



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2018 – 05:05 pm GMT

PDB ID : 1PYT
Title : TERNARY COMPLEX OF PROCARBOXYPEPTIDASE A, PROPRO-
TEINASE E, AND CHYMOTRYPSINOGEN C
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Deposited on : 1995-06-21
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

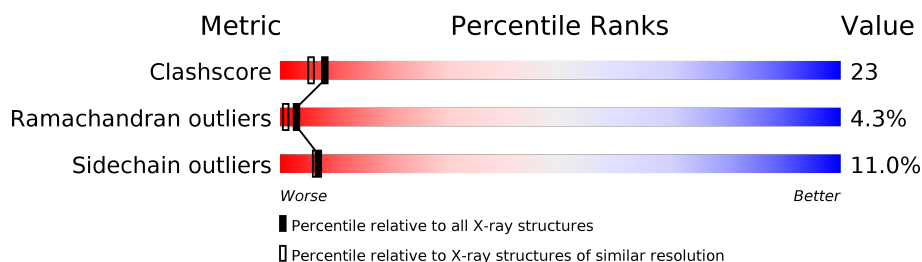
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	122078	1081 (2.36-2.36)
Ramachandran outliers	120005	1066 (2.36-2.36)
Sidechain outliers	119972	1067 (2.36-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	94	
2	B	309	
3	C	253	
4	D	251	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7411 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 PROCARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			760	480	131	147	2			

- Molecule 2 is a protein called PROCARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total	C	N	O	S	0	0	0
			2462	1579	405	473	5			

- Molecule 3 is a protein called PROPROTEINASE E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	0	0
			1880	1185	322	362	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	477	GLN	GLU	CONFLICT	UNP P05805
C	557	GLU	GLN	CONFLICT	UNP P05805
C	570A	TYR	TRP	CONFLICT	UNP P05805
C	592	ASP	ASN	CONFLICT	UNP P05805
C	639	ASN	ASP	CONFLICT	UNP P05805

- Molecule 4 is a protein called CHYMOTRYPSINOGEN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	251	Total	C	N	O	S	0	0	0
			1926	1218	330	367	11			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

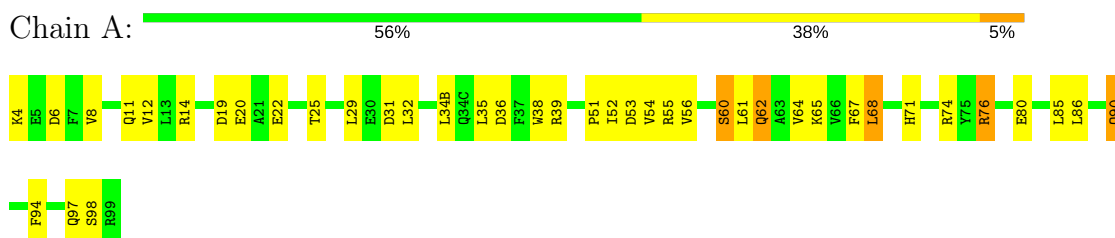
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	47	Total	O	0	0
			47	47		
7	B	161	Total	O	0	0
			161	161		
7	C	99	Total	O	0	0
			99	99		
7	D	74	Total	O	0	0
			74	74		

3 Residue-property plots

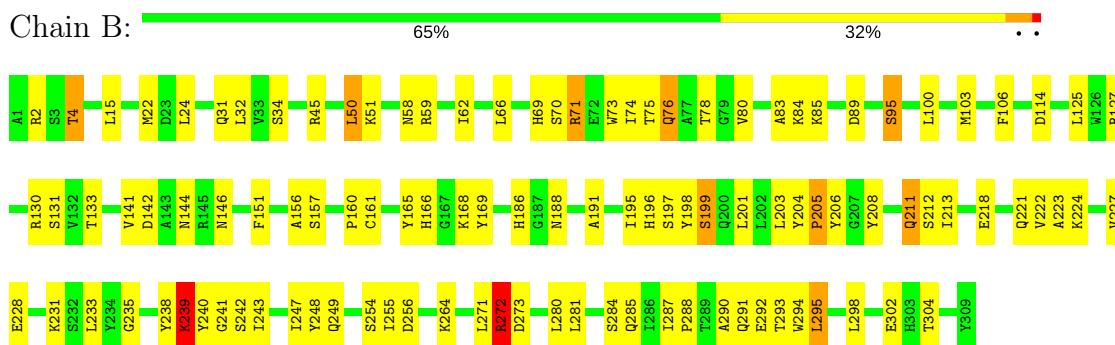
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

