



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 03:37 PM BST

PDB ID : 6EMJ  
Title : FAB Fragment. AbVance: Increasing our knowledge of antibody structural space to enable faster and better decision making in antibody drug discovery  
Authors : Benz, J.; Weigand, S.; Dengl, S.; Schlothauer, T.; Auer, J.; Ehler, A.; Kettenberger, H.; Lorenz, S.; Hirschheydt, T.; Georges, G.  
Deposited on : 2017-10-02  
Resolution : 2.30 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 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 : 2.13  
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) : 2.13

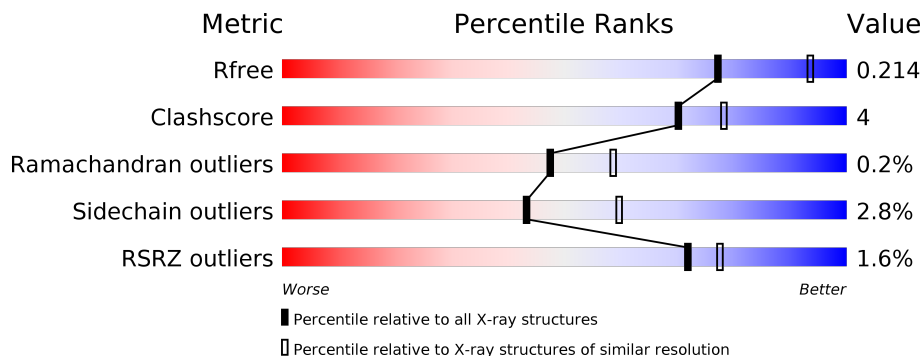
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	227	
1	H	227	
2	B	214	
2	L	214	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6915 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	212	Total 1614	C 1023	N 268	O 316	S 7	0	0	0
1	H	218	Total 1669	C 1058	N 279	O 325	S 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	213	Total 1649	C 1032	N 278	O 334	S 5	0	0	0
2	L	211	Total 1636	C 1025	N 276	O 330	S 5	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0

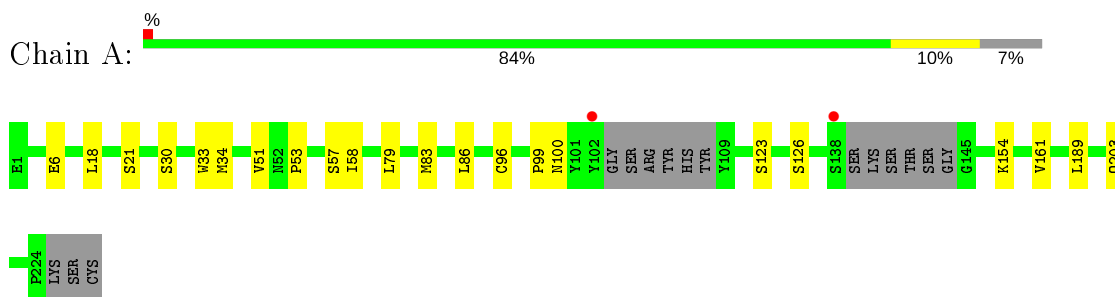
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total 101	O 101	0	0
4	B	91	Total 91	O 91	0	0
4	H	74	Total 74	O 74	0	0
4	L	80	Total 80	O 80	0	0

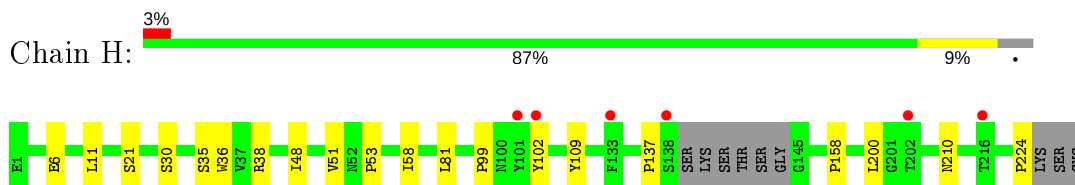
### 3 Residue-property plots [i](#)

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.

