



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:29 am BST

PDB ID : 5KKQ
Title : Homo sapiens CCCTC-binding factor (CTCF) ZnF3-7 and DNA complex structure
Authors : Hashimoto, H.; Wang, D.; Cheng, X.
Deposited on : 2016-06-22
Resolution : 1.74 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 : 2.11
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) : 2.11

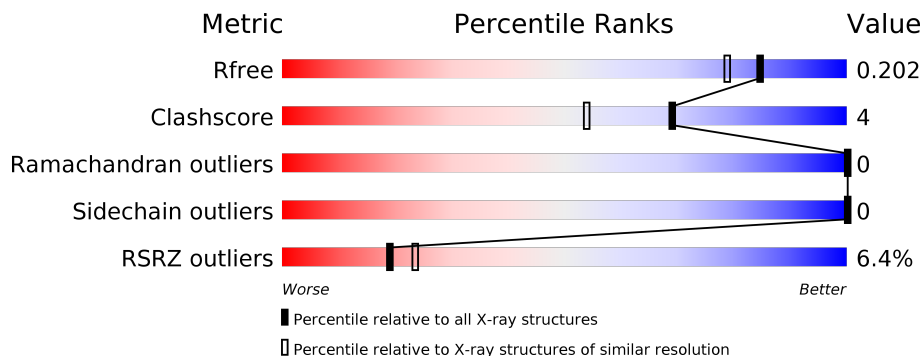
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	150	8% (red), 95% (green), 2% (yellow), 3% (grey)
1	D	150	7% (red), 93% (green), 2% (yellow), 3% (grey)
2	B	17	29% (green), 41% (yellow), 29% (orange)
2	E	17	18% (green), 76% (yellow), 6% (orange)
3	C	17	76% (green), 18% (yellow), 6% (orange)
3	F	17	65% (green), 24% (yellow), 12% (orange)

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7332 atoms, of which 3147 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	147	2366	744	1167	232	208	15	0	2	0
1	D	145	2363	743	1167	230	207	16	0	3	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	GLY	-	expression tag	UNP P49711
A	317	PRO	-	expression tag	UNP P49711
A	318	LEU	-	expression tag	UNP P49711
A	319	GLY	-	expression tag	UNP P49711
A	320	SER	-	expression tag	UNP P49711
D	316	GLY	-	expression tag	UNP P49711
D	317	PRO	-	expression tag	UNP P49711
D	318	LEU	-	expression tag	UNP P49711
D	319	GLY	-	expression tag	UNP P49711
D	320	SER	-	expression tag	UNP P49711

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	17	619	187	227	60	125	20	0	5	0
2	E	17	565	172	206	60	110	17	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	C	17	Total	C	H	N	O	P	0	0	0
			541	165	190	72	98	16			
3	F	17	Total	C	H	N	O	P	0	0	0
			541	165	190	72	98	16			

- 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		
4	D	5	Total	Zn	0	0
			5	5		

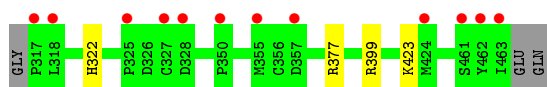
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	39	Total	O	0	0
			39	39		
5	C	41	Total	O	0	0
			41	41		
5	D	87	Total	O	0	0
			87	87		
5	E	41	Total	O	0	0
			41	41		
5	F	39	Total	O	0	0
			39	39		

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.

- Molecule 1: Transcriptional repressor CTCF



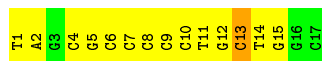
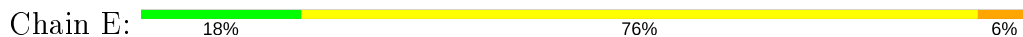
- Molecule 1: Transcriptional repressor CTCF



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



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



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



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

Chain F:  65% 24% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.99Å 44.91Å 86.80Å 98.33° 92.40° 94.80°	Depositor
Resolution (Å)	28.94 – 1.74 28.94 – 1.74	Depositor EDS
% Data completeness (in resolution range)	89.2 (28.94-1.74) 83.2 (28.94-1.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (dev_2257: ???)	Depositor
R, R_{free}	0.170 , 0.199 0.173 , 0.202	Depositor DCC
R_{free} test set	1919 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7332	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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

