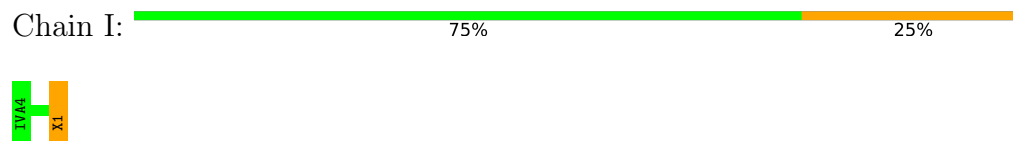
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: INHIBITOR ISOVALERYL (IVA)-VAL-VAL-LYSTA-O-ET (LYSTA IS A LYSYL SIDE CHAIN ANALOGUE OF STATIN)



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	97.57Å 46.47Å 66.39Å 90.00° 116.15° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.135 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2659	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: IVA, LTA, MAN

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	1.29	3/2420 (0.1%)	2.03	69/3304 (2.1%)
2	I	0.99	0/13	1.68	0/17
All	All	1.29	3/2433 (0.1%)	2.03	69/3321 (2.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	GLY	N-CA	5.64	1.50	1.45
1	E	267	VAL	CA-C	5.17	1.57	1.53
1	E	62	THR	CA-CB	5.14	1.62	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	117	ASN	OD1-CG-ND2	9.48	132.08	122.60
1	E	14	ASP	CA-CB-CG	7.50	120.10	112.60
1	E	55	SER	N-CA-C	-7.38	97.22	109.46
1	E	89	SER	O-C-N	7.08	131.29	123.22
1	E	307	TYR	N-CA-C	-6.71	98.31	109.24
1	E	165	TYR	N-CA-CB	6.44	120.83	110.65
1	E	164	VAL	O-C-N	6.43	130.29	123.02
1	E	267	VAL	O-C-N	6.40	126.45	121.46
1	E	228	GLN	OE1-CD-NE2	6.29	128.89	122.60
1	E	18	ILE	CB-CA-C	6.28	120.50	110.82
1	E	237	GLN	CB-CG-CD	6.26	123.24	112.60
1	E	52	SER	O-C-N	6.17	131.22	123.01
1	E	160	GLN	CG-CD-NE2	6.16	125.64	116.40
1	E	180	THR	CA-C-O	-6.16	113.67	120.38
1	E	274	TYR	CA-C-O	6.15	126.94	120.42
1	E	13	ASN	OD1-CG-ND2	6.15	128.75	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	312	SER	CA-C-O	-6.13	111.84	119.38
1	E	46	LEU	O-C-N	6.12	128.39	121.53
1	E	208	PHE	CA-CB-CG	6.10	119.90	113.80
1	E	83	GLY	O-C-N	6.10	128.86	123.80
1	E	98	HIS	CA-CB-CG	-6.04	107.76	113.80
1	E	47	PRO	CA-C-O	-6.02	114.56	121.36
1	E	23	ILE	O-C-N	5.95	129.50	123.20
1	E	5	VAL	O-C-N	5.88	129.60	123.26
1	E	89	SER	CA-C-N	-5.86	115.47	123.14
1	E	89	SER	C-N-CA	-5.86	115.47	123.14
1	E	33	ASP	N-CA-CB	-5.80	101.49	110.65
1	E	218	LEU	N-CA-CB	-5.80	101.17	110.51
1	E	240	SER	CA-C-O	-5.79	113.56	120.10
1	E	226	VAL	O-C-N	5.78	127.57	121.91
1	E	21	VAL	CA-C-O	-5.75	114.16	120.43
1	E	172	SER	CA-CB-OG	-5.66	99.78	111.10
1	E	247	PHE	CA-CB-CG	-5.60	108.20	113.80
1	E	280	GLY	O-C-N	5.56	129.93	122.70
1	E	276	PRO	O-C-N	5.56	129.63	122.85
1	E	188	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	E	19	THR	O-C-N	5.55	128.34	121.79
1	E	42	PHE	N-CA-C	-5.53	102.10	110.28
1	E	89	SER	CA-CB-OG	-5.49	100.13	111.10
1	E	159	HIS	CA-CB-CG	-5.46	108.33	113.80
1	E	22	THR	CA-CB-OG1	-5.46	101.41	109.60
1	E	317	LEU	CA-C-N	-5.40	117.56	122.80
1	E	317	LEU	C-N-CA	-5.40	117.56	122.80
1	E	9	THR	O-C-N	5.36	128.12	121.79
1	E	252	ASN	CA-C-O	-5.36	114.54	120.60
1	E	58	ASN	CB-CA-C	5.35	115.79	110.33
1	E	214	THR	O-C-N	5.35	129.60	122.43
1	E	246	VAL	O-C-N	5.34	128.88	123.00
1	E	237	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	E	13	ASN	CA-C-O	-5.30	114.11	119.78
1	E	106	GLN	N-CA-C	-5.29	107.38	113.88
1	E	58	ASN	O-C-N	5.28	126.43	120.83
1	E	306	GLN	O-C-N	5.26	129.99	123.15
1	E	89	SER	CA-C-O	-5.26	114.59	120.54
1	E	11	THR	N-CA-C	-5.25	101.72	109.86
1	E	57	TYR	O-C-N	5.25	129.25	123.16
1	E	199	THR	CA-CB-OG1	-5.18	101.82	109.60
1	E	5	VAL	CA-C-N	-5.16	115.45	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5	VAL	C-N-CA	-5.16	115.45	122.93
1	E	33	ASP	N-CA-C	5.16	117.05	108.02
1	E	267	VAL	CA-C-O	-5.14	115.45	119.20
1	E	106	GLN	OE1-CD-NE2	5.12	127.72	122.60
1	E	9	THR	CB-CA-C	-5.12	103.35	110.16
1	E	53	GLY	O-C-N	5.10	128.42	122.45
1	E	187	SER	CA-C-O	-5.08	114.36	120.10
1	E	21	VAL	O-C-N	5.05	128.53	123.07
1	E	276	PRO	CA-C-O	-5.05	115.81	121.32
1	E	221	LEU	CA-C-O	-5.04	115.74	121.58
1	E	296	SER	CA-CB-OG	-5.02	101.05	111.10

