



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:54 AM UTC

PDB ID : 1F5T / pdb_00001f5t
Title : DIPHTHERIA TOX REPRESSOR (C102D MUTANT) COMPLEXED
WITH NICKEL AND DTXR CONSENSUS BINDING SEQUENCE
Authors : Chen, S.; White, A.; Love, J.; Murphy, J.R.; Ringe, D.
Deposited on : 2000-06-15
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

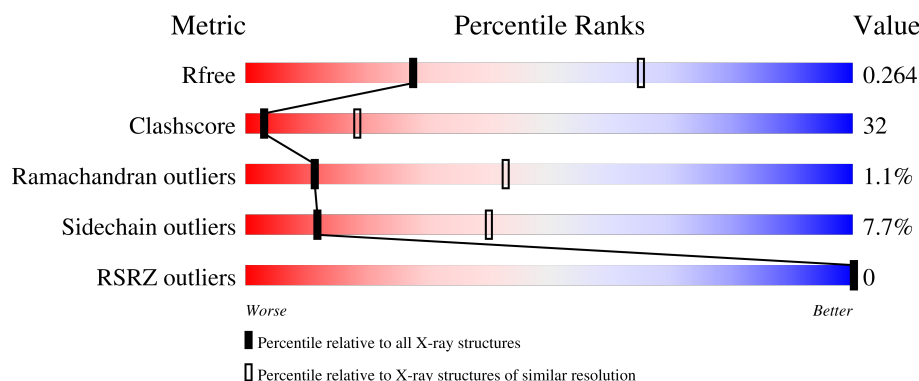
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

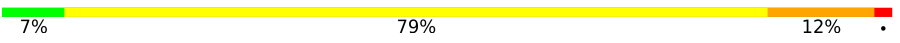
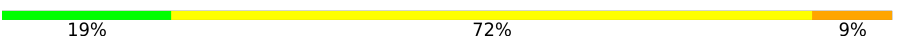
The reported resolution of this entry is 3.00 Å.

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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	43	
2	F	43	
3	A	121	
3	B	121	
3	C	121	

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Mol	Chain	Length	Quality of chain
3	D	121	 A horizontal bar chart showing the quality of chain D. The bar is divided into three segments: green (54%), yellow (36%), and orange (9%). The segments are labeled with their respective percentages: 54%, 36%, and 9%. The bar ends with a small black dot.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5621 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 DNA chain called 43MER DNA CONTAINING DXTR CONSENSUS BINDING SEQUENCE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	43	Total	C	N	O	P	0	0	0
			877	420	159	256	42			

- Molecule 2 is a DNA chain called 43MER DNA CONTAINING DXTR CONSENSUS BINDING SEQUENCE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	43	Total	C	N	O	P	0	0	0
			880	421	161	256	42			

- Molecule 3 is a protein called DIPHTHERIA TOXIN REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	120	Total	C	N	O	S	0	0	0
			963	593	178	187	5			
3	B	120	Total	C	N	O	S	0	0	0
			963	593	178	187	5			
3	C	120	Total	C	N	O	S	0	0	0
			963	593	178	187	5			
3	D	120	Total	C	N	O	S	0	0	0
			963	593	178	187	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1102	ASP	CYS	engineered mutation	UNP P33120
B	2102	ASP	CYS	engineered mutation	UNP P33120
C	3102	ASP	CYS	engineered mutation	UNP P33120
D	4102	ASP	CYS	engineered mutation	UNP P33120

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ni 2	0	0
4	B	2	Total 2	Ni 2	0	0
4	C	2	Total 2	Ni 2	0	0
4	D	2	Total 2	Ni 2	0	0

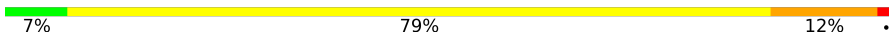
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	1	Total 1	O 1	0	0

3 Residue-property plots

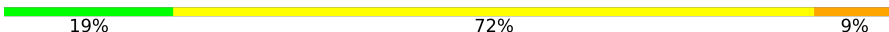
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

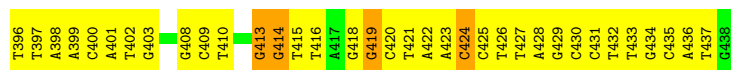
• Molecule 1: 43MER DNA CONTAINING DXTR CONSENSUS BINDING SEQUENCE

Chain E: 



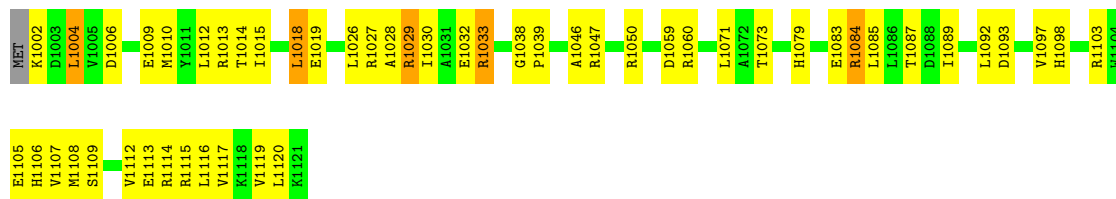
• Molecule 2: 43MER DNA CONTAINING DXTR CONSENSUS BINDING SEQUENCE

Chain F: 



