



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2016 – 07:41 PM EDT

PDB ID : 5I66
Title : X-ray structure of the Fab fragment of 8B6, a murine monoclonal antibody specific for the human serotonin transporter
Authors : Coleman, J.A.; Green, E.M.; Gouaux, E.
Deposited on : 2016-02-16
Resolution : 1.62 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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-20027457

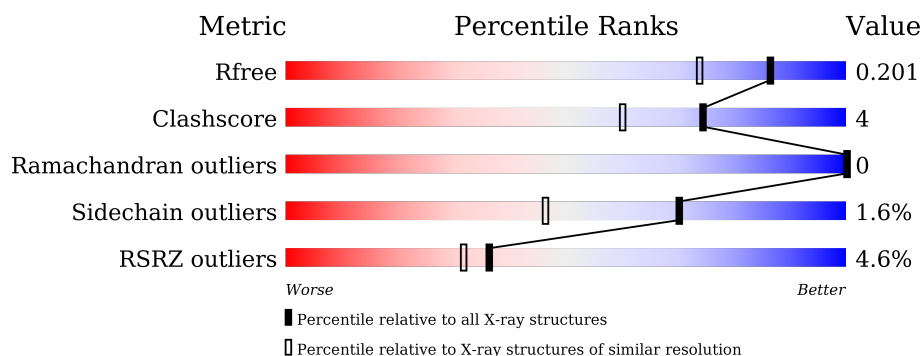
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	3202 (1.64-1.60)
Clashscore	102246	3500 (1.64-1.60)
Ramachandran outliers	100387	3411 (1.64-1.60)
Sidechain outliers	100360	3410 (1.64-1.60)
RSRZ outliers	91569	3207 (1.64-1.60)

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	221	<div> <div>7%</div> <div>88%</div> <div>10% ..</div> </div>
2	B	214	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6778 atoms, of which 3174 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 8B6 antibody, heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	H	N	O	S	0	0	0
			3240	1040	1593	266	333	8			

- Molecule 2 is a protein called 8B6 antibody, light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	213	Total	C	H	N	O	S	0	0	0
			3236	1033	1581	280	335	7			

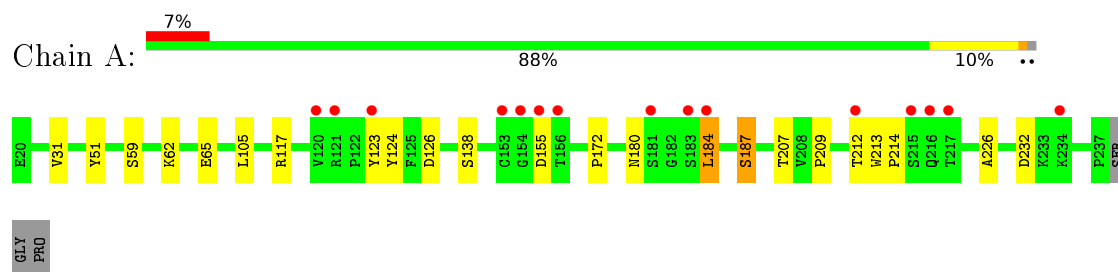
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	131	Total	O	0	0
			131	131		

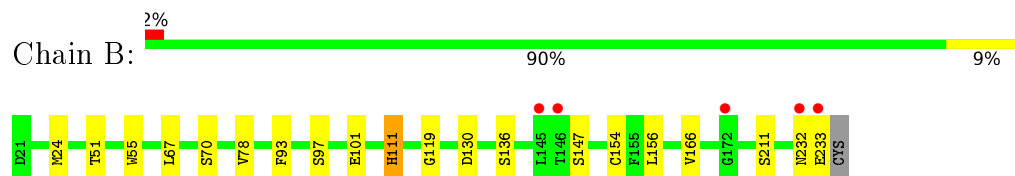
3 Residue-property plots [i](#)

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: 8B6 antibody, heavy chain



- Molecule 2: 8B6 antibody, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	81.56 Å 81.56 Å 142.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.67 – 1.62 57.67 – 1.63	Depositor EDS
% Data completeness (in resolution range)	97.0 (57.67-1.62) 97.5 (57.67-1.63)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.63 Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.178 , 0.198 0.179 , 0.201	Depositor DCC
R_{free} test set	5622 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6778	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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](#)

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	0.65	0/1692	0.71	0/2314
2	B	0.62	0/1693	0.69	0/2298
All	All	0.63	0/3385	0.70	0/4612

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 [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	1593	1594	15	0
2	B	1655	1581	1581	13	0
3	A	171	0	0	4	1
3	B	131	0	0	3	0
All	All	3604	3174	3175	26	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 4.

