wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 04:57 PM EDT

PDB ID	:	4TPI
Title	:	THE REFINED 2.2-ANGSTROMS (0.22-NM) X-RAY CRYSTAL STRUCTURE OF THE TERNARY COMPLEX FORMED BY BOVINE TRYPSINOGEN, VALINE-VALINE AND THE ARG15 ANALOGUE OF BOVINE PANCREATIC TRYPSIN INHIBITOR
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Deposited on	:	1985-06-11
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

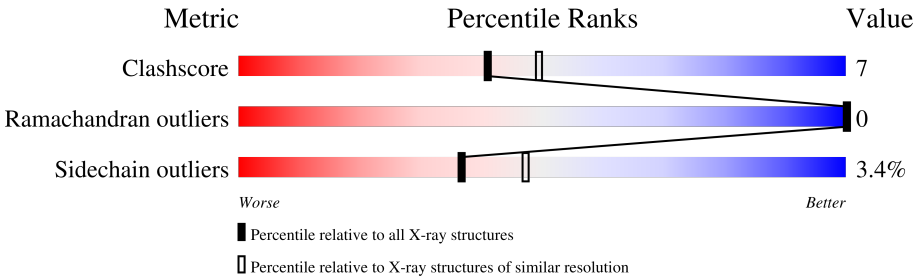
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	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 of 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	Z	229	69% 25%
2	I	58	72% 21% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2266 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 TRYPSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Z	223	1629	1012	279	324	14	65	0	0

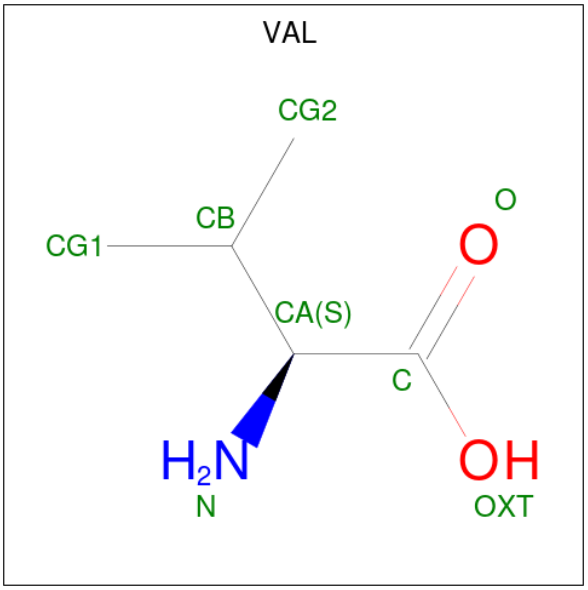
- Molecule 2 is a protein called BOVINE PANCREATIC TRYPSIN INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	58	456	284	86	79	7	34	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	15	ARG	LYS	conflict	UNP P00974

- Molecule 3 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).

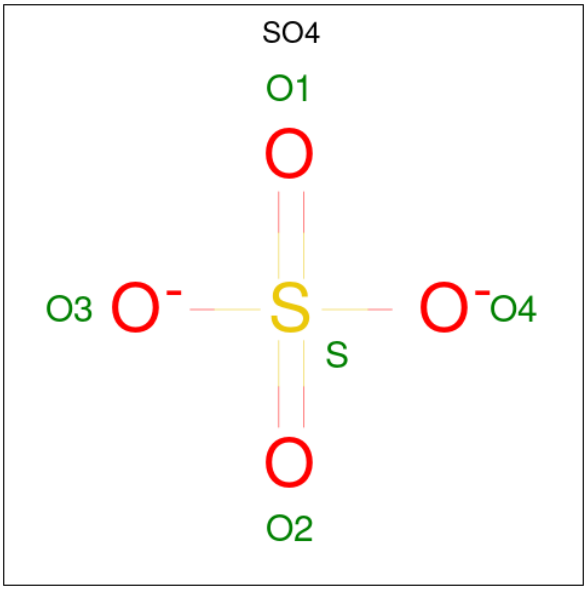


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Z	1	Total C N O 7 5 1 1	0	0
3	Z	1	Total C N O 8 5 1 2	0	0

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Z	117	Total O 117 117	0	0
6	I	38	Total O 38 38	0	0