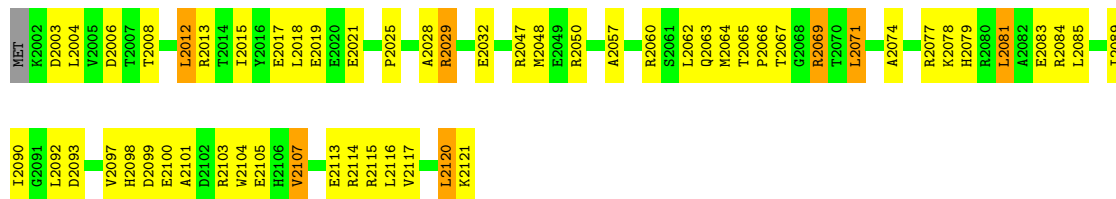
• Molecule 3: DIPHTHERIA TOXIN REPRESSOR

Chain A: 



• Molecule 3: DIPHTHERIA TOXIN REPRESSOR

Chain B: 



• Molecule 3: DIPHTHERIA TOXIN REPRESSOR

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	116.18Å 116.18Å 142.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 3.00 48.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.83-3.00) 95.9 (48.83-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.01Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.245 , 0.273 0.242 , 0.264	Depositor DCC
R_{free} test set	1877 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5621	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NI

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	0.38	0/983	0.77	1/1515 (0.1%)
2	F	0.37	0/987	0.82	0/1522
3	A	0.49	0/972	0.95	3/1310 (0.2%)
3	B	0.47	0/972	0.93	0/1310
3	C	0.48	0/972	0.99	3/1310 (0.2%)
3	D	0.49	0/972	0.97	4/1310 (0.3%)
All	All	0.45	0/5858	0.91	11/8277 (0.1%)

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	E	0	6
2	F	0	4
All	All	0	10

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4097	VAL	N-CA-C	8.80	118.87	110.42
3	C	3033	ARG	N-CA-C	7.50	119.10	111.07
3	A	1097	VAL	N-CA-C	6.57	118.16	111.00
3	C	3003	ASP	N-CA-C	-6.26	104.53	111.36
3	D	4094	ILE	N-CA-C	5.90	117.34	110.62

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	310	DG	Sidechain
1	E	311	DG	Sidechain
1	E	316	DC	Sidechain
1	E	317	DC	Sidechain
1	E	321	DC	Sidechain

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	877	0	487	92	0
2	F	880	0	487	65	0
3	A	963	0	988	45	0
3	B	963	0	988	51	0
3	C	963	0	988	47	0
3	D	963	0	988	59	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	5621	0	4926	331	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 32.

The worst 5 of 331 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:331:DG:H2''	1:E:332:DC:H5''	1.40	1.02
1:E:315:DG:H2''	1:E:316:DC:H5'	1.41	1.00
1:E:299:DT:H1'	1:E:300:DG:H5'	1.44	0.97
1:E:306:DC:H2'	1:E:307:DT:H72	1.44	0.96
1:E:328:DC:H2'	1:E:329:DT:H71	1.47	0.96

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	
3	A	118/121 (98%)	104 (88%)	14 (12%)	0	100	100
3	B	118/121 (98%)	109 (92%)	7 (6%)	2 (2%)	7	32
3	C	118/121 (98%)	105 (89%)	10 (8%)	3 (2%)	4	23
3	D	118/121 (98%)	112 (95%)	6 (5%)	0	100	100
All	All	472/484 (98%)	430 (91%)	37 (8%)	5 (1%)	11	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	2120	LEU
3	C	3057	ALA
3	C	3119	VAL
3	B	2097	VAL
3	C	3091	GLY

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	
3	A	107/108 (99%)	100 (94%)	7 (6%)	15	47
3	B	107/108 (99%)	98 (92%)	9 (8%)	10	37
3	C	107/108 (99%)	99 (92%)	8 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	107/108 (99%)	98 (92%)	9 (8%)	10	37
All	All	428/432 (99%)	395 (92%)	33 (8%)	12	40

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	4062	LEU
3	D	4071	LEU
3	D	4115	ARG
3	B	2071	LEU
3	B	2069	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	2098	HIS
3	C	3043	GLN
3	C	3098	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	43/43 (100%)	-1.29	0 100 100	25, 64, 106, 106	0
2	F	43/43 (100%)	-1.28	0 100 100	24, 66, 106, 106	0
3	A	120/121 (99%)	-1.63	0 100 100	22, 44, 75, 88	0
3	B	120/121 (99%)	-1.63	0 100 100	23, 45, 77, 85	0
3	C	120/121 (99%)	-1.61	0 100 100	23, 45, 74, 94	0
3	D	120/121 (99%)	-1.62	0 100 100	21, 45, 77, 95	0
All	All	566/570 (99%)	-1.57	0 100 100	21, 45, 92, 106	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NI	A	251	1/1	1.00	0.00	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NI	A	252	1/1	1.00	0.03	49,49,49,49	0
4	NI	B	253	1/1	1.00	0.00	49,49,49,49	0
4	NI	B	254	1/1	1.00	0.02	49,49,49,49	0
4	NI	C	255	1/1	1.00	0.00	49,49,49,49	0
4	NI	C	256	1/1	1.00	0.02	49,49,49,49	0
4	NI	D	257	1/1	1.00	0.00	49,49,49,49	0
4	NI	D	258	1/1	1.00	0.03	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.