



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 10:55 am GMT

PDB ID : 1KF9  
Title : PHAGE DISPLAY DERIVED VARIANT OF HUMAN GROWTH HORMONE COMPLEXED WITH TWO COPIES OF THE EXTRACELLULAR DOMAIN OF ITS RECEPTOR  
Authors : Schiffer, C.A.; Ultsch, M.; Walsh, S.; Somers, W.; De Vos, A.M.; Kossiakoff, A.A.  
Deposited on : 2001-11-19  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

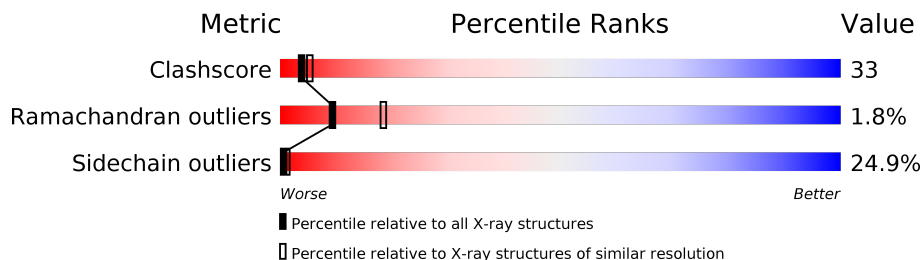
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	122078	3109 (2.60-2.60)
Ramachandran outliers	120005	3061 (2.60-2.60)
Sidechain outliers	119972	3061 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	191	
1	D	191	
2	B	238	
2	C	238	
2	E	238	
2	F	238	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8678 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 PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1284	825	211	242	6			
1	D	158	Total	C	N	O	S	0	0	0
			1264	811	208	239	6			

- Molecule 2 is a protein called EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1577	1011	258	298	10			
2	C	175	Total	C	N	O	S	0	0	0
			1419	916	229	265	9			
2	E	193	Total	C	N	O	S	0	0	0
			1576	1011	258	298	9			
2	F	184	Total	C	N	O	S	0	0	0
			1484	952	239	284	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	13	Total	O	0	0
			13	13		
3	C	28	Total	O	0	0
			28	28		
3	D	3	Total	O	0	0
			3	3		
3	E	12	Total	O	0	0
			12	12		

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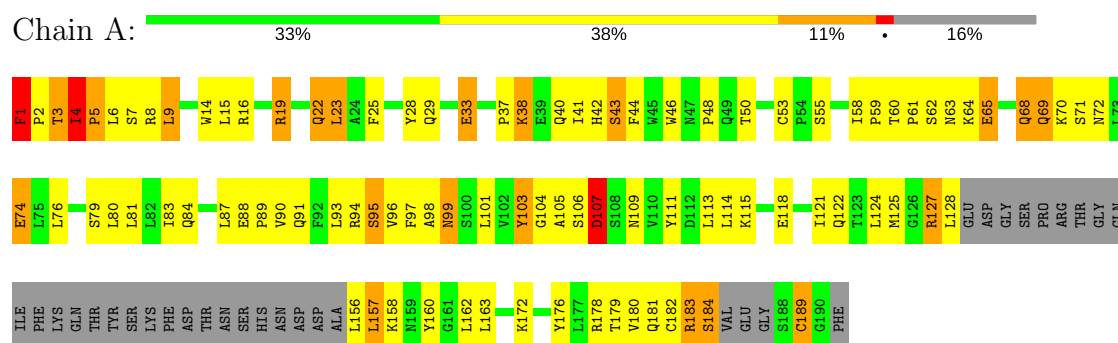
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	7	Total	O	0	0
			7	7		

### 3 Residue-property plots

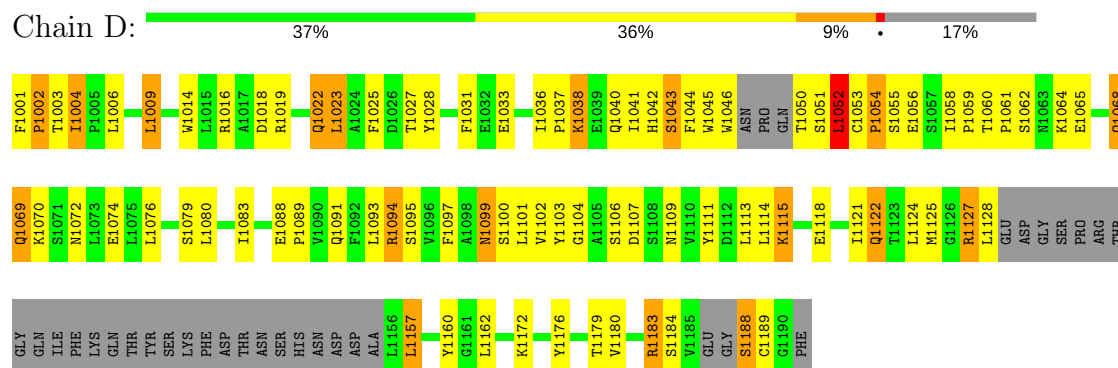
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

