



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 06:39 AM EDT

PDB ID : 6WIR  
Title : Fab antigen complex  
Authors : Antonysamy, S.  
Deposited on : 2020-04-10  
Resolution : 2.96 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

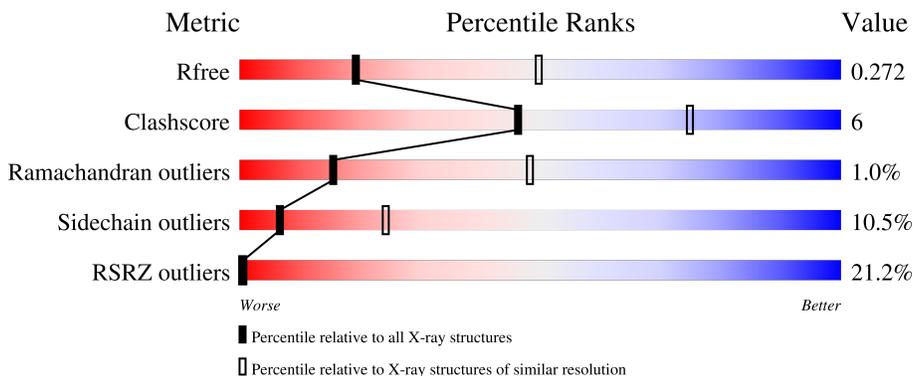
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	236	
2	B	213	
3	C	161	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4125 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1721	1095	288	331	7	0	0	0

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1610	1002	275	328	5	0	0	0

- Molecule 3 is a protein called Interleukin-17A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	89	722	452	133	131	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	133	HIS	-	expression tag	UNP Q16552
C	134	HIS	-	expression tag	UNP Q16552
C	135	HIS	-	expression tag	UNP Q16552
C	136	HIS	-	expression tag	UNP Q16552
C	137	HIS	-	expression tag	UNP Q16552
C	138	HIS	-	expression tag	UNP Q16552

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	36	Total	O	0	0
			36	36		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	2	Total	O	0	0
			2	2		



L112	L113	K114	I115	L116	V117	S118	V119	G120	T125	P126	I127	V128	H129	HIS	VAL	ALA	HIS						
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.40Å 73.40Å 326.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.61 – 2.96 71.61 – 2.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (71.61-2.96) 100.0 (71.61-2.96)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.96Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.217 , 0.260 0.227 , 0.272	Depositor DCC
$R_{free}$ test set	977 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.3	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 91.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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	0.54	0/1766	0.79	0/2411
2	B	0.54	0/1643	0.76	0/2230
3	C	0.48	0/743	0.68	0/1015
All	All	0.53	0/4152	0.76	0/5656

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	1721	0	1644	20	0
2	B	1610	0	1550	23	0
3	C	722	0	688	7	0
4	A	34	0	0	1	0
4	B	36	0	0	0	0
4	C	2	0	0	0	0
All	All	4125	0	3882	50	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.

