



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 09:31 PM EDT

PDB ID : 7KET  
Title : Factor H enhancing human antibody fragment (Fab) to meningococcal Factor H binding protein  
Authors : Beernink, P.T.; Sands, N.  
Deposited on : 2020-10-12  
Resolution : 2.00 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](mailto: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>.

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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) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

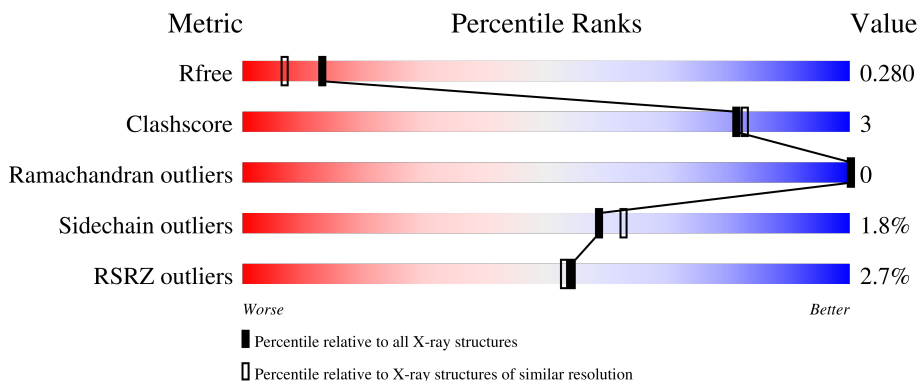
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

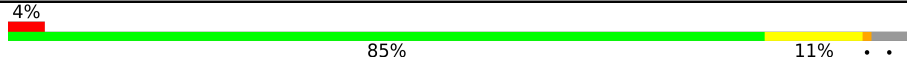
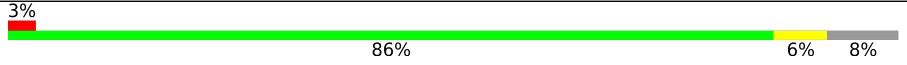

The reported resolution of this entry is 2.00 Å.

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	B	217	 4% 85% 11% 8%
2	A	235	 3% 86% 6% 8%
3	C	263	 % 88% 8%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10263 atoms, of which 5014 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 Immunoglobulin gamma, kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	209	3160	1008	1551	274	322	5	0	1	0

- Molecule 2 is a protein called Immunoglobulin gamma, heavy chain Fd fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	A	217	3260	1031	1623	276	320	10	0	4	0

- Molecule 3 is a protein called Factor H binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	242	3681	1145	1840	330	365	1	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	256	LEU	-	expression tag	UNP Q6VRZ6
C	257	GLU	-	expression tag	UNP Q6VRZ6
C	258	HIS	-	expression tag	UNP Q6VRZ6
C	259	HIS	-	expression tag	UNP Q6VRZ6
C	260	HIS	-	expression tag	UNP Q6VRZ6
C	261	HIS	-	expression tag	UNP Q6VRZ6
C	262	HIS	-	expression tag	UNP Q6VRZ6
C	263	HIS	-	expression tag	UNP Q6VRZ6

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	30	Total	O	0	0
			30	30		

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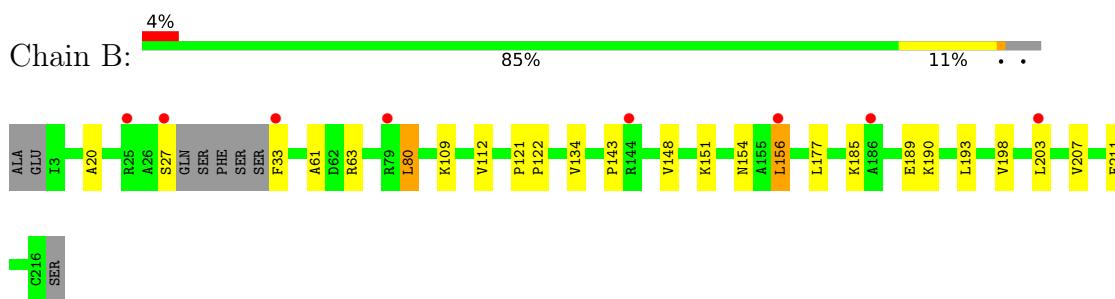
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	A	67	Total O 67 67	0	0
4	C	65	Total O 65 65	0	0

