wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 09:24 am GMT

PDB ID	:	4A6Y
Title	:	CRYSTAL STRUCTURE OF FAB FRAGMENT OF ANTI-(4-HYDROXY-3-NITROPHENYL) -ACETYL MURINE GERMLINE ANTIBODY BBE6.12H3
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Deposited on	:	2011-11-10
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

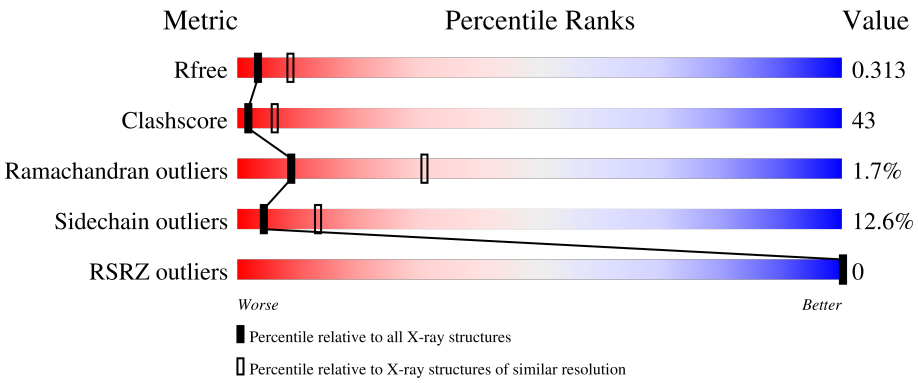
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	211	37% 55% 8%
2	B	220	43% 44% 10% •
3	H	220	35% 50% 9% • •
4	L	211	42% 49% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6593 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 ANTIBODY BBE6.12H3 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	1595	996	269	324	6	0	0	0

- Molecule 2 is a protein called ANTIBODY BBE6.12H3 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1632	1042	265	318	7	0	0	0

- Molecule 3 is a protein called ANTIBODY BBE6.12H3 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	215	1640	1047	266	320	7	0	0	0

- Molecule 4 is a protein called ANTIBODY BBE6.12H3 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	211	1596	999	268	323	6	0	0	0

- Molecule 5 is water.

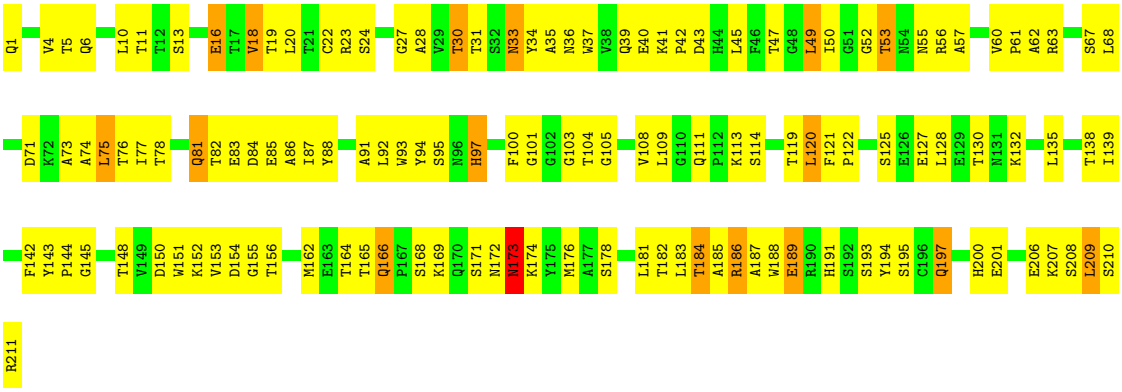
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	46	46	46	0	0
5	B	30	30	30	0	0
5	H	28	28	28	0	0
5	L	26	26	26	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

