



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2026 – 04:11 pm BST

PDB ID : 9TUW / pdb\_00009tuw  
Title : PfrIPR EGF6 and 7 bound to monoclonal antibody RP.012  
Authors : Farrell, B.; Higgins, M.K.  
Deposited on : 2026-01-10  
Resolution : 2.20 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.

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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.015 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

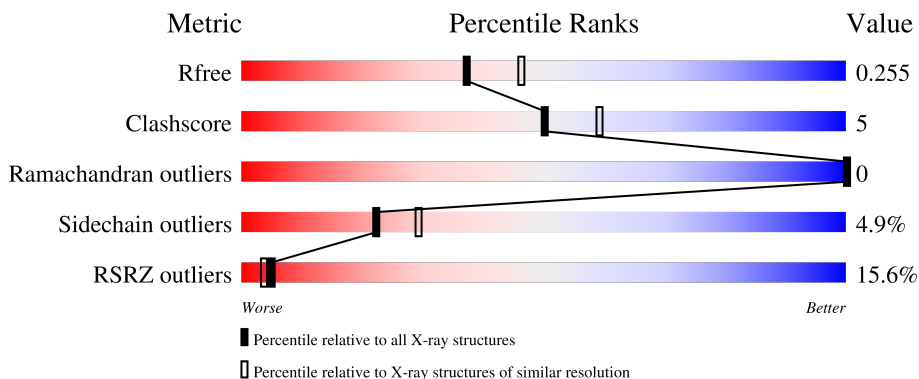
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	A	343	 4% 13% 83%
1	D	343	 2% 13% 5% 82%
2	B	241	 12% 72% 13% 14%
2	E	241	 10% 72% 13% 14%
3	C	234	 17% 80% 9% 10%

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Mol	Chain	Length	Quality of chain
3	F	234	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '16%', a large green segment labeled '79%', a yellow segment labeled '10%', and a grey segment on the far right labeled '10%'.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7553 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 Immunoglobulin gamma-1 heavy chain,Rh5-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	60	482	288	84	99	11	0	0	0
1	D	63	507	304	89	103	11	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	MET	-	initiating methionine	UNP P0DOX5
A	524	GLY	-	expression tag	UNP P0DOX5
A	525	TRP	-	expression tag	UNP P0DOX5
A	526	SER	-	expression tag	UNP P0DOX5
A	527	CYS	-	expression tag	UNP P0DOX5
A	528	ILE	-	expression tag	UNP P0DOX5
A	529	ILE	-	expression tag	UNP P0DOX5
A	530	LEU	-	expression tag	UNP P0DOX5
A	531	PHE	-	expression tag	UNP P0DOX5
A	532	LEU	-	expression tag	UNP P0DOX5
A	533	VAL	-	expression tag	UNP P0DOX5
A	534	ALA	-	expression tag	UNP P0DOX5
A	535	THR	-	expression tag	UNP P0DOX5
A	536	ALA	-	expression tag	UNP P0DOX5
A	537	THR	-	expression tag	UNP P0DOX5
A	538	GLY	-	expression tag	UNP P0DOX5
A	539	VAL	-	expression tag	UNP P0DOX5
A	540	HIS	-	expression tag	UNP P0DOX5
A	541	SER	-	expression tag	UNP P0DOX5
A	670	ASN	SER	conflict	UNP P0DOX5
A	713	ASN	TYR	conflict	UNP P0DOX5
A	754	GLY	-	linker	UNP P0DOX5
A	755	GLY	-	linker	UNP P0DOX5
A	756	GLY	-	linker	UNP P0DOX5
A	757	GLY	-	linker	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	758	SER	-	linker	UNP P0DOX5
A	759	GLY	-	linker	UNP P0DOX5
A	760	GLY	-	linker	UNP P0DOX5
A	761	GLY	-	linker	UNP P0DOX5
A	762	SER	-	linker	UNP P0DOX5
A	763	GLU	-	linker	UNP P0DOX5
A	764	ASN	-	linker	UNP P0DOX5
A	765	LEU	-	linker	UNP P0DOX5
A	766	TYR	-	linker	UNP P0DOX5
A	767	PHE	-	linker	UNP P0DOX5
A	768	GLN	-	linker	UNP P0DOX5
A	769	GLY	-	linker	UNP P0DOX5
A	770	SER	-	linker	UNP P0DOX5
A	856	GLY	-	expression tag	UNP O97302
A	857	GLY	-	expression tag	UNP O97302
A	858	THR	-	expression tag	UNP O97302
A	859	GLY	-	expression tag	UNP O97302
A	860	GLY	-	expression tag	UNP O97302
A	861	SER	-	expression tag	UNP O97302
A	862	GLU	-	expression tag	UNP O97302
A	863	PRO	-	expression tag	UNP O97302
A	864	GLU	-	expression tag	UNP O97302
A	865	ALA	-	expression tag	UNP O97302
D	523	MET	-	initiating methionine	UNP P0DOX5
D	524	GLY	-	expression tag	UNP P0DOX5
D	525	TRP	-	expression tag	UNP P0DOX5
D	526	SER	-	expression tag	UNP P0DOX5
D	527	CYS	-	expression tag	UNP P0DOX5
D	528	ILE	-	expression tag	UNP P0DOX5
D	529	ILE	-	expression tag	UNP P0DOX5
D	530	LEU	-	expression tag	UNP P0DOX5
D	531	PHE	-	expression tag	UNP P0DOX5
D	532	LEU	-	expression tag	UNP P0DOX5
D	533	VAL	-	expression tag	UNP P0DOX5
D	534	ALA	-	expression tag	UNP P0DOX5
D	535	THR	-	expression tag	UNP P0DOX5
D	536	ALA	-	expression tag	UNP P0DOX5
D	537	THR	-	expression tag	UNP P0DOX5
D	538	GLY	-	expression tag	UNP P0DOX5
D	539	VAL	-	expression tag	UNP P0DOX5
D	540	HIS	-	expression tag	UNP P0DOX5
D	541	SER	-	expression tag	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	670	ASN	SER	conflict	UNP P0DOX5
D	713	ASN	TYR	conflict	UNP P0DOX5
D	754	GLY	-	linker	UNP P0DOX5
D	755	GLY	-	linker	UNP P0DOX5
D	756	GLY	-	linker	UNP P0DOX5
D	757	GLY	-	linker	UNP P0DOX5
D	758	SER	-	linker	UNP P0DOX5
D	759	GLY	-	linker	UNP P0DOX5
D	760	GLY	-	linker	UNP P0DOX5
D	761	GLY	-	linker	UNP P0DOX5
D	762	SER	-	linker	UNP P0DOX5
D	763	GLU	-	linker	UNP P0DOX5
D	764	ASN	-	linker	UNP P0DOX5
D	765	LEU	-	linker	UNP P0DOX5
D	766	TYR	-	linker	UNP P0DOX5
D	767	PHE	-	linker	UNP P0DOX5
D	768	GLN	-	linker	UNP P0DOX5
D	769	GLY	-	linker	UNP P0DOX5
D	770	SER	-	linker	UNP P0DOX5
D	856	GLY	-	expression tag	UNP O97302
D	857	GLY	-	expression tag	UNP O97302
D	858	THR	-	expression tag	UNP O97302
D	859	GLY	-	expression tag	UNP O97302
D	860	GLY	-	expression tag	UNP O97302
D	861	SER	-	expression tag	UNP O97302
D	862	GLU	-	expression tag	UNP O97302
D	863	PRO	-	expression tag	UNP O97302
D	864	GLU	-	expression tag	UNP O97302
D	865	ALA	-	expression tag	UNP O97302

