



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:23 PM BST

PDB ID : 6LTY  
Title : DNA bound antitoxin HigA3  
Authors : Park, J.Y.; Lee, B.J.  
Deposited on : 2020-01-23  
Resolution : 3.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

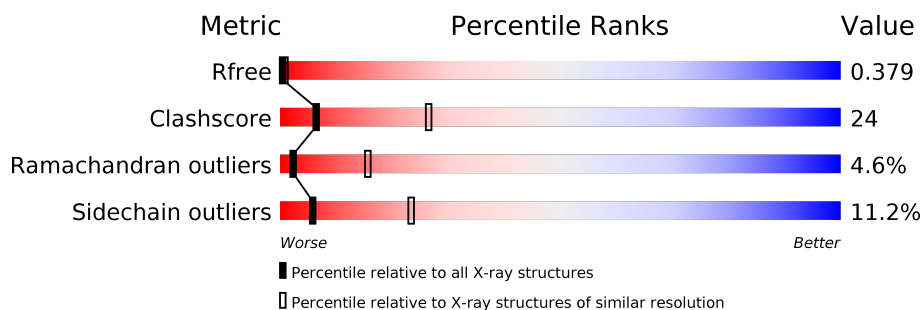
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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))
$R_{free}$	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	117	
1	B	117	
2	C	20	
3	D	20	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1988 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 Putative antitoxin HigA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			584	363	111	109	1			
1	B	78	Total	C	N	O	S	0	0	0
			584	363	111	109	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	-	expression tag	UNP O53333
A	111	GLU	-	expression tag	UNP O53333
A	112	HIS	-	expression tag	UNP O53333
A	113	HIS	-	expression tag	UNP O53333
A	114	HIS	-	expression tag	UNP O53333
A	115	HIS	-	expression tag	UNP O53333
A	116	HIS	-	expression tag	UNP O53333
A	117	HIS	-	expression tag	UNP O53333
B	110	LEU	-	expression tag	UNP O53333
B	111	GLU	-	expression tag	UNP O53333
B	112	HIS	-	expression tag	UNP O53333
B	113	HIS	-	expression tag	UNP O53333
B	114	HIS	-	expression tag	UNP O53333
B	115	HIS	-	expression tag	UNP O53333
B	116	HIS	-	expression tag	UNP O53333
B	117	HIS	-	expression tag	UNP O53333

- Molecule 2 is a DNA chain called DNA (5'-D(P\*CP\*CP\*AP\*CP\*GP\*AP\*GP\*AP\*TP\*AP\*TP\*AP\*AP\*CP\*CP\*TP\*AP\*GP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			411	195	81	115	20			

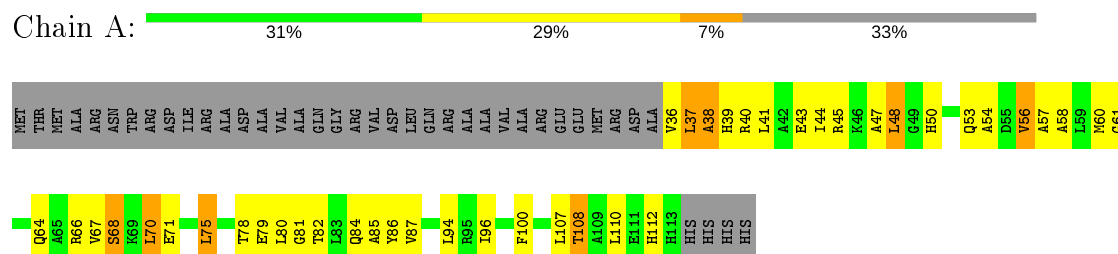
- Molecule 3 is a DNA chain called DNA (5'-D(P\*CP\*TP\*CP\*TP\*AP\*GP\*GP\*TP\*TP\*AP\*TP\*AP\*TP\*CP\*TP\*CP\*GP\*TP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total	C	N	O	P	0	0	0
			409	196	68	125	20			

