



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:56 PM GMT

PDB ID : 4QEX
Title : Crystal structure of PfEBA-175 RII in complex with a Fab fragment from inhibitory antibody R217
Authors : Chen, E.; Paing, M.M.; Salinas, N.; Sim, B.K.; Tolia, N.H.
Deposited on : 2014-05-19
Resolution : 4.50 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 : 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

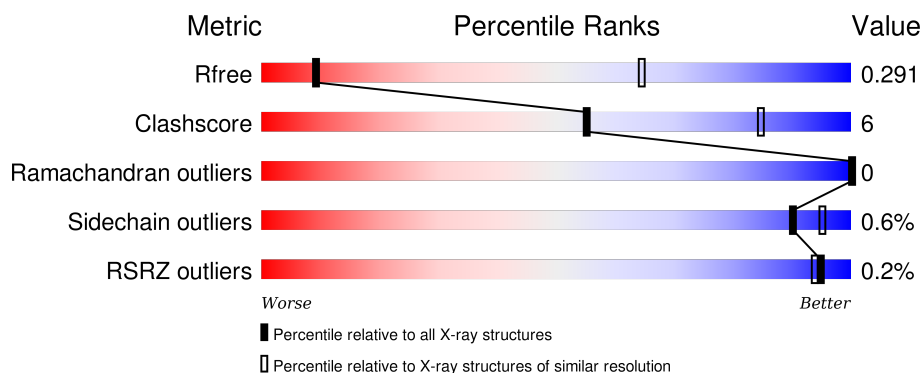
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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	602	<div> <div>81%</div> <div>12%</div> <div>7%</div> </div>
1	B	602	<div> <div>83%</div> <div>13%</div> <div>.</div> </div>
2	L	214	<div> <div>79%</div> <div>21%</div> <div>.</div> </div>
2	M	214	<div> <div>77%</div> <div>22%</div> </div>
3	H	215	<div> <div>78%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	215	 78%20%•

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 31624 atoms, of which 15595 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 Erythrocyte-binding antigen-175.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	561	Total	C	H	N	O	S	0	0	0
			9393	2994	4660	826	880	33			
1	B	580	Total	C	H	N	O	S	0	0	0
			9696	3088	4810	851	913	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLN	ASN	ENGINEERED MUTATION	UNP Q05644
A	50	ALA	SER	ENGINEERED MUTATION	UNP Q05644
A	195	ALA	SER	ENGINEERED MUTATION	UNP Q05644
A	206	ALA	THR	ENGINEERED MUTATION	UNP Q05644
B	3	GLN	ASN	ENGINEERED MUTATION	UNP Q05644
B	50	ALA	SER	ENGINEERED MUTATION	UNP Q05644
B	195	ALA	SER	ENGINEERED MUTATION	UNP Q05644
B	206	ALA	THR	ENGINEERED MUTATION	UNP Q05644

- Molecule 2 is a protein called Antibody Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	212	Total	C	H	N	O	S	0	0	0
			3201	1024	1557	284	330	6			
2	M	213	Total	C	H	N	O	S	0	0	0
			3212	1027	1562	285	332	6			

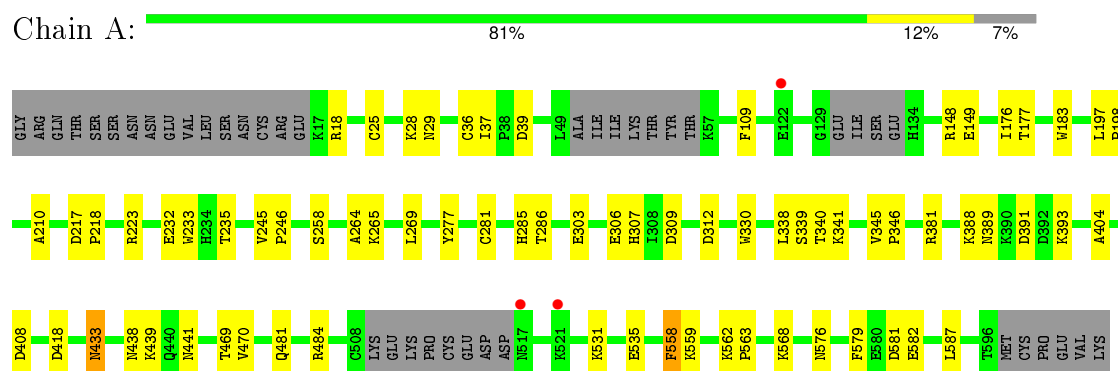
- Molecule 3 is a protein called Antibody Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	206	Total	C	H	N	O	S	0	0	0
			3040	973	1493	248	318	8			
3	I	210	Total	C	H	N	O	S	0	0	0
			3082	986	1513	252	323	8			

