



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:29 PM BST

PDB ID : 6L8T
Title : Crystal structure of the Fab fragment of a humanized HBV therapeutic anti-body
Authors : He, M.Z.; Gu, Y.; Li, S.W.
Deposited on : 2019-11-07
Resolution : 1.77 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.14.2
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)	:	2.14.2

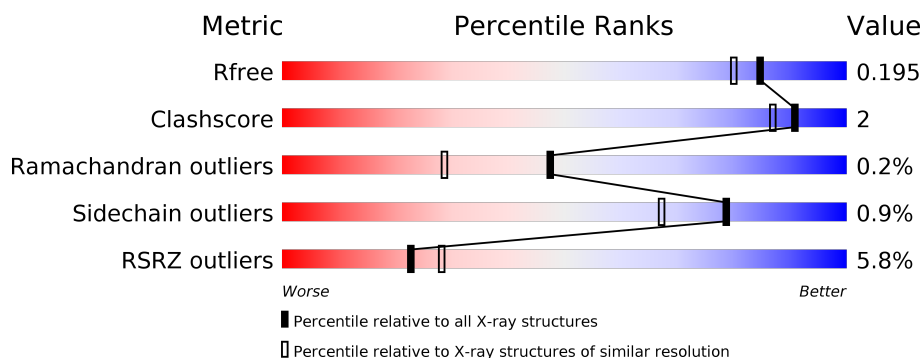
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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 $\leq 5\%$. 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	B	219	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	D	219	<div> <div>17%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	L	219	<div> <div>4%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>
2	A	220	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>
2	C	220	<div> <div>7%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
2	H	220	<div> <div>2%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21440 atoms, of which 9817 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 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	219	Total	C	H	N	O	S	0	0	0
			3342	1064	1649	284	339	6			
1	B	219	Total	C	H	N	O	S	0	0	0
			3343	1064	1650	284	339	6			
1	D	219	Total	C	H	N	O	S	0	0	0
			3342	1064	1649	284	339	6			

- Molecule 2 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	220	Total	C	H	N	O	S	0	0	0
			3289	1054	1623	275	332	5			
2	A	220	Total	C	H	N	O	S	0	0	0
			3289	1054	1623	275	332	5			
2	C	220	Total	C	H	N	O	S	0	0	0
			3288	1054	1623	275	331	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	197	Total	O	0	0
			197	197		
3	H	249	Total	O	0	0
			249	249		
3	B	343	Total	O	0	0
			343	343		
3	A	343	Total	O	0	0
			343	343		
3	D	157	Total	O	0	0
			157	157		
3	C	258	Total	O	0	0
			258	258		

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.

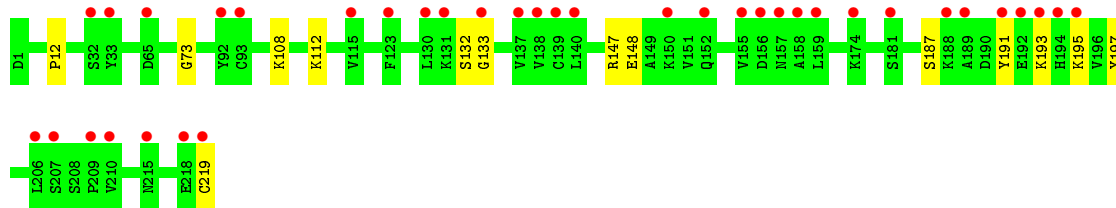
- Molecule 1: Antibody light chain



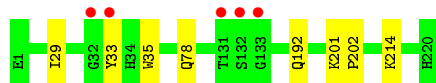
- Molecule 1: Antibody light chain



- Molecule 1: Antibody light chain

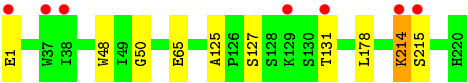


- Molecule 2: Antibody heavy chain

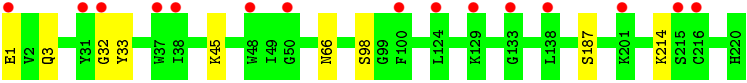


- Molecule 2: Antibody heavy chain





● Molecule 2: Antibody heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.94Å 75.94Å 137.55Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	26.54 – 1.77 26.54 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.3 (26.54-1.77) 99.3 (26.54-1.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.165 , 0.192 0.169 , 0.195	Depositor DCC
R_{free} test set	7493 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21440	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.333 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	B	0.33	0/1732	0.52	0/2352
1	D	0.26	0/1732	0.46	0/2352
1	L	0.27	0/1732	0.47	0/2352
2	A	0.34	0/1710	0.57	0/2333
2	C	0.29	0/1709	0.50	0/2333
2	H	0.29	0/1710	0.49	0/2333
All	All	0.30	0/10325	0.50	0/14055

