



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 23, 2018 – 10:09 AM EST

PDB ID : 5NQX  
Title : Structure of a fHbp(V1.1):PorA(P1.16) chimera. Fusion at fHbp position 294.  
Authors : Johnson, S.; Jongerius, I.; Lea, S.M.; Tang, C.M.  
Deposited on : 2017-04-21  
Resolution : 3.66 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

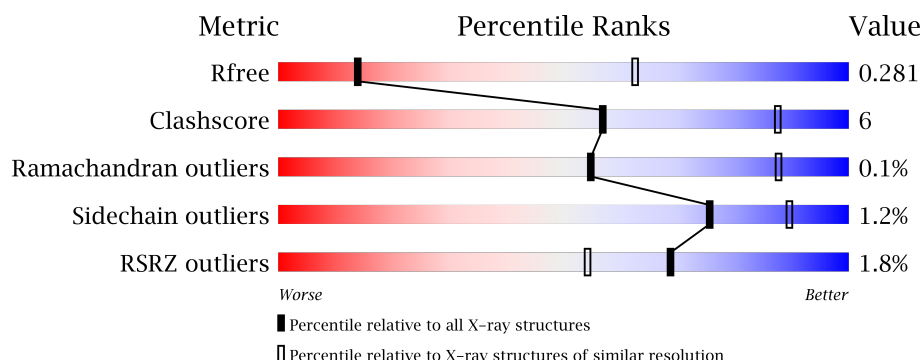
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.66 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))
$R_{free}$	100719	1134 (3.82-3.50)
Clashscore	112137	1267 (3.82-3.50)
Ramachandran outliers	110173	1219 (3.82-3.50)
Sidechain outliers	110143	1218 (3.82-3.50)
RSRZ outliers	101464	1160 (3.82-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	269	<div> <div>0.1%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
1	B	269	<div> <div>0.1%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
1	C	269	<div> <div>0.1%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>
1	D	269	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>
1	E	269	<div> <div>0.1%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9572 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 Factor H binding protein, Major outer membrane protein P.IA, Factor H binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	250	Total	C	N	O	S	0	0	0
			1903	1186	338	378	1			
1	A	255	Total	C	N	O	S	0	0	0
			1941	1208	346	386	1			
1	B	247	Total	C	N	O		0	0	0
			1881	1174	335	372				
1	D	255	Total	C	N	O	S	0	0	0
			1941	1208	346	386	1			
1	E	250	Total	C	N	O	S	0	0	0
			1906	1189	339	377	1			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	72	MET	GLY	conflict	UNP Q9JXV4
C	321	LEU	-	expression tag	UNP Q9JXV4
C	322	GLU	-	expression tag	UNP Q9JXV4
C	323	HIS	-	expression tag	UNP Q9JXV4
C	324	HIS	-	expression tag	UNP Q9JXV4
C	325	HIS	-	expression tag	UNP Q9JXV4
C	326	HIS	-	expression tag	UNP Q9JXV4
C	327	HIS	-	expression tag	UNP Q9JXV4
C	328	HIS	-	expression tag	UNP Q9JXV4
A	72	MET	GLY	conflict	UNP Q9JXV4
A	321	LEU	-	expression tag	UNP Q9JXV4
A	322	GLU	-	expression tag	UNP Q9JXV4
A	323	HIS	-	expression tag	UNP Q9JXV4
A	324	HIS	-	expression tag	UNP Q9JXV4
A	325	HIS	-	expression tag	UNP Q9JXV4
A	326	HIS	-	expression tag	UNP Q9JXV4
A	327	HIS	-	expression tag	UNP Q9JXV4
A	328	HIS	-	expression tag	UNP Q9JXV4