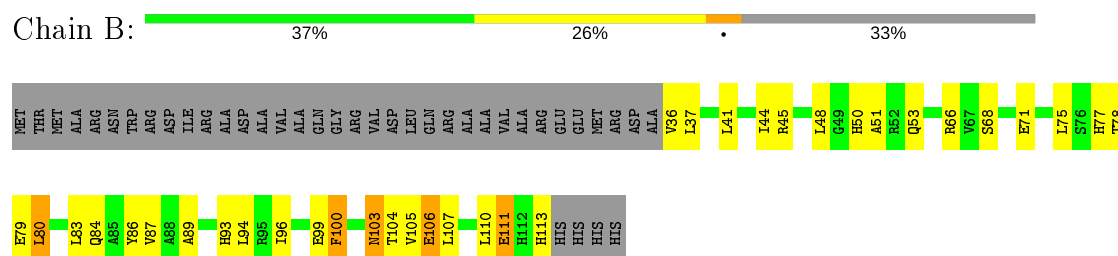
### 3 Residue-property plots [i](#)

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.

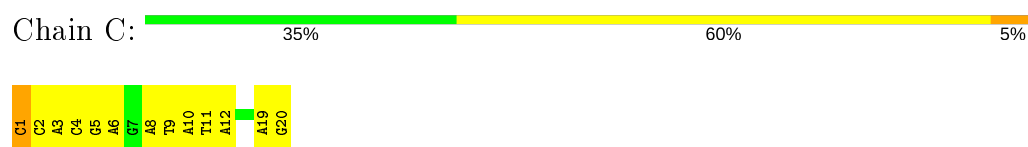
#### • Molecule 1: Putative antitoxin HigA3



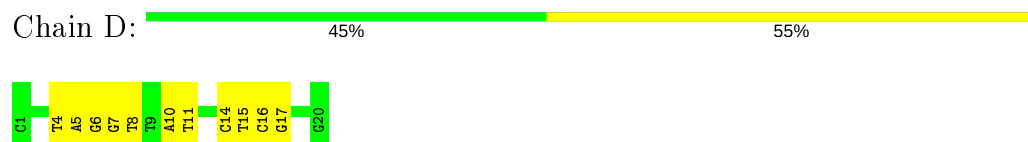
#### • Molecule 1: Putative antitoxin HigA3



#### • Molecule 2: DNA (5'-D(P\*CP\*CP\*AP\*CP\*GP\*AP\*GP\*AP\*TP\*AP\*TP\*AP\*AP\*CP\*CP\*T P\*AP\*GP\*AP\*G)-3')



#### • Molecule 3: DNA (5'-D(P\*CP\*TP\*CP\*TP\*AP\*GP\*GP\*TP\*TP\*AP\*TP\*AP\*TP\*CP\*TP\*C P\*GP\*TP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.61Å 101.81Å 58.03Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	41.79 – 3.28 41.79 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.79-3.28) 99.3 (41.79-3.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.277 , 0.326 0.302 , 0.379	Depositor DCC
$R_{free}$ test set	338 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.8	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 314.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.115 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	1988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.82	0/591	0.97	0/798
1	B	0.82	0/591	0.92	0/798
2	C	0.44	0/462	0.83	1/710 (0.1%)
3	D	0.38	0/456	0.77	0/702
All	All	0.68	0/2100	0.88	1/3008 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	DC	C1'-O4'-C4'	-5.46	104.64	110.10

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	A	584	0	590	46	0
1	B	584	0	590	37	0
2	C	411	0	224	12	0
3	D	409	0	229	9	0
All	All	1988	0	1633	83	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 24.