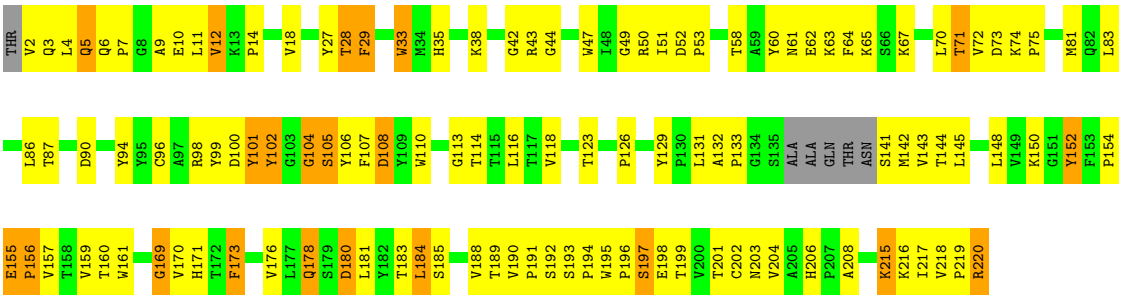
- Molecule 1: ANTIBODY BBE6.12H3 LIGHT CHAIN

Chain A: 37% 55% 8%



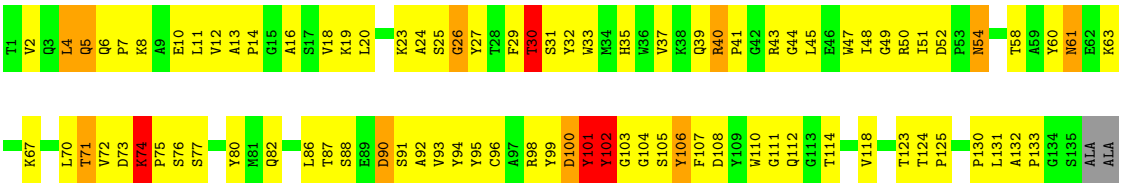
- Molecule 2: ANTIBODY BBE6.12H3 HEAVY CHAIN

Chain B: 43% 44% 10%



- Molecule 3: ANTIBODY BBE6.12H3 HEAVY CHAIN

Chain H: 35% 50% 9%



GLN THR ASN S141 T144 L145 G146 C147 L148 V149 Y152 F153 P154 E155 P156 V157 T158 V159 T160 W161 N162 S165 L166 G169 V170 H171 T172 F173 V176 L177 Q178 S179 D180 L181 Y182 T183 L184 S185 S186 S187 V188 T189 V190 P191 S192 S193 P194 W195 P196 S197 E198 T199 V200 T201

P207 A208 K215 K216 I217 V218 P219 R220

• Molecule 4: ANTIBODY BBE6.12H3 LIGHT CHAIN

Chain L: 42% 49% 9%

Q1 A2 V3 V4 E7 L10 T11 T12 S13 E16 T19 L20 K21 C22 A23 S24 G27 A28 Y34 A35 N36 W37 V38 Q39 E40 K41 P42 D43 H44 L45 F46 T47 G48 L49 I50 G51 N54 N55 R56 A57 V60 P61 A62 R63 L68 D71 K72 A73 A74 L75

T76 Q81 T82 E83 D84 E85 A86 T87 Y88 F89 L92 W93 Y94 S95 N96 H97 W98 V99 T104 T107 V108 L109 S114 V118 T119 L120 F121 P122 P123 E127 L128 E129 T130 N131 K132 A133 T134 L135 T138 I139 T140 D141 F142 Y143 P144 G145 V146 V147 T148 V149 K152

V153 D154 G155 T156 T165 Q166 K169 Q170 S171 N172 N173 K174 Y175 M176 A177 S178 S179 Y180 L181 T182 L183 T184 A185 R186 E189 R190 H191 S192 S195 C196 Q197 V198 T199 H200 E201 G202 H203 T204 V205 E206 K207 S208 L209 S210 R211

