



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 10, 2024 – 07:21 AM EST

PDB ID : 3EOB  
Title : Crystal structure the Fab fragment of Efalizumab in complex with LFA-1 I domain, Form II  
Authors : Li, S.; Ding, J.  
Deposited on : 2008-09-26  
Resolution : 3.60 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.

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)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

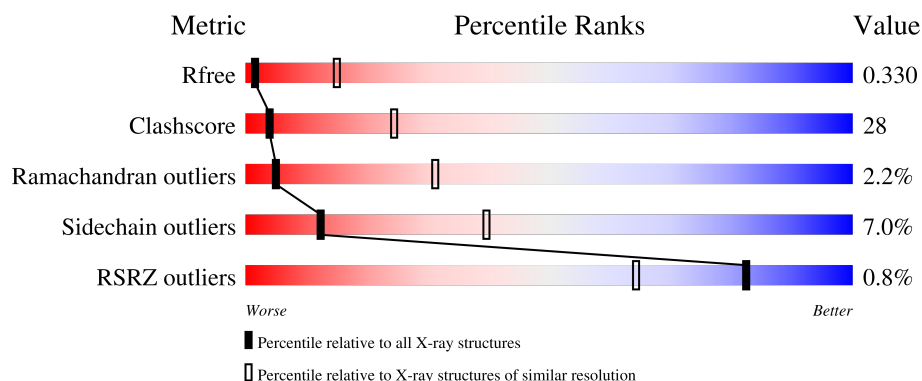
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

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	214	<div> <div>55%</div> <div>41%</div> <div>.</div> </div>
1	L	214	<div> <div>50%</div> <div>43%</div> <div>7%</div> </div>
2	B	220	<div> <div>2%</div> <div>56%</div> <div>37%</div> <div>5%</div> <div>.</div> </div>
2	H	220	<div> <div>49%</div> <div>44%</div> <div>5%</div> <div>.</div> </div>
3	I	181	<div> <div>51%</div> <div>40%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	181	 A horizontal bar chart showing the quality of chain J. The bar is divided into three segments: green (47%), yellow (46%), and orange (6%). The segments are labeled with their respective percentages: 47%, 46%, and 6%.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9454 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 Efalizumab Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1647	1030	276	335	6			
1	A	214	Total	C	N	O	S	0	0	0
			1647	1030	276	335	6			

- Molecule 2 is a protein called Efalizumab Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1641	1043	273	318	7			
2	B	215	Total	C	N	O	S	0	0	0
			1641	1043	273	318	7			

- Molecule 3 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	179	Total	C	N	O	S	0	0	0
			1438	929	231	274	4			
3	J	179	Total	C	N	O	S	0	0	0
			1438	929	231	274	4			

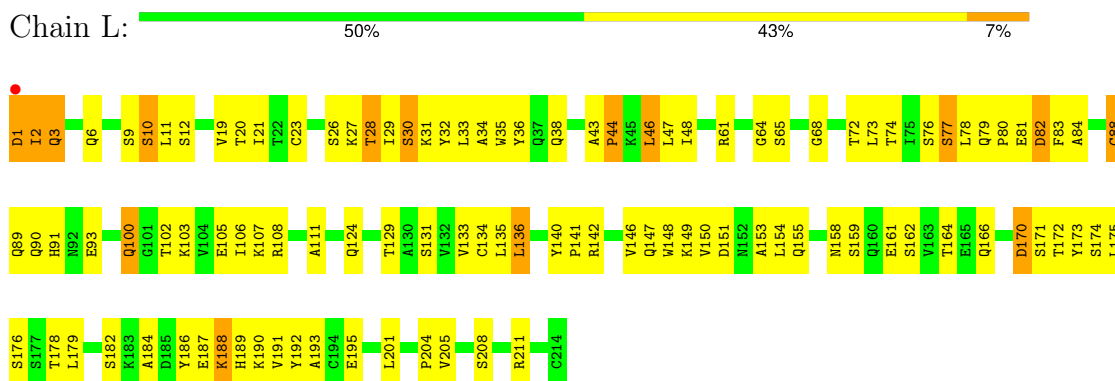
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		