All (83) 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:A:100:PHE:CD1	1:B:48:LEU:HD11	2.19	0.77
1:A:87:VAL:HG11	1:A:94:LEU:HB2	1.67	0.74
2:C:8:DA:H2'	2:C:9:DT:C6	2.23	0.73
1:B:45:ARG:HG3	1:B:51:ALA:HB3	1.70	0.73
2:C:19:DA:H2''	2:C:20:DG:H8	1.54	0.72
1:B:100:PHE:HB2	1:B:103:ASN:O	1.90	0.71
1:A:100:PHE:CE1	1:B:48:LEU:HD11	2.27	0.69
1:A:68:SER:HB2	3:D:4:DT:OP2	1.98	0.64
1:A:44:ILE:HD13	1:B:105:VAL:HG21	1.79	0.63
1:A:66:ARG:NH2	2:C:12:DA:OP2	2.31	0.63
1:B:99:GLU:HA	1:B:104:THR:HG23	1.81	0.62
1:A:80:LEU:HD12	1:B:78:THR:HB	1.82	0.61
1:A:79:GLU:OE1	1:B:77:HIS:HA	2.02	0.60
1:A:54:ALA:HA	1:A:64:GLN:HG2	1.83	0.60
1:A:45:ARG:NH1	1:A:71:GLU:OE2	2.33	0.59
1:A:41:LEU:O	1:A:44:ILE:HG22	2.03	0.59
3:D:6:DG:H2'	3:D:7:DG:C8	2.39	0.58
1:B:45:ARG:NH2	1:B:53:GLN:HE21	2.02	0.57
1:B:86:TYR:O	1:B:89:ALA:HB3	2.05	0.56
1:A:81:GLY:HA2	1:A:84:GLN:HB3	1.87	0.56
1:B:80:LEU:H	1:B:80:LEU:HD23	1.71	0.56
1:B:41:LEU:HB2	1:B:71:GLU:HG2	1.88	0.55
1:A:44:ILE:CD1	1:B:105:VAL:HG21	2.36	0.55
1:A:70:LEU:HD21	1:A:82:THR:CG2	2.37	0.54
1:B:84:GLN:HA	1:B:84:GLN:OE1	2.07	0.54
1:B:45:ARG:NH1	1:B:71:GLU:OE2	2.34	0.54
1:A:82:THR:O	1:A:85:ALA:HB3	2.07	0.54
1:A:66:ARG:HE	2:C:12:DA:C2'	2.20	0.54
1:A:68:SER:O	1:A:71:GLU:N	2.42	0.53
1:B:66:ARG:NH2	3:D:14:DC:O5'	2.41	0.53
1:A:96:ILE:CD1	1:B:96:ILE:HG12	2.39	0.53
2:C:5:DG:H2''	2:C:6:DA:C5'	2.41	0.51
1:B:36:VAL:O	1:B:36:VAL:HG22	2.09	0.51
1:B:87:VAL:HG21	1:B:94:LEU:HB2	1.93	0.51
1:B:86:TYR:O	1:B:89:ALA:N	2.44	0.51
1:B:66:ARG:HD3	3:D:15:DT:H73	1.92	0.51
1:A:75:LEU:HD11	1:B:107:LEU:HD12	1.93	0.51
1:A:100:PHE:CE1	1:B:48:LEU:CD1	2.95	0.49
1:A:78:THR:O	1:B:79:GLU:HA	2.12	0.49
1:B:45:ARG:HH22	1:B:53:GLN:HE21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:O	1:A:61:GLY:N	2.46	0.49
1:A:38:ALA:HA	1:B:106:GLU:O	2.13	0.49
1:A:44:ILE:HD12	1:A:47:ALA:HB3	1.95	0.49
2:C:4:DC:H2''	2:C:5:DG:H5''	1.94	0.49
3:D:14:DC:C5	3:D:15:DT:H72	2.48	0.49
1:B:50:HIS:O	1:B:50:HIS:CG	2.65	0.48
2:C:5:DG:H2''	2:C:6:DA:H5'	1.94	0.48
1:B:41:LEU:O	1:B:44:ILE:HG12	2.14	0.48
2:C:1:DC:H6	2:C:2:DC:C5	2.32	0.48
1:B:80:LEU:O	1:B:83:LEU:HB3	2.13	0.48
3:D:16:DC:H2'	3:D:17:DG:C8	2.49	0.47
1:A:108:THR:OG1	1:A:108:THR:O	2.32	0.47
