



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:52 pm BST

PDB ID : 2HAP
Title : STRUCTURE OF A HAP1-18/DNA COMPLEX REVEALS THAT PROTEIN/DNA INTERACTIONS CAN HAVE DIRECT ALLOSTERIC EFFECTS ON TRANSCRIPTIONAL ACTIVATION
Authors : King, D.A.; Zhang, L.; Guarente, L.; Marmorstein, R.
Deposited on : 1998-09-17
Resolution : 2.50 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)	:	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)	:	2.11

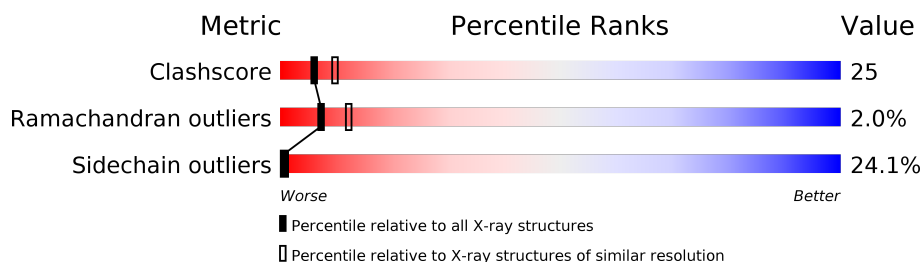
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	20	
2	B	20	
3	C	81	
3	D	81	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2148 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(*AP*CP*GP*CP*TP*AP*TP*TP*AP*TP*CP*GP*CP*TP*AP*TP*TP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	P	0	0	0
			404	196	68	121	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			410	197	79	115	19			

- Molecule 3 is a protein called PROTEIN (HEME ACTIVATOR PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	76	Total	C	N	O	S	0	0	0
			636	392	128	109	7			
3	D	75	Total	C	N	O	S	0	0	0
			619	381	123	108	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	Zn	0	0
			3	3		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total 11	O 11	0	0
5	C	25	Total 25	O 25	0	0
5	D	16	Total 16	O 16	0	0

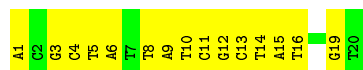
3 Residue-property plots

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. 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.

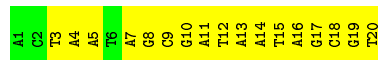
- Molecule 1: DNA (5'-D(*AP*CP*GP*CP*TP*AP*TP*TP*AP*TP*CP*GP*CP*TP*AP*TP*TP*AP*GP*T)-3')

Chain A: 



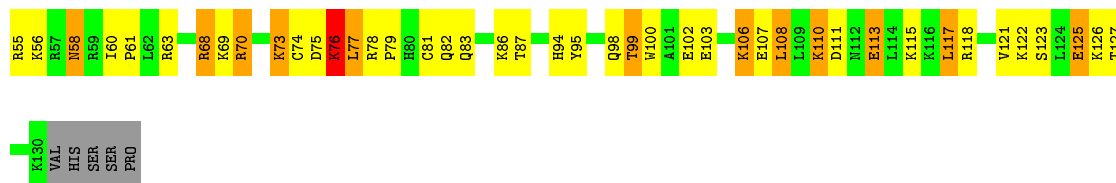
- Molecule 2: DNA (5'-D(*AP*CP*TP*AP*AP*TP*AP*GP*CP*GP*AP*TP*AP*AP*TP*AP*GP*CP*GP*T)-3')

Chain B: 



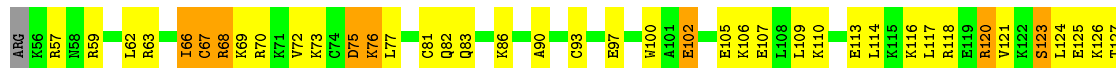
- Molecule 3: PROTEIN (HEME ACTIVATOR PROTEIN)

Chain C: 



- Molecule 3: PROTEIN (HEME ACTIVATOR PROTEIN)

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.50 Å 92.50 Å 86.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	91.9 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.248 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2148	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	0.47	0/451	0.80	0/694
2	B	0.51	0/461	0.79	0/710
3	C	0.42	0/643	0.64	0/853
3	D	0.43	0/626	0.76	1/832 (0.1%)
All	All	0.45	0/2181	0.75	1/3089 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	75	ASP	N-CA-C	-5.21	96.94	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	DG	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	A	404	0	230	20	0
2	B	410	0	227	22	0
3	C	636	0	675	37	0
3	D	619	0	644	33	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	A	22	0	0	0	0
5	B	11	0	0	1	0
5	C	25	0	0	6	0
5	D	16	0	0	1	0
All	All	2148	0	1776	94	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 25.