All (26) 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:232:ASP:OD2	3:A:301:HOH:O	1.99	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:OE1	3:A:303:HOH:O	2.02	0.78
1:A:155:ASP:OD1	3:A:302:HOH:O	2.01	0.77
2:B:232:ASN:OD1	2:B:233:GLU:N	2.18	0.76
2:B:130:ASP:OD1	3:B:301:HOH:O	2.09	0.69
1:A:31:VAL:HG21	1:A:105:LEU:HD13	1.76	0.68
1:A:65:GLU:OE2	3:A:304:HOH:O	2.11	0.67
1:A:209:PRO:O	1:A:212:THR:HG22	2.03	0.58
1:A:59:SER:HB2	1:A:62:LYS:HD3	1.88	0.56
2:B:55:TRP:CD2	2:B:93:PHE:HB2	2.43	0.54
1:A:123:TYR:HB3	2:B:111:HIS:CG	2.47	0.50
2:B:101:GLU:HB3	3:B:346:HOH:O	2.11	0.50
1:A:123:TYR:HB3	2:B:111:HIS:CD2	2.46	0.50
2:B:97:SER:OG	3:B:302:HOH:O	2.20	0.48
2:B:51:THR:O	2:B:70:SER:HA	2.14	0.47
1:A:180:ASN:HB2	1:A:184:LEU:HD22	1.98	0.45
1:A:124:TYR:CE1	1:A:126:ASP:HB3	2.52	0.44
2:B:55:TRP:CE2	2:B:93:PHE:HB2	2.53	0.42
2:B:156:LEU:HD21	2:B:166:VAL:HG22	2.02	0.42
2:B:24:MET:O	2:B:119:GLY:HA2	2.20	0.42
1:A:51:TYR:HB3	1:A:117:ARG:HG3	2.02	0.41
1:A:187:SER:HB3	1:A:207:THR:O	2.20	0.41
2:B:67:LEU:HA	2:B:78:VAL:HG21	2.03	0.41
1:A:172:PRO:HD2	1:A:226:ALA:CB	2.51	0.41
1:A:213:TRP:CG	1:A:214:PRO:HA	2.56	0.41
2:B:136:SER:O	2:B:154:CYS:HA	2.20	0.41

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)
3:A:409:HOH:O	3:A:409:HOH:O[7_556]	1.92	0.28

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	216/221 (98%)	212 (98%)	4 (2%)	0	100	100
2	B	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
All	All	427/435 (98%)	419 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	191/193 (99%)	188 (98%)	3 (2%)	70	46
2	B	188/190 (99%)	185 (98%)	3 (2%)	70	46
All	All	379/383 (99%)	373 (98%)	6 (2%)	70	46

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	184	LEU
1	A	187	SER
2	B	111	HIS
2	B	147	SER
2	B	211	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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

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	218/221 (98%)	0.29	15 (6%) 20 17	22, 34, 69, 82	0
2	B	213/214 (99%)	0.09	5 (2%) 64 62	23, 38, 66, 101	0
All	All	431/435 (99%)	0.19	20 (4%) 36 32	22, 36, 67, 101	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	LEU	5.1
1	A	216	GLN	4.2
2	B	232	ASN	4.2
1	A	153	CYS	4.2
1	A	212	THR	4.1
1	A	155	ASP	4.1
1	A	183	SER	4.0
1	A	154	GLY	3.2
1	A	217	THR	3.1
1	A	123	TYR	2.9
1	A	181	SER	2.7
1	A	215	SER	2.7
2	B	233	GLU	2.4
1	A	121	ARG	2.3
1	A	156	THR	2.3
2	B	146	THR	2.3
1	A	234	LYS	2.3
1	A	120	VAL	2.0
2	B	145	LEU	2.0
2	B	172	GLY	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.