

# Full wwPDB X-ray Structure Validation Report (i)

Apr 5, 2022 – 01:18 pm BST

PDB ID :	D : 7AW9
Title :	e : CCAAT-binding complex and HapX bound to Aspergillus fumigatus cccA
	DNA
Authors :	s : Huber, E.M.; Groll, M.
eposited on :	n : 2020-11-06
Resolution :	n : 3.50 Å (reported)
eposited on :	s : Huber, E.M.; Groll, M. n : 2020-11-06

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

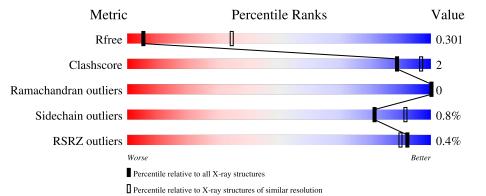
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 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	А	64	86% • 12%
2	В	92	97% •
3	С	119	% 94% 5% •
4	D	98	90% 5% 5%
4	Е	98	62% · 34%

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Mol	Chain	Length	Quality of chain	
5	F	37	78%	22%
6	G	37	81%	19%



 $\mathbf{2}$ 

# Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5013 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 HapB.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	56	Total 479	C 299	N 107	0 72	S 1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	230	MET	-	initiating methionine	UNP G5EAZ0

• Molecule 2 is a protein called Transcription factor HapC (Eurofung).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	92	Total 741	C 469	N 123	0 142	S 7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	41	MET	-	initiating methionine	UNP Q5B5Z6

• Molecule 3 is a protein called CBFD\_NFYB\_HMF domain-containing protein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	118	Total 950	C 603	N 170	0 172	${S \atop 5}$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Cha	n Residue	Modelled	Actual	Comment	Reference
C	46	MET	-	initiating methionine	UNP Q5AYY8

• Molecule 4 is a protein called BZIP domain-containing protein.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	П	93	Total	С	Ν	0	S	0	0	0
4		95	774	476	156	140	2	0	0	0
4	F	65	Total	С	Ν	0	S	0	0	0
4	Ľ	05	551	335	113	101	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	92	LYS	CYS	engineered mutation	UNP G5EAX9
D	129	SER	CYS	engineered mutation	UNP G5EAX9
Е	92	LYS	CYS	engineered mutation	UNP G5EAX9
Е	129	SER	CYS	engineered mutation	UNP G5EAX9

• Molecule 5 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
5	F	37	Total 767	C 365	N 139	0 226	Р 37	0	0	0

• Molecule 6 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
6	G	37	Total 750	C 358	N 137	0 218	Р 37	0	0	0

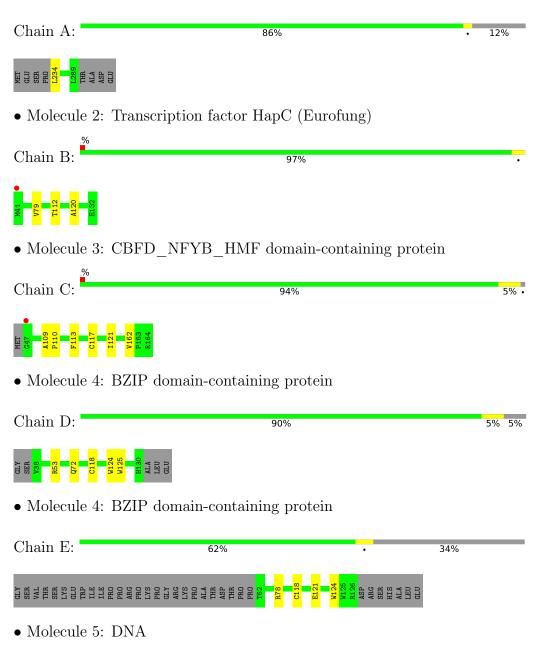
• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Cl 1 1	0	0



# 3 Residue-property plots (i)

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 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: HapB



Chain F:	78%	22%
11 126 130 130 130 131 137 137		
• Molecule 6: DNA		
Chain G:	81%	19%
A1 C3 C3 A3 A3 A3 A3 A3 A3 A3 A3 A3 A		



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	76.84Å 127.66Å 198.98Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	30.00 - 3.50	Depositor
Resolution (A)	47.67 - 3.50	EDS
% Data completeness	97.8 (30.00-3.50)	Depositor
(in resolution range)	$98.0\ (47.67-3.50)$	EDS
R <sub>merge</sub>	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.82 (at 3.48 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
B B.	0.245 , $0.291$	Depositor
$R, R_{free}$	0.249 , $0.301$	DCC
$R_{free}$ test set	624 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	156.3	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5013	wwPDB-VP
Average B, all atoms $(Å^2)$	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: CL