All (94) 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:7:DA:H1'	2:B:8:DG:H5'	1.56	0.85
1:A:1:DA:H2	2:B:20:DT:H3	1.25	0.84
1:A:3:DG:H1'	1:A:4:DC:H5'	1.65	0.78
3:C:63:ARG:CZ	3:C:68:ARG:HG2	2.16	0.76
1:A:13:DC:H2''	1:A:14:DT:OP2	1.86	0.75
3:C:63:ARG:NE	3:C:68:ARG:HG2	2.05	0.72
3:C:56:LYS:HE2	3:C:58:ASN:OD1	1.89	0.72
2:B:11:DA:H1'	2:B:12:DT:H5'	1.71	0.71
2:B:12:DT:H2''	2:B:13:DA:OP2	1.92	0.68
3:C:75:ASP:OD2	3:C:82:GLN:HB3	1.93	0.68
3:C:118:ARG:HD3	3:D:113:GLU:OE2	1.93	0.67
3:C:98:GLN:HE22	3:C:106:LYS:HE3	1.59	0.67
2:B:10:DG:H2''	2:B:11:DA:OP2	1.95	0.67
3:D:66:ILE:HG22	3:D:67:CYS:N	2.11	0.62
3:C:94:HIS:HA	5:C:162:HOH:O	2.00	0.61
2:B:8:DG:H2''	2:B:9:DC:OP2	2.00	0.61
3:D:82:GLN:O	3:D:86:LYS:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:GLU:OE1	3:D:102:GLU:HA	2.01	0.60
2:B:9:DC:H1'	2:B:10:DG:H5'	1.84	0.59
1:A:9:DA:H2''	1:A:10:DT:H71	1.85	0.58
1:A:1:DA:H2	2:B:20:DT:N3	2.01	0.58
1:A:10:DT:H2''	1:A:11:DC:H5'	1.85	0.57
1:A:4:DC:H2''	1:A:5:DT:OP2	2.03	0.57
3:C:121:VAL:HG22	3:D:121:VAL:HG23	1.87	0.57
3:C:99:THR:HG22	3:C:102:GLU:H	1.70	0.56
3:C:70:ARG:HD2	3:D:100:TRP:CE2	2.40	0.56
3:C:117:LEU:HD13	3:D:117:LEU:HB3	1.87	0.56
3:D:129:SER:O	3:D:130:LYS:O	2.24	0.56
3:D:63:ARG:HH21	3:D:68:ARG:HG2	1.71	0.56
2:B:3:DT:H2''	2:B:4:DA:OP2	2.06	0.55
3:C:94:HIS:HB2	5:C:143:HOH:O	2.06	0.55
2:B:17:DG:H2''	2:B:18:DC:OP2	2.06	0.54
1:A:11:DC:H2''	1:A:12:DG:OP2	2.08	0.54
3:C:82:GLN:O	3:C:86:LYS:HG2	2.08	0.54
1:A:15:DA:C8	1:A:16:DT:H72	2.43	0.54
3:C:125:GLU:OE2	3:D:120:ARG:NH1	2.41	0.53
3:D:123:SER:O	3:D:126:LYS:HG2	2.09	0.52
1:A:5:DT:H2''	1:A:6:DA:OP2	2.09	0.52
3:C:108:LEU:O	3:C:111:ASP:HB2	2.09	0.51
3:C:77:LEU:HB2	5:C:161:HOH:O	2.10	0.51
1:A:8:DT:H5'	5:B:26:HOH:O	2.10	0.50
2:B:11:DA:H2''	2:B:12:DT:O5'	2.12	0.50
3:D:75:ASP:CG	3:D:75:ASP:O	2.51	0.50
3:C:78:ARG:HB3	3:C:79:PRO:HA	1.95	0.49
1:A:8:DT:H2''	1:A:9:DA:C8	2.48	0.48
3:C:113:GLU:O	3:C:117:LEU:HB2	2.13	0.48
1:A:12:DG:H1'	1:A:13:DC:H5'	1.95	0.48
3:C:99:THR:HG23	3:C:100:TRP:N	2.28	0.48
2:B:13:DA:H1'	2:B:14:DA:H5'	1.95	0.47
3:D:62:LEU:O	3:D:76:LYS:HG2	2.14	0.47
3:C:81:CYS:HB3	3:C:95:TYR:OH	2.15	0.47
2:B:7:DA:H2''	2:B:8:DG:O5'	2.15	0.47
2:B:5:DA:OP1	3:C:55:ARG:HG2	2.15	0.47
3:C:113:GLU:HG2	5:C:156:HOH:O	2.14	0.46
3:C:121:VAL:CG2	3:D:121:VAL:HG23	2.44	0.46
1:A:14:DT:H1'	1:A:15:DA:H5'	1.97	0.46
3:D:62:LEU:HD12	5:D:153:HOH:O	2.15	0.46
3:D:90:ALA:O	3:D:93:CYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:70:ARG:O	3:D:72:VAL:HG13	2.16	0.46
3:C:77:LEU:HD22	5:C:161:HOH:O	2.15	0.45
3:C:87:THR:O	3:D:62:LEU:HD22	2.15	0.45
2:B:14:DA:H2''	2:B:15:DT:OP2	2.16	0.45
2:B:17:DG:H3'	3:D:73:LYS:HG3	1.98	0.45
3:D:124:LEU:O	3:D:127:THR:HB	2.16	0.45
1:A:13:DC:C2'	1:A:14:DT:OP2	2.60	0.45
3:C:99:THR:CG2	3:C:100:TRP:N	2.79	0.45
3:D:125:GLU:HA	3:D:128:LEU:HB2	1.99	0.44
3:C:74:CYS:C	3:C:76:LYS:H	2.19	0.44
2:B:16:DA:OP1	3:D:63:ARG:HG3	2.17	0.44
2:B:19:DG:H2''	2:B:20:DT:OP2	2.18	0.43
2:B:9:DC:H2''	2:B:10:DG:O5'	2.18	0.43
3:C:60:ILE:HA	3:C:61:PRO:HD2	1.81	0.43
3:C:126:LYS:O	3:C:127:THR:C	2.57	0.43
3:C:77:LEU:CB	5:C:161:HOH:O	2.66	0.43
3:C:73:LYS:O	3:C:83:GLN:HG2	2.19	0.43
1:A:10:DT:H5'	3:D:59:ARG:HG3	1.99	0.43
3:D:63:ARG:NH2	3:D:68:ARG:HG2	2.34	0.43
1:A:3:DG:H2''	1:A:4:DC:O5'	2.19	0.42
2:B:16:DA:H1'	2:B:17:DG:H5'	2.02	0.42
3:C:110:LYS:HZ3	3:C:110:LYS:HG2	1.71	0.42
3:D:127:THR:C	3:D:129:SER:N	2.73	0.42
3:C:107:GLU:OE1	3:D:110:LYS:HE3	2.19	0.42
3:D:123:SER:HA	3:D:126:LYS:CE	2.50	0.41
2:B:12:DT:C1'	3:D:57:ARG:HH22	2.33	0.41
2:B:7:DA:C1'	2:B:8:DG:H5'	2.40	0.41
3:C:68:ARG:HE	3:C:68:ARG:HB3	1.26	0.41
1:A:10:DT:OP2	3:C:70:ARG:NH1	2.50	0.41
1:A:10:DT:H2''	1:A:11:DC:C5'	2.49	0.41
3:D:114:LEU:O	3:D:118:ARG:HG3	2.20	0.41
1:A:10:DT:C2'	1:A:11:DC:H5'	2.51	0.41
3:D:75:ASP:O	3:D:81:CYS:HB2	2.21	0.41
3:C:113:GLU:CD	3:D:118:ARG:HH12	2.23	0.41
3:C:111:ASP:OD1	3:D:110:LYS:HD3	2.20	0.40
3:D:77:LEU:HB3	3:D:81:CYS:HA	2.04	0.40

