wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:26 AM GMT

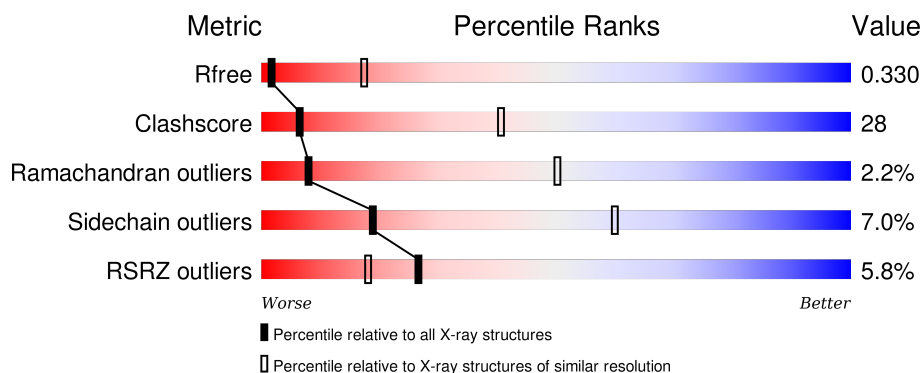|		
PDB ID	:	3EOB
Title	:	Crystal structure the Fab fragment of Efalizumab in complex with LFA-1 I domain, Form II
Authors	:	Li, S.; Ding, J.
Deposited on	:	2008-09-26
Resolution	:	3.60 Å(reported)

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 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	Percentile Ranks	Value
Rfree		0.330
Clashscore		28
Ramachandran outliers		2.2%
Sidechain outliers		7.0%
RSRZ outliers		5.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 <=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	11% / 55% / 41% / •
1	L	214	2% / 50% / 43% / 7%
2	B	220	15% / 56% / 37% / 5% •
2	H	220	2% / 49% / 44% / 5% •
3	I	181	2% / 51% / 40% / 8% •

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Mol	Chain	Length	Quality of chain
3	J	181	

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 1647	C 1030	N 276	O 335	S 6	0	0	0
1	A	214	Total 1647	C 1030	N 276	O 335	S 6	0	0	0

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

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

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

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

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

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

3 Residue-property plots ⓘ

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 1: Efalizumab Fab fragment, light chain

• Molecule 2: Efalizumab Fab fragment, heavy chain

D152 Y153 F154 P155 E156 P157 V158 S161 W162 F174 P175 A176 V177 L178 Q179 S180 S181 G182 L183 Y184 L185 L186 S187 V189 V190 T191 V192 P193 S196 L197 G198 T199 Q200 Y201 Y202 I203 C204 N205 V206 N207 H208 K209 P210 K217 K218 V219 E220

• Molecule 2: Efalizumab Fab fragment, heavy chain

Chain B:

15%

56% 37% 5%

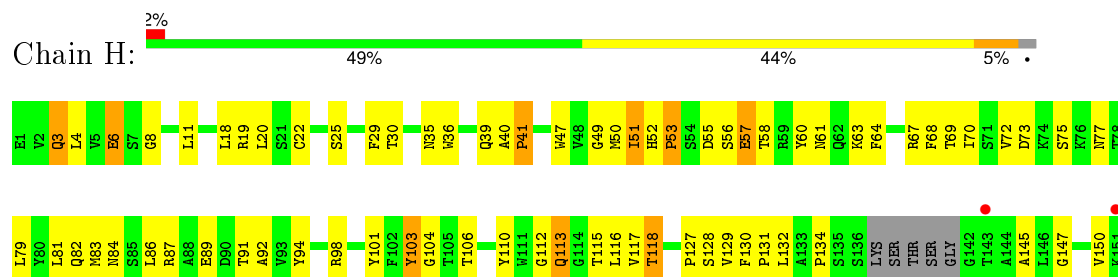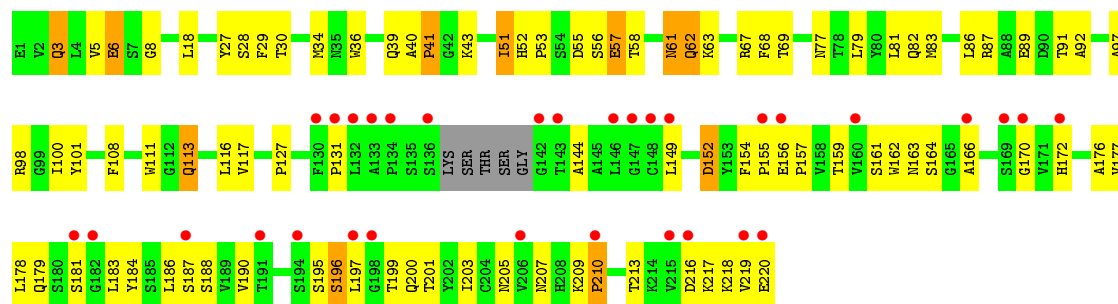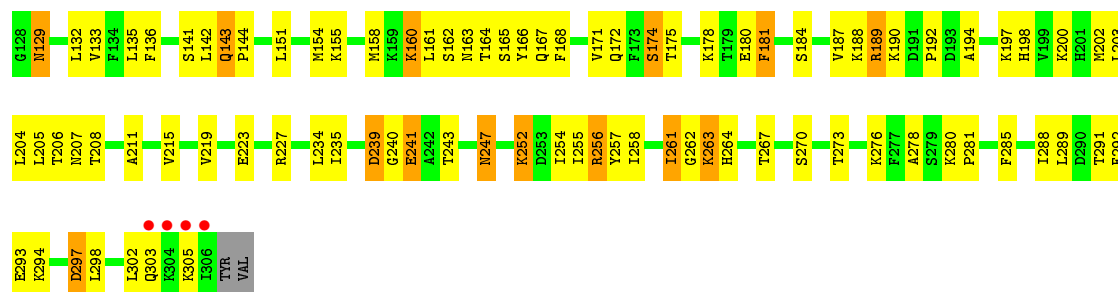E1 V2 Q3 L4 V5 E6 S7 G8 L18 Y27 S28 F29 T30 M34 N35 W36 Q39 A40 P41 G42 K43 I51 H52 P53 S54 D55 S56 E57 T58 N61 Q62 K63 R67 F68 T69 N77 T78 L79 Y80 L81 Q82 M83 L86 R87 A88 E89 D90 T91 A92 A97

R98 G99 I100 Y101 F108 W111 G112 Q113 L116 V117 P127 F130 P131 L132 A133 P134 S135 S136 LYS SER THR SER GLY G142 T143 A144 A145 L146 G147 C148 L149 D152 Y153 F154 P155 E156 P157 V158 T159 V160 S161 W162 N163 S164 G165 A166 S169 G170 V171 H172 A176 V177

L178 Q179 S180 S181 G182 L183 Y184 L185 L186 S187 S188 V189 V190 T191 S194 S195 S196 L197 G198 T199 Q200 T201 Y202 C204 N205 V206 N207 H208 K209 P210 T213 V214 V215 D216 K217 K218 V219 E220

• Molecule 3: Integrin alpha-L

Chain I:

2%

51% 40% 8%

G128 N129 L132 V133 F134 L135 F136 S141 L142 Q143 P144 L151 M154 K155 M158 K159 K160 L161 S162 N163 T164 S165 Y166 Q167 F168 V171 Q172 F173 S174 T175 R178 T179 E180 F181 S184 V187 K188 R189 K190 D191 P192 D193 A194 K197 H198 V199 K200 H201 M202 L203

L204 L205 T206 N207 T208 A211 V215 V219 E223 R227 L234 I235 D239 G240 E241 A242 T243 N247 K252 D253 I254 I255 R256 Y257 I258 I261 G262 K263 H264 T267 S270 T273 K276 F277 A278 S279 K280 P281 F285 I288 L289 D290 T291 F292

