Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 03:38 PM EST

PDB ID	:	1G2D
Title	:	STRUCTURE OF A CYS2HIS2 ZINC FINGER/TATA BOX COMPLEX (CLONE #2)
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Deposited on	:	2000-10-18
Resolution	:	2.20 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:

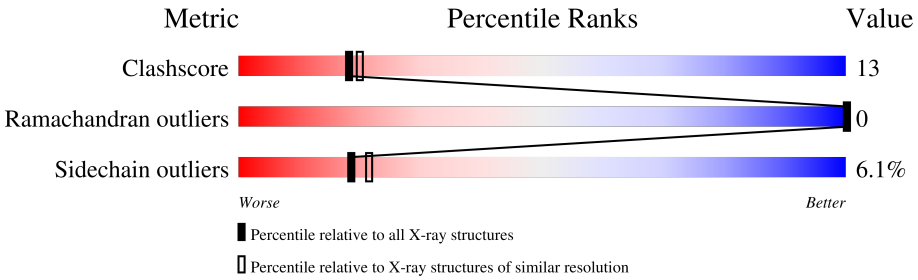
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	16	62% 38%
1	D	16	62% 38%
2	B	16	56% 44%
2	E	16	56% 44%
3	C	90	73% 23% ••
3	F	90	68% 29% ••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2997 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 5'-D(*GP*AP*CP*GP*CP*TP*AP*TP*AP*AP*AP*AP*GP*GP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	16	Total	C	N	O	P	0	0	0
			332	158	70	89	15			
1	D	16	Total	C	N	O	P	0	0	0
			332	158	70	89	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	P	0	0	0
			318	155	49	99	15			
2	E	16	Total	C	N	O	P	0	0	0
			318	155	49	99	15			

- Molecule 3 is a protein called TATA BOX ZINC FINGER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	89	Total	C	N	O	S	0	0	0
			738	452	153	125	8			
3	F	88	Total	C	N	O	S	0	0	0
			729	446	151	124	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	Zn	0	0
			3	3		
4	F	3	Total	Zn	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	28	Total O 28 28	0	0
5	B	34	Total O 34 34	0	0
5	D	26	Total O 26 26	0	0
5	E	35	Total O 35 35	0	0
5	C	50	Total O 50 50	0	0
5	F	51	Total O 51 51	0	0

3 Residue-property plots

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.

Note EDS was not executed.

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

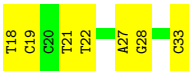
Chain A:

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

Chain D:

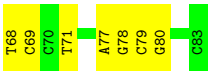
• Molecule 2: 5'-D(*TP*CP*CP*TP*TP*TP*TP*AP*TP*AP*GP*CP*GP*TP*CP*C)-3'

Chain B:



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

Chain E:

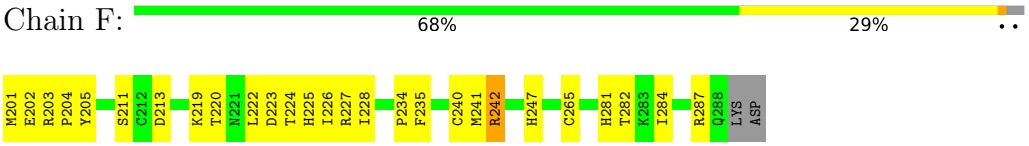


• Molecule 3: TATA BOX ZINC FINGER PROTEIN

Chain C:

• Molecule 3: TATA BOX ZINC FINGER PROTEIN

Chain F:


68%
29%
M201
E202
R203
P204
Y205
S211
C212
D213
K219
T220
N221
L222
D223
T224
H225
I226
R227
I228
P234
F235
C240
M241
R242
H247
C265
H281
T282
K283
I284
R287
Q288
LYS
ASP

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	105.10Å 105.10Å 104.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	94.6 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	6.60	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.225 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2997	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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	A	0.43	0/375	0.78	0/578
1	D	0.41	0/375	0.71	0/578
2	B	0.39	0/353	0.75	0/542
2	E	0.42	0/353	0.76	0/542
3	C	0.34	0/755	0.59	0/1011
3	F	0.36	0/746	0.62	0/1000
All	All	0.38	0/2957	0.69	0/4251

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	332	0	180	11	0
1	D	332	0	180	6	0
2	B	318	0	185	15	0
2	E	318	0	185	8	0
3	C	738	0	724	16	0
3	F	729	0	711	15	0
4	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	3	0	0	0	0
5	A	28	0	0	0	0
5	B	34	0	0	1	0
5	C	50	0	0	1	0
5	D	26	0	0	0	0
5	E	35	0	0	3	0
5	F	51	0	0	1	0
All	All	2997	0	2165	66	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 13.

