



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:40 pm BST

PDB ID : 1TMQ
Title : STRUCTURE OF TENEBRIO MOLITOR LARVAL ALPHA-AMYLASE IN
COMPLEX WITH RAGI BIFUNCTIONAL INHIBITOR
Authors : Gomis-Rueth, F.X.; Strobl, S.; Glockshuber, R.
Deposited on : 1998-01-13
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

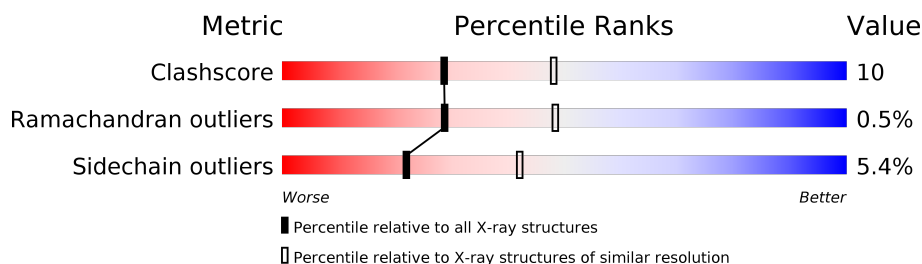
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	
2	B	117	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4820 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 PROTEIN (ALPHA-AMYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3606	2241	627	718	20			

- Molecule 2 is a protein called PROTEIN (RAGI BIFUNCTIONAL INHIBITOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			881	544	164	160	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	570	SER	PRO	conflict	UNP P01087

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	298	Total	O	0	0
			298	298		

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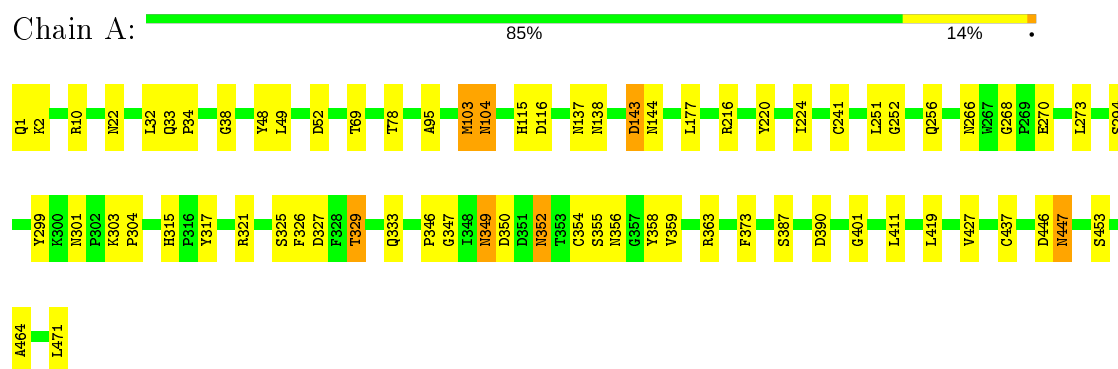
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	33	Total	O	0	0
			33	33		

3 Residue-property plots [i](#)

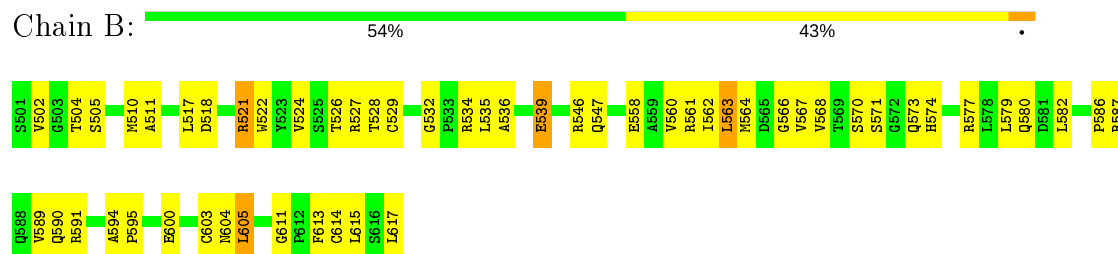
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



• Molecule 2: PROTEIN (RAGI BIFUNCTIONAL INHIBITOR)



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.16 Å 186.87 Å 111.54 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.191 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4820	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: CA, PCA, CL

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	0.46	0/3684	0.71	0/5003
2	B	0.43	0/898	0.71	0/1217
All	All	0.45	0/4582	0.71	0/6220

There are no bond length outliers.

There are no bond angle outliers.