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	
3	C	74/81 (91%)	68 (92%)	5 (7%)	1 (1%)	11	20
3	D	73/81 (90%)	65 (89%)	6 (8%)	2 (3%)	5	7
All	All	147/162 (91%)	133 (90%)	11 (8%)	3 (2%)	7	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	76	LYS
3	C	76	LYS
3	D	128	LEU

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	
3	C	72/77 (94%)	54 (75%)	18 (25%)	0	1
3	D	69/77 (90%)	53 (77%)	16 (23%)	1	1
All	All	141/154 (92%)	107 (76%)	34 (24%)	0	1

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	58	ASN
3	C	68	ARG
3	C	69	LYS

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Mol	Chain	Res	Type
3	C	70	ARG
3	C	73	LYS
3	C	76	LYS
3	C	77	LEU
3	C	99	THR
3	C	103	GLU
3	C	106	LYS
3	C	108	LEU
3	C	110	LYS
3	C	113	GLU
3	C	115	LYS
3	C	117	LEU
3	C	122	LYS
3	C	123	SER
3	C	125	GLU
3	D	66	ILE
3	D	67	CYS
3	D	68	ARG
3	D	69	LYS
3	D	83	GLN
3	D	97	GLU
3	D	102	GLU
3	D	105	GLU
3	D	106	LYS
3	D	107	GLU
3	D	109	LEU
3	D	116	LYS
3	D	120	ARG
3	D	123	SER
3	D	128	LEU
3	D	130	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	98	GLN
3	D	82	GLN
3	D	83	GLN

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 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 [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.