



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:46 AM GMT

PDB ID : 2W81  
Title : STRUCTURE OF A COMPLEX BETWEEN NEISSERIA MENINGITIDIS  
FACTOR H BINDING PROTEIN AND CCPS 6-7 OF HUMAN COMPLE-  
MENT FACTOR H  
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Q.; Quoraishi, S.; Lovett, J.E.; Deane, J.E.; Sim, R.B.; Roversi, P.; Johnson,  
S.; Tang, C.M.; Lea, S.M.  
Deposited on : 2009-01-08  
Resolution : 2.35 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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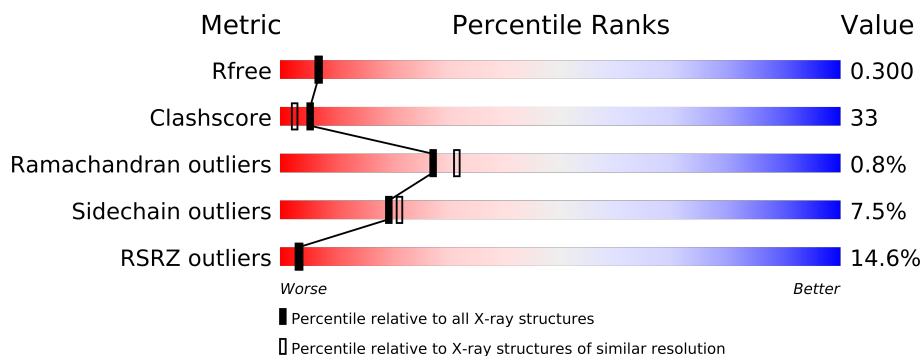
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	123	
1	B	123	
1	E	123	
2	C	253	
2	D	253	
2	F	253	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8836 atoms, of which 0 are hydrogen and 0 are deuterium.

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 COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			943	602	162	169	10			
1	B	121	Total	C	N	O	S	0	0	0
			984	629	169	176	10			
1	E	122	Total	C	N	O	S	0	0	0
			992	635	170	177	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	TYR	VARIANT	UNP P08603
B	402	HIS	TYR	VARIANT	UNP P08603
E	402	HIS	TYR	VARIANT	UNP P08603

- Molecule 2 is a protein called FACTOR H BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	242	Total	C	N	O	S	0	0	0
			1832	1137	329	365	1			
2	D	243	Total	C	N	O	S	0	0	0
			1845	1146	330	368	1			
2	F	240	Total	C	N	O	S	0	0	0
			1816	1127	327	361	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	55	Total	O	0	0
			55	55		

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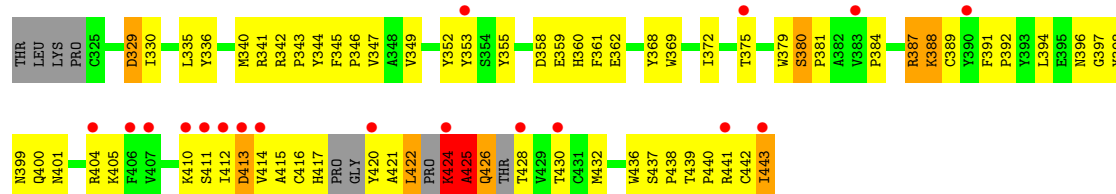
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	98	Total 98	O 98	0	0
3	D	99	Total 99	O 99	0	0
3	E	46	Total 46	O 46	0	0
3	F	90	Total 90	O 90	0	0

### 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 errors 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.

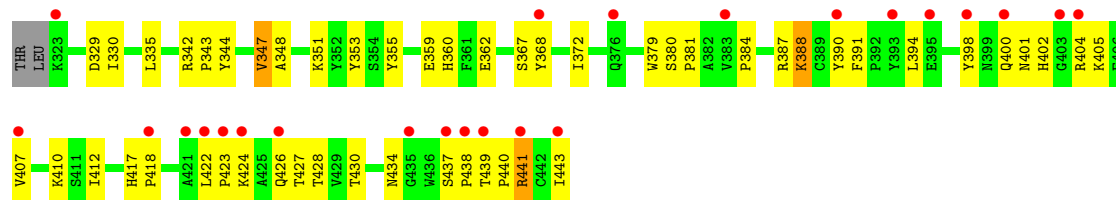
#### • Molecule 1: COMPLEMENT FACTOR H

Chain A: 