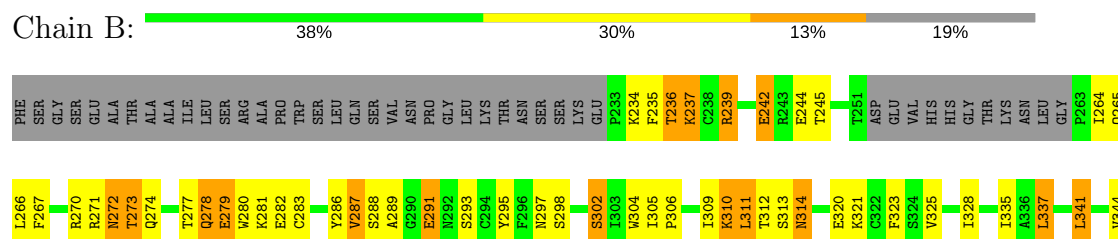
#### • Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE

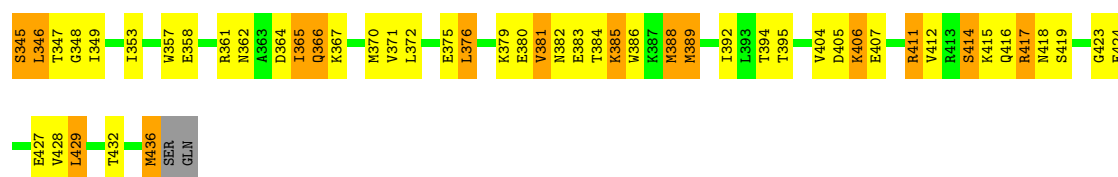


#### • Molecule 1: PHAGE DISPLAY DERIVED VARIANT HUMAN GROWTH HORMONE



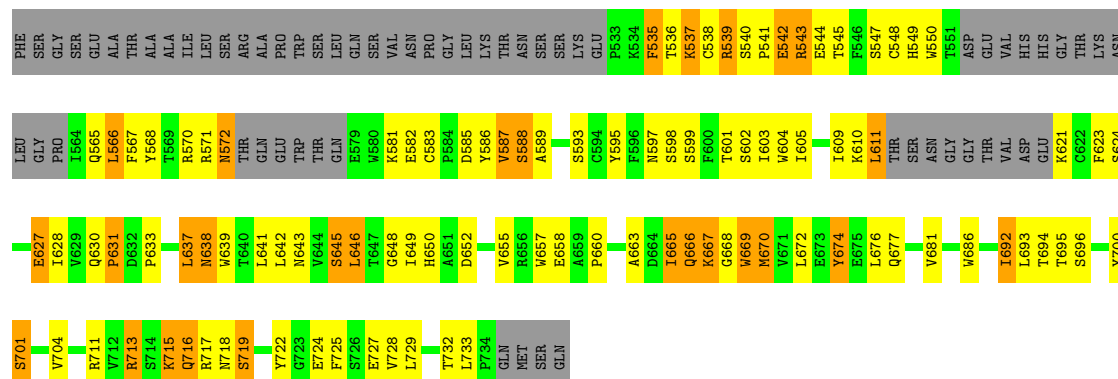
#### • Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)





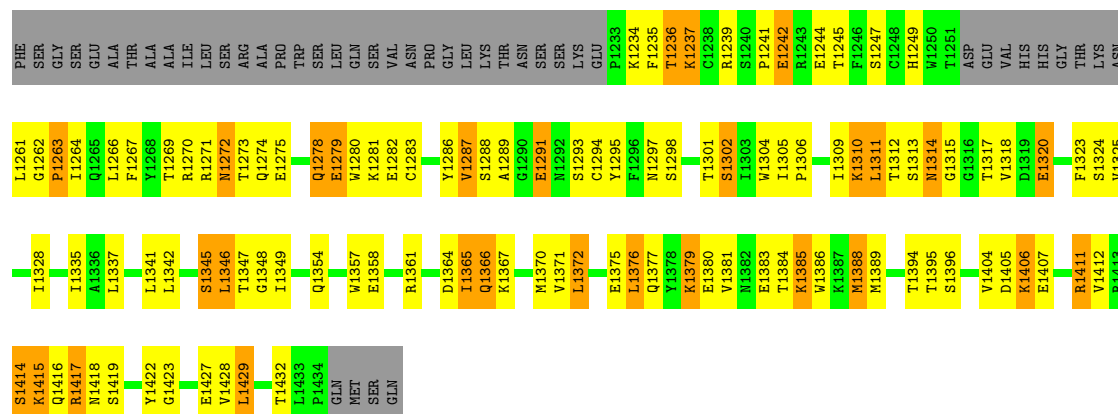
- Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain C: 30% 32% 12% 26%