E293 K294 D297 L298 L302 Q303 K304 K305 I306 TYR VAL

• Molecule 3: Integrin alpha-L

Chain J:

2%

47% 46% 6%

G128 N129 V130 D131 L132 V133 F134 L135 F136 S139 M140 S141 L142 Q143 P144 K149 I150 L151 M154 K155 K160 L161 S162 N163 T164 S165 Y166 Q167 F168 A169 V171 Q172 T175 S176 Y177 R178 T179 E180 F181 D182 F183 S184 V187 K188 R189 K190 A194 L195 L196 K197 H198 V199

M202 L203 L204 L205 T206 N207 G210 N213 Y214 V215 V219 E222 E223 G225 A226 R227 K232 V233 L234 I235 I236 D239 G240 E241 A242 D244 S245 G246 N247 I248 K252 D253 R256 Y257 I258 I259 G260 I261 G262 K263 H264 Q271 E272 A278 S279 F285

I288 T291 F292 E293 K294 L295 K296 D297 L298 F299 T300 E301 L302 Q303 K304 K305 I306 TYR VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	111.10Å 111.10Å 470.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.60 47.84 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.60) 97.8 (47.84-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$<I/\sigma(I)>$ [1]	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%)	DCC
Wilson B-factor (Å^2)	99.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\lvert L \rvert> = 0.46, <L^2> = 0.29$	Xtriage
Outliers	0 of 20630 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:
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(^{o})	Ideal(^{o})
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%)	21	67
1	L	212/214 (99%)	182 (86%)	22 (10%)	8 (4%)	4	37
2	B	211/220 (96%)	183 (87%)	22 (10%)	6 (3%)	6	45
2	H	211/220 (96%)	191 (90%)	16 (8%)	4 (2%)	10	53
3	I	177/181 (98%)	157 (89%)	16 (9%)	4 (2%)	8	50
3	J	177/181 (98%)	158 (89%)	16 (9%)	3 (2%)	11	55
All	All	1200/1230 (98%)	1064 (89%)	109 (9%)	27 (2%)	8	50

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%)	12	49
1	L	189/189 (100%)	178 (94%)	11 (6%)	25	66
2	B	182/186 (98%)	176 (97%)	6 (3%)	45	80
2	H	182/186 (98%)	168 (92%)	14 (8%)	16	56
3	I	159/161 (99%)	148 (93%)	11 (7%)	19	60
3	J	159/161 (99%)	144 (91%)	15 (9%)	11	47
All	All	1060/1072 (99%)	986 (93%)	74 (7%)	19	60

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

Mol	Chain	Res	Type
3	I	263	LYS
1	A	30	SER
3	J	247	ASN
3	I	288	ILE
1	A	3	GLN

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	137	ASN
3	J	143	GLN
1	A	38	GLN
1	A	89	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 carbohydrates 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, 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	A	214/214 (100%)	0.59	23 (10%)	8	6	54, 102, 134, 155	0
1	L	214/214 (100%)	0.18	5 (2%)	64	48	72, 101, 129, 144	0
2	B	215/220 (97%)	0.69	32 (14%)	3	3	52, 104, 132, 159	0
2	H	215/220 (97%)	0.18	4 (1%)	70	56	53, 95, 121, 136	0
3	I	179/181 (98%)	0.15	4 (2%)	65	50	26, 91, 122, 137	0
3	J	179/181 (98%)	0.10	3 (1%)	73	59	26, 86, 118, 137	0
All	All	1216/1230 (98%)	0.33	71 (5%)	26	18	26, 96, 130, 159	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	306	ILE	8.7
3	I	304	LYS	7.7
1	A	129	THR	5.6
1	A	214	CYS	5.3
2	B	142	GLY	4.7

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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors($Å^2$)	Q<0.9
4	ZN	J	2	1/1	0.97	0.25	0.53	99,99,99,99	0
4	ZN	I	1	1/1	0.85	0.28	0.52	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.