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	0.67	0/1235	0.74	3/1655 (0.2%)
1	D	0.72	0/1234	0.78	3/1652 (0.2%)
2	B	1.78	6/488 (1.2%)	1.44	8/749 (1.1%)
2	E	1.62	4/426 (0.9%)	1.45	3/655 (0.5%)
3	C	1.52	1/395 (0.3%)	1.27	4/609 (0.7%)
3	F	1.62	4/395 (1.0%)	1.39	5/609 (0.8%)
All	All	1.18	15/4173 (0.4%)	1.09	26/5929 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5[A]	DG	C3'-O3'	7.20	1.53	1.44
2	B	5[B]	DG	C3'-O3'	7.20	1.53	1.44
3	F	6	DC	C3'-O3'	-6.83	1.35	1.44
3	F	7	DA	P-OP1	-6.12	1.38	1.49
2	B	12	DG	C3'-O3'	-6.09	1.36	1.44
2	E	13	DC	C3'-O3'	-5.99	1.36	1.44
3	F	8	DG	C3'-O3'	-5.63	1.36	1.44
2	E	15[A]	DG	C5-C4	-5.60	1.34	1.38
2	E	15[B]	DG	C5-C4	-5.60	1.34	1.38
2	B	13	DC	C3'-O3'	-5.44	1.36	1.44
2	B	1	DT	C3'-O3'	-5.38	1.36	1.44
3	C	9	DG	C8-N7	-5.22	1.27	1.30
2	B	7	DC	C3'-O3'	-5.11	1.37	1.44
2	E	11	DT	C2-N3	-5.09	1.33	1.37
3	F	6	DC	P-O5'	-5.06	1.54	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	10	DG	O5'-P-OP2	-11.06	95.75	105.70
1	A	399	ARG	NE-CZ-NH2	-7.71	116.44	120.30
2	B	11	DT	O5'-P-OP2	-6.66	99.71	105.70
1	A	399	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	B	13	DC	O5'-P-OP1	6.38	118.36	110.70
1	D	399	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	B	11	DT	OP1-P-OP2	6.29	129.03	119.60
3	F	10	DG	O4'-C1'-N9	5.93	112.15	108.00
3	C	10	DG	O5'-P-OP2	-5.87	100.42	105.70
3	F	10	DG	C1'-O4'-C4'	-5.82	104.28	110.10
1	A	377	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	E	12	DG	O5'-P-OP2	-5.78	100.50	105.70
3	F	4	DA	OP2-P-O3'	5.77	117.89	105.20
2	B	6[A]	DC	O4'-C1'-N1	5.52	111.86	108.00
2	B	6[B]	DC	O4'-C1'-N1	5.52	111.86	108.00
3	F	4	DA	OP1-P-OP2	5.50	127.85	119.60
2	B	9[A]	DC	O5'-P-OP2	-5.43	100.81	105.70
2	B	9[B]	DC	O5'-P-OP2	-5.43	100.81	105.70
2	E	11	DT	O5'-P-OP2	-5.38	100.86	105.70
3	C	4	DA	OP2-P-O3'	5.37	117.01	105.20
2	B	12	DG	O4'-C1'-N9	5.29	111.70	108.00
3	C	10	DG	O4'-C1'-N9	5.25	111.68	108.00
3	C	6	DC	OP2-P-O3'	5.11	116.44	105.20
1	D	396	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	399	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	E	7	DC	O5'-P-OP2	-5.00	101.20	105.70