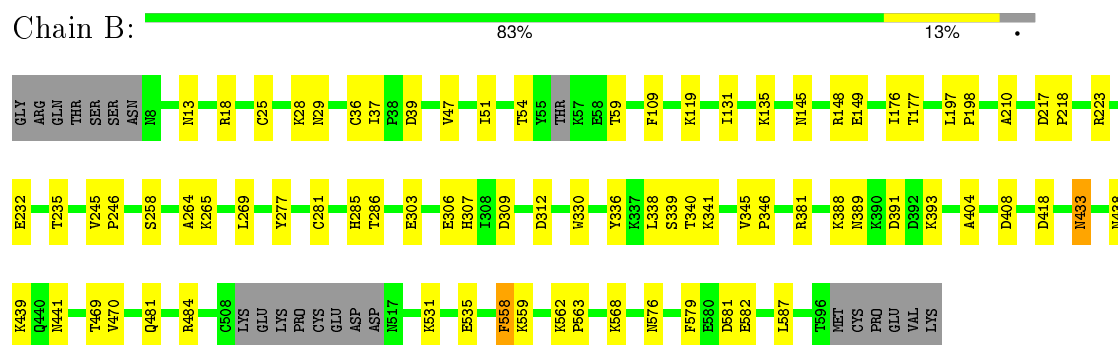
3 Residue-property plots [i](#)

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.

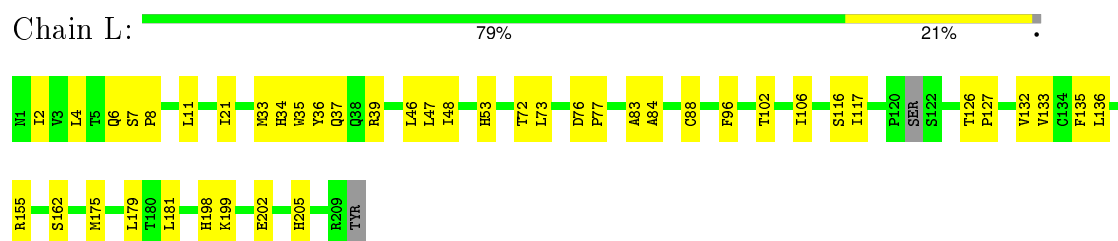
• Molecule 1: Erythrocyte-binding antigen-175



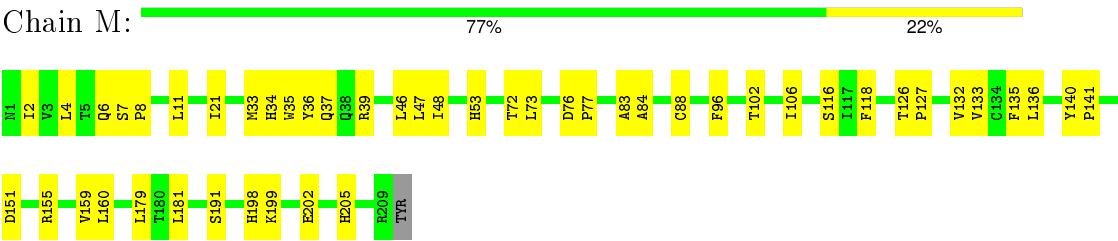
• Molecule 1: Erythrocyte-binding antigen-175