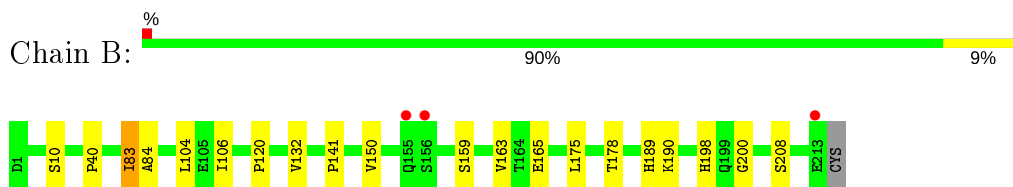
- Molecule 1: fAB heavy chain



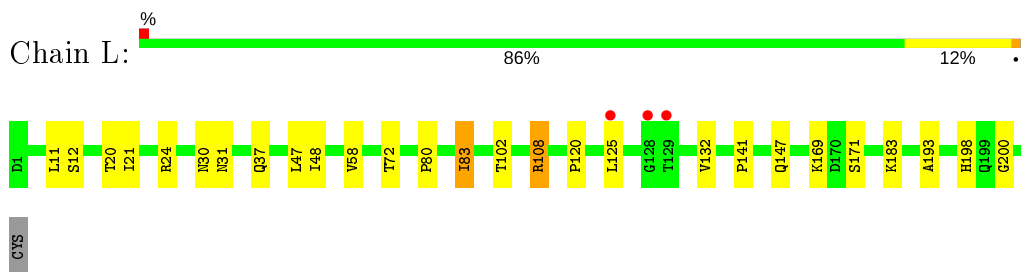
- Molecule 1: fAB heavy chain



- Molecule 2: fAb light chain



- Molecule 2: fAb light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.48Å 73.87Å 76.92Å 69.34° 78.05° 70.20°	Depositor
Resolution (Å)	45.79 – 2.30 45.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.79-2.30) 100.0 (45.79-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.29Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.165 , 0.211 0.169 , 0.214	Depositor DCC
$R_{free}$ test set	2221 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.8	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	0.97	EDS
Total number of atoms	6915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.53	0/1655	0.72	0/2260
1	H	0.49	0/1714	0.72	0/2341
2	B	0.49	0/1685	0.70	0/2287
2	L	0.51	0/1672	0.70	0/2270
All	All	0.51	0/6726	0.71	0/9158

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	1614	0	1565	10	0
1	H	1669	0	1612	9	0
2	B	1649	0	1601	12	0
2	L	1636	0	1592	16	0
3	A	1	0	0	0	0
4	A	101	0	0	0	0
4	B	91	0	0	0	0
4	H	74	0	0	0	0
4	L	80	0	0	0	0
All	All	6915	0	6370	47	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 4.

