W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:33 am BST

PDB ID	:	1LTO
Title	:	Human alpha1-tryptase
Authors	:	Marquardt, U.; Zettl, F.; Huber, R.; Bode, W.; Sommerhoff, C.P.
Deposited on	:	2002-05-20
Resolution	:	2.20 Å(reported)

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	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1   Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Clashscore		18
Ramachandran outliers		0.5%
Sidechain outliers		4.1%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
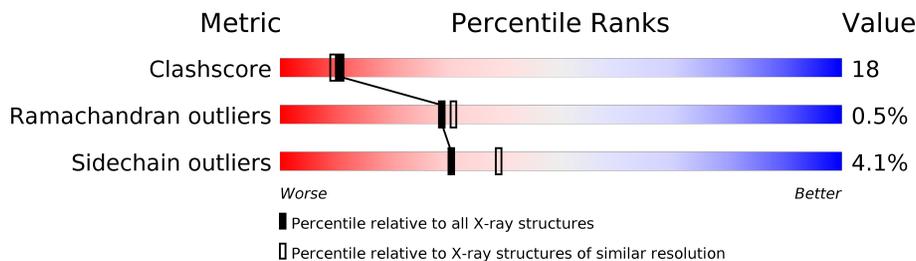
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	67% 30% ··
1	B	245	70% 27% ··
1	C	245	69% 29% ··
1	D	245	69% 27% ··

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8351 atoms, of which 8 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 tryptase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	243	Total 1937	C 1239	H 2	N 338	O 345	S 13	66	0	0
1	B	243	Total 1937	C 1239	H 2	N 338	O 345	S 13	42	0	0
1	C	243	Total 1937	C 1239	H 2	N 338	O 345	S 13	72	0	0
1	D	243	Total 1937	C 1239	H 2	N 338	O 345	S 13	76	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	153	Total 153	O 153	0	0
2	B	220	Total 220	O 220	0	0
2	C	96	Total 96	O 96	0	0
2	D	134	Total 134	O 134	0	0

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. 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: alpha tryptase I
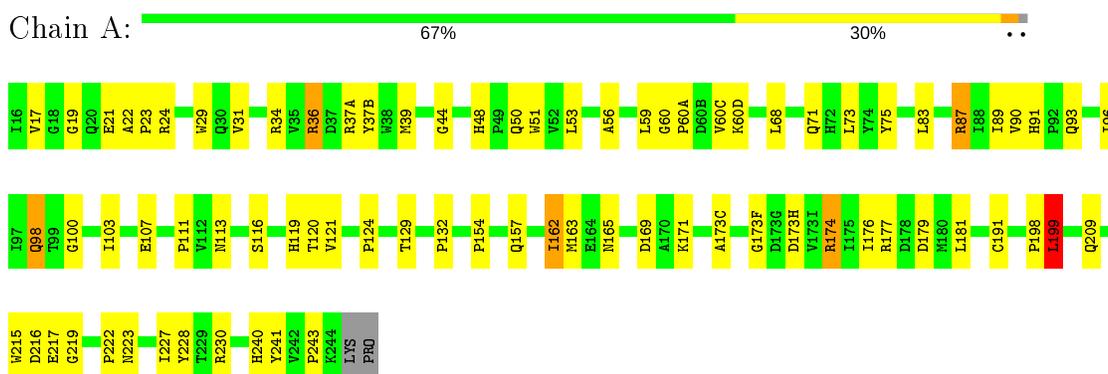
Chain A:

- Molecule 1: alpha tryptase I

Chain B:

- Molecule 1: alpha tryptase I

Chain C:

V231 T232 V242 P243 K244 LYS PRO

• Molecule 1: alpha tryptase I

Chain D:

69%   27%

I16 V17 Q20 E21 R24 W27 P28 W29 Q30 V31 V35 R36 W38 G44 S45 L46 I47 H48 P49 Q50 W51 V52 L53 L59 G60 P60A K60D D60E L61 A62 T63 L68 R69 E70 Q71 H72 L73 Y74 Y75 Q79 D80 Q81 L82 L83 P84 V85 I89 V90 H91 P92

Q93 Q98 I103 H119 T120 V121 P124 E128 T129 F130 P131 P132 V138 W141 P152A P152B F153 P154 I162 H166 Y173D T173E G173F V173I R174 I175 I176 L181 C191 K192 P198 L199 N204 L208 W215 D216 E217 R224 H239 H240

