wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:17 PM GMT

PDB ID	:	1A0L
Title	:	HUMAN BETA-TRYPTASE: A RING-LIKE TETRAMER WITH ACTIVE SITES FACING A CENTRAL PORE
Authors	:	Pereira, P.J.B.; Bergner, A.; Macedo-Ribeiro, S.; Huber, R.; Matschiner, G.; Fritz, H.; Sommerhoff, C.P.; Bode, W.
Deposited on	:	1997-12-03
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

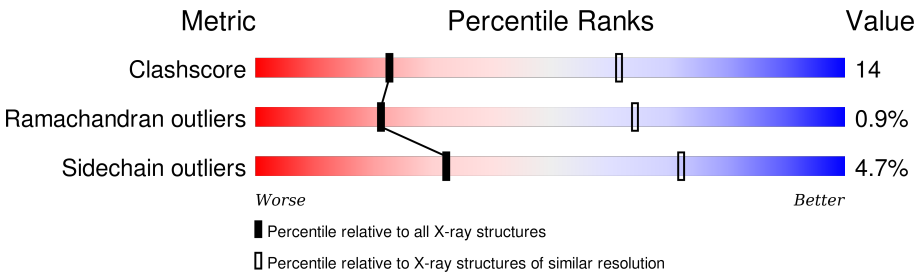
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 <=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	244	70% 27% •
1	B	244	73% 25% •
1	C	244	65% 33% •
1	D	244	66% 31% • •

2 Entry composition (i)

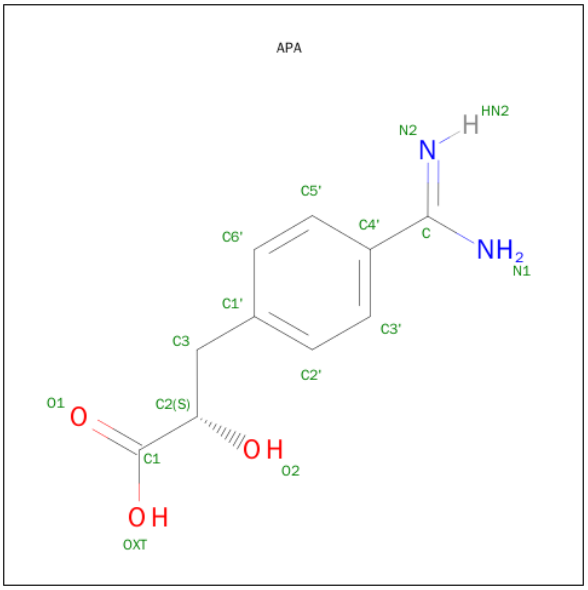
There are 3 unique types of molecules in this entry. The entry contains 7872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-TRYPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	1929	1236	340	341	12	0	0	0
1	B	244	1929	1236	340	341	12	0	0	0
1	C	244	1929	1236	340	341	12	0	0	0
1	D	244	1929	1236	340	341	12	0	0	0

- Molecule 2 is (2S)-3-(4-CARBAMIMIDOYLPHENYL)-2-HYDROXYPROPANOIC ACID (three-letter code: APA) (formula: $C_{10}H_{12}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	10	2	3	0	0
2	B	1	15	10	2	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	15	10	2	3	0	0
			Total	C	N	O		
2	D	1	15	10	2	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	26	26	26	0	0
			Total	O		
3	B	25	25	25	0	0
			Total	O		
3	C	17	17	17	0	0
			Total	O		
3	D	28	28	28	0	0

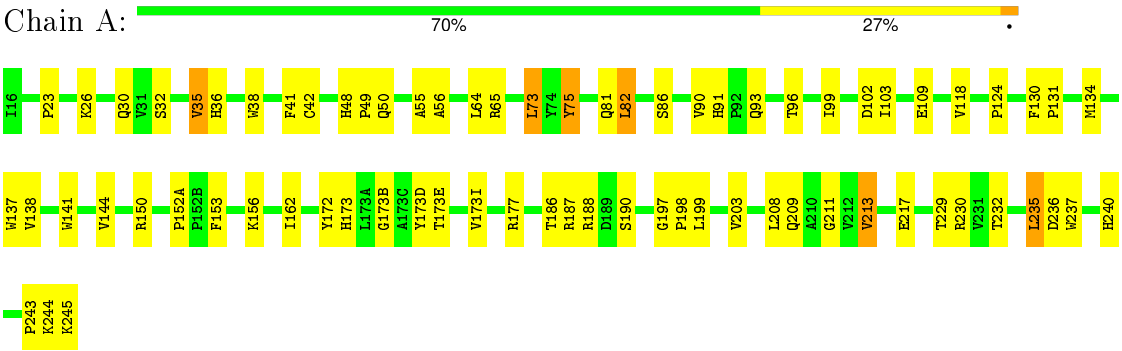
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

