wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 05:04 PM EDT

PDB ID	:	1TET
Title	:	CRYSTAL STRUCTURE OF AN ANTICHOLERA TOXIN PEPTIDE COMPLEX AT 2.3 ANGSTROMS
Authors	:	Shoham, M.
Deposited on	:	1993-06-21
Resolution	:	2.30 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:

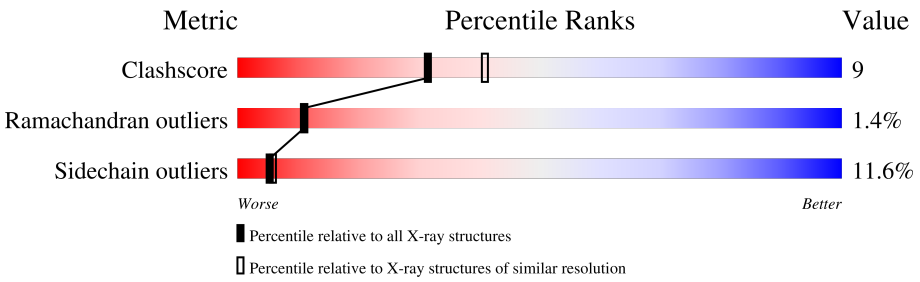
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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	L	216	68% 28% • •
2	H	210	68% 24% 6% •
3	P	15	47% 33% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3541 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 IGG1 TE33 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	216	1681	1059	278	338	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	24	LYS	ARG	conflict	PIR PC4203
L	31A	SER	THR	conflict	PIR PC4203
L	31B	SER	ASN	conflict	PIR PC4203
L	33	PHE	LEU	conflict	PIR PC4203
L	94	ILE	VAL	conflict	PIR PC4203
L	96	PHE	ARG	conflict	PIR PC4203
L	100	SER	GLY	conflict	PIR PC4203
L	188	TRP	ARG	conflict	PIR PC4203

- Molecule 2 is a protein called IGG1 TE33 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	210	1604	1026	262	309	7	0	0	1

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	13	THR	LYS	conflict	GB 2072131
H	26	GLY	ASP	conflict	GB 2072131
H	28	THR	SER	conflict	GB 2072131
H	30	THR	MET	conflict	GB 2072131
H	32	TYR	SER	conflict	GB 2072131
H	35	SER	GLN	conflict	GB 2072131
H	38	LYS	GLN	conflict	GB 2072131
H	40	THR	MET	conflict	GB 2072131

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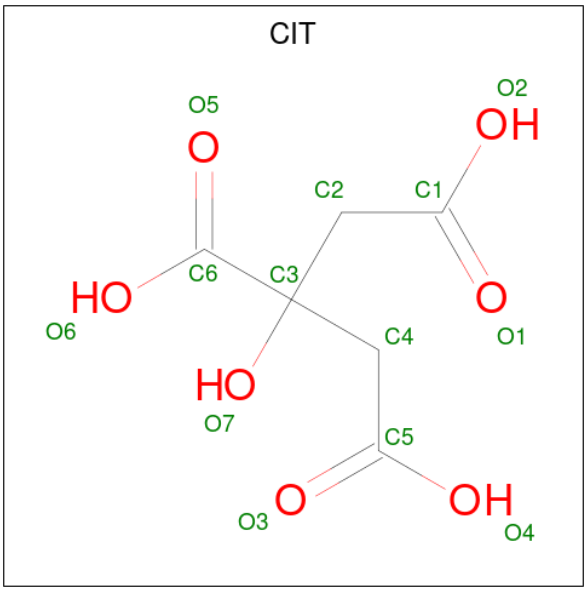
Chain	Residue	Modelled	Actual	Comment	Reference
H	45	PHE	LEU	conflict	GB 2072131
H	48	MET	ILE	conflict	GB 2072131
H	51	ILE	LEU	conflict	GB 2072131
H	53	TYR	GLN	conflict	GB 2072131
H	58	THR	GLU	conflict	GB 2072131
H	61	ASP	GLU	conflict	GB 2072131
H	76	SER	THR	conflict	GB 2072131
H	?	-	THR	deletion	GB 2072131
H	?	-	TRP	deletion	GB 2072131
H	?	-	GLY	deletion	GB 2072131
H	94	ARG	GLY	conflict	GB 2072131
H	95	ARG	ASN	conflict	GB 2072131
H	100A	TRP	ALA	conflict	GB 2072131
H	100C	PHE	-	insertion	GB 2072131
H	101	ASP	-	insertion	GB 2072131
H	102	VAL	-	insertion	GB 2072131
H	105	THR	GLN	conflict	GB 2072131
H	109	VAL	LEU	conflict	GB 2072131
H	?	-	SER	deletion	GB 2072131
H	?	-	ALA	deletion	GB 2072131
H	?	-	ALA	deletion	GB 2072131
H	?	-	GLN	deletion	GB 2072131
H	?	-	THR	deletion	GB 2072131
H	?	-	ASN	deletion	GB 2072131
H	187	PRO	THR	conflict	GB 2072131
H	188	ARG	TRP	conflict	GB 2072131

- Molecule 3 is a protein called CHOLERA TOXIN PEPTIDE 3 (CTP3).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	12	92	56	18	18	0	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	66	Total O 66 66	0	0
5	H	78	Total O 78 78	0	0
5	P	7	Total O 7 7	0	0

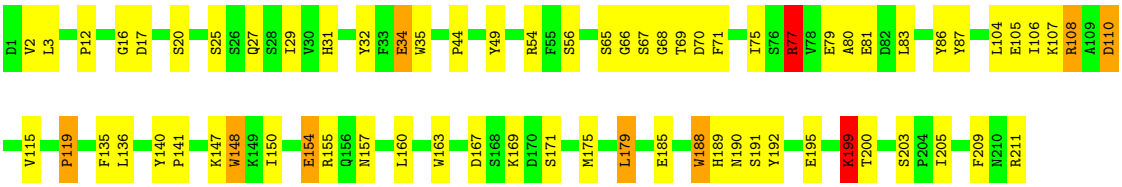
3 Residue-property plots (i)

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.

