wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 05:14 am BST

PDB ID	:	1FY8
Title	:	CRYSTAL STRUCTURE OF THE DELTAILE16VAL17 RAT ANIONIC TRYPSINOGEN-BPTI COMPLEX
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Deposited on	:	2000-09-28
Resolution	:	1.70 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 (i) symbol.

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

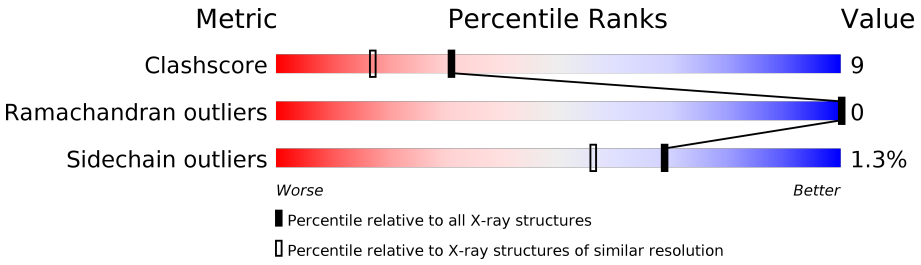
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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	E	231	82% 10% • 7%
2	I	58	79% 17% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2305 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 TRYPSIN II, ANIONIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	215	Total	C	N	O	S	0	3	0
			1627	1017	281	315	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	6	GLU	VAL	CONFLICT	UNP P00763
E	?	-	ILE	deletion	UNP P00763
E	?	-	VAL	deletion	UNP P00763

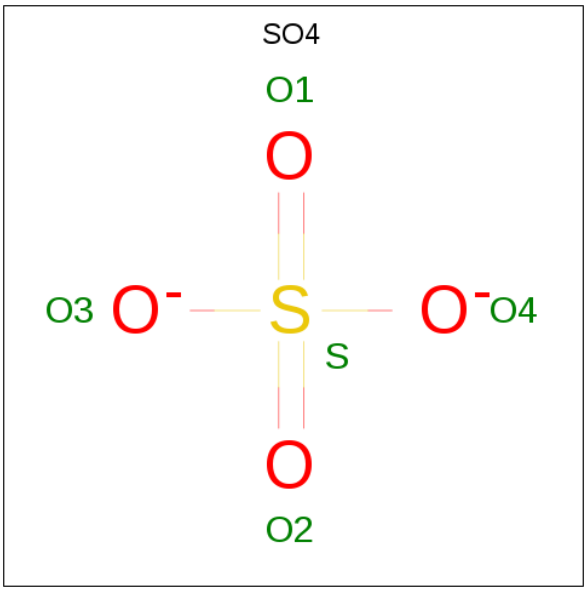
- Molecule 2 is a protein called PANCREATIC TRYPSIN INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	56	Total	C	N	O	S	0	0	0
			444	279	82	76	7			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	172	Total O 172 172	0	0
5	I	46	Total O 46 46	0	0

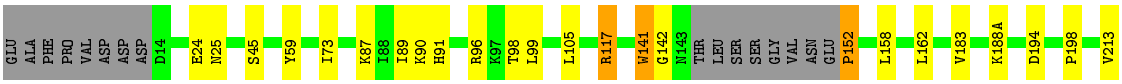
3 Residue-property plots (i)

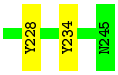
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

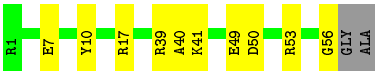
Chain E:





- Molecule 2: PANCREATIC TRYPSIN INHIBITOR

Chain I:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.60Å 92.60Å 62.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.70	Depositor
% Data completeness (in resolution range)	95.2 (10.00-1.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , 0.214	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2305	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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: CA, SO4

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	0.44	2/1673 (0.1%)	0.75	2/2273 (0.1%)
2	I	0.37	0/455	0.67	1/610 (0.2%)
All	All	0.43	2/2128 (0.1%)	0.73	3/2883 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	152	PRO	N-CA	5.74	1.57	1.47
1	E	141	TRP	C-N	-5.07	1.24	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	96[A]	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	E	96[B]	ARG	NE-CZ-NH2	7.64	124.12	120.30
2	I	17	ARG	NE-CZ-NH1	-6.27	117.16	120.30

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	1627	0	1567	27	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	444	0	430	9	1
3	E	1	0	0	0	0
4	I	15	0	0	0	0
5	E	172	0	0	11	3
5	I	46	0	0	5	1
All	All	2305	0	1997	37	4

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 9.

The worst 5 of 37 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:234:TYR:HE1	5:E:646:HOH:O	0.88	1.22
2:I:40:ALA:CB	5:I:611:HOH:O	1.93	1.14
2:I:56:GLY:N	5:I:622:HOH:O	1.83	0.92
1:E:117:ARG:HH11	1:E:117:ARG:CG	1.83	0.91
1:E:117:ARG:HH11	1:E:117:ARG:HG3	1.35	0.91

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ILE:CD1	5:E:545:HOH:O[6_444]	1.76	0.44
1:E:105:LEU:CD1	5:E:556:HOH:O[6_444]	1.77	0.43
5:E:617:HOH:O	5:E:712:HOH:O[6_444]	1.82	0.38
2:I:7:GLU:OE2	5:I:633:HOH:O[6_344]	1.92	0.28

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	214/231 (93%)	210 (98%)	4 (2%)	0	100	100
2	I	54/58 (93%)	54 (100%)	0	0	100	100
All	All	268/289 (93%)	264 (98%)	4 (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	181/192 (94%)	180 (99%)	1 (1%)	86	80
2	I	46/46 (100%)	44 (96%)	2 (4%)	29	11
All	All	227/238 (95%)	224 (99%)	3 (1%)	69	56

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	117	ARG
2	I	50	ASP
2	I	53	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	30	GLN
1	E	93	ASN
1	E	101	ASN
1	E	165	GLN
1	E	224	ASN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
4	SO4	I	992	-	4,4,4	0.82	0	6,6,6	0.48	0
4	SO4	I	990	-	4,4,4	0.82	0	6,6,6	0.47	0
4	SO4	I	991	-	4,4,4	0.82	0	6,6,6	0.48	0

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.