



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 07:51 PM GMT

PDB ID : 1XTC
Title : CHOLERA TOXIN
Authors : Zhang, R.-G.; Westbrook, E.
Deposited on : 1996-01-10
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

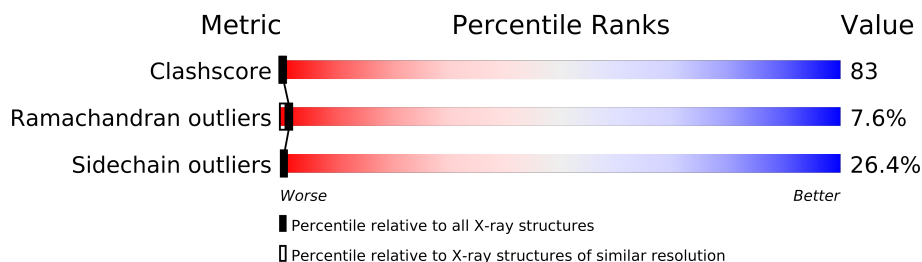
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	
2	C	46	
3	D	103	
3	E	103	
3	F	103	
3	G	103	
3	H	103	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6135 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CHOLERA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1532	961	279	288	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	LEU	ILE	CONFLICT	UNP P01555
A	88	LEU	ILE	CONFLICT	UNP P01555

- Molecule 2 is a protein called CHOLERA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	45	Total	C	N	O	S	0	0	0
			370	227	64	78	1			

- Molecule 3 is a protein called CHOLERA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	E	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	F	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	G	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	H	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	54	SER	GLY	CONFLICT	UNP P01556
D	87	THR	VAL	CONFLICT	UNP P01556
E	54	SER	GLY	CONFLICT	UNP P01556
E	87	THR	VAL	CONFLICT	UNP P01556
F	54	SER	GLY	CONFLICT	UNP P01556
F	87	THR	VAL	CONFLICT	UNP P01556
G	54	SER	GLY	CONFLICT	UNP P01556
G	87	THR	VAL	CONFLICT	UNP P01556
H	54	SER	GLY	CONFLICT	UNP P01556
H	87	THR	VAL	CONFLICT	UNP P01556

- Molecule 4 is water.

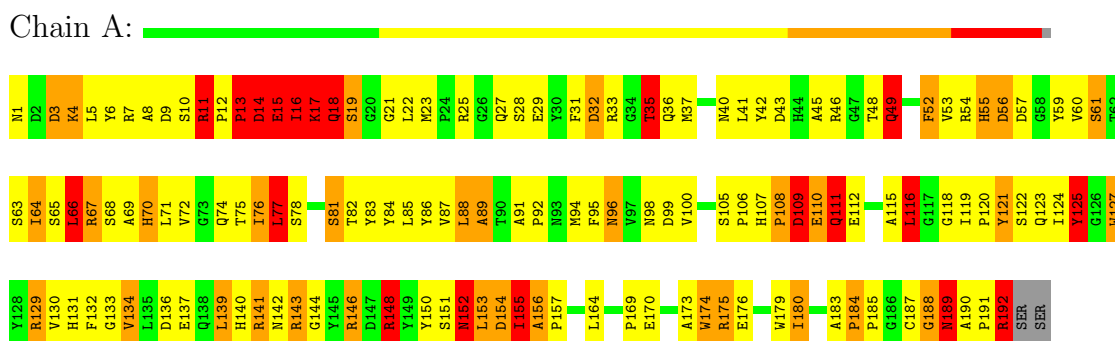
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	C	4	Total O 4 4	0	0
4	D	24	Total O 24 24	0	0
4	E	19	Total O 19 19	0	0
4	F	19	Total O 19 19	0	0
4	G	19	Total O 19 19	0	0
4	H	18	Total O 18 18	0	0