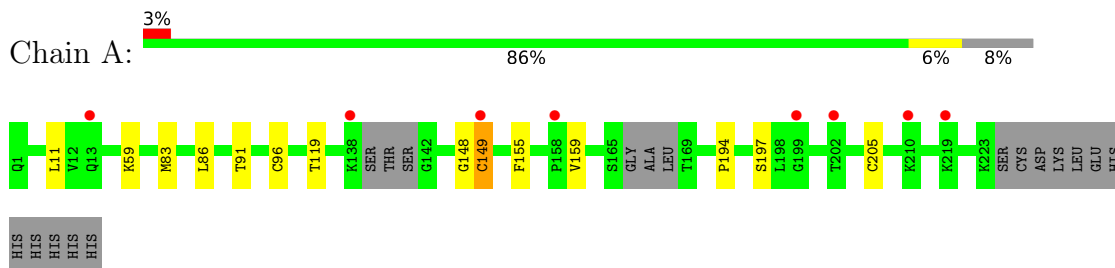
### 3 Residue-property plots [i](#)

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.

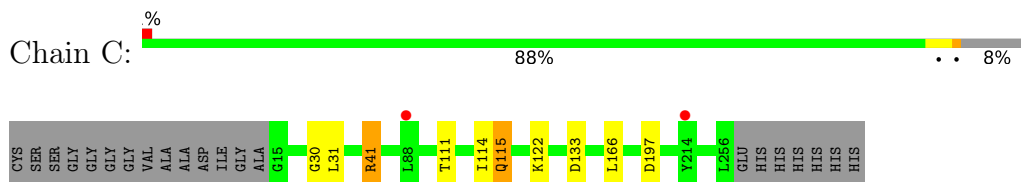
- Molecule 1: Immunoglobulin gamma, kappa light chain



- Molecule 2: Immunoglobulin gamma, heavy chain Fd fragment



- Molecule 3: Factor H binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.58Å 86.03Å 107.89Å 90.00° 96.91° 90.00°	Depositor
Resolution (Å)	107.11 – 2.00 107.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (107.11-2.00) 95.0 (107.11-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.00Å)	Xtrriage
Refinement program	Coot 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.234 , 0.281 0.242 , 0.280	Depositor DCC
$R_{free}$ test set	1571 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtrriage
Anisotropy	0.254	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10263	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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	B	0.39	0/1646	0.62	0/2233
2	A	0.47	1/1685 (0.1%)	0.62	0/2290
3	C	0.44	2/1872 (0.1%)	0.65	0/2512
All	All	0.44	3/5203 (0.1%)	0.63	0/7035

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	B	0	4
3	C	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	115[A]	GLN	C-O	6.33	1.35	1.23
3	C	115[B]	GLN	C-O	6.33	1.35	1.23
2	A	148	GLY	C-O	-5.32	1.15	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	177	LEU	Mainchain
1	B	33	PHE	Peptide
1	B	80	LEU	Mainchain
3	C	166	LEU	Mainchain

## 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	B	1609	1551	1568	10	1
2	A	1637	1623	1628	10	0
3	C	1841	1840	1840	5	1
4	A	67	0	0	0	0
4	B	30	0	0	1	0
4	C	65	0	0	0	0
All	All	5249	5014	5036	25	1

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 3.