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	3606	0	3332	44	0
2	B	881	0	876	41	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	298	0	0	7	0
5	B	33	0	0	1	0
All	All	4820	0	4208	84	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 10.

All (84) 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:137:ASN:H	1:A:144:ASN:HD21	1.20	0.87
1:A:143:ASP:HB3	5:A:1161:HOH:O	1.85	0.76
2:B:614:CYS:HB3	2:B:617:LEU:HD22	1.73	0.71
2:B:615:LEU:HD21	5:B:1134:HOH:O	1.92	0.69
1:A:266:ASN:HD22	1:A:270:GLU:HG2	1.60	0.67
2:B:528:THR:HG22	2:B:529:CYS:SG	2.35	0.67
2:B:518:ASP:HB3	2:B:547:GLN:HE22	1.60	0.67
2:B:586:PRO:O	2:B:589:VAL:HG12	1.96	0.66
1:A:329:THR:H	1:A:333:GLN:HE22	1.45	0.65
1:A:315:HIS:HE1	5:A:1249:HOH:O	1.82	0.63
2:B:527:ARG:HB3	2:B:527:ARG:NH1	2.13	0.63
1:A:303:LYS:HB3	1:A:304:PRO:HD3	1.81	0.61
1:A:352:ASN:O	1:A:363:ARG:HD3	2.03	0.58
2:B:614:CYS:CB	2:B:617:LEU:HD22	2.33	0.58
2:B:561:ARG:NH2	2:B:566:GLY:O	2.39	0.56
1:A:137:ASN:N	1:A:144:ASN:HD21	1.97	0.55
2:B:591:ARG:NH1	2:B:591:ARG:HG2	2.20	0.55
1:A:315:HIS:HD2	1:A:317:TYR:H	1.53	0.55
1:A:411:LEU:O	1:A:453:SER:HA	2.06	0.55
1:A:266:ASN:ND2	1:A:270:GLU:HG2	2.22	0.55
1:A:359:VAL:HG22	5:A:1269:HOH:O	2.06	0.54
2:B:591:ARG:HG2	2:B:591:ARG:HH11	1.72	0.54
1:A:104:ASN:HD22	1:A:104:ASN:N	2.05	0.54
1:A:104:ASN:HD21	1:A:116:ASP:H	1.54	0.54
1:A:270:GLU:HB2	5:A:1252:HOH:O	2.07	0.54
2:B:536:ALA:O	2:B:539:GLU:HB3	2.08	0.54
2:B:594:ALA:HB3	2:B:595:PRO:HD3	1.90	0.53
2:B:524:VAL:O	2:B:528:THR:HB	2.07	0.53
2:B:526:THR:CG2	2:B:532:GLY:HA3	2.38	0.53
2:B:603:CYS:HB3	2:B:605:LEU:HD22	1.91	0.52
2:B:564:MET:O	2:B:577:ARG:HA	2.11	0.51
1:A:347:GLY:O	1:A:354:CYS:HA	2.11	0.51
2:B:527:ARG:HB3	2:B:527:ARG:HH11	1.74	0.50
1:A:437:CYS:SG	1:A:471:LEU:HD11	2.52	0.50
2:B:577:ARG:NH1	2:B:580:GLN:HE22	2.09	0.50
2:B:522:TRP:CZ3	2:B:582:LEU:HD21	2.47	0.50
2:B:561:ARG:HA	2:B:564:MET:HE2	1.94	0.49
2:B:568:VAL:HG22	2:B:574:HIS:ND1	2.27	0.49
1:A:355:SER:O	1:A:356:ASN:HB2	2.13	0.48
2:B:600:GLU:HA	2:B:604:ASN:HB2	1.95	0.48
1:A:427:VAL:HG22	1:A:464:ALA:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:PCA:HB2	5:A:1054:HOH:O	2.13	0.48
1:A:447:ASN:OD1	1:A:447:ASN:N	2.45	0.48
2:B:567:VAL:O	2:B:574:HIS:HA	2.12	0.48
1:A:273:LEU:HB3	1:A:317:TYR:OH	2.14	0.48
1:A:349:ASN:HD22	1:A:349:ASN:C	2.17	0.47
2:B:560:VAL:CG2	2:B:617:LEU:HD21	2.44	0.46
1:A:78:THR:HG22	1:A:177:LEU:HD22	1.97	0.46
2:B:558:GLU:OE2	2:B:561:ARG:NH1	2.48	0.46
2:B:517:LEU:HB2	2:B:563:LEU:HG	1.98	0.46
1:A:329:THR:H	1:A:333:GLN:NE2	2.10	0.46
2:B:558:GLU:O	2:B:562:ILE:HG13	2.15	0.46
1:A:224:ILE:HD12	2:B:504:THR:HG22	1.99	0.45
2:B:560:VAL:O	2:B:564:MET:HG3	2.16	0.45
2:B:571:SER:OG	2:B:573:GLN:HG3	2.17	0.45
1:A:33:GLN:HB3	1:A:34:PRO:HD3	1.98	0.45
2:B:526:THR:HG23	2:B:532:GLY:HA3	1.97	0.45
1:A:2:LYS:HB3	1:A:241:CYS:SG	2.57	0.44
1:A:48:TYR:CE2	1:A:69:THR:HB	2.52	0.44
1:A:95:ALA:HA	5:A:1103:HOH:O	2.16	0.44
1:A:252:GLY:O	1:A:256:GLN:HG3	2.18	0.44
2:B:521:ARG:NH2	2:B:590:GLN:OE1	2.50	0.44
2:B:510:MET:HB3	2:B:511:ALA:H	1.67	0.44
1:A:10:ARG:HB3	1:A:38:GLY:HA2	2.00	0.44
2:B:579:LEU:O	2:B:587:ARG:HG3	2.18	0.42
2:B:611:GLY:HA3	2:B:613:PHE:CE2	2.54	0.42
2:B:603:CYS:CB	2:B:605:LEU:HD22	2.49	0.42
2:B:600:GLU:HA	2:B:604:ASN:ND2	2.34	0.42
2:B:577:ARG:HH12	2:B:580:GLN:HE22	1.67	0.42
1:A:326:PHE:HA	1:A:358:TYR:HA	2.01	0.42
1:A:1:PCA:HG2	1:A:216:ARG:CB	2.49	0.41
1:A:299:TYR:OH	1:A:327:ASP:HA	2.20	0.41
2:B:528:THR:HG23	2:B:589:VAL:HG22	2.02	0.41
1:A:373:PHE:CD1	1:A:373:PHE:C	2.94	0.41
1:A:346:PRO:HB3	1:A:358:TYR:CD1	2.55	0.41
2:B:600:GLU:CD	2:B:600:GLU:H	2.23	0.41
1:A:268:GLY:HA2	1:A:273:LEU:HD12	2.03	0.41
1:A:49:LEU:CD2	1:A:103:MET:SD	3.09	0.41
2:B:587:ARG:NH2	2:B:591:ARG:HD2	2.36	0.41
1:A:138:ASN:H	1:A:144:ASN:ND2	2.19	0.41
1:A:22:ASN:HB2	5:A:1076:HOH:O	2.20	0.41
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:N	1:A:419:LEU:HD21	2.37	0.40
1:A:137:ASN:H	1:A:144:ASN:ND2	2.00	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	A	469/471 (100%)	443 (94%)	24 (5%)	2 (0%)	34	54
2	B	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	17	31
All	All	584/588 (99%)	548 (94%)	33 (6%)	3 (0%)	29	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ASP
1	A	390	ASP
2	B	502	VAL