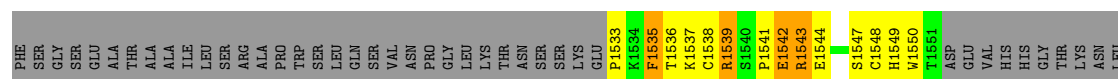
- Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain E: 34% 35% 12% 19%



- Molecule 2: EXTRACELLULAR DOMAIN HUMAN GROWTH HORMONE RECEPTOR (1-238)

Chain F: 29% 36% 12% 23%



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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.29Å 111.94Å 95.29Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	90.5 (20.00-2.60)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.234 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP



## 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	0.67	0/1312	0.84	2/1781 (0.1%)
1	D	0.71	0/1289	0.84	2/1747 (0.1%)
2	B	0.70	0/1622	0.87	0/2208
2	C	0.67	0/1459	0.86	1/1987 (0.1%)
2	E	0.69	0/1621	0.86	1/2208 (0.0%)
2	F	0.65	0/1525	0.84	0/2078
All	All	0.68	0/8828	0.85	6/12009 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	THR	N-CA-C	-9.03	86.61	111.00
1	D	1107	ASP	CB-CG-OD1	6.76	124.39	118.30
2	C	668	GLY	N-CA-C	-6.00	98.09	113.10
2	E	1324	SER	N-CA-C	-5.23	96.87	111.00
1	A	1	PHE	C-N-CD	5.20	139.32	128.40

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	1284	0	1257	102	0
1	D	1264	0	1241	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1577	0	1506	91	0
2	C	1419	0	1338	99	0
2	E	1576	0	1508	104	0
2	F	1484	0	1395	115	0
3	A	11	0	0	2	0
3	B	13	0	0	1	0
3	C	28	0	0	2	0
3	D	3	0	0	0	0
3	E	12	0	0	1	0
3	F	7	0	0	0	0
All	All	8678	0	8245	550	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 33.

The worst 5 of 550 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:104:GLY:CA	2:C:666:GLN:HB3	1.65	1.26
2:E:1346:LEU:HB2	2:F:1701:SER:HB3	1.24	1.17
1:A:104:GLY:HA2	2:C:666:GLN:HB3	1.25	1.14
2:F:1581:LYS:HZ3	2:F:1581:LYS:HB2	1.08	1.09
1:A:104:GLY:HA3	2:C:666:GLN:HB3	1.41	1.02

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	154/191 (81%)	129 (84%)	19 (12%)	6 (4%)	<b>3</b> <b>4</b>
1	D	150/191 (78%)	129 (86%)	17 (11%)	4 (3%)	<b>5</b> <b>9</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	189/238 (79%)	168 (89%)	20 (11%)	1 (0%)	31	56
2	C	167/238 (70%)	144 (86%)	21 (13%)	2 (1%)	14	30
2	E	189/238 (79%)	171 (90%)	16 (8%)	2 (1%)	16	33
2	F	178/238 (75%)	155 (87%)	20 (11%)	3 (2%)	10	20
All	All	1027/1334 (77%)	896 (87%)	113 (11%)	18 (2%)	9	18

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	107	ASP
2	B	274	GLN
1	D	1002	PRO
2	E	1274	GLN

### 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	143/175 (82%)	112 (78%)	31 (22%)	1	2
1	D	142/175 (81%)	112 (79%)	30 (21%)	1	2
2	B	177/218 (81%)	130 (73%)	47 (27%)	0	1
2	C	157/218 (72%)	113 (72%)	44 (28%)	0	1
2	E	177/218 (81%)	134 (76%)	43 (24%)	1	1
2	F	165/218 (76%)	121 (73%)	44 (27%)	0	1
All	All	961/1222 (79%)	722 (75%)	239 (25%)	0	1

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	672	LEU
1	D	1055	SER

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Mol	Chain	Res	Type
2	F	1658	GLU
2	C	692	ILE
2	C	729	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	716	GLN
1	D	1122	GLN
2	F	1643	ASN
1	D	1068	GLN
1	D	1099	ASN

### 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](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.