



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:46 PM BST

PDB ID : 6VI2  
Title : Structure of the unaligned Fab4  
Authors : Cingolani, G.; Lokareddy, R.; Ko, Y.  
Deposited on : 2020-01-11  
Resolution : 1.15 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.

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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	:	2.14.2
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)	:	2.14.2

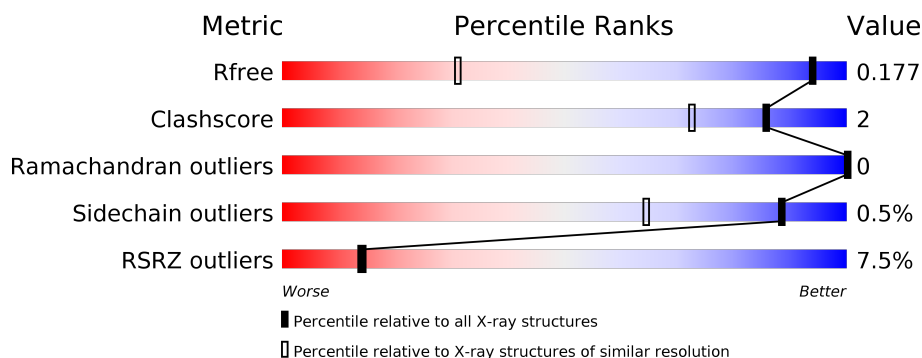
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.15 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	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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 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	215	<div> <div>4%</div> <div>95%</div> <div>5%</div> </div>
1	C	215	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
2	B	243	<div> <div>8%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
2	D	243	<div> <div>13%</div> <div>92%</div> <div>5%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14565 atoms, of which 6591 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 FAB4 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	H	N	O	S	0	0	0
			3237	1021	1601	275	334	6			
1	C	215	Total	C	H	N	O	S	0	0	0
			3237	1021	1601	275	334	6			

- Molecule 2 is a protein called FAB4 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	231	Total	C	H	N	O	S	0	0	0
			3419	1108	1681	286	338	6			
2	D	236	Total	C	H	N	O	S	0	0	0
			3483	1129	1708	291	348	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	322	Total	O	0	0
			322	322		
3	B	270	Total	O	0	0
			270	270		
3	C	323	Total	O	0	0
			323	323		
3	D	274	Total	O	0	0
			274	274		

### 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.

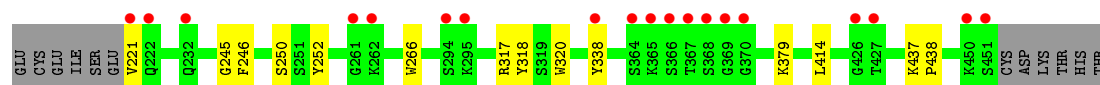
- Molecule 1: FAB4 light chain



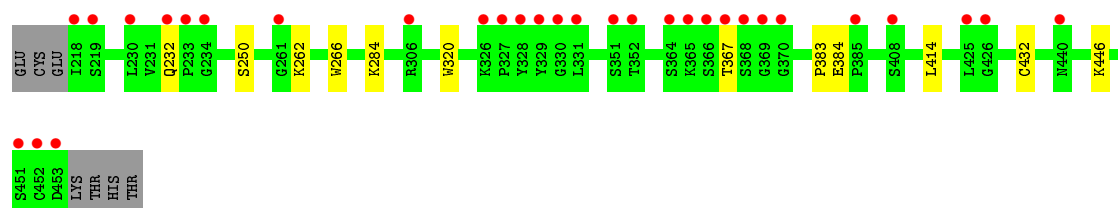
- Molecule 1: FAB4 light chain



- Molecule 2: FAB4 heavy chain



- Molecule 2: FAB4 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.77Å 65.84Å 107.42Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	14.99 – 1.15 14.99 – 1.15	Depositor EDS
% Data completeness (in resolution range)	93.5 (14.99-1.15) 93.5 (14.99-1.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 1.15Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.158 , 0.171 0.160 , 0.177	Depositor DCC
$R_{free}$ test set	1996 reflections (0.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	14565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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	0.43	0/1670	0.64	0/2265
1	C	0.43	0/1670	0.72	4/2265 (0.2%)
2	B	0.41	0/1789	0.67	0/2443
2	D	0.54	3/1826 (0.2%)	0.71	0/2493
All	All	0.46	3/6955 (0.0%)	0.69	4/9466 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	232	GLN	C-N	9.41	1.52	1.34
2	D	384	GLU	C-N	8.49	1.50	1.34
2	D	432	CYS	CB-SG	-5.61	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ARG	O-C-N	8.08	135.62	122.70
1	C	17	ASP	O-C-N	-6.99	111.51	122.70
1	C	17	ASP	C-N-CA	6.94	139.05	121.70
1	C	18	ARG	CA-C-N	-6.12	103.73	117.20

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	1636	1601	1601	7	0
1	C	1636	1601	1600	7	0
2	B	1738	1681	1681	11	0
2	D	1775	1708	1712	7	0
3	A	322	0	0	2	0
3	B	270	0	0	1	0
3	C	323	0	0	3	0
3	D	274	0	0	3	0
All	All	7974	6591	6594	30	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 2.

