



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:15 PM GMT

PDB ID : 4XZU
Title : Crystal Structure of the Human Factor VIII C2 Domain in Complex with Murine 3E6 Inhibitory Antibody
Authors : Spiegel, P.C.; Wuerth, M.E.
Deposited on : 2015-02-05
Resolution : 2.61 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
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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

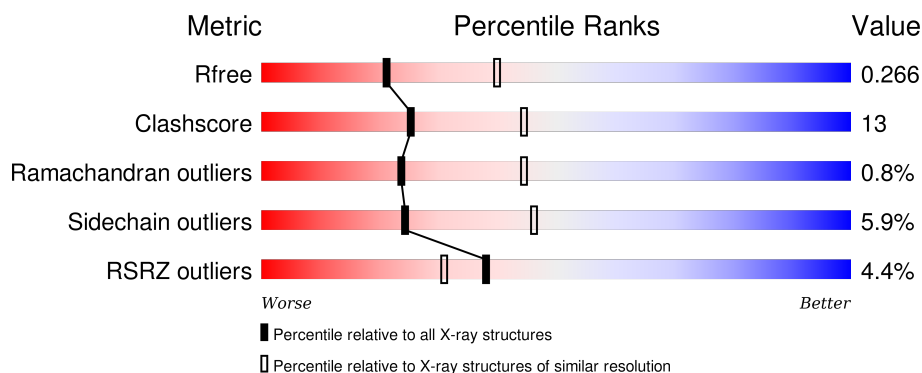
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	A	219	
1	E	219	
2	B	213	
2	F	213	
3	G	154	

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Mol	Chain	Length	Quality of chain
3	M	154	<div><div>%</div><div><div></div><div>84%</div><div>16%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9034 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 3E6 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1619	1029	265	319	6			
1	E	208	Total	C	N	O	S	0	0	0
			1581	1007	257	312	5			

- Molecule 2 is a protein called 3E6 antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1633	1016	271	337	9			
2	F	195	Total	C	N	O	S	0	0	0
			1495	937	244	306	8			

- Molecule 3 is a protein called Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	154	Total	C	N	O	S	0	0	0
			1231	785	214	224	8			
3	G	154	Total	C	N	O	S	0	0	0
			1231	785	214	224	8			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		

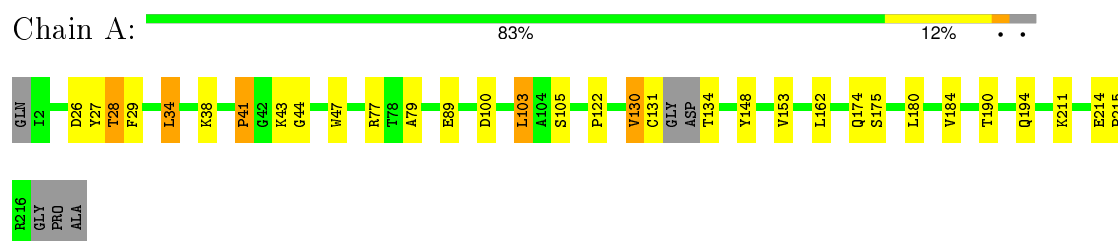
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total 73	O 73	0	0
5	B	49	Total 49	O 49	0	0
5	M	30	Total 30	O 30	0	0
5	E	41	Total 41	O 41	0	0
5	F	27	Total 27	O 27	0	0
5	G	21	Total 21	O 21	0	0

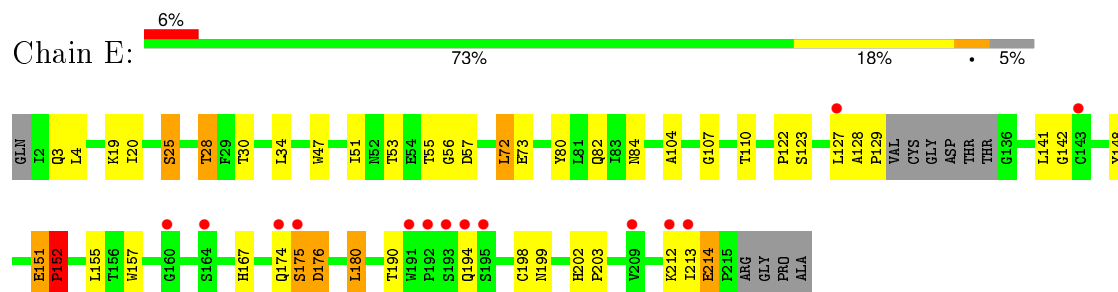
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

