



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 AM GMT

PDB ID : 3EO9
Title : Crystal structure the Fab fragment of Efalizumab
Authors : Li, S.; Ding, J.
Deposited on : 2008-09-26
Resolution : 1.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

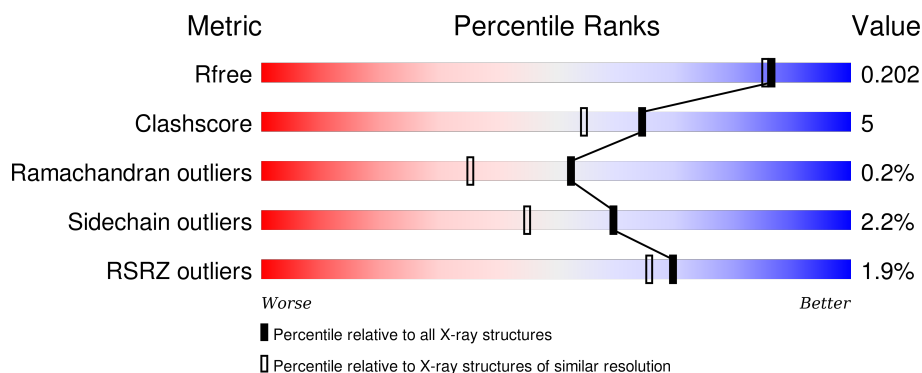
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	L	214	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 10% . </div> </div>
2	H	219	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 86% 9% . . </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3899 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	213	Total	C	N	O	S	23	0	0
			1640	1027	275	333	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	24	1	0
			1634	1040	272	315	7			

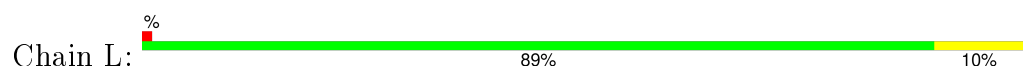
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	295	Total	O	1	0
			295	295		
3	L	330	Total	O	2	0
			330	330		

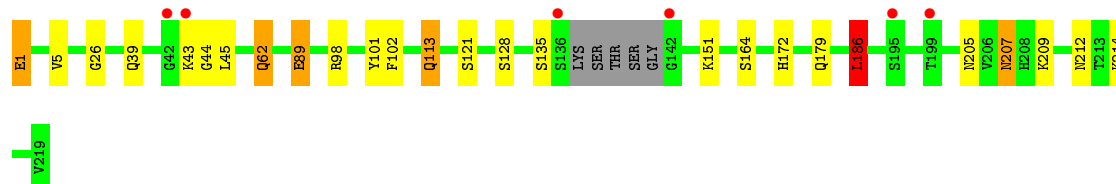
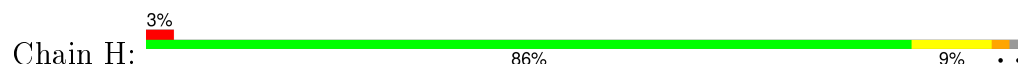
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 2: Efalizumab Fab fragment, heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.20 Å 87.20 Å 117.22 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.80 17.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-1.80) 98.0 (17.97-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.80 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.189 , 0.217 0.192 , 0.202	Depositor DCC
R_{free} test set	2401 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 47314 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3899	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	L	0.54	1/1675 (0.1%)	0.56	3/2272 (0.1%)
2	H	1.21	9/1680 (0.5%)	0.88	13/2287 (0.6%)
All	All	0.94	10/3355 (0.3%)	0.74	16/4559 (0.4%)

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	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	89	GLU	CG-CD	25.72	1.90	1.51
2	H	214	LYS	CE-NZ	20.93	2.01	1.49
2	H	1	GLU	CD-OE2	-20.50	1.03	1.25
2	H	212	ASN	CG-OD1	19.06	1.65	1.24
1	L	126	LYS	CD-CE	-13.24	1.18	1.51
2	H	209	LYS	CG-CD	-8.14	1.24	1.52
2	H	207	ASN	CG-ND2	7.93	1.52	1.32
2	H	212	ASN	CB-CG	7.50	1.68	1.51
2	H	214	LYS	CB-CG	-6.32	1.35	1.52
2	H	98	ARG	CD-NE	5.37	1.55	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	GLU	OE1-CD-OE2	-13.47	107.14	123.30
2	H	62	GLN	OE1-CD-NE2	-11.75	94.88	121.90
2	H	89	GLU	CG-CD-OE1	-11.24	95.83	118.30
2	H	89	GLU	CG-CD-OE2	-11.10	96.11	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	212	ASN	CB-CG-OD1	9.77	141.14	121.60
2	H	1	GLU	CG-CD-OE2	7.97	134.25	118.30
2	H	209	LYS	CB-CG-CD	7.79	131.84	111.60
2	H	209	LYS	CD-CE-NZ	-7.35	94.80	111.70
2	H	207	ASN	CB-CG-ND2	-6.50	101.11	116.70
2	H	186	LEU	CA-CB-CG	6.41	130.03	115.30
1	L	126	LYS	CG-CD-CE	6.40	131.10	111.90
2	H	212	ASN	CB-CG-ND2	-6.26	101.68	116.70
2	H	89	GLU	CB-CG-CD	5.97	130.32	114.20
2	H	214	LYS	CA-CB-CG	5.81	126.18	113.40
1	L	154	LEU	CB-CG-CD2	5.41	120.19	111.00
1	L	181	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	207	ASN	Sidechain
2	H	62	GLN	Sidechain
2	H	89	GLU	Sidechain

