



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2017 – 08:52 pm GMT

PDB ID : 2DRP
Title : THE CRYSTAL STRUCTURE OF A TWO ZINC-FINGER PEPTIDE REVEALS AN EXTENSION TO THE RULES FOR ZINC-FINGER/DNA RECOGNITION
Authors : Fairall, L.; Schwabe, J.W.R.; Chapman, L.; Finch, J.T.; Rhodes, D.
Deposited on : 1994-06-06
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

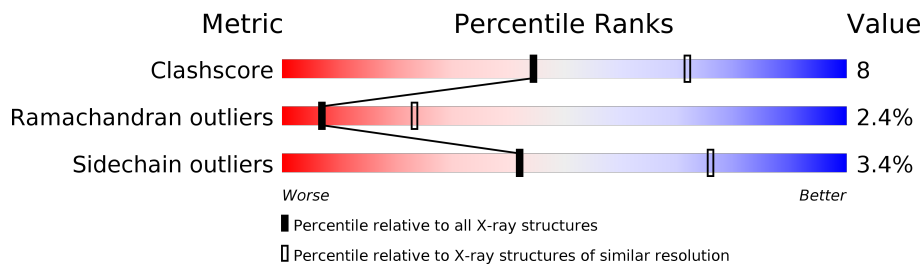
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	19	
1	E	19	
2	C	19	
2	F	19	
3	A	66	
3	D	66	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2670 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 DNA (5'-D(*CP*TP*AP*AP*TP*AP*AP*GP*GP*AP*TP*AP*AP*CP*GP*TP*C P*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	19	Total	C	N	O	P	0	0	0
			388	186	75	109	18			
1	E	19	Total	C	N	O	P	0	0	0
			388	186	75	109	18			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*GP*GP*AP*CP*GP*TP*TP*AP*TP*CP*CP*TP*TP*AP*T P*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	0	0
			383	186	63	116	18			
2	F	19	Total	C	N	O	P	0	0	0
			383	186	63	116	18			

- Molecule 3 is a protein called PROTEIN (TRAMTRACK DNA-BINDING DOMAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	63	Total	C	N	O	S	0	0	0
			525	335	99	85	6			
3	D	65	Total	C	N	O	S	0	0	0
			542	345	101	90	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is water.

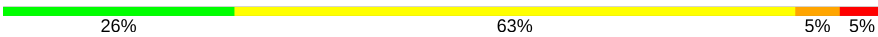
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	B	12	Total 12	O 12	0	0
5	C	9	Total 9	O 9	0	0
5	D	7	Total 7	O 7	0	0
5	E	8	Total 8	O 8	0	0
5	F	11	Total 11	O 11	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*TP*AP*AP*GP*GP*AP*TP*AP*AP*CP*GP*TP*C P*CP*G)-3')

Chain B: 



- Molecule 1: DNA (5'-D(*CP*TP*AP*AP*TP*AP*AP*GP*GP*AP*TP*AP*AP*CP*GP*TP*C P*CP*G)-3')

Chain E: 

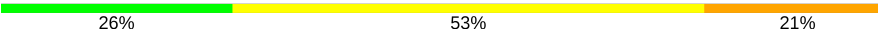


- Molecule 2: DNA (5'-D(*TP*CP*GP*GP*AP*CP*GP*TP*TP*AP*TP*CP*CP*TP*TP*AP*T P*TP*A)-3')

Chain C: 



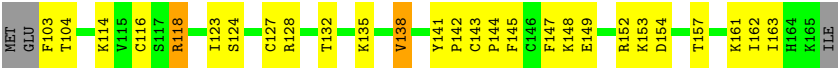
- Molecule 2: DNA (5'-D(*TP*CP*GP*GP*AP*CP*GP*TP*TP*AP*TP*CP*CP*TP*TP*AP*T P*TP*A)-3')

Chain F: 

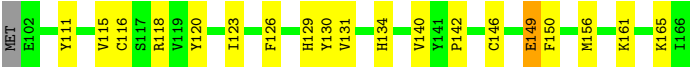


- Molecule 3: PROTEIN (TRAMTRACK DNA-BINDING DOMAIN)

Chain A: 



● Molecule 3: PROTEIN (TRAMTRACK DNA-BINDING DOMAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.70Å 64.60Å 117.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.2 (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2670	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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	B	1.29	1/436 (0.2%)	2.10	24/671 (3.6%)
1	E	1.21	2/436 (0.5%)	2.08	31/671 (4.6%)
2	C	1.29	1/427 (0.2%)	2.20	36/657 (5.5%)
2	F	1.31	2/427 (0.5%)	2.19	27/657 (4.1%)
3	A	0.50	0/541	0.68	0/725
3	D	0.54	0/558	0.65	0/750
All	All	1.05	6/2825 (0.2%)	1.76	118/4131 (2.9%)

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	B	0	1
3	D	0	1
All	All	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	DT	C5-C7	6.01	1.53	1.50
2	F	34	DT	C2'-C1'	-5.72	1.46	1.52
1	E	11	DT	C5-C7	5.59	1.53	1.50
1	E	16	DT	C5-C7	5.42	1.53	1.50
2	F	21	DT	C5-C7	5.15	1.53	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	28	DT	C1'-O4'-C4'	-9.44	100.66	110.10
1	E	16	DT	C1'-O4'-C4'	-9.31	100.78	110.10
1	B	14	DC	O4'-C4'-C3'	-9.13	100.52	106.00
1	B	17	DC	O4'-C1'-C2'	-9.13	98.60	105.90
2	F	34	DT	O4'-C4'-C3'	-9.11	100.53	106.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	DC	Sidechain
3	D	120	TYR	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	B	388	0	215	2	0
1	E	388	0	215	0	0
2	C	383	0	219	1	0
2	F	383	0	219	2	0
3	A	525	0	506	20	0
3	D	542	0	520	10	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	10	0	0	0	0
5	B	12	0	0	0	0
5	C	9	0	0	0	0
5	D	7	0	0	0	0
5	E	8	0	0	0	0
5	F	11	0	0	0	0
All	All	2670	0	1894	34	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 8.

The worst 5 of 34 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)
3:A:116:CYS:SG	3:A:118:ARG:HD3	2.01	0.99
3:A:118:ARG:HG2	3:A:118:ARG:HH11	1.48	0.79
3:D:130:TYR:CE1	3:D:134:HIS:HB2	2.24	0.71
3:D:142:PRO:HA	3:D:149:GLU:HA	1.74	0.70
3:D:130:TYR:CD1	3:D:134:HIS:HB2	2.28	0.69

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	61/66 (92%)	54 (88%)	7 (12%)	0	100	100
3	D	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	8
All	All	124/132 (94%)	108 (87%)	13 (10%)	3 (2%)	7	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	146	CYS
3	D	165	LYS
3	D	115	VAL

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	58/64 (91%)	56 (97%)	2 (3%)	42	76
3	D	61/64 (95%)	59 (97%)	2 (3%)	43	77
All	All	119/128 (93%)	115 (97%)	4 (3%)	42	76

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	118	ARG
3	A	138	VAL
3	D	140	VAL
3	D	149	GLU

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.