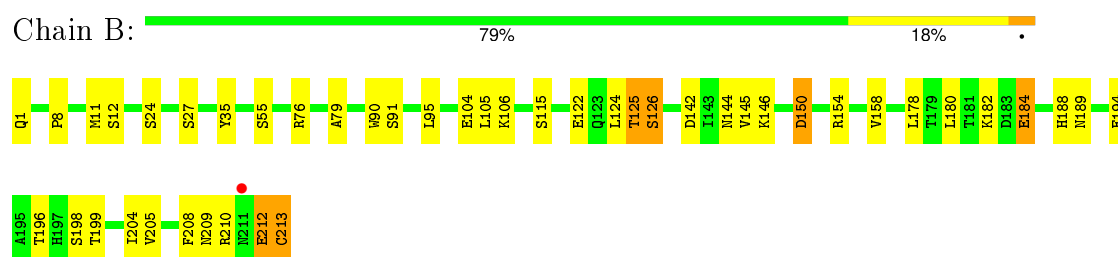
- Molecule 1: 3E6 antibody Fab heavy chain



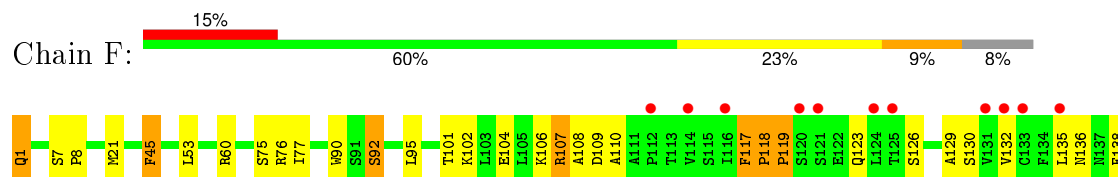
- Molecule 1: 3E6 antibody Fab heavy chain

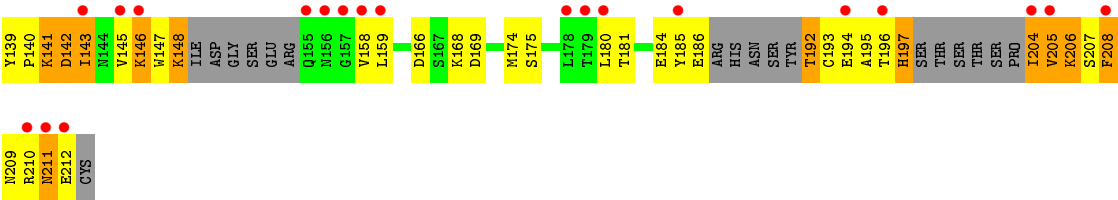


- Molecule 2: 3E6 antibody Fab light chain

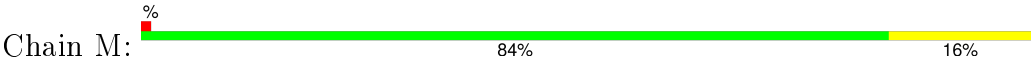


- Molecule 2: 3E6 antibody Fab light chain

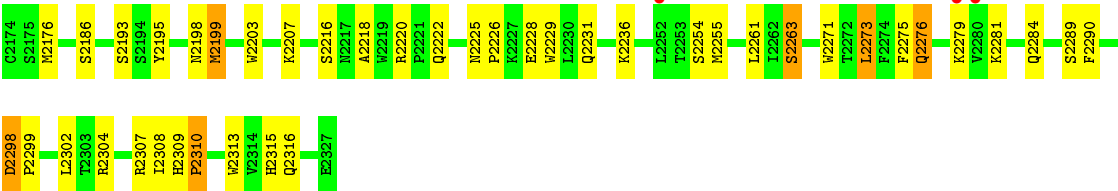




● Molecule 3: Coagulation factor VIII



● Molecule 3: Coagulation factor VIII



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	43.23Å 148.49Å 188.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 2.61 39.77 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.78-2.61) 95.0 (39.77-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.199 , 0.267 0.198 , 0.266	Depositor DCC
R_{free} test set	1821 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36886 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9034	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/1660	0.64	2/2266 (0.1%)
1	E	0.69	1/1622 (0.1%)	0.73	6/2214 (0.3%)
2	B	0.49	0/1672	0.61	0/2274
2	F	0.62	2/1528 (0.1%)	0.72	2/2074 (0.1%)
3	G	0.42	0/1263	0.62	0/1713
3	M	0.46	0/1263	0.61	0/1713
All	All	0.55	3/9008 (0.0%)	0.66	10/12254 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	119	PRO	N-CD	5.71	1.55	1.47
2	F	118	PRO	N-CD	5.19	1.55	1.47
1	E	129	PRO	N-CD	5.01	1.54	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	28	THR	N-CA-C	-7.11	91.81	111.00
1	E	152	PRO	CA-N-CD	-6.31	102.66	111.50
2	F	117	PHE	C-N-CD	6.25	141.52	128.40
1	E	214	GLU	C-N-CD	6.06	141.13	128.40
1	E	128	ALA	C-N-CD	6.03	141.07	128.40

There are no chirality outliers.