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	B	1693	1650	1649	6	0
1	D	1693	1649	1649	6	0
1	L	1693	1649	1649	4	0
2	A	1666	1623	1623	6	0
2	C	1665	1623	1623	7	0
2	H	1666	1623	1623	6	0
3	A	343	0	0	2	3
3	B	343	0	0	2	1
3	C	258	0	0	5	2
3	D	157	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	249	0	0	3	1
3	L	197	0	0	3	1
All	All	11623	9817	9816	34	5

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 2.

All (34) 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:A:65:GLU:OE2	3:A:301:HOH:O	1.89	0.90
2:H:214:LYS:O	3:H:301:HOH:O	1.93	0.86
2:C:32:GLY:O	3:C:301:HOH:O	1.98	0.82
2:A:1:GLU:OE2	3:A:302:HOH:O	1.99	0.81
2:C:45:LYS:NZ	3:C:302:HOH:O	2.15	0.78
2:C:214:LYS:NZ	3:C:303:HOH:O	2.18	0.75
2:C:66:ASN:ND2	3:C:304:HOH:O	2.22	0.73
1:L:218:GLU:O	3:L:301:HOH:O	2.08	0.71
2:H:78:GLN:NE2	3:H:304:HOH:O	2.25	0.69
2:H:192:GLN:OE1	3:H:302:HOH:O	2.15	0.63
2:C:1:GLU:O	2:C:3:GLN:NE2	2.31	0.62
1:L:108:LYS:NZ	3:L:303:HOH:O	2.28	0.57
1:L:194:HIS:ND1	3:L:304:HOH:O	2.33	0.56
1:B:7:SER:OG	1:B:22:SER:OG	2.24	0.54
1:L:218:GLU:HA	1:L:219:CYS:CB	2.38	0.53
1:D:132:SER:OG	1:D:133:GLY:N	2.44	0.50
1:D:147:ARG:NE	3:D:301:HOH:O	2.24	0.50
1:D:108:LYS:NZ	3:D:312:HOH:O	2.45	0.49
1:B:124:PRO:HG2	2:A:214:LYS:HE2	1.98	0.46
1:D:191:TYR:O	1:D:197:TYR:OH	2.32	0.46
2:H:29:ILE:HA	2:H:35:TRP:CZ2	2.51	0.46
1:D:148:GLU:N	1:D:148:GLU:OE1	2.47	0.44
2:C:33:TYR:CD2	2:C:98:SER:HB2	2.52	0.44
1:B:191:TYR:CZ	1:B:216:ARG:HG3	2.53	0.44
2:C:66:ASN:ND2	3:C:316:HOH:O	2.51	0.43
2:H:201:LYS:N	2:H:202:PRO:CD	2.82	0.43
2:H:33:TYR:HB2	2:H:35:TRP:CE2	2.53	0.43
1:B:152:GLN:NE2	3:B:306:HOH:O	2.46	0.42
1:B:157:ASN:ND2	3:B:312:HOH:O	2.51	0.42
2:A:48:TRP:CZ2	2:A:50:GLY:HA2	2.54	0.42
2:A:127:SER:O	2:A:131:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:125:ALA:HB3	2:A:214:LYS:HE3	2.02	0.41
1:D:12:PRO:HB2	1:D:112:LYS:HE2	2.03	0.40
1:B:195:LYS:HE3	1:B:196:VAL:HG23	2.04	0.40

All (5) 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:598:HOH:O	3:A:604:HOH:O[2_444]	2.05	0.15
3:L:459:HOH:O	3:C:465:HOH:O[1_455]	2.11	0.09
3:A:404:HOH:O	3:A:598:HOH:O[2_454]	2.13	0.07
3:H:511:HOH:O	3:C:480:HOH:O[2_545]	2.14	0.06
3:B:620:HOH:O	3:A:592:HOH:O[2_544]	2.14	0.06

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	B	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
1	D	217/219 (99%)	211 (97%)	5 (2%)	1 (0%)	29	12
1	L	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
2	A	218/220 (99%)	211 (97%)	6 (3%)	1 (0%)	29	12
2	C	218/220 (99%)	214 (98%)	4 (2%)	0	100	100
2	H	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
All	All	1305/1317 (99%)	1276 (98%)	27 (2%)	2 (0%)	47	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	215	SER