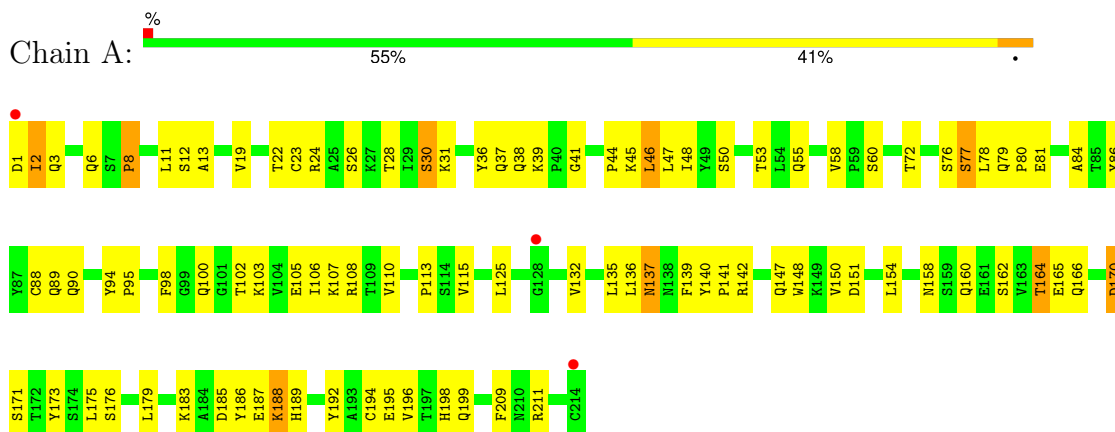
### 3 Residue-property plots

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.

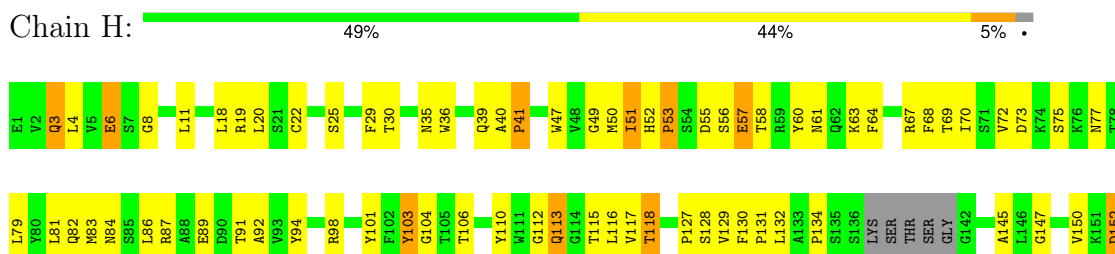
- Molecule 1: Efalizumab Fab fragment, light chain



- Molecule 1: Efalizumab Fab fragment, light chain



- Molecule 2: Efalizumab Fab fragment, heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.10Å 111.10Å 470.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.60) 97.7 (50.00-3.60)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.267 , 0.333 0.267 , 0.330	Depositor DCC
$R_{free}$ test set	1026 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

### 5.1 Standard geometry

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

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	0.48	0/1682	0.73	2/2280 (0.1%)
1	L	0.45	0/1682	0.73	0/2280
2	B	0.54	2/1684 (0.1%)	0.75	1/2291 (0.0%)
2	H	0.58	2/1684 (0.1%)	0.78	2/2291 (0.1%)
3	I	0.63	3/1465 (0.2%)	0.83	4/1970 (0.2%)
3	J	0.60	0/1465	0.85	1/1970 (0.1%)
All	All	0.55	7/9662 (0.1%)	0.78	10/13082 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
3	I	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	241	GLU	CG-CD	7.92	1.63	1.51
3	I	141	SER	CA-CB	-7.37	1.41	1.52
2	H	57	GLU	CB-CG	7.21	1.65	1.52
2	H	57	GLU	CG-CD	6.78	1.62	1.51
2	B	57	GLU	CB-CG	6.61	1.64	1.52