All (25) 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:A:149[A]:CYS:HG	2:A:205:CYS:HG	1.41	0.68
2:A:11:LEU:CD1	2:A:155:PHE:HE2	2.11	0.64
2:A:91:THR:HG23	2:A:119:THR:HA	1.82	0.60
2:A:11:LEU:HD11	2:A:155:PHE:HE2	1.71	0.55
3:C:111[B]:THR:HG21	3:C:114:ILE:CG2	2.40	0.52
3:C:111[B]:THR:HG21	3:C:114:ILE:HG23	1.92	0.51
2:A:149[B]:CYS:HB3	2:A:205:CYS:HG	1.76	0.51
3:C:115[A]:GLN:NE2	3:C:122:LYS:O	2.45	0.50
2:A:83:MET:HB3	2:A:86:LEU:HD21	1.94	0.49
2:A:194:PRO:HG2	2:A:197:SER:OG	2.13	0.49
1:B:20:ALA:HB2	1:B:80:LEU:HD11	1.96	0.48
1:B:122:PRO:HD3	1:B:134:VAL:HG22	1.98	0.45
3:C:41:ARG:HA	3:C:41:ARG:HD2	1.52	0.43
2:A:149[B]:CYS:HB3	2:A:205:CYS:SG	2.59	0.43
2:A:11:LEU:CD1	2:A:155:PHE:CE2	2.98	0.42
1:B:112:VAL:HG22	1:B:143:PRO:HD3	2.01	0.41
1:B:203:LEU:HD13	1:B:207:VAL:HG23	2.02	0.41
1:B:109:LYS:NZ	4:B:306:HOH:O	2.53	0.41
1:B:148:VAL:HG22	1:B:198:VAL:HG12	2.01	0.41
1:B:121:PRO:HB3	1:B:211:PHE:CE1	2.56	0.41
2:A:11:LEU:HD13	2:A:155:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:GLY:HA2	3:C:31:LEU:C	2.42	0.41
1:B:185:LYS:HE3	1:B:189:GLU:OE1	2.21	0.41
1:B:61:ALA:HB3	1:B:63:ARG:HG3	2.04	0.40
1:B:151:LYS:HE2	1:B:156:LEU:HG	2.03	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HZ1	3:C:197:ASP:OD1[1_656]	1.50	0.10

## 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	B	206/217 (95%)	194 (94%)	12 (6%)	0	100	100
2	A	215/235 (92%)	209 (97%)	6 (3%)	0	100	100
3	C	242/263 (92%)	229 (95%)	13 (5%)	0	100	100
All	All	663/715 (93%)	632 (95%)	31 (5%)	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	B	181/187 (97%)	177 (98%)	4 (2%)	52	55
2	A	188/200 (94%)	182 (97%)	6 (3%)	39	38
3	C	191/202 (95%)	189 (99%)	2 (1%)	76	81
All	All	560/589 (95%)	548 (98%)	12 (2%)	59	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	SER
1	B	154	ASN
1	B	156	LEU
1	B	193	LEU
2	A	59	LYS
2	A	96[A]	CYS
2	A	96[B]	CYS
2	A	149[A]	CYS
2	A	149[B]	CYS
2	A	159	VAL
3	C	41	ARG
3	C	133	ASP

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

Mol	Chain	Res	Type
1	B	154	ASN
2	A	208	ASN
3	C	32	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](#)

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	B	209/217 (96%)	0.27	8 (3%) 40 39	44, 69, 99, 122	0
2	A	217/235 (92%)	0.15	8 (3%) 41 41	31, 55, 91, 117	0
3	C	242/263 (92%)	0.07	2 (0%) 86 85	34, 54, 87, 121	0
All	All	668/715 (93%)	0.16	18 (2%) 54 53	31, 59, 94, 122	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	138	LYS	3.5
2	A	202	THR	3.4
3	C	214	TYR	3.1
2	A	149[A]	CYS	2.9
3	C	88	LEU	2.8
1	B	33	PHE	2.7
2	A	219	LYS	2.6
1	B	79	ARG	2.5
2	A	199	GLY	2.5
1	B	186	ALA	2.3
2	A	158	PRO	2.3
1	B	203	LEU	2.3
1	B	25	ARG	2.3
2	A	210	LYS	2.2
1	B	156	LEU	2.1
1	B	27	SER	2.1
1	B	144	ARG	2.0
2	A	13	GLN	2.0

### 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 monosaccharides 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.