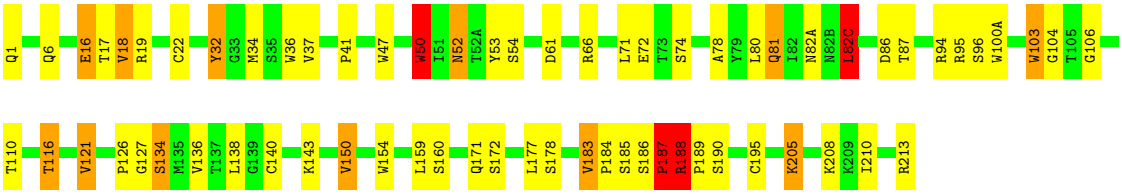
• Molecule 1: IGG1 TE33 FAB (LIGHT CHAIN)

Chain L: 68% 28%



• Molecule 2: IGG1 TE33 FAB (HEAVY CHAIN)

Chain H: 68% 24% 6%



• Molecule 3: CHOLERA TOXIN PEPTIDE 3 (CTP3)

Chain P: 47% 33% 20%

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 2	Depositor
Cell constants a, b, c, α, β, γ	104.15Å 110.61Å 40.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3541	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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: CIT

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	L	0.85	0/1723	1.68	33/2337 (1.4%)
2	H	0.92	2/1651 (0.1%)	1.77	39/2258 (1.7%)
3	P	0.79	0/93	1.87	2/123 (1.6%)
All	All	0.89	2/3467 (0.1%)	1.73	74/4718 (1.6%)

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
2	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	50	TRP	CG-CD2	-5.21	1.34	1.43
2	H	126	PRO	C-N	-5.04	1.24	1.33

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	188	TRP	CG-CD2-CE3	13.54	146.08	133.90
2	H	188	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	L	108	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	L	188	TRP	CB-CG-CD1	-11.38	112.21	127.00
1	L	175	MET	CG-SD-CE	-9.34	85.25	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	186	SER	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	L	1681	0	1617	27	0
2	H	1604	0	1570	33	1
3	P	92	0	92	3	0
4	L	13	0	5	1	0
5	H	78	0	0	7	0
5	L	66	0	0	2	1
5	P	7	0	0	0	0
All	All	3541	0	3284	60	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 9.

The worst 5 of 60 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)
2:H:116:THR:CG2	5:H:268:HOH:O	1.82	1.26
2:H:116:THR:HG21	5:H:268:HOH:O	1.43	1.07
2:H:143:LYS:NZ	5:H:267:HOH:O	1.80	1.04
2:H:116:THR:HG22	5:H:268:HOH:O	1.57	0.88
1:L:141:PRO:HD2	1:L:199:LYS:HD3	1.63	0.80

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)
2:H:159:LEU:CD1	5:L:256:HOH:O[1_556]	2.14	0.06

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	L	214/216 (99%)	202 (94%)	8 (4%)	4 (2%)	8 7
2	H	206/210 (98%)	194 (94%)	10 (5%)	2 (1%)	15 17
3	P	10/15 (67%)	8 (80%)	2 (20%)	0	100 100
All	All	430/441 (98%)	404 (94%)	20 (5%)	6 (1%)	11 11

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	68	GLY
2	H	172	SER
1	L	77	ARG
1	L	199	LYS
2	H	41	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	L	194/194 (100%)	174 (90%)	20 (10%)	7 8
2	H	182/182 (100%)	158 (87%)	24 (13%)	4 4
3	P	11/13 (85%)	10 (91%)	1 (9%)	9 11
All	All	387/389 (100%)	342 (88%)	45 (12%)	5 6

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	74	SER
2	H	140	CYS
2	H	80	LEU
2	H	121	VAL
2	H	160	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	L	38	GLN
1	L	42	GLN
2	H	6	GLN
2	H	52	ASN
2	H	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
4	CIT	L	212	-	12,12,12	1.43	2 (16%)	17,17,17	4.15	11 (64%)

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
4	CIT	L	212	-	-	4/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	212	CIT	O7-C3	-2.12	1.39	1.43
4	L	212	CIT	O4-C5	-2.04	1.23	1.30

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	212	CIT	C4-C3-C2	-10.00	83.07	109.16
4	L	212	CIT	O7-C3-C4	-6.99	93.03	109.40
4	L	212	CIT	O7-C3-C2	6.98	125.73	109.40
4	L	212	CIT	O7-C3-C6	4.60	115.33	108.86
4	L	212	CIT	C3-C4-C5	3.85	123.12	113.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	212	CIT	C2-C3-C6-O5
4	L	212	CIT	C2-C3-C6-O6
4	L	212	CIT	C1-C2-C3-O7
4	L	212	CIT	C3-C4-C5-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	212	CIT	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 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.