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	2366	0	2182	9	0
2	I	35	0	46	1	0
3	E	11	0	10	0	0
4	E	244	0	0	1	0
4	I	3	0	0	0	0
All	All	2659	0	2238	9	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 2.

All (9) 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:233:VAL:HG13	1:E:251:THR:HG21	1.91	0.51
1:E:239:ASP:OD1	1:E:279:ASP:OD2	2.31	0.49
1:E:211:ILE:HD11	2:I:1:LTA:H102	1.96	0.47
1:E:306:GLN:C	1:E:322:GLN:HG3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:GLN:NE2	4:E:571:HOH:O	2.51	0.44
1:E:218:LEU:O	1:E:299:GLY:HA3	2.21	0.41
1:E:150:GLN:O	1:E:168:GLY:HA2	2.21	0.40
1:E:71:TRP:CE2	1:E:103:GLN:HB3	2.55	0.40
1:E:203:GLN:OE1	1:E:228:GLN:HG2	2.22	0.40

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	E	321/323 (99%)	316 (98%)	5 (2%)	0	100	100
2	I	2/4 (50%)	2 (100%)	0	0	100	100
All	All	323/327 (99%)	318 (98%)	5 (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	E	259/259 (100%)	251 (97%)	8 (3%)	35	23
2	I	2/2 (100%)	2 (100%)	0	100	100
All	All	261/261 (100%)	253 (97%)	8 (3%)	35	23

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	ILE
1	E	28	LEU
1	E	39	LEU
1	E	64	LYS
1	E	107	GLN
1	E	195	VAL
1	E	228	GLN
1	E	237	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	31	ASN
1	E	98	HIS
1	E	133	GLN
1	E	188	GLN
1	E	228	GLN
1	E	306	GLN

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	$\# Z > 2$
2	LTA	I	1	2	14,14,14	1.97	1 (7%)	15,16,16	2.67	6 (40%)

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
2	LTA	I	1	2	-	4/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	LTA	O-C	-6.26	1.30	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	LTA	C2-C-CA	-4.84	105.45	112.93
2	I	1	LTA	O2-C1-C2	-4.52	102.84	111.17
2	I	1	LTA	O1-C1-C2	-4.19	114.92	124.65
2	I	1	LTA	CB-CA-C	-3.77	106.62	112.66
2	I	1	LTA	O-C-CA	3.04	115.25	109.48
2	I	1	LTA	CG-CB-CA	2.86	121.27	113.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	LTA	CA-C-C2-C1
2	I	1	LTA	O-C-C2-C1
2	I	1	LTA	C2-C1-O2-C9
2	I	1	LTA	O1-C1-O2-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	LTA	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand 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	MAN	E	334	1	11,11,12	0.88	0	15,15,17	1.11	1 (6%)

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	MAN	E	334	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	334	MAN	O2-C2-C1	-3.01	102.33	109.22

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

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.