All (66) 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:2:DG:H2"	1:A:3:DA:H5'	1.17	1.11
1:A:2:DG:H2"	1:A:3:DA:C5'	1.86	1.04
2:B:27:DA:H2"	2:B:28:DG:H5"	1.43	0.98
1:D:57:DT:H2"	1:D:58:DA:H5'	1.53	0.90
1:A:5:DG:H2"	1:A:6:DC:H5'	1.50	0.89
2:B:27:DA:H2"	2:B:28:DG:C5'	2.02	0.89
2:B:27:DA:C2'	2:B:28:DG:H5"	2.05	0.86
2:E:77:DA:H2"	2:E:78:DG:H5"	1.59	0.84
1:D:57:DT:H2"	1:D:58:DA:C5'	2.14	0.76
1:A:7:DT:H2"	1:A:8:DA:H5'	1.67	0.75
2:B:18:DT:H6	2:B:18:DT:H5'	1.49	0.75
3:F:265:CYS:SG	3:F:282:THR:HG22	2.29	0.72
2:E:69:DC:H5"	5:E:1040:HOH:O	1.90	0.72
1:A:5:DG:C2'	1:A:6:DC:H5'	2.20	0.71
2:B:21:DT:H2"	2:B:22:DT:C5'	2.21	0.70
1:D:55:DG:H2"	1:D:56:DC:H5'	1.73	0.69
2:E:77:DA:C2'	2:E:78:DG:H5"	2.25	0.67
1:A:7:DT:H2"	1:A:8:DA:C5'	2.25	0.66
3:C:105:TYR:HB3	3:C:122:LEU:HD22	1.78	0.65
1:A:2:DG:C2'	1:A:3:DA:C5'	2.70	0.64
2:B:21:DT:H2"	2:B:22:DT:H5"	1.82	0.61
2:E:79:DC:H2"	2:E:80:DG:C8	2.36	0.60
3:C:181:HIS:O	3:C:184:ILE:HG12	2.01	0.60
2:B:21:DT:H2"	2:B:22:DT:H5'	1.84	0.59
3:C:127:ARG:NH1	3:C:145:SER:O	2.36	0.59
3:F:205:TYR:HB3	3:F:222:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:DA:H2"	1:D:61:DA:H5'	1.86	0.58
1:A:7:DT:H5"	3:C:142:ARG:HH12	1.68	0.57
3:F:225:HIS:O	3:F:228:ILE:HG12	2.05	0.56
2:B:18:DT:H5'	2:B:18:DT:C6	2.38	0.55
2:B:21:DT:C2'	2:B:22:DT:H5"	2.37	0.54
1:D:55:DG:C2'	1:D:56:DC:H5'	2.38	0.54
3:C:124:THR:HG23	3:C:127:ARG:HH12	1.73	0.54
3:F:202:GLU:C	3:F:204:PRO:HD3	2.29	0.53
3:F:240:CYS:SG	3:F:242:ARG:HB2	2.49	0.52
2:B:21:DT:H73	3:C:120:THR:HG21	1.92	0.52
2:B:21:DT:H73	3:C:120:THR:CG2	2.40	0.51
2:B:33:DC:O3'	2:E:68:DT:H5'	2.10	0.51
3:F:222:LEU:O	3:F:226:ILE:HG12	2.11	0.51
2:E:77:DA:H2"	2:E:78:DG:C5'	2.37	0.51
3:F:224:THR:HG23	3:F:227:ARG:NH1	2.25	0.51
3:F:281:HIS:O	3:F:284:ILE:HG12	2.11	0.50
5:E:1244:HOH:O	3:F:247:HIS:HE1	1.95	0.50
3:C:125:HIS:O	3:C:128:ILE:HG12	2.11	0.49
3:C:114:ARG:HG2	3:C:116:PHE:CZ	2.47	0.49
2:B:27:DA:H2"	2:B:28:DG:H5'	1.90	0.49
3:C:110:GLU:HG3	3:C:111:SER:N	2.27	0.49
2:B:18:DT:H2'	2:B:19:DC:C6	2.48	0.48
3:F:202:GLU:O	3:F:204:PRO:HD3	2.14	0.47
5:E:1023:HOH:O	3:F:247:HIS:HD2	1.97	0.46
1:D:56:DC:H2"	1:D:57:DT:OP2	2.15	0.46
1:A:2:DG:C2'	1:A:3:DA:H5"	2.45	0.44
3:F:242:ARG:HG3	5:F:1316:HOH:O	2.17	0.44
2:E:71:DT:O4	3:F:220:THR:HG21	2.19	0.43
3:F:219:LYS:HE3	3:F:223:ASP:OD1	2.18	0.43
2:B:18:DT:H2'	2:B:19:DC:C5	2.54	0.43
3:C:115:ARG:CG	3:C:115:ARG:HH11	2.32	0.43
3:C:124:THR:HG23	3:C:127:ARG:NH1	2.34	0.42
3:C:137:CYS:O	3:C:141:MET:HA	2.19	0.42
1:A:5:DG:H1'	1:A:6:DC:H5'	2.00	0.42
2:E:78:DG:H2"	2:E:79:DC:C6	2.54	0.42
5:B:1233:HOH:O	3:C:147:HIS:HE1	2.02	0.41
3:C:148:THR:O	3:C:152:GLN:HG3	2.20	0.41
3:C:149:GLY:HA3	5:C:1205:HOH:O	2.20	0.40
3:F:234:PRO:HG2	3:F:235:PHE:CD1	2.56	0.40
1:A:5:DG:C1'	1:A:6:DC:H5'	2.50	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	
3	C	87/90 (97%)	85 (98%)	2 (2%)	0	100	100
3	F	86/90 (96%)	84 (98%)	2 (2%)	0	100	100
All	All	173/180 (96%)	169 (98%)	4 (2%)	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	
3	C	82/83 (99%)	79 (96%)	3 (4%)	34	43
3	F	81/83 (98%)	74 (91%)	7 (9%)	10	10
All	All	163/166 (98%)	153 (94%)	10 (6%)	18	21

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	110	GLU
3	C	115	ARG
3	C	138	ARG
3	F	201	MET
3	F	203	ARG
3	F	211	SER
3	F	213	ASP
3	F	241	MET

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Mol	Chain	Res	Type
3	F	242	ARG
3	F	287	ARG

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

Mol	Chain	Res	Type
3	F	247	HIS
3	F	251	ASN

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 6 ligands modelled in this entry, 6 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 (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.