- Molecule 2 is a protein called RP.012 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	208	1575	998	262	309	6	0	1	0
2	E	207	1555	988	257	304	6	0	0	0

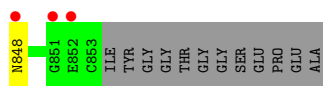
- Molecule 3 is a protein called RP.012 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	210	Total 1633	C 1018	N 273	O 334	S 8	0	0	0
3	F	211	Total 1644	C 1024	N 277	O 335	S 8	0	0	0

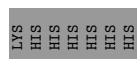
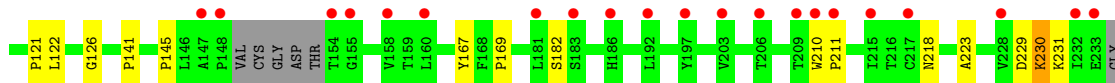
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	43	Total 43	O 43	0	0
4	C	23	Total 23	O 23	0	0
4	D	16	Total 16	O 16	0	0
4	E	35	Total 35	O 35	0	0
4	F	28	Total 28	O 28	0	0

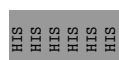




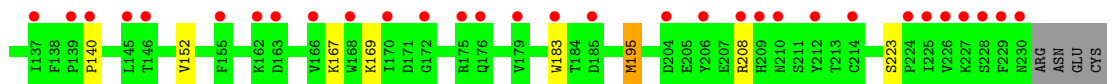
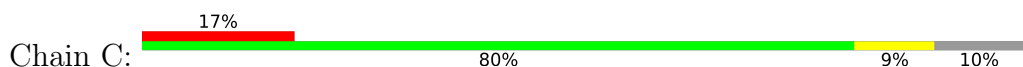
- Molecule 2: RP.012 heavy chain