All (30) 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:221:VAL:HG11	2:B:338:TYR:CD2	2.15	0.81
1:C:109:LYS:HE2	3:C:378:HOH:O	1.96	0.65
1:A:22:THR:HG23	3:A:431:HOH:O	2.00	0.60
2:B:221:VAL:HG13	2:B:246:PHE:CD1	2.39	0.56
2:B:379:LYS:HE3	3:B:545:HOH:O	2.05	0.56
2:D:367:THR:HG22	2:D:367:THR:O	2.06	0.56
2:B:221:VAL:HG11	2:B:338:TYR:CE2	2.41	0.55
2:B:221:VAL:HG13	2:B:246:PHE:HD1	1.73	0.54
1:C:165:VAL:HG22	1:C:177:LEU:HD12	1.90	0.54
2:D:414:LEU:HA	3:D:597:HOH:O	2.10	0.50
1:A:0:SER:O	1:A:0:SER:OG	2.29	0.48
2:B:414:LEU:C	2:B:414:LEU:HD12	2.33	0.48
1:C:12:SER:CB	1:C:107:GLU:OE2	2.63	0.47
2:D:446:LYS:HD3	3:D:755:HOH:O	2.14	0.47
1:C:214:GLY:OXT	3:C:301:HOH:O	2.20	0.47
2:D:414:LEU:C	2:D:414:LEU:HD12	2.35	0.47
2:B:252:TYR:HB2	2:B:318:TYR:HB2	1.97	0.46
2:D:262:LYS:NZ	3:D:505:HOH:O	2.40	0.45
1:A:45:LYS:NZ	3:A:303:HOH:O	2.32	0.45
1:C:97:PRO:HA	2:D:266:TRP:CZ3	2.52	0.44
1:C:45:LYS:HD3	3:C:332:HOH:O	2.17	0.44
1:A:97:PRO:HA	2:B:266:TRP:CZ3	2.53	0.43
2:D:250:SER:O	2:D:320:TRP:HB2	2.19	0.43
2:B:250:SER:O	2:B:320:TRP:HB2	2.20	0.41
1:A:107:GLU:HG2	1:A:108:ILE:N	2.35	0.41
2:B:437:LYS:N	2:B:438:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ALA:O	1:A:90:GLN:HA	2.21	0.41
2:B:221:VAL:HG22	2:B:245:GLY:O	2.20	0.41
1:A:40:PRO:HG2	1:A:167:GLU:HG3	2.03	0.40
1:C:126:GLN:HG2	1:C:131:THR:O	2.21	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	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
1	C	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
2	B	229/243 (94%)	225 (98%)	4 (2%)	0	100	100
2	D	234/243 (96%)	226 (97%)	8 (3%)	0	100	100
All	All	889/916 (97%)	867 (98%)	22 (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	189/189 (100%)	189 (100%)	0	100	100
1	C	189/189 (100%)	188 (100%)	1 (0%)	88	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	193/205 (94%)	192 (100%)	1 (0%)	88	64
2	D	198/205 (97%)	196 (99%)	2 (1%)	76	42
All	All	769/788 (98%)	765 (100%)	4 (0%)	88	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	317	ARG
1	C	107	GLU
2	D	284	LYS
2	D	383	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

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	215/215 (100%)	0.26	8 (3%) 41 41	12, 18, 33, 49	0
1	C	215/215 (100%)	0.26	9 (4%) 36 35	12, 19, 32, 49	0
2	B	231/243 (95%)	0.73	19 (8%) 11 12	13, 23, 42, 65	0
2	D	236/243 (97%)	1.02	31 (13%) 3 4	13, 23, 48, 64	0
All	All	897/916 (97%)	0.58	67 (7%) 14 14	12, 20, 40, 65	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	452	CYS	16.1
2	B	367	THR	15.1
2	D	366	SER	13.4
2	B	368	SER	13.2
2	D	368	SER	11.1
2	D	453	ASP	11.0
2	D	367	THR	10.2
2	B	369	GLY	10.1
2	D	329	TYR	8.8
2	D	369	GLY	8.7
2	D	365	LYS	8.4
2	B	451	SER	8.3
2	D	364	SER	7.9
2	B	366	SER	7.5
2	D	326	LYS	6.6
1	C	214	GLY	6.5
2	B	221	VAL	6.1
2	D	218	ILE	6.1
2	D	219	SER	5.8
2	D	331	LEU	5.8
2	D	328	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
2	D	451	SER	5.3
2	B	364	SER	5.3
2	B	365	LYS	5.1
1	C	171	LYS	4.6
2	B	426	GLY	4.6
2	D	306	ARG	4.5
2	D	426	GLY	4.4
1	A	0	SER	4.3
2	D	230	LEU	4.1
2	D	440	ASN	4.0
2	B	370	GLY	4.0
2	D	408	SER	3.6
1	A	214	GLY	3.6
2	D	327	PRO	3.6
1	C	170	SER	3.4
1	A	154	ASN	3.3
1	A	41	GLY	3.3
2	D	370	GLY	3.3
1	A	156	LEU	3.3
2	D	330	GLY	3.2
2	B	261	GLY	3.1
1	C	156	LEU	3.1
2	D	385	PRO	3.0
1	C	0	SER	3.0
2	B	222	GLN	2.9
2	D	233	PRO	2.9
2	B	232	GLN	2.8
2	B	338	TYR	2.8
1	C	154	ASN	2.8
2	B	427	THR	2.7
2	D	232	GLN	2.7
2	B	450	LYS	2.6
1	A	1	ASP	2.6
2	D	351	SER	2.6
2	B	294	SER	2.5
1	A	170	SER	2.4
1	C	102	GLN	2.4
2	D	352	THR	2.3
1	C	1	ASP	2.3
2	B	262	LYS	2.3
2	B	295	LYS	2.2
1	C	129	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	261	GLY	2.2
1	A	40	PRO	2.2
2	D	234	GLY	2.1
2	D	425	LEU	2.1

## 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.