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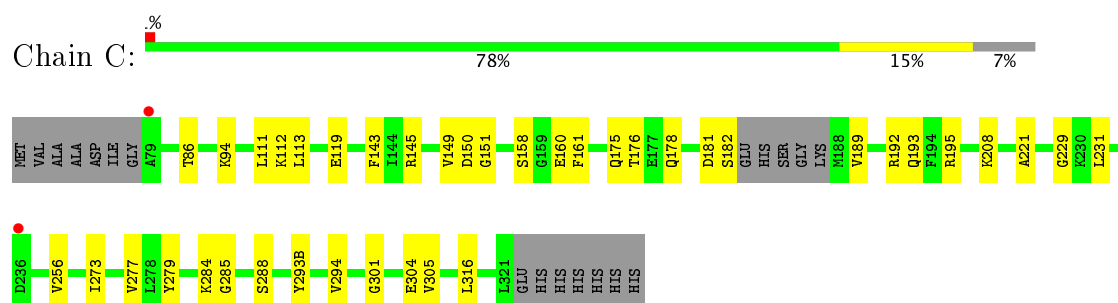
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Chain	Residue	Modelled	Actual	Comment	Reference
B	72	MET	GLY	conflict	UNP Q9JXV4
B	321	LEU	-	expression tag	UNP Q9JXV4
B	322	GLU	-	expression tag	UNP Q9JXV4
B	323	HIS	-	expression tag	UNP Q9JXV4
B	324	HIS	-	expression tag	UNP Q9JXV4
B	325	HIS	-	expression tag	UNP Q9JXV4
B	326	HIS	-	expression tag	UNP Q9JXV4
B	327	HIS	-	expression tag	UNP Q9JXV4
B	328	HIS	-	expression tag	UNP Q9JXV4
D	72	MET	GLY	conflict	UNP Q9JXV4
D	321	LEU	-	expression tag	UNP Q9JXV4
D	322	GLU	-	expression tag	UNP Q9JXV4
D	323	HIS	-	expression tag	UNP Q9JXV4
D	324	HIS	-	expression tag	UNP Q9JXV4
D	325	HIS	-	expression tag	UNP Q9JXV4
D	326	HIS	-	expression tag	UNP Q9JXV4
D	327	HIS	-	expression tag	UNP Q9JXV4
D	328	HIS	-	expression tag	UNP Q9JXV4
E	72	MET	GLY	conflict	UNP Q9JXV4
E	321	LEU	-	expression tag	UNP Q9JXV4
E	322	GLU	-	expression tag	UNP Q9JXV4
E	323	HIS	-	expression tag	UNP Q9JXV4
E	324	HIS	-	expression tag	UNP Q9JXV4
E	325	HIS	-	expression tag	UNP Q9JXV4
E	326	HIS	-	expression tag	UNP Q9JXV4
E	327	HIS	-	expression tag	UNP Q9JXV4
E	328	HIS	-	expression tag	UNP Q9JXV4

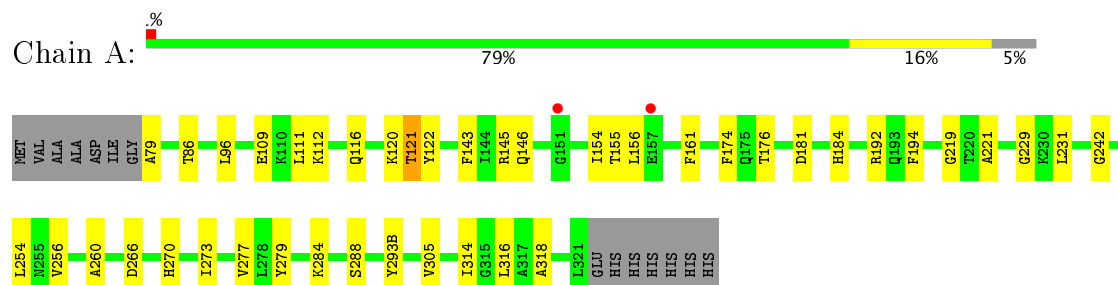
### 3 Residue-property plots [i](#)

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.

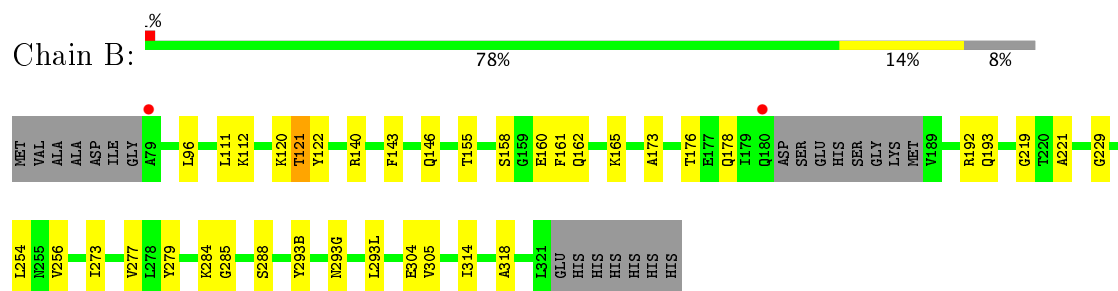
- Molecule 1: Factor H binding protein, Major outer membrane protein P.IA, Factor H binding protein




- Molecule 1: Factor H binding protein, Major outer membrane protein P.IA, Factor H binding protein

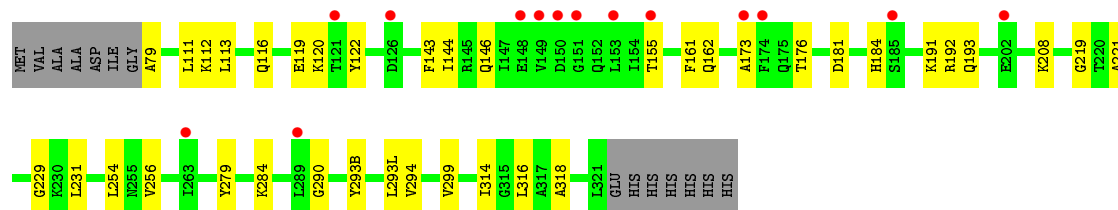


- Molecule 1: Factor H binding protein, Major outer membrane protein P.IA, Factor H binding protein