3 Residue-property plots

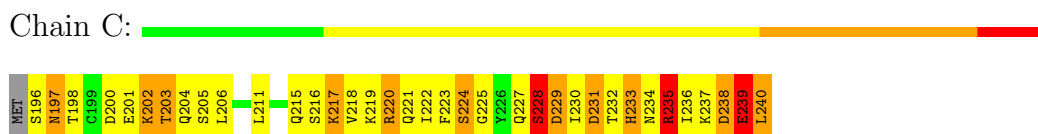
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

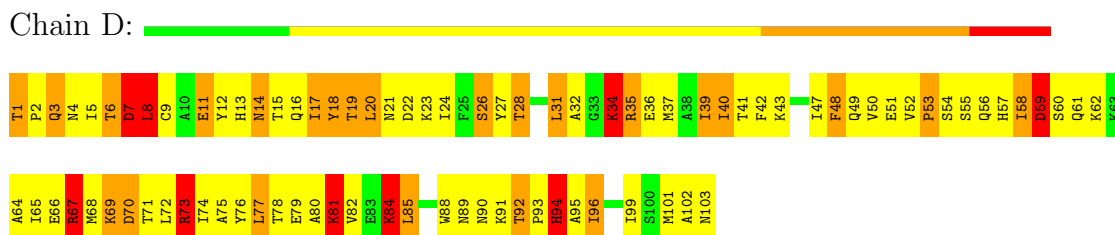
• Molecule 1: CHOLERA TOXIN



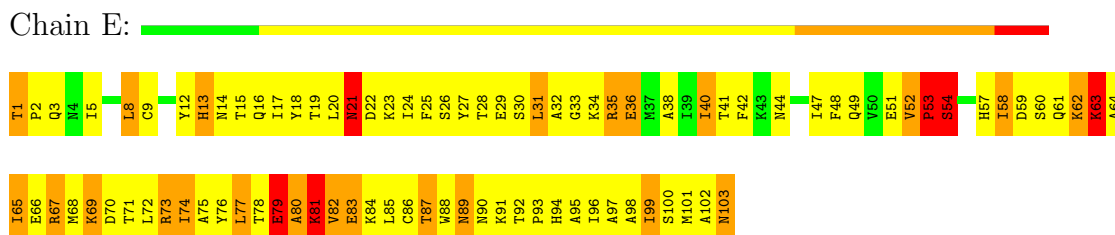
• Molecule 2: CHOLERA TOXIN



• Molecule 3: CHOLERA TOXIN



• Molecule 3: CHOLERA TOXIN



• Molecule 3: CHOLERA TOXIN

Chain F: 



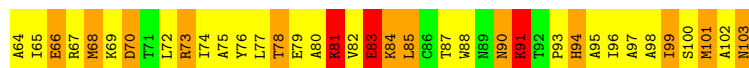
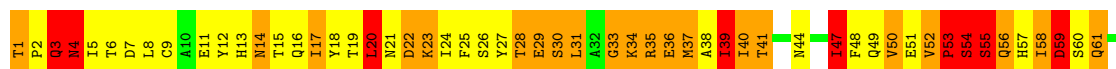
• Molecule 3: CHOLERA TOXIN

Chain G: 



• Molecule 3: CHOLERA TOXIN

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.00Å 92.20Å 60.60Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6135	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.97	2/1581 (0.1%)	1.87	42/2153 (2.0%)
2	C	1.04	0/374	1.51	5/498 (1.0%)
3	D	0.95	0/833	1.71	9/1125 (0.8%)
3	E	0.99	0/833	1.75	12/1125 (1.1%)
3	F	0.96	0/833	1.72	11/1125 (1.0%)
3	G	1.15	2/833 (0.2%)	1.79	22/1125 (2.0%)
3	H	0.98	1/833 (0.1%)	1.91	17/1125 (1.5%)
All	All	1.00	5/6120 (0.1%)	1.79	118/8276 (1.4%)