Y241 K244 LYS PRO
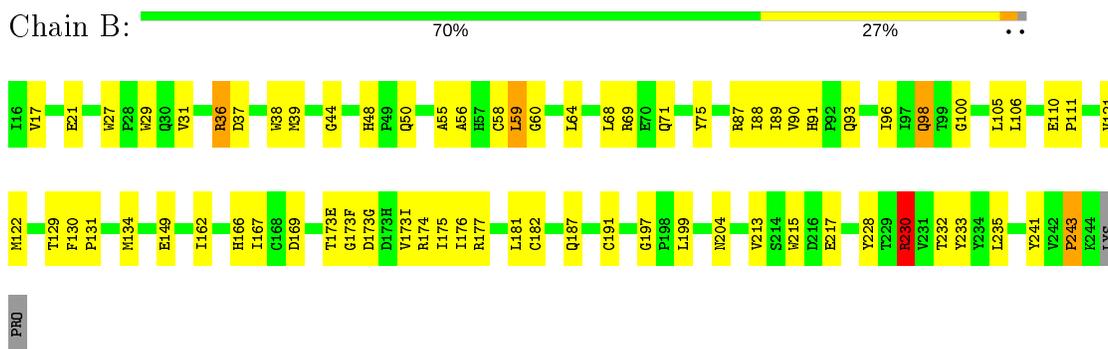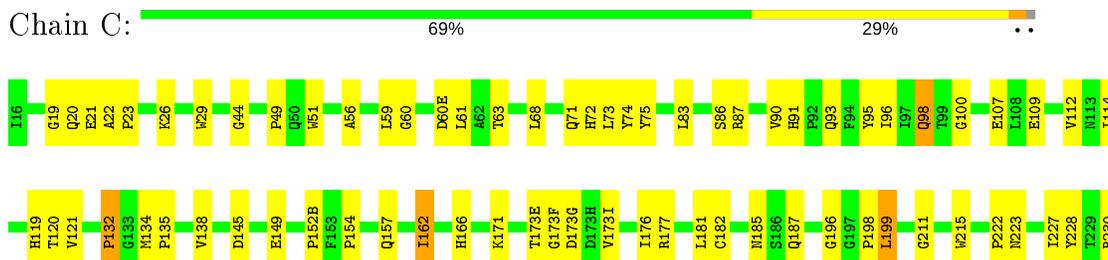
4 Data and refinement statistics (i)

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	91.44Å 110.69Å 130.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.94 – 2.20	Depositor
% Data completeness (in resolution range)	94.7 (23.94-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8351	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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	A	0.48	0/1998	0.75	1/2735 (0.0%)
1	B	0.59	0/1998	0.79	1/2735 (0.0%)
1	C	0.43	0/1998	0.70	1/2735 (0.0%)
1	D	0.44	0/1998	0.74	2/2735 (0.1%)
All	All	0.49	0/7992	0.75	5/10940 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	129	THR	N-CA-C	-6.56	93.29	111.00
1	C	176	ILE	CB-CG1-CD1	6.14	131.10	113.90
1	D	224	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	199	LEU	N-CA-C	-5.97	94.87	111.00
1	B	230	ARG	NE-CZ-NH1	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1935	2	1876	73	0
1	B	1935	2	1876	78	0
1	C	1935	2	1876	60	0
1	D	1935	2	1876	65	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	153	0	0	12	0
2	B	220	0	0	19	0
2	C	96	0	0	8	0
2	D	134	0	0	10	0
All	All	8343	8	7504	268	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 18.

The worst 5 of 268 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:B:169:ASP:HB2	1:B:176:ILE:CG1	1.67	1.24
1:A:98:GLN:H	1:A:98:GLN:NE2	1.50	1.09
1:A:60:GLY:HA3	2:A:315:HOH:O	1.55	1.04
1:B:98:GLN:H	1:B:98:GLN:NE2	1.62	0.96
1:D:91:HIS:HD2	1:D:93:GLN:H	1.15	0.93

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	241/245 (98%)	223 (92%)	17 (7%)	1 (0%)	34	37
1	B	241/245 (98%)	226 (94%)	14 (6%)	1 (0%)	34	37
1	C	241/245 (98%)	221 (92%)	19 (8%)	1 (0%)	34	37
1	D	241/245 (98%)	219 (91%)	20 (8%)	2 (1%)	19	19
All	All	964/980 (98%)	889 (92%)	70 (7%)	5 (0%)	29	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	75	TYR
1	A	243	PRO
1	B	243	PRO
1	D	81	GLN
1	C	132	PRO

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	212/214 (99%)	203 (96%)	9 (4%)	30	38
1	B	212/214 (99%)	203 (96%)	9 (4%)	30	38
1	C	212/214 (99%)	205 (97%)	7 (3%)	38	49
1	D	212/214 (99%)	202 (95%)	10 (5%)	26	33
All	All	848/856 (99%)	813 (96%)	35 (4%)	30	39

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	187	GLN
1	C	61	LEU
1	D	181	LEU
1	B	199	LEU
1	B	230	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	221(A)	GLN
1	C	50	GLN
1	D	221(A)	GLN
1	B	223	ASN
1	C	81	GLN

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)

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.