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Mol	Chain	Res	Type
1	D	73	GLY

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	B	196/196 (100%)	195 (100%)	1 (0%)	88	83
1	D	196/196 (100%)	192 (98%)	4 (2%)	55	34
1	L	196/196 (100%)	193 (98%)	3 (2%)	65	49
2	A	192/192 (100%)	190 (99%)	2 (1%)	76	63
2	C	192/192 (100%)	191 (100%)	1 (0%)	88	83
2	H	192/192 (100%)	192 (100%)	0	100	100
All	All	1164/1164 (100%)	1153 (99%)	11 (1%)	78	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	SER
1	L	22	SER
1	L	219	CYS
1	B	110	GLU
2	A	178	LEU
2	A	214	LYS
1	D	187	SER
1	D	193	LYS
1	D	195	LYS
1	D	219	CYS
2	C	187	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	192	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 ⓘ

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	B	219/219 (100%)	-0.19	4 (1%) 68 76	15, 26, 49, 94	0
1	D	219/219 (100%)	0.78	37 (16%) 1 2	25, 46, 90, 109	0
1	L	219/219 (100%)	0.04	9 (4%) 37 44	22, 42, 60, 80	0
2	A	220/220 (100%)	-0.05	7 (3%) 47 54	14, 23, 53, 73	0
2	C	220/220 (100%)	0.16	15 (6%) 17 22	21, 34, 62, 87	0
2	H	220/220 (100%)	-0.11	5 (2%) 60 67	18, 33, 60, 75	0
All	All	1317/1317 (100%)	0.10	77 (5%) 23 28	14, 34, 69, 109	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	219	CYS	8.7
1	D	33	TYR	8.5
1	B	219	CYS	8.0
1	D	189	ALA	5.8
1	D	159	LEU	5.6
1	D	206	LEU	5.5
1	D	157	ASN	5.3
1	B	33	TYR	5.0
2	H	132	SER	4.7
1	D	131	LYS	4.7
2	C	32	GLY	4.6
1	D	219	CYS	4.5
2	H	133	GLY	4.5
1	D	130	LEU	4.5
1	D	138	VAL	4.4
1	D	210	VAL	4.4
2	C	1	GLU	4.4
1	D	209	PRO	4.0
1	D	139	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	L	33	TYR	3.9
2	H	33	TYR	3.9
2	A	215	SER	3.7
2	H	131	THR	3.7
1	D	32	SER	3.6
1	D	195	LYS	3.5
1	D	193	LYS	3.5
1	D	207	SER	3.4
1	D	133	GLY	3.4
1	D	191	TYR	3.4
1	D	158	ALA	3.3
1	D	65	ASP	3.2
1	D	192	GLU	3.1
1	L	131	LYS	3.1
1	L	218	GLU	3.1
2	C	133	GLY	3.1
2	C	216	CYS	3.0
1	D	174	LYS	2.9
2	C	37	TRP	2.9
1	L	82	ARG	2.9
1	D	188	LYS	2.8
1	D	194	HIS	2.8
1	L	9	LEU	2.7
2	A	1	GLU	2.7
1	D	140	LEU	2.6
2	C	201	LYS	2.6
1	D	123	PHE	2.5
2	C	100	PHE	2.5
1	D	155	VAL	2.5
1	D	156	ASP	2.5
2	C	38	ILE	2.5
2	A	38	ILE	2.5
2	A	37	TRP	2.5
1	L	24	ARG	2.4
2	C	129	LYS	2.4
1	D	93	CYS	2.4
1	D	218	GLU	2.4
2	C	215	SER	2.4
1	D	150	LYS	2.4
1	B	218	GLU	2.3
1	D	115	VAL	2.3
1	D	181	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	92	TYR	2.2
2	C	50	GLY	2.2
1	D	152	GLN	2.2
1	D	215	ASN	2.1
1	L	65	ASP	2.1
2	C	31	TYR	2.1
1	D	137	VAL	2.1
2	C	138	LEU	2.1
2	A	129	LYS	2.1
1	B	159	LEU	2.1
2	A	131	THR	2.1
1	L	123	PHE	2.1
2	H	32	GLY	2.1
2	A	214	LYS	2.0
2	C	48	TRP	2.0
2	C	124	LEU	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 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.