



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8SSU
Title : ZnFs 3-11 of CCCTC-binding factor (CTCF) Complexed with 19mer DNA
Authors : Horton, J.R.; Yang, J.; Cheng, X.
Deposited on : 2023-05-08
Resolution : 2.89 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 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

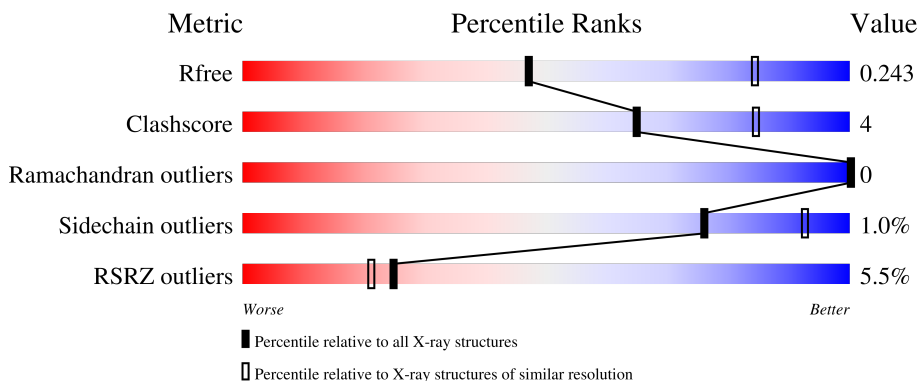
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	A	345	 4% 62% 6% 32%
2	B	19	 68% 32%
3	C	19	 5% 84% 11% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	101	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2711 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 Transcriptional repressor CTCF, LIM domain-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1887	1172	370	320	25	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	583	GLY	-	linker	UNP P49711
A	584	SER	-	linker	UNP P49711
A	585	GLY	-	linker	UNP P49711
A	586	GLY	-	linker	UNP P49711
A	587	HIS	-	linker	UNP P49711
A	588	MET	-	linker	UNP P49711
A	589	GLY	-	linker	UNP P49711
A	590	SER	-	linker	UNP P49711
A	591	GLY	-	linker	UNP P49711
A	592	GLY	-	linker	UNP P49711
A	593	LEU	-	linker	UNP P49711
A	594	VAL	-	linker	UNP P49711
A	595	PRO	-	linker	UNP P49711
A	596	ARG	-	linker	UNP P49711
A	597	GLY	-	linker	UNP P49711
A	598	SER	-	linker	UNP P49711
A	599	GLY	-	linker	UNP P49711
A	600	GLY	-	linker	UNP P49711

- Molecule 2 is a DNA chain called DNA (19-MER) Strand I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	19	407	196	62	129	20	0	3	0

- Molecule 3 is a DNA chain called DNA (19-MER) Strand II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	19	395	185	85	107	18	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
4	C	1	4	2	2	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	8	8	8	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	3	3	3	0	0
6	B	1	1	1	0	0
6	C	2	2	2	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.46Å 80.46Å 187.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 – 2.89 34.84 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.34-2.89) 90.4 (34.84-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.240 0.203 , 0.243	Depositor DCC
R_{free} test set	807 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtrriage
Anisotropy	1.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2711	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/1944	0.49	0/2613
2	B	0.51	0/482	0.92	0/740
3	C	0.54	0/446	0.80	1/688 (0.1%)
All	All	0.36	0/2872	0.65	1/4041 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	DG	O4'-C4'-C3'	-5.13	102.45	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1887	0	1766	14	0
2	B	407	0	222	5	0
3	C	395	0	211	4	0
4	A	4	0	6	0	0
4	C	4	0	6	0	0
5	A	8	0	0	0	0
6	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	2	0	0	0	0
All	All	2711	0	2211	20	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 4.

All (20) 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:390:ASP:HB3	1:A:393:LYS:HG2	1.72	0.69
1:A:504:CYS:SG	1:A:505:ARG:N	2.74	0.60
3:C:14:DG:C8	3:C:14:DG:H5'	2.39	0.57
1:A:426:ILE:HA	1:A:430:HIS:HD2	1.71	0.55
3:C:14:DG:H5'	3:C:14:DG:H8	1.72	0.53
1:A:390:ASP:OD1	1:A:391:THR:N	2.44	0.51
1:A:371:ARG:HA	1:A:374:THR:HG22	1.92	0.51
1:A:374:THR:HG23	1:A:376:GLU:H	1.76	0.51
1:A:448:ARG:HH21	3:C:6:DC:H2'	1.79	0.48
1:A:393:LYS:NZ	3:C:12:DG:O6	2.48	0.47
1:A:497:CYS:SG	1:A:513:HIS:HD2	2.25	0.46
1:A:375:GLY:HA2	1:A:389:ARG:HH21	1.83	0.43
1:A:497:CYS:HB2	1:A:510:MET:HE3	2.01	0.42
2:B:13:DT:H2''	2:B:14:DG:C8	2.54	0.42
1:A:395:LYS:NZ	2:B:6:DC:OP2	2.50	0.41
2:B:6:DC:H2''	2:B:7[A]:DC:O4'	2.20	0.41
1:A:375:GLY:HA2	1:A:389:ARG:HE	1.85	0.41
2:B:3[B]:DC:H2''	2:B:4:DG:C8	2.56	0.41
2:B:3[A]:DC:H2''	2:B:4:DG:C8	2.56	0.40
1:A:504:CYS:SG	1:A:509:HIS:HB2	2.62	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	232/345 (67%)	223 (96%)	9 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	201/308 (65%)	199 (99%)	2 (1%)	76	92

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

Mol	Chain	Res	Type
1	A	415	ARG
1	A	473	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	HIS

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 [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	701	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	C	101	-	3,3,3	0.48	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	701	-	-	0/1/1/1	-
4	EDO	C	101	-	-	0/1/1/1	-

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

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	233/345 (67%)	0.43	14 (6%) 21 18	64, 96, 129, 144	0
2	B	19/19 (100%)	0.59	0 100 100	66, 90, 96, 101	0
3	C	19/19 (100%)	0.79	1 (5%) 26 22	68, 79, 93, 93	0
All	All	271/383 (70%)	0.46	15 (5%) 25 21	64, 94, 128, 144	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	ALA	4.1
1	A	491	ASN	3.7
1	A	501	ASP	2.8
1	A	512	MET	2.8
1	A	446	ILE	2.7
1	A	433	ASN	2.6
1	A	506	GLN	2.6
1	A	438	HIS	2.6
1	A	539	ASP	2.4
1	A	437	PHE	2.4
1	A	551	VAL	2.3
1	A	434	VAL	2.2
1	A	535	LYS	2.1
3	C	1	DA	2.0
1	A	410	TYR	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(\AA^2)	Q<0.9
4	EDO	C	101	4/4	0.54	0.40	71,78,78,83	0
4	EDO	A	701	4/4	0.73	0.25	86,89,90,102	0
5	ZN	A	707	1/1	0.96	0.05	135,135,135,135	0
5	ZN	A	705	1/1	0.97	0.06	114,114,114,114	0
5	ZN	A	702	1/1	0.97	0.08	97,97,97,97	0
5	ZN	A	708	1/1	0.97	0.08	117,117,117,117	0
5	ZN	A	704	1/1	0.98	0.07	81,81,81,81	0
5	ZN	A	709	1/1	0.98	0.07	73,73,73,73	0
5	ZN	A	706	1/1	0.99	0.08	76,76,76,76	0
5	ZN	A	703	1/1	0.99	0.08	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.