All (50) 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:B:38:GLN:HB2	2:B:48:LEU:HD11	1.60	0.83
2:B:18:ARG:HG3	2:B:77:SER:HA	1.69	0.73
1:A:67:ARG:HH12	1:A:87:ARG:HG3	1.55	0.71
2:B:164:VAL:HG22	2:B:176:LEU:HD12	1.74	0.69
3:C:101:ARG:HD3	3:C:106:CYS:H	1.57	0.68
1:A:12:VAL:HG21	1:A:18:LEU:HG	1.74	0.68
2:B:109:ARG:NH2	2:B:112:ALA:HB2	2.12	0.64
1:A:160:PHE:HB2	1:A:189:LEU:HD23	1.80	0.63
2:B:108:LYS:HA	2:B:141:TYR:OH	2.02	0.60
3:C:63:PRO:HD2	3:C:98:VAL:HG22	1.85	0.58
1:A:50:ALA:HB3	1:A:59:TYR:HB2	1.86	0.57
1:A:214:HIS:CE1	1:A:217:SER:HB3	2.41	0.55
2:B:41:PRO:HG3	2:B:166:GLU:HG2	1.88	0.55
1:A:58:LYS:HE3	1:A:70:ILE:O	2.07	0.54
1:A:214:HIS:CD2	1:A:216:PRO:HD2	2.42	0.54
2:B:191:LYS:O	2:B:209:ASN:HA	2.07	0.54
2:B:164:VAL:CG2	2:B:176:LEU:HD12	2.36	0.54
2:B:148:GLN:HB3	2:B:155:LEU:HD11	1.90	0.52
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.93	0.51
2:B:21:LEU:HD22	2:B:74:LEU:HD23	1.93	0.51
1:A:156:VAL:HG13	1:A:212:VAL:HG11	1.94	0.49
2:B:109:ARG:HH22	2:B:112:ALA:HB2	1.77	0.49
2:B:2:ILE:HG12	2:B:27:GLN:HB2	1.95	0.48
1:A:32:TYR:HB2	1:A:34:MET:HE2	1.95	0.48
3:C:50:PRO:HB2	3:C:72:ARG:HH11	1.80	0.47
1:A:133:PRO:HB3	1:A:159:TYR:HB3	1.97	0.47
1:A:17:SER:HA	1:A:83:MET:O	2.15	0.46
2:B:116:VAL:HG12	2:B:206:LYS:HG3	1.97	0.46
1:A:214:HIS:ND1	1:A:217:SER:HB3	2.30	0.45
1:A:137:PRO:HB2	1:A:225:VAL:HG13	1.98	0.45
3:C:96:ILE:HG13	3:C:97:LEU:H	1.81	0.45
2:B:120:PRO:HB3	2:B:208:PHE:CZ	2.52	0.44
2:B:190:HIS:HB2	2:B:193:TYR:OH	2.18	0.44
2:B:48:LEU:HD23	2:B:59:ILE:HD12	2.00	0.43
3:C:50:PRO:HB2	3:C:72:ARG:HD2	2.01	0.43
3:C:58:ASP:HB3	3:C:61:ARG:HB2	1.99	0.43
1:A:198:VAL:HG11	1:A:208:TYR:CE1	2.55	0.42
1:A:67:ARG:NH1	1:A:87:ARG:HG3	2.29	0.42
2:B:60:PRO:HG2	2:B:63:PHE:HD1	1.83	0.42
3:C:101:ARG:HG3	3:C:104:PRO:HA	2.02	0.42
2:B:11:LEU:HG	2:B:13:LEU:HD13	2.02	0.42
2:B:137:LEU:HD11	2:B:197:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:HA	1:A:82:GLN:O	2.21	0.41
2:B:121:PRO:HB3	2:B:132:SER:H	1.85	0.41
2:B:137:LEU:HD22	2:B:176:LEU:HD22	2.03	0.41
2:B:118:ILE:HG22	2:B:206:LYS:HB3	2.03	0.41
2:B:135:CYS:HB2	2:B:149:TRP:CH2	2.56	0.41
1:A:27:PHE:HB2	4:A:317:HOH:O	2.21	0.41
1:A:209:THR:HA	1:A:223:LYS:O	2.21	0.41
1:A:33:TRP:HB2	1:A:99:ASP:HB2	2.03	0.40

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	225/236 (95%)	201 (89%)	21 (9%)	3 (1%)	12	41
2	B	210/213 (99%)	196 (93%)	13 (6%)	1 (0%)	29	64
3	C	87/161 (54%)	76 (87%)	10 (12%)	1 (1%)	14	46
All	All	522/610 (86%)	473 (91%)	44 (8%)	5 (1%)	15	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
2	B	139	ASN
1	A	145	THR
1	A	144	SER
3	C	107	PRO

### 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	186/203 (92%)	169 (91%)	17 (9%)	9	31
2	B	179/184 (97%)	157 (88%)	22 (12%)	4	18
3	C	83/150 (55%)	75 (90%)	8 (10%)	8	28
All	All	448/537 (83%)	401 (90%)	47 (10%)	7	24

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	28	THR
1	A	43	LYS
1	A	52	ASN
1	A	71	SER
1	A	89	GLU
1	A	112	TRP
1	A	126	SER
1	A	162	GLU
1	A	167	SER
1	A	170	SER
1	A	173	LEU
1	A	191	SER
1	A	192	LEU
1	A	210	CYS
1	A	217	SER
1	A	224	ARG
2	B	10	THR
2	B	15	PRO
2	B	20	THR
2	B	22	SER
2	B	30	SER
2	B	34	LEU
2	B	57	THR
2	B	71	ASP
2	B	78	ARG

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Mol	Chain	Res	Type
2	B	80	GLU
2	B	106	GLU
2	B	109	ARG
2	B	115	SER
2	B	123	ASP
2	B	128	SER
2	B	133	VAL
2	B	177	SER
2	B	181	THR
2	B	189	LYS
2	B	199	GLN
2	B	204	VAL
2	B	207	SER
3	C	45	ASN
3	C	66	ILE
3	C	88	ASN
3	C	98	VAL
3	C	100	ARG
3	C	102	GLU
3	C	110	PHE
3	C	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
2	B	27	GLN
2	B	138	ASN
3	C	45	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 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