There are no planarity outliers.

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	A	1619	0	1587	23	0
1	E	1581	0	1548	48	0
2	B	1633	0	1554	28	0
2	F	1495	0	1429	99	0
3	G	1231	0	1218	29	0
3	M	1231	0	1218	18	0
4	A	1	0	0	0	0
4	F	1	0	0	0	0
4	M	1	0	0	0	0
5	A	73	0	0	0	1
5	B	49	0	0	1	0
5	E	41	0	0	6	0
5	F	27	0	0	1	0
5	G	21	0	0	2	0
5	M	30	0	0	3	1
All	All	9034	0	8554	219	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 13.

The worst 5 of 219 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:F:186:GLU:HA	2:F:210:ARG:NH2	1.21	1.41
2:F:185:TYR:CE2	2:F:210:ARG:HD2	1.65	1.30
2:F:186:GLU:CA	2:F:210:ARG:NH2	1.94	1.30
2:F:185:TYR:CZ	2:F:210:ARG:HD2	1.71	1.24
1:E:167:HIS:HD2	2:F:136:ASN:ND2	1.37	1.19

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)
5:A:438:HOH:O	5:M:2526:HOH:O[1_455]	2.15	0.05

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	A	209/219 (95%)	193 (92%)	15 (7%)	1 (0%)	34	58
1	E	204/219 (93%)	188 (92%)	15 (7%)	1 (0%)	34	58
2	B	211/213 (99%)	203 (96%)	6 (3%)	2 (1%)	21	41
2	F	187/213 (88%)	166 (89%)	17 (9%)	4 (2%)	9	15
3	G	152/154 (99%)	128 (84%)	23 (15%)	1 (1%)	26	49
3	M	152/154 (99%)	140 (92%)	12 (8%)	0	100	100
All	All	1115/1172 (95%)	1018 (91%)	88 (8%)	9 (1%)	24	44

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	205	VAL
2	F	142	ASP
2	F	143	ILE
2	B	212	GLU
2	B	125	THR

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	A	183/186 (98%)	176 (96%)	7 (4%)	40	68
1	E	178/186 (96%)	171 (96%)	7 (4%)	39	67
2	B	188/188 (100%)	175 (93%)	13 (7%)	19	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	171/188 (91%)	150 (88%)	21 (12%)	6	10
3	G	139/139 (100%)	132 (95%)	7 (5%)	30	55
3	M	139/139 (100%)	135 (97%)	4 (3%)	50	76
All	All	998/1026 (97%)	939 (94%)	59 (6%)	24	46

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	84	ASN
2	F	75	SER
3	G	2263	SER
1	E	123	SER
1	E	176	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	167	HIS
1	E	194	GLN
2	F	136	ASN
3	G	2222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 ⓘ

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, 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	213/219 (97%)	-0.55	0 100 100	25, 33, 55, 79	0
1	E	208/219 (94%)	0.12	14 (6%) 21 16	31, 47, 96, 114	0
2	B	213/213 (100%)	-0.38	1 (0%) 91 90	25, 37, 71, 97	0
2	F	195/213 (91%)	0.48	31 (15%) 3 1	30, 50, 130, 163	0
3	G	154/154 (100%)	-0.01	3 (1%) 70 65	38, 56, 74, 84	0
3	M	154/154 (100%)	-0.44	1 (0%) 90 88	25, 38, 60, 72	0
All	All	1137/1172 (97%)	-0.13	50 (4%) 38 31	25, 42, 99, 163	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	155	GLN	8.1
1	E	193	SER	7.8
2	F	156	ASN	7.3
2	F	212	GLU	5.8
1	E	192	PRO	5.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
4	MG	A	301	1/1	0.72	0.23	-	75,75,75,75	0
4	MG	F	301	1/1	0.72	0.10	-	96,96,96,96	0
4	MG	M	2401	1/1	0.92	0.31	-	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.