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	381/381 (100%)	364 (96%)	17 (4%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	98/98 (100%)	89 (91%)	9 (9%)	9 18
All	All	479/479 (100%)	453 (95%)	26 (5%)	22 42

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	52	ASP
1	A	103	MET
1	A	104	ASN
1	A	115	HIS
1	A	143	ASP
1	A	220	TYR
1	A	294	SER
1	A	301	ASN
1	A	321	ARG
1	A	325	SER
1	A	329	THR
1	A	349	ASN
1	A	352	ASN
1	A	387	SER
1	A	446	ASP
1	A	447	ASN
2	B	505	SER
2	B	521	ARG
2	B	534	ARG
2	B	535	LEU
2	B	539	GLU
2	B	546	ARG
2	B	563	LEU
2	B	570	SER
2	B	605	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	99	HIS
1	A	104	ASN
1	A	144	ASN
1	A	263	ASN

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Mol	Chain	Res	Type
1	A	301	ASN
1	A	315	HIS
1	A	331	ASN
1	A	333	GLN
1	A	349	ASN
1	A	414	ASN
1	A	468	ASN
2	B	515	ASN
2	B	580	GLN
2	B	604	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	PCA	A	1	1	7,8,9	1.28	1 (14%)	9,10,12	1.72	3 (33%)

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	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CB-CG	2.69	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CG-CD	-2.69	100.07	104.40
1	A	1	PCA	CG-CD-N	2.27	114.26	108.39
1	A	1	PCA	OE-CD-CG	-2.08	123.12	126.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	2	0

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

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.