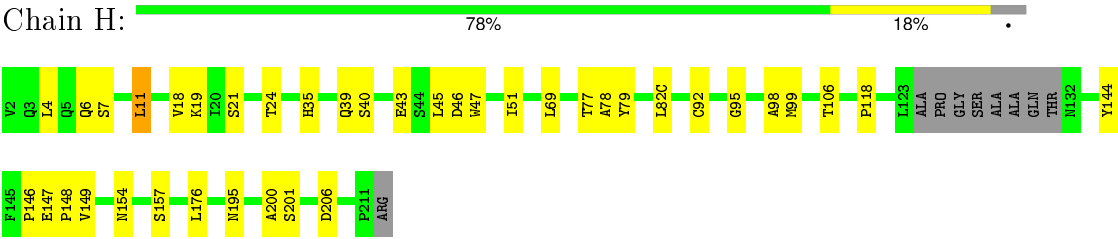
• Molecule 2: Antibody Light Chain



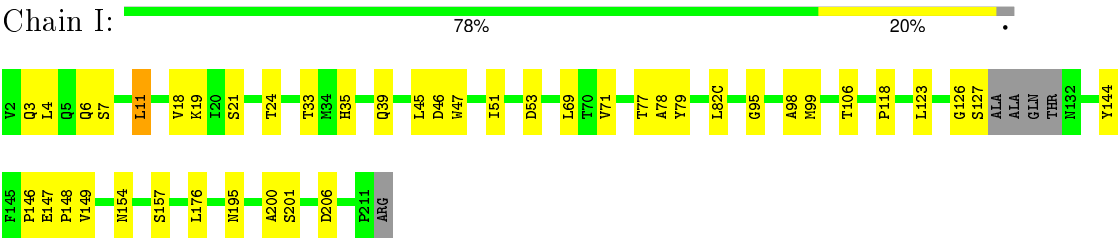
• Molecule 2: Antibody Light Chain



● Molecule 3: Antibody Heavy Chain



● Molecule 3: Antibody Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.10Å 101.26Å 117.59Å 90.00° 102.86° 90.00°	Depositor
Resolution (Å)	19.84 – 4.50 19.84 – 4.50	Depositor EDS
% Data completeness (in resolution range)	94.0 (19.84-4.50) 94.0 (19.84-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 4.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.232 , 0.285 0.234 , 0.291	Depositor DCC
R_{free} test set	665 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	118.4	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 72.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 13322 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	31624	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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	A	0.23	0/4831	0.37	0/6468
1	B	0.23	0/4986	0.37	0/6679
2	L	0.23	0/1683	0.43	0/2284
2	M	0.23	0/1690	0.42	0/2295
3	H	0.24	0/1585	0.45	0/2166
3	I	0.24	0/1608	0.45	0/2198
All	All	0.23	0/16383	0.40	0/22090

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

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	4733	4660	4670	41	0
1	B	4886	4810	4820	53	0
2	L	1644	1557	1562	28	0
2	M	1650	1562	1568	31	0
3	H	1547	1493	1497	25	0
3	I	1569	1513	1517	31	0
All	All	16029	15595	15634	198	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 6.

The worst 5 of 198 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)
3:I:6:GLN:HG3	3:I:106:THR:OG1	1.86	0.76
3:H:6:GLN:HG3	3:H:106:THR:OG1	1.86	0.76
2:M:34:HIS:CD2	3:I:98:ALA:HB2	2.22	0.73
1:B:433:ASN:N	1:B:433:ASN:OD1	2.23	0.71
3:I:147:GLU:HB2	3:I:148:PRO:HA	1.72	0.71

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	553/602 (92%)	526 (95%)	27 (5%)	0	100	100
1	B	574/602 (95%)	546 (95%)	28 (5%)	0	100	100
2	L	208/214 (97%)	192 (92%)	16 (8%)	0	100	100
2	M	211/214 (99%)	195 (92%)	16 (8%)	0	100	100
3	H	202/215 (94%)	185 (92%)	17 (8%)	0	100	100
3	I	206/215 (96%)	188 (91%)	18 (9%)	0	100	100
All	All	1954/2062 (95%)	1832 (94%)	122 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	530/569 (93%)	527 (99%)	3 (1%)	90	95
1	B	548/569 (96%)	545 (100%)	3 (0%)	92	96
2	L	182/184 (99%)	182 (100%)	0	100	100
2	M	183/184 (100%)	183 (100%)	0	100	100
3	H	182/187 (97%)	180 (99%)	2 (1%)	80	90
3	I	184/187 (98%)	182 (99%)	2 (1%)	80	90
All	All	1809/1880 (96%)	1799 (99%)	10 (1%)	90	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	46	ASP
1	B	433	ASN
1	B	558	PHE
3	H	11	LEU
1	B	439	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	HIS
2	L	34	HIS
1	B	371	HIS
1	B	436	HIS
2	M	34	HIS

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 [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	A	561/602 (93%)	-0.21	3 (0%) 91 88	78, 159, 211, 254	0
1	B	580/602 (96%)	-0.19	0 100 100	77, 160, 211, 254	0
2	L	212/214 (99%)	-0.30	0 100 100	78, 124, 180, 228	0
2	M	213/214 (99%)	-0.32	0 100 100	78, 123, 180, 227	0
3	H	206/215 (95%)	-0.35	0 100 100	70, 129, 172, 192	0
3	I	210/215 (97%)	-0.28	0 100 100	67, 130, 171, 192	0
All	All	1982/2062 (96%)	-0.25	3 (0%) 95 94	67, 144, 205, 254	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	ASN	2.6
1	A	521	LYS	2.2
1	A	122	GLU	2.0

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 [i](#)

There are no such residues in this entry.