5.2 Too-close contacts ⓘ

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	L	1640	0	1603	12	0
2	H	1634	0	1590	23	0
3	H	295	0	0	4	0
3	L	330	0	0	1	0
All	All	3899	0	3193	32	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.

All (32) 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:H:164:SER:H	2:H:205:ASN:HD21	1.22	0.84
1:L:106:ILE:H	1:L:166:GLN:HE22	1.23	0.81
2:H:39:GLN:HB2	2:H:45:LEU:HD13	1.64	0.80
2:H:43:LYS:HD2	3:H:368:HOH:O	1.86	0.76
2:H:43:LYS:HD3	2:H:44:GLY:N	2.01	0.75
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.33	0.75
1:L:142:ARG:NH1	3:L:357:HOH:O	2.24	0.69
2:H:151:LYS:NZ	2:H:179:GLN:HE22	1.92	0.68
2:H:43:LYS:HD3	2:H:44:GLY:H	1.58	0.68
1:L:155:GLN:HE21	1:L:158:ASN:HD21	1.44	0.65
1:L:137:ASN:HD21	2:H:172:HIS:CD2	2.17	0.63
1:L:6:GLN:H	1:L:100:GLN:HE22	1.48	0.61
2:H:39:GLN:HB2	2:H:45:LEU:CD1	2.32	0.60
1:L:137:ASN:HD21	2:H:172:HIS:HD2	1.48	0.59
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.89	0.53
2:H:151:LYS:HZ2	2:H:179:GLN:HE22	1.59	0.51
2:H:164:SER:H	2:H:205:ASN:ND2	2.01	0.48
2:H:5:VAL:HA	2:H:113:GLN:HE22	1.80	0.47
2:H:43:LYS:CD	2:H:44:GLY:H	2.26	0.47
2:H:121:SER:HB2	3:H:227:HOH:O	2.14	0.47
1:L:145:LYS:HB3	1:L:197:THR:HB	1.97	0.46
1:L:149:LYS:NZ	1:L:195:GLU:OE1	2.37	0.46
2:H:151:LYS:HZ3	2:H:179:GLN:HE22	1.61	0.45
1:L:32:TYR:HD1	1:L:92:ASN:HD22	1.64	0.45
2:H:151:LYS:NZ	2:H:179:GLN:NE2	2.64	0.45
2:H:113:GLN:H	2:H:113:GLN:HE21	1.63	0.45
2:H:151:LYS:HE3	3:H:419:HOH:O	2.17	0.44
2:H:1:GLU:O	2:H:26:GLY:HA3	2.18	0.43
1:L:163:VAL:HG22	1:L:175:LEU:HD12	2.01	0.43
2:H:43:LYS:CD	2:H:44:GLY:N	2.77	0.42
2:H:151:LYS:HZ3	2:H:179:GLN:NE2	2.19	0.41
2:H:186:LEU:HA	3:H:222:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	L	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
2	H	211/219 (96%)	208 (99%)	2 (1%)	1 (0%)	34	17
All	All	422/433 (98%)	415 (98%)	6 (1%)	1 (0%)	52	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	102	PHE

5.3.2 Protein sidechains ⓘ

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	L	188/189 (100%)	185 (98%)	3 (2%)	70	59
2	H	182/185 (98%)	177 (97%)	5 (3%)	52	36
All	All	370/374 (99%)	362 (98%)	8 (2%)	60	45

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	24	ARG
1	L	100	GLN
1	L	181	LEU
2	H	101	TYR
2	H	113	GLN
2	H	128	SER
2	H	135	SER
2	H	186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	100	GLN
1	L	124	GLN
1	L	137	ASN
1	L	152	ASN
1	L	155	GLN
1	L	166	GLN
1	L	199	GLN
2	H	39	GLN
2	H	62	GLN
2	H	113	GLN
2	H	179	GLN
2	H	205	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 carbohydrates 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, 95th 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 ²)	Q<0.9
1	L	213/214 (99%)	-0.27	2 (0%) 85 83	13, 19, 27, 59	13 (6%)
2	H	214/219 (97%)	-0.13	6 (2%) 56 51	12, 18, 32, 53	16 (7%)
All	All	427/433 (98%)	-0.20	8 (1%) 70 66	12, 19, 29, 59	29 (6%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	42	GLY	4.5
1	L	212	GLY	4.5
2	H	199	THR	3.5
2	H	136	SER	3.4
2	H	43	LYS	3.0
1	L	24	ARG	2.9
2	H	195	SER	2.6
2	H	142	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.