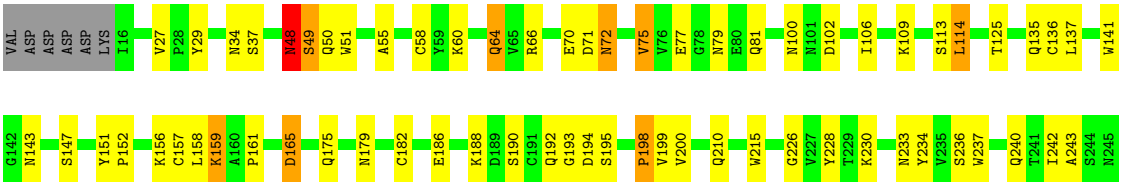
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

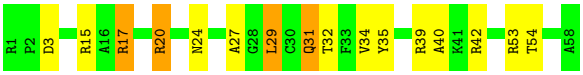
• Molecule 1: TRYPSINOGEN

Chain Z:



• Molecule 2: BOVINE 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	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	75.51Å 85.45Å 122.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2266	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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	Z	1.12	5/1660 (0.3%)	1.36	4/2250 (0.2%)
2	I	1.07	0/467	1.58	8/625 (1.3%)
All	All	1.11	5/2127 (0.2%)	1.41	12/2875 (0.4%)

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	Z	0	27
2	I	0	3
All	All	0	30

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	51	TRP	NE1-CE2	-8.30	1.26	1.37
1	Z	215	TRP	NE1-CE2	-7.64	1.27	1.37
1	Z	237	TRP	NE1-CE2	-6.76	1.28	1.37
1	Z	141	TRP	NE1-CE2	-6.68	1.28	1.37
1	Z	186	GLU	CD-OE2	5.95	1.32	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	17	ARG	NE-CZ-NH1	12.07	126.34	120.30
1	Z	165	ASP	CB-CG-OD2	-11.21	108.21	118.30
2	I	53	ARG	NE-CZ-NH2	-10.37	115.12	120.30
2	I	42	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	75	VAL	CA-CB-CG2	6.08	120.02	110.90

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Z	27	VAL	Mainchain
1	Z	34	ASN	Mainchain
1	Z	48	ASN	Sidechain
1	Z	60	LYS	Mainchain
1	Z	64	GLN	Sidechain

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	Z	1629	0	1588	25	1
2	I	456	0	438	5	1
3	Z	15	0	17	0	0
4	Z	1	0	0	0	0
5	I	10	0	0	0	0
6	I	38	0	0	0	0
6	Z	117	0	0	2	0
All	All	2266	0	2043	28	1

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 7.

The worst 5 of 28 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:Z:64:GLN:HE21	1:Z:66:ARG:HE	1.37	0.73
1:Z:193:GLY:HA2	2:I:17:ARG:HB2	1.78	0.65
1:Z:48:ASN:HD22	1:Z:50:GLN:H	1.45	0.63
1:Z:137:LEU:HD11	1:Z:157:CYS:HB3	1.83	0.60
1:Z:100:ASN:HD21	1:Z:179:ASN:HD22	1.54	0.56

All (1) 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:Z:109:LYS:NZ	2:I:54:THR:O[2_575]	1.59	0.61

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	Z	221/229 (96%)	212 (96%)	9 (4%)	0	100	100
2	I	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
All	All	277/287 (96%)	266 (96%)	11 (4%)	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	Z	184/190 (97%)	180 (98%)	4 (2%)	52	65
2	I	46/46 (100%)	43 (94%)	3 (6%)	17	19
All	All	230/236 (98%)	223 (97%)	7 (3%)	37	53

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	242	ILE
2	I	3	ASP
2	I	31	GLN
2	I	29	LEU
1	Z	195	SER

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

Mol	Chain	Res	Type
1	Z	30	GLN
1	Z	48	ASN
1	Z	64	GLN
1	Z	100	ASN
1	Z	175	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	SO4	I	60	-	4,4,4	0.73	0	6,6,6	0.35	0
5	SO4	I	59	-	4,4,4	0.64	0	6,6,6	0.26	0
3	VAL	Z	1016	3	4,6,7	0.88	0	6,7,9	1.05	0
3	VAL	Z	1017	3	5,7,7	1.00	0	7,9,9	1.56	2 (28%)

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
3	VAL	Z	1016	3	-	4/5/6/8	-
3	VAL	Z	1017	3	-	1/8/8/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	1017	VAL	OXT-C-O	-2.78	117.78	124.09
3	Z	1017	VAL	CB-CA-C	-2.19	104.99	110.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Z	1016	VAL	N-CA-CB-CG1
3	Z	1016	VAL	N-CA-CB-CG2
3	Z	1016	VAL	C-CA-CB-CG1
3	Z	1016	VAL	C-CA-CB-CG2
3	Z	1017	VAL	OXT-C-CA-N

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.