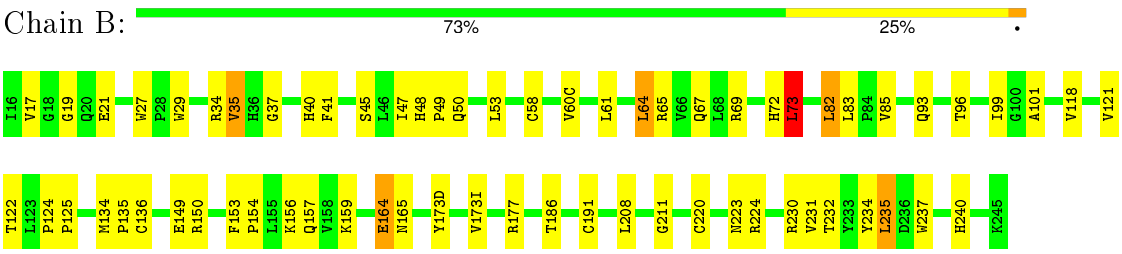
- Molecule 1: BETA-TRYPTASE

Chain A:



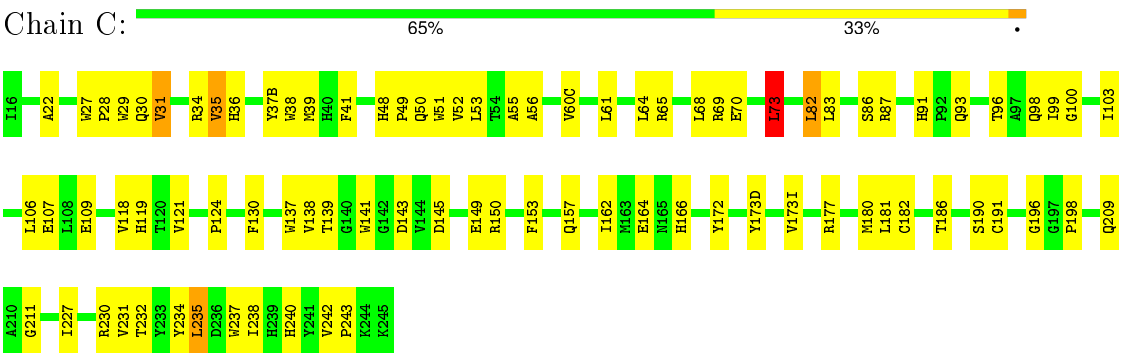
- Molecule 1: BETA-TRYPTASE

Chain B:



- Molecule 1: BETA-TRYPTASE

Chain C:



- Molecule 1: BETA-TRYPTASE

Chain D:

66%
31%

I16 E21 R24 W27 P28 W29 Q30 V31 R34 V35 H36 W38 M39 H40 F41 G44 H48 P49 Q50 W51 V52 L53 A56 D60B V60C K60D R65 R69 L73 Y74 Y75 Q79 D80 Q81 L82 S86 I89 V90 H91 P92 Q93 I103 E109
V118 H119 P124 T129 F130 P131 M134 P135 C136 W137 V138 W141 D145 E149 R150 L151 P152 P152A P152B F153 P154 I162 M163 T173E V173I R177 M180 T186 R187 R188 D189 S190 C191 D194 S195 G196 G197 P198 Q209 A210 G211 N223 R224 T229
R230 V231 T232 L235 D236 W237 H240 Y241 K244 K245

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	82.93Å 82.93Å 172.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.3 (10.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7872	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: APA