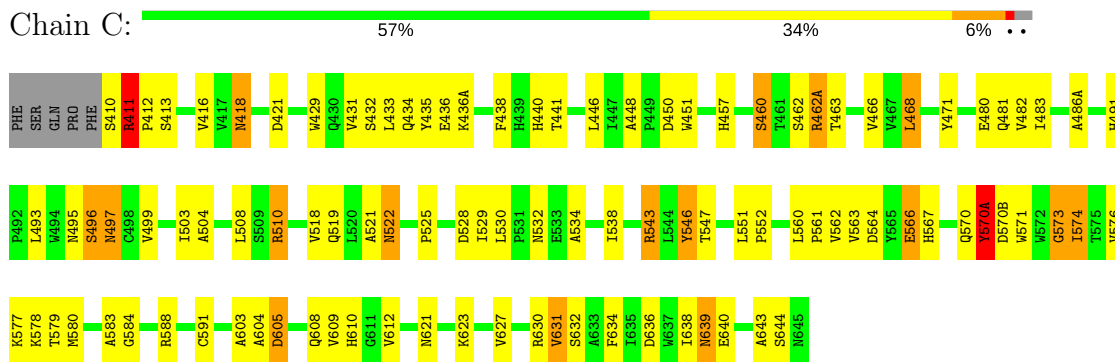
• Molecule 1: PROCARBOXYPEPTIDASE A



• Molecule 2: PROCARBOXYPEPTIDASE A

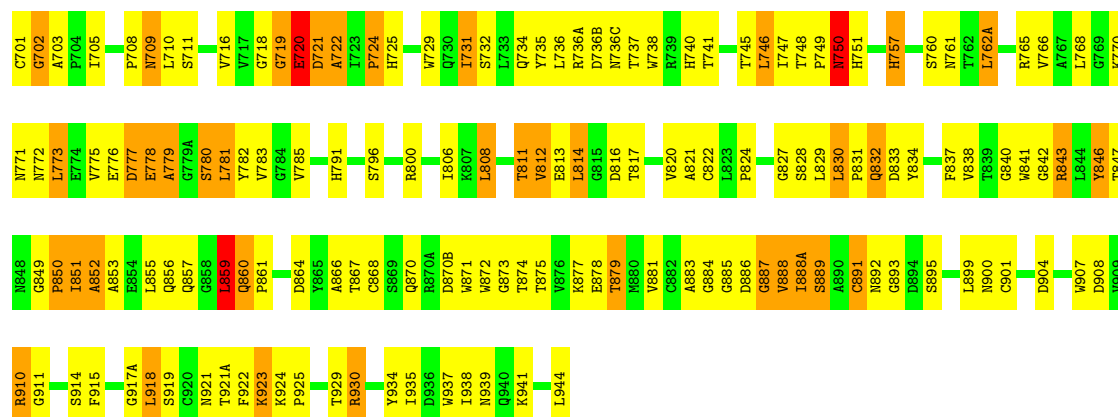


• Molecule 3: PROPROTEINASE E



• Molecule 4: CHYMOTRYPSINOGEN C

Chain D:



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	188.50Å 188.50Å 82.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.35)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7411	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: ZN, 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	0.60	0/775	0.79	0/1048
2	B	0.63	0/2529	0.79	3/3437 (0.1%)
3	C	0.56	0/1932	0.83	0/2642
4	D	0.56	0/1974	0.86	1/2698 (0.0%)
All	All	0.59	0/7210	0.82	4/9825 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	859	LEU	CA-CB-CG	6.05	129.22	115.30
2	B	69	HIS	N-CA-C	-5.79	95.37	111.00
2	B	239	LYS	N-CA-C	-5.18	97.02	111.00
2	B	70	SER	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	ARG	Peptide

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	A	760	0	739	35	0
2	B	2462	0	2367	69	0
3	C	1880	0	1785	80	0
4	D	1926	0	1853	143	0
5	B	1	0	0	1	0
6	C	1	0	0	0	0
7	A	47	0	0	2	0
7	B	161	0	0	5	0
7	C	99	0	0	3	0
7	D	74	0	0	5	0
All	All	7411	0	6744	315	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 23.

The worst 5 of 315 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)
3:C:468:LEU:HD11	3:C:483:ILE:HD12	1.53	0.91
3:C:460:SER:HB3	3:C:462(A):ARG:HG3	1.52	0.91
3:C:525:PRO:HG2	3:C:528:ASP:HB2	1.52	0.90
3:C:411:ARG:HB3	3:C:412:PRO:HD2	1.52	0.90
2:B:196:HIS:ND1	7:B:351:HOH:O	2.08	0.86

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	A	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	16	15
2	B	307/309 (99%)	281 (92%)	23 (8%)	3 (1%)	17	16
3	C	246/253 (97%)	215 (87%)	25 (10%)	6 (2%)	6	4
4	D	249/251 (99%)	179 (72%)	42 (17%)	28 (11%)	0	0
All	All	894/907 (99%)	762 (85%)	94 (10%)	38 (4%)	3	1

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	SER
3	C	411	ARG
3	C	605	ASP
4	D	702	GLY
4	D	721	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	A	83/83 (100%)	76 (92%)	7 (8%)	12	11
2	B	266/266 (100%)	245 (92%)	21 (8%)	13	13
3	C	205/210 (98%)	182 (89%)	23 (11%)	6	6
4	D	209/209 (100%)	176 (84%)	33 (16%)	3	2
All	All	763/768 (99%)	679 (89%)	84 (11%)	7	6

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	510	ARG
3	C	621	ASN
4	D	891	CYS
3	C	543	ARG

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Mol	Chain	Res	Type
3	C	570(A)	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	465	GLN
3	C	570	GLN
4	D	870	GLN
3	C	532	ASN
3	C	610	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.