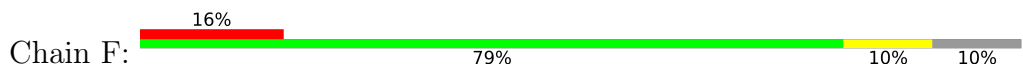
- Molecule 2: RP.012 heavy chain

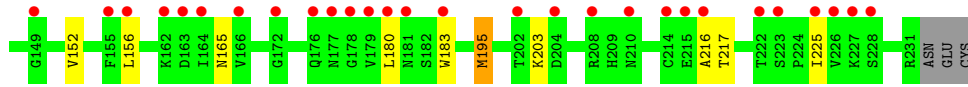


- Molecule 3: RP.012 light chain



- Molecule 3: RP.012 light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.16Å 50.98Å 109.78Å 76.82° 83.26° 76.50°	Depositor
Resolution (Å)	48.66 – 2.20 48.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.66-2.20) 98.2 (48.66-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.20Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, $R_{free}$	0.241 , 0.256 0.238 , 0.255	Depositor DCC
$R_{free}$ test set	2699 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.7	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	0.95	EDS
Total number of atoms	7553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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	0.67	0/486	0.94	0/644
1	D	0.72	0/512	0.98	0/680
2	B	0.70	0/1615	0.92	0/2206
2	E	0.67	0/1595	0.93	0/2179
3	C	0.64	0/1669	0.94	0/2264
3	F	0.64	0/1680	0.94	0/2278
All	All	0.67	0/7557	0.93	0/10251

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	482	0	439	10	0
1	D	507	0	470	12	0
2	B	1575	0	1561	19	0
2	E	1555	0	1544	21	0
3	C	1633	0	1560	11	0
3	F	1644	0	1573	10	0
4	A	12	0	0	0	0
4	B	43	0	0	0	0
4	C	23	0	0	0	0
4	D	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	35	0	0	0	0
4	F	28	0	0	0	0
All	All	7553	0	7147	77	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 5.

The worst 5 of 77 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)
3:C:167:LYS:HD2	3:C:169:LYS:HZ1	1.18	1.03
3:C:167:LYS:HD2	3:C:169:LYS:NZ	1.78	0.98
3:F:216:ALA:HB3	3:F:225:ILE:HB	1.62	0.82
2:B:103:LEU:HB3	2:B:106:LEU:HD21	1.80	0.64
2:E:103:LEU:HB3	2:E:106:LEU:HD21	1.80	0.63

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	54/343 (16%)	53 (98%)	1 (2%)	0	100	100
1	D	59/343 (17%)	57 (97%)	2 (3%)	0	100	100
2	B	205/241 (85%)	202 (98%)	3 (2%)	0	100	100
2	E	203/241 (84%)	201 (99%)	2 (1%)	0	100	100
3	C	208/234 (89%)	203 (98%)	5 (2%)	0	100	100
3	F	209/234 (89%)	203 (97%)	6 (3%)	0	100	100
All	All	938/1636 (57%)	919 (98%)	19 (2%)	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	A	58/307 (19%)	53 (91%)	5 (9%)	10	10
1	D	61/307 (20%)	56 (92%)	5 (8%)	10	12
2	B	180/208 (86%)	173 (96%)	7 (4%)	28	39
2	E	178/208 (86%)	169 (95%)	9 (5%)	21	27
3	C	187/209 (90%)	180 (96%)	7 (4%)	30	41
3	F	188/209 (90%)	179 (95%)	9 (5%)	23	30
All	All	852/1448 (59%)	810 (95%)	42 (5%)	22	29

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	122	LEU
3	F	80	ASP
2	E	137	LYS
2	E	230	LYS
3	F	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	58	GLN
1	D	783	ASN
3	F	58	GLN
2	E	59	GLN
2	B	59	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 oligosaccharides 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	60/343 (17%)	1.30	13 (21%) 2 1	45, 60, 127, 130	0
1	D	63/343 (18%)	1.04	7 (11%) 10 8	45, 58, 103, 108	0
2	B	208/241 (86%)	1.06	28 (13%) 7 5	28, 58, 98, 107	1 (0%)
2	E	207/241 (85%)	1.16	25 (12%) 8 6	44, 61, 79, 88	0
3	C	210/234 (89%)	1.29	39 (18%) 3 2	38, 65, 103, 112	0
3	F	211/234 (90%)	1.35	38 (18%) 3 2	46, 70, 92, 108	0
All	All	959/1636 (58%)	1.21	150 (15%) 5 4	28, 63, 98, 130	1 (0%)

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	215	GLU	5.1
3	C	183	TRP	4.9
3	F	172	GLY	4.4
3	F	216	ALA	4.4
2	E	116	CYS	4.2

### 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 oligosaccharides 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.