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	0/1994	0.73	1/2731 (0.0%)
1	B	0.49	0/1994	0.74	2/2731 (0.1%)
1	C	0.48	0/1994	0.74	1/2731 (0.0%)
1	D	0.47	0/1994	0.72	2/2731 (0.1%)
All	All	0.48	0/7976	0.73	6/10924 (0.1%)

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
1	B	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	LEU	N-CA-C	6.66	128.99	111.00
1	A	73	LEU	N-CA-C	6.14	127.59	111.00
1	B	35	VAL	CB-CA-C	-5.77	100.43	111.40
1	D	73	LEU	N-CA-C	5.42	125.65	111.00
1	C	73	LEU	N-CA-C	5.40	125.57	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	37	GLY	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	1929	0	1867	48	0
1	B	1929	0	1867	46	0
1	C	1929	0	1867	62	0
1	D	1929	0	1867	62	0
2	A	15	0	9	1	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
3	A	26	0	0	1	0
3	B	25	0	0	2	0
3	C	17	0	0	1	0
3	D	28	0	0	5	0
All	All	7872	0	7504	207	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 14.

The worst 5 of 207 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:D:65:ARG:HG2	1:D:82:LEU:HB3	1.40	1.02
1:A:65:ARG:HG2	1:A:82:LEU:HB3	1.49	0.93
1:B:65:ARG:HG2	1:B:82:LEU:HB3	1.58	0.85
1:A:232:THR:HA	1:A:235:LEU:HD22	1.58	0.84
1:C:65:ARG:HG2	1:C:82:LEU:HB3	1.62	0.82

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	242/244 (99%)	221 (91%)	19 (8%)	2 (1%)	24	66
1	B	242/244 (99%)	221 (91%)	19 (8%)	2 (1%)	24	66
1	C	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	24	66
1	D	242/244 (99%)	218 (90%)	21 (9%)	3 (1%)	16	56
All	All	968/976 (99%)	882 (91%)	77 (8%)	9 (1%)	21	64

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	73	LEU
1	A	213	VAL
1	B	73	LEU
1	D	38	TRP
1	B	49	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	209/209 (100%)	199 (95%)	10 (5%)	31	71
1	B	209/209 (100%)	200 (96%)	9 (4%)	35	75
1	C	209/209 (100%)	200 (96%)	9 (4%)	35	75
1	D	209/209 (100%)	198 (95%)	11 (5%)	28	67
All	All	836/836 (100%)	797 (95%)	39 (5%)	32	72

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	230	ARG
1	C	64	LEU
1	D	186	THR

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Mol	Chain	Res	Type
1	B	235	LEU
1	C	31	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	240	HIS
1	C	30	GLN
1	D	48	HIS
1	B	91	HIS
1	C	240	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)

4 ligands are 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	APA	A	301	1	11,15,15	1.56	2 (18%)	14,20,20	3.04	8 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	APA	B	301	1	11,15,15	1.44	2 (18%)	14,20,20	2.95	8 (57%)
2	APA	C	301	1	11,15,15	1.59	3 (27%)	14,20,20	3.00	9 (64%)
2	APA	D	301	1	11,15,15	1.26	3 (27%)	14,20,20	2.98	7 (50%)

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	APA	A	301	1	-	0/8/12/12	0/1/1/1
2	APA	B	301	1	-	0/8/12/12	0/1/1/1
2	APA	C	301	1	-	0/8/12/12	0/1/1/1
2	APA	D	301	1	-	0/8/12/12	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	APA	C4'-C	-3.80	1.41	1.47
2	C	301	APA	C4'-C	-2.91	1.42	1.47
2	B	301	APA	C4'-C	-2.82	1.42	1.47
2	D	301	APA	C4'-C	-2.27	1.43	1.47
2	D	301	APA	C3'-C4'	2.02	1.42	1.39

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	APA	C2'-C3'-C4'	-4.40	115.67	120.76
2	B	301	APA	C3-C2-C1	-4.38	104.91	111.19
2	C	301	APA	C2'-C3'-C4'	-4.29	115.79	120.76
2	D	301	APA	C2'-C3'-C4'	-3.97	116.16	120.76
2	B	301	APA	C2'-C3'-C4'	-3.96	116.17	120.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	APA	1	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.