### 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	227/236 (96%)	0.99	39 (17%) <b>1</b> <b>1</b>	68, 99, 130, 145	0
2	B	212/213 (99%)	0.79	27 (12%) <b>3</b> <b>2</b>	71, 100, 125, 145	0
3	C	89/161 (55%)	2.54	46 (51%) <b>0</b> <b>0</b>	97, 132, 244, 259	0
All	All	528/610 (86%)	1.17	112 (21%) <b>0</b> <b>0</b>	68, 103, 190, 259	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	112	LEU	7.5
3	C	67	TRP	7.4
3	C	93	GLN	7.4
3	C	115	ILE	7.3
3	C	116	LEU	7.1
3	C	65	VAL	6.9
3	C	96	ILE	6.6
3	C	53	LEU	5.9
3	C	97	LEU	5.8
3	C	120	GLY	5.7
3	C	59	PRO	5.6
3	C	92	ILE	5.6
3	C	90	VAL	5.5
3	C	113	GLU	5.4
3	C	98	VAL	5.2
3	C	70	LYS	5.2
1	A	112	TRP	4.9
3	C	119	VAL	4.8
2	B	37	TYR	4.7
1	A	50	ALA	4.6
3	C	55	ARG	4.6
1	A	97	VAL	4.3
1	A	48	VAL	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	94	GLN	4.1
1	A	36	TRP	3.9
3	C	129	HIS	3.8
1	A	34	MET	3.7
3	C	66	ILE	3.7
1	A	37	VAL	3.7
2	B	47	LEU	3.7
3	C	114	LYS	3.6
3	C	99	LEU	3.6
3	C	68	GLU	3.5
1	A	47	TRP	3.5
3	C	89	SER	3.5
1	A	41	PRO	3.5
1	A	33	TRP	3.4
1	A	114	PHE	3.4
1	A	20	LEU	3.4
3	C	117	VAL	3.4
1	A	79	LEU	3.4
1	A	111	TYR	3.3
2	B	49	ILE	3.2
3	C	43	TYR	3.2
2	B	126	LEU	3.2
2	B	97	CYS	3.1
2	B	92	TYR	3.1
3	C	58	ASP	3.1
3	C	48	THR	3.0
1	A	58	LYS	3.0
3	C	107	PRO	3.0
3	C	128	VAL	2.9
3	C	69	ALA	2.9
1	A	122	LEU	2.9
3	C	91	PRO	2.9
1	A	4	LEU	2.9
1	A	81	LEU	2.9
3	C	60	GLU	2.9
2	B	116	VAL	2.9
2	B	35	ALA	2.9
3	C	105	HIS	2.9
1	A	95	TYR	2.8
1	A	70	ILE	2.8
2	B	36	TRP	2.8
3	C	126	PRO	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	117	TRP	2.7
1	A	45	LEU	2.7
2	B	180	LEU	2.7
2	B	140	PHE	2.6
3	C	127	ILE	2.6
2	B	148	GLN	2.5
1	A	113	TYR	2.5
1	A	49	ALA	2.5
2	B	45	PRO	2.5
1	A	60	TYR	2.5
2	B	182	LEU	2.5
3	C	87	MET	2.5
2	B	136	LEU	2.5
1	A	38	ARG	2.5
3	C	51	TRP	2.5
1	A	64	VAL	2.4
3	C	125	THR	2.4
2	B	124	GLU	2.4
3	C	86	HIS	2.4
1	A	166	VAL	2.4
1	A	59	TYR	2.3
2	B	114	PRO	2.3
1	A	51	ILE	2.3
1	A	68	PHE	2.3
3	C	52	ASN	2.3
1	A	80	TYR	2.3
2	B	32	SER	2.2
2	B	34	LEU	2.2
2	B	133	VAL	2.2
2	B	11	LEU	2.2
2	B	134	VAL	2.2
3	C	106	CYS	2.2
3	C	54	HIS	2.2
1	A	164	VAL	2.1
3	C	108	ASN	2.1
1	A	24	ALA	2.1
3	C	95	GLU	2.1
1	A	39	GLN	2.1
1	A	135	VAL	2.1
2	B	52	ALA	2.1
2	B	151	VAL	2.1
2	B	93	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	176	LEU	2.0
1	A	151	ALA	2.0
2	B	96	PRO	2.0
1	A	192	LEU	2.0
1	A	125	VAL	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.