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
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.63	0/489	0.71	0/649
2	В	0.65	0/751	0.70	0/1004
3	С	0.65	0/970	0.70	0/1313
4	D	0.62	0/791	0.69	0/1065
4	Е	0.65	0/558	0.70	0/744
5	F	0.30	0/860	0.73	0/1328
6	G	0.29	0/840	0.72	0/1291
All	All	0.55	0/5259	0.71	0/7394

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 (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	А	479	0	505	0	0
2	В	741	0	749	2	0
3	С	950	0	953	3	0
4	D	774	0	773	3	0
4	Е	551	0	545	4	0
5	F	767	0	420	4	0

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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 2.

All (18) 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)
4:E:78:ARG:NH1	6:G:25:DG:H5'	2.20	0.57
5:F:36:DA:H2"	5:F:37:DT:C6	2.42	0.54
5:F:26:DT:H2"	5:F:27:DG:C8	2.43	0.53
5:F:30:DT:H2"	5:F:31:DG:C8	2.42	0.53
3:C:109:ALA:HB3	3:C:110:PRO:HD3	1.92	0.52
4:D:72:GLN:HE22	6:G:31:DC:N4	2.09	0.50
4:D:118:CYS:SG	4:E:118:CYS:HB3	2.52	0.50
4:E:78:ARG:HH12	6:G:25:DG:H5'	1.78	0.48
3:C:113:PHE:O	3:C:117:CYS:N	2.46	0.48
6:G:25:DG:H2'	6:G:26:DA:C8	2.50	0.47
4:D:124:TRP:HE3	4:D:125:TRP:CD1	2.34	0.45
5:F:19:DG:H2"	5:F:20:DA:C8	2.51	0.45
6:G:36:DA:C8	6:G:37:DT:H72	2.53	0.43
6:G:34:DC:H2"	6:G:35:DA:C8	2.54	0.42
4:E:121:GLU:O	4:E:124:TRP:HB3	2.20	0.42
6:G:34:DC:H2"	6:G:35:DA:H8	1.85	0.42
2:B:112:THR:HG23	2:B:120:ALA:CB	2.50	0.41
2:B:79:VAL:HG21	3:C:121:ILE:HD11	2.02	0.41

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.



Chain Non-H H(model) H(added) Clashes Symm-Clashes Mol 6 G 750 0 0 416 7 7  $\overline{\mathbf{C}}$ 0 0 0 1 0 All All 50130 4361 18 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	54/64~(84%)	52 (96%)	2~(4%)	0	100 100
2	В	90/92~(98%)	88~(98%)	2(2%)	0	100 100
3	С	116/119~(98%)	109 (94%)	7~(6%)	0	100 100
4	D	91/98~(93%)	89 (98%)	2(2%)	0	100 100
4	Е	63/98~(64%)	62 (98%)	1 (2%)	0	100 100
All	All	414/471 (88%)	400 (97%)	14 (3%)	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	А	49/56~(88%)	48 (98%)	1 (2%)	55 79
2	В	80/80~(100%)	80 (100%)	0	100 100
3	С	102/103~(99%)	101 (99%)	1 (1%)	76 88
4	D	82/85~(96%)	81 (99%)	1 (1%)	71 87
4	Ε	56/85~(66%)	56 (100%)	0	100 100
All	All	369/409~(90%)	366~(99%)	3~(1%)	81 91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	234	LEU
3	С	162	VAL
4	D	53	ARG

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

Mol	Chain	Res	Type	
4	D	72	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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,  $95^{th}$  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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	56/64~(87%)	-0.18	0 100 100	169, 203, 244, 252	0
2	В	92/92~(100%)	0.22	1 (1%) 80 75	117, 146, 200, 223	0
3	С	118/119~(99%)	0.16	1 (0%) 86 81	111, 157, 224, 231	0
4	D	93/98~(94%)	-0.16	0 100 100	148, 186, 223, 249	0
4	Е	65/98~(66%)	-0.28	0 100 100	171, 194, 223, 257	0
5	F	37/37~(100%)	-0.82	0 100 100	152, 200, 238, 257	0
6	G	37/37~(100%)	-0.69	0 100 100	163, 191, 273, 300	0
All	All	498/545~(91%)	-0.12	2 (0%) 92 90	111, 184, 234, 300	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	47	GLY	3.7
2	В	41	MET	2.9

### 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,  $95^{th}$  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
7	CL	С	201	1/1	0.15	0.39	169, 169, 169, 169, 169	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