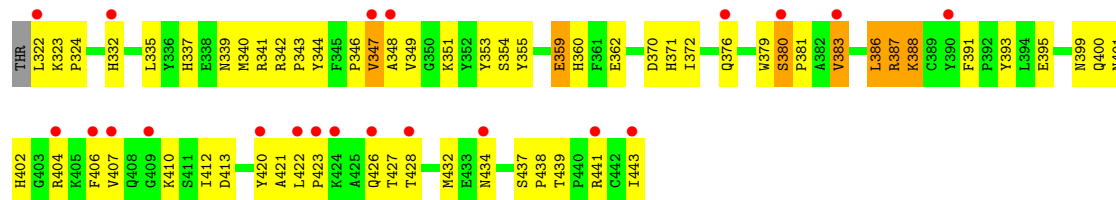
#### • Molecule 1: COMPLEMENT FACTOR H

Chain B: 



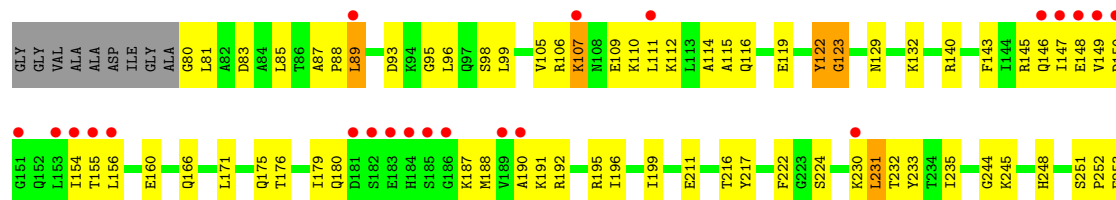
#### • Molecule 1: COMPLEMENT FACTOR H

Chain E: 



#### • Molecule 2: FACTOR H BINDING PROTEIN

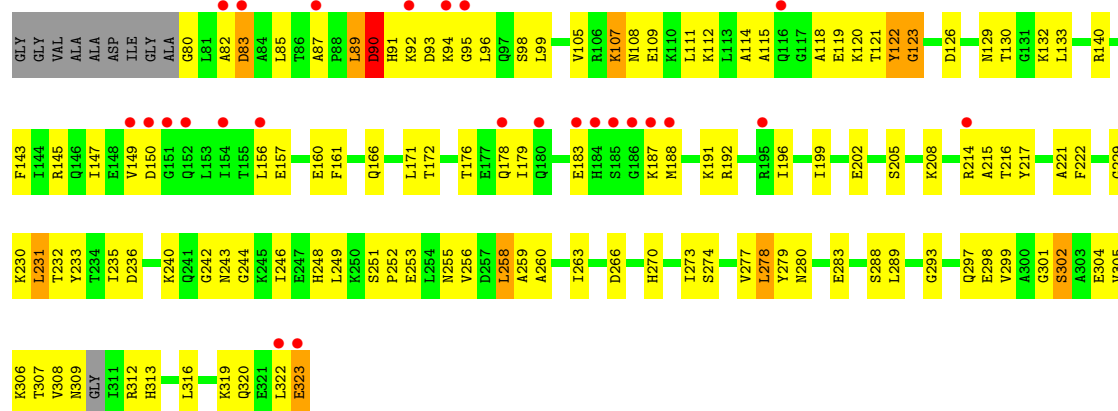
Chain C: 





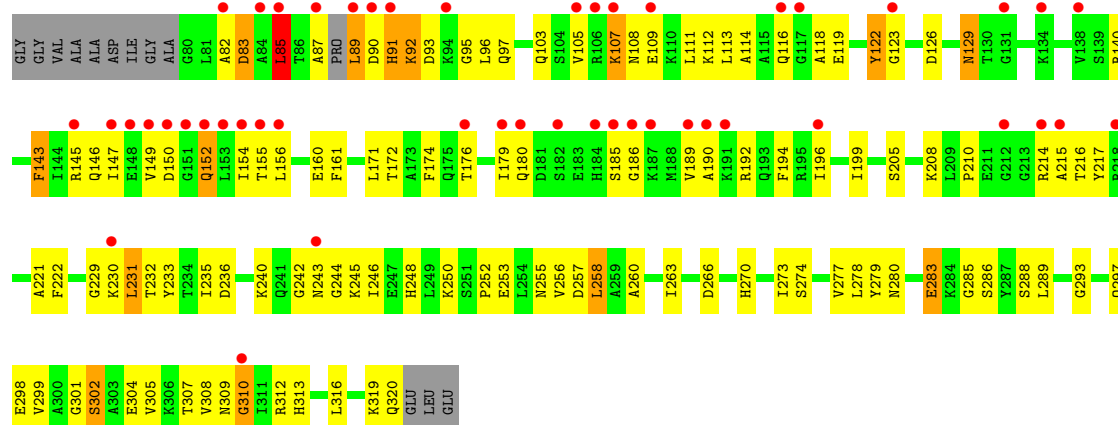
• Molecule 2: FACTOR H BINDING PROTEIN

Chain D:



• Molecule 2: FACTOR H BINDING PROTEIN

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.52Å 52.21Å 128.78Å 90.00° 118.19° 90.00°	Depositor
Resolution (Å)	38.81 – 2.35 38.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.81-2.35) 94.0 (38.82-2.35)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.34Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, $R_{free}$	0.274 , 0.283 0.290 , 0.300	Depositor DCC
$R_{free}$ test set	2187 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 24.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43085 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.63	1/977 (0.1%)	0.87	5/1325 (0.4%)
1	B	0.39	0/1024	0.55	0/1396
1	E	0.46	0/1032	0.65	0/1407
2	C	0.35	0/1857	0.55	0/2491
2	D	0.38	0/1869	0.63	3/2506 (0.1%)
2	F	0.35	0/1839	0.54	1/2464 (0.0%)
All	All	0.41	1/8598 (0.0%)	0.62	9/11589 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	LYS	CB-CG	-5.26	1.38	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	90	ASP	N-CA-C	-9.07	86.52	111.00
1	A	422	LEU	CA-CB-CG	-7.56	97.92	115.30
2	D	83	ASP	CB-CA-C	-5.71	98.97	110.40
2	D	91	HIS	N-CA-CB	-5.47	100.75	110.60
1	A	425	ALA	CA-C-N	-5.32	105.50	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	424	LYS	Mainchain,Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	943	0	850	81	1
1	B	984	0	897	58	0
1	E	992	0	908	92	0
2	C	1832	0	1820	93	0
2	D	1845	0	1833	112	0
2	F	1816	0	1806	129	1
3	A	36	0	0	9	0
3	B	55	0	0	17	0
3	C	98	0	0	15	0
3	D	99	0	0	17	0
3	E	46	0	0	20	0
3	F	90	0	0	25	0
All	All	8836	0	8114	539	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 539 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:TYR:CD1	1:A:443:ILE:HG12	1.84	1.13
1:E:407:VAL:HG12	1:E:410:LYS:HG3	1.21	1.12
1:A:375:THR:HG21	1:B:418:PRO:HD2	1.40	1.02
1:E:322:LEU:HG	1:E:324:PRO:HD3	1.44	0.97
1:E:362:GLU:HG3	1:E:388:LYS:HZ2	1.28	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:ILE:O	2:F:214:ARG:NH2[4_454]	2.18	0.02

## 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	
1	A	107/123 (87%)	99 (92%)	7 (6%)	1 (1%)	25	27
1	B	119/123 (97%)	110 (92%)	9 (8%)	0	100	100
1	E	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
2	C	240/253 (95%)	219 (91%)	18 (8%)	3 (1%)	18	17
2	D	239/253 (94%)	219 (92%)	18 (8%)	2 (1%)	27	31
2	F	236/253 (93%)	217 (92%)	17 (7%)	2 (1%)	27	31
All	All	1061/1128 (94%)	977 (92%)	76 (7%)	8 (1%)	27	31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ALA
2	C	129	ASN
2	D	129	ASN
2	F	129	ASN
2	C	310	GLY

### 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	
1	A	101/108 (94%)	92 (91%)	9 (9%)	14	14
1	B	106/108 (98%)	99 (93%)	7 (7%)	24	26
1	E	107/108 (99%)	98 (92%)	9 (8%)	16	17
2	C	189/194 (97%)	177 (94%)	12 (6%)	25	29
2	D	191/194 (98%)	177 (93%)	14 (7%)	20	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	187/194 (96%)	172 (92%)	15 (8%)	17	19
All	All	881/906 (97%)	815 (92%)	66 (8%)	19	21

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	90	ASP
2	D	231	LEU
2	F	152	GLN
2	D	94	LYS
2	D	122	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	175	GLN
2	F	175	GLN
2	D	166	GLN
2	C	166	GLN
2	C	309	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	115/123 (93%)	1.22	18 (15%) <b>3</b> <b>3</b>	26, 40, 68, 91	3 (2%)
1	B	121/123 (98%)	0.95	24 (19%) <b>2</b> <b>2</b>	20, 35, 61, 79	2 (1%)
1	E	122/123 (99%)	1.17	21 (17%) <b>2</b> <b>2</b>	24, 40, 65, 82	2 (1%)
2	C	242/253 (95%)	0.59	22 (9%) <b>9</b> <b>11</b>	14, 31, 66, 81	1 (0%)
2	D	243/253 (96%)	0.73	25 (10%) <b>7</b> <b>8</b>	18, 38, 70, 96	2 (0%)
2	F	240/253 (94%)	1.18	48 (20%) <b>2</b> <b>1</b>	27, 47, 79, 93	1 (0%)
All	All	1083/1128 (96%)	0.92	158 (14%) <b>3</b> <b>3</b>	14, 39, 70, 96	11 (1%)

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	151	GLY	11.0
2	C	147	ILE	8.4
2	C	154	ILE	7.4
2	C	156	LEU	7.3
2	C	153	LEU	7.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.