



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:39 AM BST

PDB ID : 6ML2
Title : ZBTB24 Zinc Fingers 4-8 with 19+1mer DNA Oligonucleotide (Sequence 1)
Authors : Horton, J.R.; Cheng, X.; Ren, R.
Deposited on : 2018-09-26
Resolution : 1.87 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

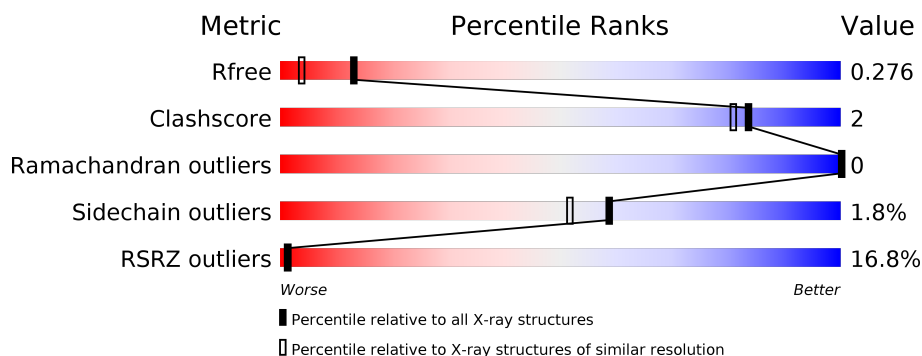
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	A	151	
2	E	20	
3	F	20	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1892 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 Zinc finger and BTB domain-containing protein 24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1048	651	197	187	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	GLY	-	expression tag	UNP Q80X44
A	371	PRO	-	expression tag	UNP Q80X44
A	372	LEU	-	expression tag	UNP Q80X44
A	373	GLY	-	expression tag	UNP Q80X44
A	374	SER	-	expression tag	UNP Q80X44
A	520	TYR	-	expression tag	UNP Q80X44

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			408	194	79	116	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	20	Total	C	N	O	P	0	0	0
			406	194	73	120	19			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Zn	0	0
			5	5		

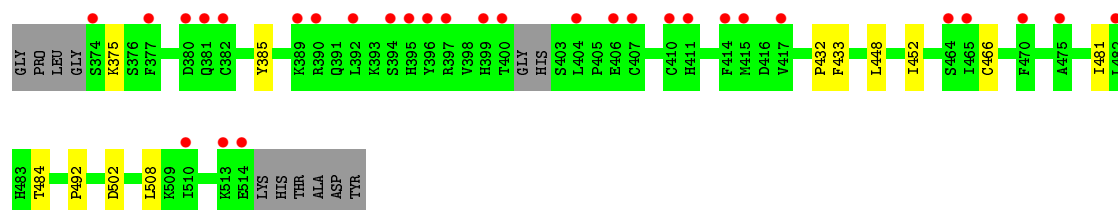
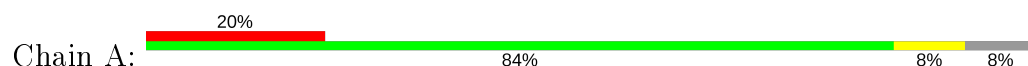
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total 16	O 16	0	0
5	E	8	Total 8	O 8	0	0
5	F	1	Total 1	O 1	0	0

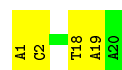
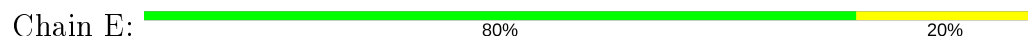
3 Residue-property plots [i](#)

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 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: Zinc finger and BTB domain-containing protein 24



- Molecule 2: DNA (5'-D(*AP*CP*GP*CP*AP*GP*GP*TP*CP*CP*TP*GP*GP*CP*AP*GP*CP*TP*AP*A)-3')



- Molecule 3: DNA (5'-D(*TP*TP*TP*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP*AP*CP*CP*TP*GP*CP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.06Å 68.62Å 49.48Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	38.23 – 1.87 34.31 – 1.87	Depositor EDS
% Data completeness (in resolution range)	73.7 (38.23-1.87) 67.4 (34.31-1.87)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, R_{free}	0.251 , 0.278 0.251 , 0.276	Depositor DCC
R_{free} test set	956 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1892	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.00% 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: ZN

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	0.27	0/1074	0.43	0/1438
2	E	0.61	0/458	0.88	0/705
3	F	0.59	0/454	0.92	0/699
All	All	0.45	0/1986	0.70	0/2842

There are no bond length outliers.

There are no bond angle outliers.

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	1048	0	958	5	0
2	E	408	0	225	2	0
3	F	406	0	227	1	0
4	A	5	0	0	0	0
5	A	16	0	0	0	0
5	E	8	0	0	0	0
5	F	1	0	0	0	0
All	All	1892	0	1410	8	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 2.

All (8) 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:E:1:DA:H4'	2:E:2:DC:H5'	1.88	0.55
1:A:492:PRO:HD2	1:A:508:LEU:HD21	1.96	0.48
3:F:3:DT:H2''	3:F:4:DA:C8	2.49	0.48
1:A:375:LYS:HB3	1:A:385:TYR:HB3	1.95	0.47
2:E:18:DT:H2''	2:E:19:DA:C8	2.49	0.47
1:A:448:LEU:O	1:A:452:ILE:HG12	2.17	0.44
1:A:481:ILE:O	1:A:484:THR:OG1	2.25	0.43
1:A:432:PRO:HG2	1:A:433:PHE:CE1	2.54	0.41

There are no symmetry-related clashes.

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	135/151 (89%)	133 (98%)	2 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	110/136 (81%)	108 (98%)	2 (2%)	59	52

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	466	CYS
1	A	502	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 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	A	139/151 (92%)	1.37	30 (21%) 0 0	35, 57, 94, 111	0
2	E	20/20 (100%)	0.55	0 100 100	35, 56, 89, 92	0
3	F	20/20 (100%)	0.39	0 100 100	43, 56, 85, 85	0
All	All	179/191 (93%)	1.17	30 (16%) 1 1	35, 57, 92, 111	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	LEU	7.2
1	A	415	MET	5.7
1	A	400	THR	5.0
1	A	397	ARG	4.5
1	A	465	ILE	4.3
1	A	390	ARG	4.2
1	A	396	TYR	3.9
1	A	392	LEU	3.9
1	A	380	ASP	3.8
1	A	406	GLU	3.6
1	A	399	HIS	3.4
1	A	514	GLU	3.2
1	A	394	SER	2.9
1	A	510	ILE	2.8
1	A	417	VAL	2.8
1	A	389	LYS	2.5
1	A	407	CYS	2.5
1	A	395	HIS	2.4
1	A	374	SER	2.4
1	A	381	GLN	2.3
1	A	414	PHE	2.3
1	A	464	SER	2.2
1	A	513	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	411	HIS	2.1
1	A	377	PHE	2.1
1	A	470	PHE	2.1
1	A	382	CYS	2.1
1	A	482	LEU	2.1
1	A	475	ALA	2.1
1	A	410	CYS	2.0

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 monosaccharides 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	ZN	A	603	1/1	0.95	0.13	44,44,44,44	0
4	ZN	A	604	1/1	0.95	0.10	59,59,59,59	0
4	ZN	A	602	1/1	0.97	0.13	52,52,52,52	0
4	ZN	A	605	1/1	0.98	0.12	48,48,48,48	0
4	ZN	A	601	1/1	0.99	0.07	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.