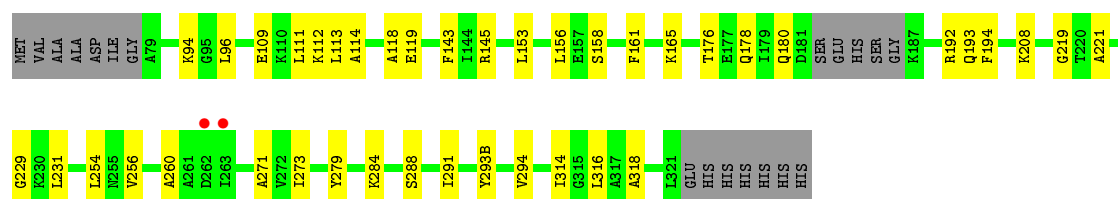
- Molecule 1: Factor H binding protein, Major outer membrane protein P.IA, Factor H binding protein

Chain D: 



- Molecule 1: Factor H binding protein, Major outer membrane protein P.IA, Factor H binding protein

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.85Å 114.90Å 160.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.64 – 3.66 81.64 – 3.66	Depositor EDS
% Data completeness (in resolution range)	99.2 (81.64-3.66) 99.2 (81.64-3.66)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.232 , 0.281 0.232 , 0.281	Depositor DCC
$R_{free}$ test set	975 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0/1968	0.45	0/2645
1	B	0.25	0/1906	0.46	0/2562
1	C	0.24	0/1928	0.45	0/2591
1	D	0.24	0/1968	0.44	0/2645
1	E	0.24	0/1931	0.44	0/2594
All	All	0.24	0/9701	0.45	0/13037

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	A	1941	0	1932	25	0
1	B	1881	0	1879	22	0
1	C	1903	0	1897	22	0
1	D	1941	0	1932	23	0
1	E	1906	0	1905	22	0
All	All	9572	0	9545	109	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 6.

The worst 5 of 109 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:176:THR:O	1:A:192:ARG:HA	1.80	0.80
1:B:176:THR:O	1:B:192:ARG:HA	1.85	0.77
1:A:221:ALA:O	1:A:229:GLY:HA3	1.88	0.73
1:C:86:THR:HG22	1:D:293(L):LEU:HD11	1.70	0.73
1:B:221:ALA:O	1:B:229:GLY:HA3	1.90	0.71

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	253/269 (94%)	248 (98%)	5 (2%)	0	100	100
1	B	243/269 (90%)	238 (98%)	5 (2%)	0	100	100
1	C	246/269 (91%)	242 (98%)	3 (1%)	1 (0%)	38	76
1	D	253/269 (94%)	246 (97%)	7 (3%)	0	100	100
1	E	246/269 (91%)	240 (98%)	6 (2%)	0	100	100
All	All	1241/1345 (92%)	1214 (98%)	26 (2%)	1 (0%)	55	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	ASP

### 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	202/213 (95%)	199 (98%)	3 (2%)	70	88
1	B	195/213 (92%)	192 (98%)	3 (2%)	70	88
1	C	198/213 (93%)	196 (99%)	2 (1%)	80	91
1	D	202/213 (95%)	201 (100%)	1 (0%)	91	96
1	E	198/213 (93%)	195 (98%)	3 (2%)	70	88
All	All	995/1065 (93%)	983 (99%)	12 (1%)	75	89

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	THR
1	B	293(B)	TYR
1	E	94	LYS
1	A	293(B)	TYR
1	D	293(B)	TYR

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

Mol	Chain	Res	Type
1	D	116	GLN
1	D	193	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](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	255/269 (94%)	0.23	2 (0%) 86 75	55, 91, 158, 218	0
1	B	247/269 (91%)	0.18	2 (0%) 86 75	53, 98, 155, 200	0
1	C	250/269 (92%)	0.24	2 (0%) 86 75	56, 94, 139, 185	0
1	D	255/269 (94%)	0.43	14 (5%) 26 17	74, 134, 200, 284	0
1	E	250/269 (92%)	0.40	2 (0%) 86 75	59, 118, 185, 234	0
All	All	1257/1345 (93%)	0.29	22 (1%) 69 54	53, 105, 178, 284	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	153	LEU	4.3
1	E	262	ASP	3.7
1	A	151	GLY	3.5
1	B	180	GLN	3.2
1	D	155	THR	3.0

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.