2:C:3:DA:C4	2:C:4:DC:C5	3.02	0.47
1:A:57:ALA:HB2	1:A:67:VAL:HG21	1.96	0.47
1:A:40:ARG:O	1:A:43:GLU:HB2	2.15	0.47
1:B:106:GLU:OE1	1:B:107:LEU:N	2.48	0.46
1:A:56:VAL:O	1:A:57:ALA:C	2.54	0.46
1:A:66:ARG:HE	2:C:12:DA:H2'	1.81	0.45
1:A:70:LEU:HD21	1:A:82:THR:HG21	1.99	0.45
1:B:110:LEU:O	1:B:111:GLU:CB	2.65	0.45
3:D:7:DG:H2''	3:D:8:DT:H5''	1.99	0.44
1:A:53:GLN:O	1:A:57:ALA:HB2	2.17	0.44
1:B:99:GLU:O	1:B:100:PHE:CD1	2.71	0.44
1:A:80:LEU:HD12	1:B:78:THR:O	2.18	0.43
1:A:41:LEU:HB2	1:A:71:GLU:HG2	2.00	0.43
1:A:39:HIS:HB2	1:A:43:GLU:OE2	2.18	0.42
3:D:5:DA:H2''	3:D:6:DG:OP2	2.19	0.42
1:A:80:LEU:CD2	1:B:80:LEU:HB3	2.49	0.42
1:A:56:VAL:O	1:A:58:ALA:N	2.52	0.42
1:B:99:GLU:O	1:B:100:PHE:CG	2.72	0.42
1:A:96:ILE:HD12	1:B:96:ILE:HG12	2.01	0.42
1:A:37:LEU:HG	1:A:38:ALA:H	1.84	0.42
1:A:68:SER:O	1:A:70:LEU:N	2.52	0.42
2:C:1:DC:C6	2:C:2:DC:C5	3.08	0.42
1:A:45:ARG:HH12	1:A:71:GLU:CD	2.20	0.42
1:A:44:ILE:O	1:A:47:ALA:HB3	2.21	0.41
1:A:60:MET:HE1	1:A:86:TYR:HD1	1.84	0.41
1:A:107:LEU:HD12	1:B:75:LEU:CD2	2.51	0.41
2:C:10:DA:H1'	2:C:11:DT:C4	2.56	0.41
1:A:44:ILE:HA	1:A:47:ALA:HB3	2.02	0.41
1:A:44:ILE:O	1:A:48:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:DA:H2''	3:D:11:DT:C5	2.56	0.40
1:A:110:LEU:C	1:A:110:LEU:HD13	2.42	0.40

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	
1	A	76/117 (65%)	52 (68%)	20 (26%)	4 (5%)	2	12
1	B	76/117 (65%)	61 (80%)	12 (16%)	3 (4%)	3	19
All	All	152/234 (65%)	113 (74%)	32 (21%)	7 (5%)	2	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	GLU
1	A	37	LEU
1	A	112	HIS
1	B	37	LEU
1	A	38	ALA
1	A	48	LEU
1	B	100	PHE

### 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	A	58/88 (66%)	51 (88%)	7 (12%)	5	21
1	B	58/88 (66%)	52 (90%)	6 (10%)	7	26
All	All	116/176 (66%)	103 (89%)	13 (11%)	6	23

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	50	HIS
1	A	56	VAL
1	A	68	SER
1	A	70	LEU
1	A	75	LEU
1	A	108	THR
1	B	68	SER
1	B	80	LEU
1	B	93	HIS
1	B	103	ASN
1	B	106	GLU
1	B	113	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	53	GLN
1	B	64	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

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 [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.