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	A	0	15
2	C	0	2
3	D	0	8
3	E	0	2
3	F	0	4
3	G	0	9
3	H	0	10
All	All	0	50

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	THR	C-N	12.81	1.58	1.34
1	A	19	SER	C-N	10.39	1.51	1.33
3	H	53	PRO	C-N	-5.56	1.21	1.34
1	A	16	ILE	C-N	-5.27	1.22	1.34
3	G	45	GLY	N-CA	-5.01	1.38	1.46

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	53	PRO	C-N-CA	19.24	169.80	121.70
3	H	54	SER	C-N-CA	18.47	167.88	121.70
1	A	15	GLU	O-C-N	-17.35	94.94	122.70
3	F	73	ARG	CD-NE-CZ	15.69	145.56	123.60
1	A	13	PRO	C-N-CA	14.48	157.89	121.70

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain
1	A	13	PRO	Peptide
1	A	14	ASP	Mainchain
1	A	16	ILE	Mainchain
1	A	17	LYS	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1532	0	1419	201	2
2	C	370	0	355	93	0
3	D	819	0	823	209	0
3	E	819	0	822	226	2
3	F	819	0	823	158	0
3	G	819	0	823	117	0
3	H	819	0	821	133	0
4	A	35	0	0	6	0
4	C	4	0	0	1	0
4	D	24	0	0	6	0
4	E	19	0	0	1	0
4	F	19	0	0	1	0
4	G	19	0	0	4	0
4	H	18	0	0	0	0
All	All	6135	0	5886	983	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 83.

The worst 5 of 983 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:ARG:NH2	1:A:131:HIS:HB3	1.25	1.47
2:C:235:ARG:HH22	2:C:239:GLU:CB	1.35	1.37
3:F:70:ASP:O	3:F:74:ILE:HG23	1.20	1.32
2:C:235:ARG:NH2	2:C:239:GLU:CB	1.90	1.30
1:A:170:GLU:HB3	1:A:192:ARG:NH2	1.47	1.29

All (2) 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	Distance(Å)	Clash(Å)
1:A:192:ARG:O	3:E:14:ASN:ND2[1_655]	1.74	0.46
1:A:192:ARG:CD	3:E:13:HIS:NE2[1_655]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	190/194 (98%)	149 (78%)	22 (12%)	19 (10%)	1	0
2	C	43/46 (94%)	40 (93%)	2 (5%)	1 (2%)	10	10
3	D	101/103 (98%)	81 (80%)	11 (11%)	9 (9%)	1	0
3	E	101/103 (98%)	73 (72%)	18 (18%)	10 (10%)	1	0
3	F	101/103 (98%)	87 (86%)	8 (8%)	6 (6%)	2	1
3	G	101/103 (98%)	80 (79%)	15 (15%)	6 (6%)	2	1
3	H	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	3	2
All	All	738/755 (98%)	593 (80%)	89 (12%)	56 (8%)	2	0

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	49	GLN
1	A	77	LEU
1	A	111	GLN
1	A	155	ILE

5.3.2 Protein sidechains ⓘ

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	158/160 (99%)	123 (78%)	35 (22%)	1	1
2	C	43/44 (98%)	27 (63%)	16 (37%)	0	0
3	D	90/90 (100%)	67 (74%)	23 (26%)	1	1
3	E	90/90 (100%)	70 (78%)	20 (22%)	1	1
3	F	90/90 (100%)	65 (72%)	25 (28%)	0	0
3	G	90/90 (100%)	73 (81%)	17 (19%)	2	2
3	H	90/90 (100%)	54 (60%)	36 (40%)	0	0
All	All	651/654 (100%)	479 (74%)	172 (26%)	1	0

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	16	GLN
3	F	15	THR
3	H	59	ASP
3	E	35	ARG
3	E	81	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	103	ASN
3	E	44	ASN
3	H	57	HIS
3	E	13	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	14	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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