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.28Å 81.42Å 128.91Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	23.02 – 2.90 23.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.5 (23.02-2.90) 83.4 (23.02-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.49 (at 2.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.240 , 0.260 0.257 , 0.313	Depositor DCC
R_{free} test set	1841 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.86	9/1633 (0.6%)	0.85	3/2232 (0.1%)
2	B	0.53	2/1681 (0.1%)	0.90	5/2297 (0.2%)
3	H	1.00	11/1689 (0.7%)	1.07	16/2309 (0.7%)
4	L	0.65	5/1634 (0.3%)	1.00	9/2232 (0.4%)
All	All	0.78	27/6637 (0.4%)	0.96	33/9070 (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	B	0	1
3	H	0	2
All	All	0	3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLU	CD-OE1	-18.18	1.05	1.25
3	H	153	PHE	CE1-CZ	-15.52	1.07	1.37
3	H	153	PHE	CE2-CZ	-15.48	1.07	1.37
3	H	153	PHE	CG-CD2	-12.90	1.19	1.38
3	H	153	PHE	CG-CD1	-11.39	1.21	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	198	GLU	N-CA-CB	16.94	141.09	110.60
2	B	101	TYR	CB-CA-C	16.59	143.59	110.40
4	L	83	GLU	CB-CA-C	-11.73	86.95	110.40
3	H	198	GLU	N-CA-C	-11.71	79.37	111.00
4	L	1	GLN	O-C-N	10.93	140.18	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	152	TYR	Sidechain
3	H	102	TYR	Sidechain
3	H	74	LYS	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	1595	0	1535	137	0
2	B	1632	0	1586	145	0
3	H	1640	0	1598	176	0
4	L	1596	0	1543	131	0
5	A	46	0	0	4	0
5	B	30	0	0	0	0
5	H	28	0	0	3	0
5	L	26	0	0	0	0
All	All	6593	0	6262	546	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 43.

The worst 5 of 546 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:H:132:ALA:HB2	3:H:217:ILE:CG2	1.67	1.25
3:H:52:ASP:OD1	3:H:54:ASN:HB2	1.34	1.24
3:H:74:LYS:HD2	3:H:74:LYS:O	1.37	1.21
2:B:18:VAL:HG22	2:B:86:LEU:HD11	1.31	1.07
2:B:176:VAL:HG23	2:B:178:GLN:HE22	1.19	1.06

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	209/211 (99%)	190 (91%)	16 (8%)	3 (1%)	11 36
2	B	210/220 (96%)	187 (89%)	21 (10%)	2 (1%)	15 45
3	H	211/220 (96%)	182 (86%)	22 (10%)	7 (3%)	4 15
4	L	209/211 (99%)	186 (89%)	21 (10%)	2 (1%)	15 45
All	All	839/862 (97%)	745 (89%)	80 (10%)	14 (2%)	9 31

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	156	PRO
3	H	101	TYR
3	H	103	GLY
3	H	198	GLU
1	A	155	GLY

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	178/178 (100%)	160 (90%)	18 (10%)	7 23
2	B	184/188 (98%)	157 (85%)	27 (15%)	3 9
3	H	185/188 (98%)	164 (89%)	21 (11%)	5 17
4	L	178/178 (100%)	153 (86%)	25 (14%)	3 10
All	All	725/732 (99%)	634 (87%)	91 (13%)	4 13

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	106	TYR
4	L	47	THR
3	H	180	ASP
3	H	215	LYS
4	L	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	112	GLN
4	L	97	HIS
4	L	197	GLN
4	L	160	GLN
4	L	81	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 monosaccharides 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	211/211 (100%)	-0.87	0	100	100	10, 26, 41, 52	1 (0%)
2	B	214/220 (97%)	-0.73	0	100	100	14, 32, 59, 71	0
3	H	215/220 (97%)	-0.76	0	100	100	14, 32, 58, 68	0
4	L	211/211 (100%)	-0.88	0	100	100	9, 26, 42, 52	2 (0%)
All	All	851/862 (98%)	-0.81	0	100	100	9, 29, 55, 71	3 (0%)

There are no RSRZ outliers to report.

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 monosaccharides 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.