The worst 5 of 10 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	239	ASP	CB-CG-OD1	-9.41	109.83	118.30
3	I	141	SER	CA-CB-OG	-8.05	89.47	111.20
3	I	239	ASP	CB-CG-OD1	-7.86	111.22	118.30
2	H	61	ASN	N-CA-C	-6.77	92.71	111.00
2	B	61	ASN	N-CA-C	-6.25	94.13	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	103	TYR	Sidechain
3	I	261	ILE	Peptide

## 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	1647	0	1608	69	1
1	L	1647	0	1608	105	0
2	B	1641	0	1591	88	0
2	H	1641	0	1591	99	0
3	I	1438	0	1449	90	0
3	J	1438	0	1449	97	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
All	All	9454	0	9296	516	1

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 28.

The worst 5 of 516 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:115:VAL:HG21	1:A:196:VAL:HG21	1.38	1.05
1:L:1:ASP:O	1:L:2:ILE:HG13	1.59	1.03
1:L:175:LEU:HD23	1:L:176:SER:N	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:143:GLN:HG3	3:J:144:PRO:HD2	1.49	0.94
1:L:80:PRO:HA	1:L:106:ILE:HD13	1.50	0.94

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:OD2	1:A:1:ASP:OD2[9_554]	2.06	0.14

## 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	212/214 (99%)	193 (91%)	17 (8%)	2 (1%)	14	48
1	L	212/214 (99%)	182 (86%)	22 (10%)	8 (4%)	2	22
2	B	211/220 (96%)	183 (87%)	22 (10%)	6 (3%)	4	27
2	H	211/220 (96%)	191 (90%)	16 (8%)	4 (2%)	6	35
3	I	177/181 (98%)	157 (89%)	16 (9%)	4 (2%)	5	31
3	J	177/181 (98%)	158 (89%)	16 (9%)	3 (2%)	7	37
All	All	1200/1230 (98%)	1064 (89%)	109 (9%)	27 (2%)	5	31

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	28	THR
2	H	152	ASP
2	B	152	ASP
2	B	196	SER

### 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%)	172 (91%)	17 (9%)	8	32
1	L	189/189 (100%)	178 (94%)	11 (6%)	17	46
2	B	182/186 (98%)	176 (97%)	6 (3%)	33	61
2	H	182/186 (98%)	168 (92%)	14 (8%)	10	36
3	I	159/161 (99%)	148 (93%)	11 (7%)	13	40
3	J	159/161 (99%)	144 (91%)	15 (9%)	7	30
All	All	1060/1072 (99%)	986 (93%)	74 (7%)	12	40

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	113	GLN
3	J	263	LYS
3	J	129	ASN
3	J	189	ARG
2	H	177	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	205	ASN
3	J	129	ASN
3	J	266	GLN
3	I	247	ASN
3	I	167	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](#)

Of 2 ligands modelled in this entry, 2 are 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 [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	214/214 (100%)	-0.04	3 (1%) 73 52	54, 102, 134, 155	0
1	L	214/214 (100%)	-0.24	1 (0%) 87 72	72, 101, 129, 144	0
2	B	215/220 (97%)	-0.07	4 (1%) 66 45	52, 104, 132, 159	0
2	H	215/220 (97%)	-0.32	0 100 100	53, 95, 121, 136	0
3	I	179/181 (98%)	-0.29	2 (1%) 77 57	26, 91, 122, 137	0
3	J	179/181 (98%)	-0.27	0 100 100	26, 86, 118, 137	0
All	All	1216/1230 (98%)	-0.20	10 (0%) 82 64	26, 96, 130, 159	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ASP	4.0
2	B	170	GLY	2.8
3	I	306	ILE	2.7
2	B	219	VAL	2.5
1	A	128	GLY	2.3

### 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( $\text{\AA}^2$ )	Q<0.9
4	ZN	I	1	1/1	0.96	0.12	99,99,99,99	0
4	ZN	J	2	1/1	0.97	0.10	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.