All (47) 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:L:30:ASN:ND2	2:L:31:ASN:H	1.88	0.72
1:H:11:LEU:HB2	1:H:158:PRO:HG3	1.74	0.70
2:B:198:HIS:CD2	2:B:200:GLY:H	2.16	0.64
1:H:30:SER:O	1:H:53:PRO:HB3	1.99	0.62
1:A:33:TRP:O	1:A:99:PRO:HD2	2.04	0.57
2:B:150:VAL:HG12	2:B:189:HIS:HB3	1.85	0.57
2:L:108:ARG:HG2	2:L:171:SER:HB2	1.85	0.57
2:L:198:HIS:CD2	2:L:200:GLY:H	2.23	0.56
2:B:198:HIS:HD2	2:B:200:GLY:H	1.51	0.56
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.88	0.56
2:L:125:LEU:HB3	2:L:183:LYS:HE3	1.89	0.55
2:L:30:ASN:ND2	2:L:31:ASN:N	2.56	0.54
1:A:30:SER:O	1:A:53:PRO:HB3	2.10	0.52
1:A:79:LEU:HD23	1:A:96:CYS:HB2	1.91	0.51
2:L:80:PRO:O	2:L:83:ILE:HG22	2.10	0.51
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.92	0.51
1:H:51:VAL:HG23	1:H:58:ILE:HG12	1.93	0.50
1:H:137:PRO:HG2	1:H:224:PRO:HB3	1.93	0.50
2:L:20:THR:HG23	2:L:72:THR:HG23	1.94	0.49
1:H:38:ARG:HB3	1:H:48:ILE:HD11	1.95	0.48
1:A:18:LEU:HD23	1:A:83:MET:HE3	1.94	0.47
2:B:150:VAL:CG1	2:B:189:HIS:CB	2.92	0.47
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.95	0.47
2:B:40:PRO:HB3	2:B:165:GLU:HG3	1.95	0.47
1:A:161:VAL:HG22	1:A:189:LEU:HD21	1.97	0.46
2:B:150:VAL:HG12	2:B:189:HIS:CB	2.45	0.46
2:L:198:HIS:HD2	2:L:200:GLY:H	1.64	0.45
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.98	0.45
2:L:141:PRO:O	2:L:198:HIS:HE1	1.99	0.45
1:A:51:VAL:HG23	1:A:58:ILE:HG12	1.99	0.44
2:B:159:SER:HA	2:B:178:THR:O	2.18	0.44
1:H:99:PRO:HB3	1:H:109:TYR:CD1	2.52	0.44
2:L:30:ASN:HD22	2:L:31:ASN:H	1.62	0.44
2:B:120:PRO:HD3	2:B:132:VAL:HG22	2.00	0.44
2:B:163:VAL:HG22	2:B:175:LEU:HD12	2.00	0.43
2:L:21:ILE:HG12	2:L:102:THR:HG21	2.00	0.42
1:A:18:LEU:HD23	1:A:83:MET:CE	2.50	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HA	1:A:21:SER:O	2.21	0.41
2:L:30:ASN:CG	2:L:31:ASN:N	2.72	0.41
2:B:83:ILE:O	2:B:84:ALA:HB2	2.21	0.41
1:H:6:GLU:HA	1:H:21:SER:O	2.21	0.41
2:L:47:LEU:HA	2:L:58:VAL:HG21	2.02	0.41
1:H:36:TRP:CE2	1:H:81:LEU:HB2	2.56	0.41
2:L:193:ALA:HB2	2:L:208:SER:HB3	2.03	0.41
1:H:99:PRO:HB3	1:H:109:TYR:CG	2.56	0.41
2:B:83:ILE:HD12	2:B:104:LEU:O	2.20	0.40
2:B:141:PRO:O	2:B:198:HIS:HE1	2.04	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	206/227 (91%)	200 (97%)	6 (3%)	0	100	100
1	H	214/227 (94%)	206 (96%)	6 (3%)	2 (1%)	17	20
2	B	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	L	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
All	All	840/882 (95%)	813 (97%)	25 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	102	TYR
1	H	200	LEU



### 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	182/195 (93%)	176 (97%)	6 (3%)	38	53
1	H	187/195 (96%)	185 (99%)	2 (1%)	73	86
2	B	189/190 (100%)	184 (97%)	5 (3%)	46	63
2	L	188/190 (99%)	180 (96%)	8 (4%)	29	40
All	All	746/770 (97%)	725 (97%)	21 (3%)	43	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	100	ASN
1	A	123	SER
1	A	126	SER
1	A	154	LYS
1	A	203	GLN
2	B	10	SER
2	B	83	ILE
2	B	106	ILE
2	B	190	LYS
2	B	208	SER
1	H	35	SER
1	H	210	ASN
2	L	11	LEU
2	L	12	SER
2	L	24	ARG
2	L	48	ILE
2	L	83	ILE
2	L	108	ARG
2	L	147	GLN
2	L	169	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
2	B	124	GLN
2	B	198	HIS
2	B	199	GLN
1	H	100	ASN
1	H	210	ASN
2	L	30	ASN
2	L	124	GLN
2	L	198	HIS
2	L	210	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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 [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	212/227 (93%)	-0.17	2 (0%) 84 88	29, 44, 72, 132	0
1	H	218/227 (96%)	0.06	6 (2%) 53 60	33, 51, 80, 95	0
2	B	213/214 (99%)	-0.14	3 (1%) 75 80	31, 46, 72, 118	0
2	L	211/214 (98%)	0.00	3 (1%) 75 80	32, 47, 82, 102	0
All	All	854/882 (96%)	-0.06	14 (1%) 72 77	29, 47, 79, 132	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	TYR	4.8
1	H	101	TYR	4.6
2	L	129	THR	4.2
2	B	156	SER	3.8
1	H	216	THR	3.4
2	L	125	LEU	3.1
1	H	202	THR	3.0
2	L	128	GLY	2.5
2	B	213	GLU	2.4
1	A	138	SER	2.4
1	H	133	PHE	2.3
2	B	155	GLN	2.2
1	H	102	TYR	2.2
1	H	138	SER	2.2

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	A	301	1/1	0.83	0.14	65,65,65,65	0

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

There are no such residues in this entry.