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	1199	1167	1154	2	0
1	D	1196	1167	1154	3	0
2	B	392	227	207	12	0
2	E	359	206	197	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	351	190	190	1	0
3	F	351	190	190	2	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	80	0	0	1	0
5	B	39	0	0	2	0
5	C	41	0	0	1	0
5	D	87	0	0	0	0
5	E	41	0	0	1	0
5	F	39	0	0	0	0
All	All	4185	3147	3092	26	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 (26) 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:B:15:DG:OP2	5:B:101:HOH:O	1.75	1.05
2:B:12:DG:OP2	5:B:102:HOH:O	1.88	0.90
2:E:10:DC:OP1	5:E:101:HOH:O	2.04	0.74
3:C:4:DA:OP2	5:C:101:HOH:O	2.05	0.74
2:B:5[A]:DG:H2''	2:B:6[A]:DC:H5''	1.72	0.72
1:A:322:HIS:ND1	5:A:601:HOH:O	2.27	0.66
1:D:333:THR:HG22	1:D:336:GLU:OE1	2.01	0.60
2:B:5[A]:DG:H2''	2:B:6[A]:DC:C5'	2.34	0.57
2:B:5[A]:DG:C2'	2:B:6[A]:DC:C5'	2.82	0.57
2:B:5[A]:DG:C2'	2:B:6[A]:DC:H5'	2.35	0.56
1:A:423:LYS:NZ	2:B:9[A]:DC:OP1	2.34	0.54
2:B:5[A]:DG:H2'	2:B:6[A]:DC:H5'	1.94	0.49
2:E:4:DC:H2'	2:E:5:DG:C8	2.50	0.46
2:E:1:DT:H2'	2:E:2:DA:C8	2.52	0.44
1:D:393:LYS:NZ	3:F:9:DG:N7	2.67	0.42
2:B:4[A]:DC:H2'	2:B:5[A]:DG:O4'	2.20	0.42
2:E:5:DG:H2'	2:E:6:DC:C6	2.55	0.41
2:B:8[A]:DC:H2''	2:B:9[A]:DC:O5'	2.20	0.41
1:D:390:ASP:OD2	1:D:393:LYS:HG2	2.21	0.41
2:E:5:DG:H2''	2:E:6:DC:H5'	2.03	0.41
2:E:8:DC:H2''	2:E:9:DC:H5'	2.03	0.41
3:F:6:DC:H2''	3:F:7:DA:C8	2.55	0.40
2:B:13:DC:H2''	2:B:14:DT:H5'	2.03	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	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
1	D	145/150 (97%)	143 (99%)	2 (1%)	0	100	100
All	All	291/300 (97%)	287 (99%)	4 (1%)	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	135/137 (98%)	135 (100%)	0	100	100
1	D	135/137 (98%)	135 (100%)	0	100	100
All	All	270/274 (98%)	270 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 10 ligands modelled in this entry, 10 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 [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	147/150 (98%)	0.29	12 (8%) 11 15	23, 39, 63, 85	0
1	D	145/150 (96%)	0.37	11 (7%) 13 18	23, 39, 65, 95	0
2	B	17/17 (100%)	-0.04	0 100 100	28, 37, 57, 60	0
2	E	17/17 (100%)	-0.11	0 100 100	27, 36, 61, 65	0
3	C	17/17 (100%)	-0.05	0 100 100	23, 29, 57, 61	0
3	F	17/17 (100%)	-0.02	0 100 100	24, 31, 54, 61	0
All	All	360/368 (97%)	0.26	23 (6%) 19 23	23, 38, 64, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	ILE	9.8
1	D	465	GLN	7.8
1	A	462	TYR	5.1
1	A	318	LEU	4.1
1	D	463	ILE	3.6
1	A	328	ASP	3.3
1	D	332	VAL	3.3
1	A	317	PRO	3.1
1	D	329[A]	MET	3.1
1	A	355	MET	2.9
1	D	325	PRO	2.7
1	D	327	CYS	2.6
1	A	461	SER	2.5
1	A	357	ASP	2.4
1	D	333	THR	2.3
1	A	327	CYS	2.3
1	D	323	LYS	2.2
1	D	411	ILE	2.2
1	D	412	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	350	PRO	2.1
1	D	328	ASP	2.1
1	A	424	MET	2.1
1	A	325	PRO	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 carbohydrates 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	503	1/1	0.92	0.04	37,37,37,37	0
4	ZN	A	501	1/1	0.93	0.05	55,55,55,55	0
4	ZN	D	505	1/1	0.95	0.05	30,30,30,30	0
4	ZN	D	501	1/1	0.95	0.03	46,46,46,46	0
4	ZN	A	504	1/1	0.96	0.05	32,32,32,32	0
4	ZN	A	502	1/1	0.97	0.04	37,37,37,37	0
4	ZN	A	505	1/1	0.97	0.06	33,33,33,33	0
4	ZN	D	502	1/1	0.97	0.05	34,34,34,34	0
4	ZN	D	503	1/1	0.98	0.03	32,32,32,32	0
4	ZN	D	504	1/1	0.99	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.