



Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2022 – 02:54 PM EDT

PDB ID : 7SO5
Title : Novel structural insights for a pair of monoclonal antibodies recognizing non-overlapping epitopes of the glucosyltransferase domain of Clostridium difficile toxin B
Authors : Liu, J.
Deposited on : 2021-10-29
Resolution : 1.80 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	:	2.28.1
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)	:	2.28.1

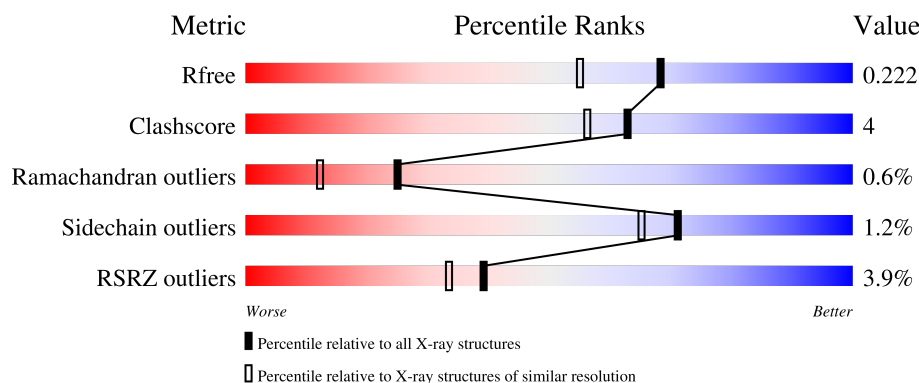
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 $\leq 5\%$. 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	H	215	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	L	216	<div> <div>%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
3	A	541	<div> <div>5%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8436 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 Fab B2 HC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	0	0	0
			1610	1023	275	307	5			

- Molecule 2 is a protein called Fab B2 LC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	216	Total	C	N	O	S	0	0	0
			1655	1039	281	329	6			

- Molecule 3 is a protein called Toxin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	539	Total	C	N	O	S	0	0	0
			4419	2805	716	882	16			

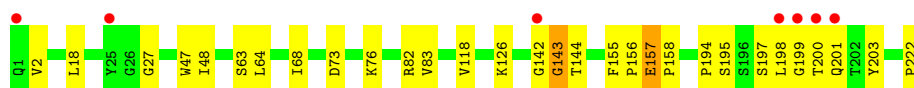
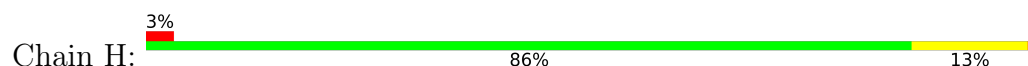
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	187	Total	O	0	0
			187	187		
4	L	175	Total	O	0	0
			175	175		
4	A	390	Total	O	0	0
			390	390		

3 Residue-property plots

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.

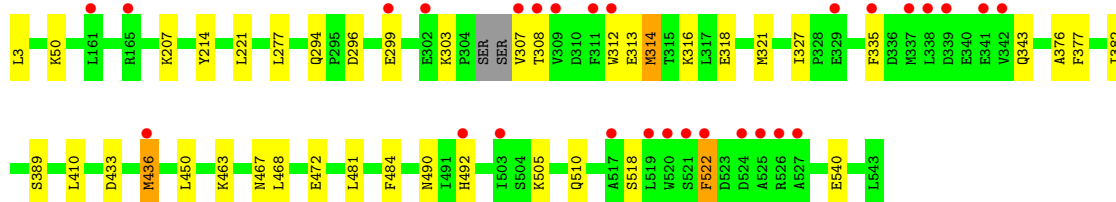
• Molecule 1: Fab B2 HC



• Molecule 2: Fab B2 LC



• Molecule 3: Toxin B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.17Å 110.72Å 83.06Å 90.00° 99.33° 90.00°	Depositor
Resolution (Å)	52.87 – 1.80 52.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (52.87-1.80) 93.8 (52.87-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.185 , 0.223 0.185 , 0.222	Depositor DCC
R_{free} test set	4684 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8436	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

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	H	0.41	0/1651	0.62	0/2252
2	L	0.40	0/1692	0.61	2/2301 (0.1%)
3	A	0.38	0/4499	0.52	0/6070
All	All	0.39	0/7842	0.56	2/10623 (0.0%)

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
1	H	0	3
2	L	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	145	TYR	C-N-CD	-6.98	105.25	120.60
2	L	38	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	155	PHE	Mainchain,Peptide
1	H	157	GLU	Peptide
2	L	145	TYR	Peptide

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	H	1610	0	1585	20	0
2	L	1655	0	1628	16	0
3	A	4419	0	4299	31	0
4	A	390	0	0	9	0
4	H	187	0	0	6	1
4	L	175	0	0	2	1
All	All	8436	0	7512	65	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 (65) 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:A:463:LYS:HE3	3:A:467:ASN:HD21	1.31	0.95
3:A:313:GLU:OE2	4:A:601:HOH:O	1.91	0.88
3:A:321:MET:CE	3:A:327:ILE:H	1.98	0.77
1:H:2:VAL:HG22	1:H:27:GLY:HA3	1.67	0.75
3:A:303:LYS:NZ	4:A:606:HOH:O	2.19	0.74
2:L:150:LYS:NZ	4:L:301:HOH:O	2.21	0.73
1:H:82:ARG:NH2	4:H:301:HOH:O	2.21	0.71
1:H:126:LYS:NZ	4:H:303:HOH:O	2.28	0.66
3:A:540:GLU:OE2	4:A:603:HOH:O	2.14	0.64
1:H:143:GLY:N	4:H:304:HOH:O	2.29	0.62
3:A:296:ASP:HA	3:A:299:GLU:HG3	1.80	0.62
3:A:313:GLU:OE1	4:A:604:HOH:O	2.16	0.61
3:A:207:LYS:HG2	3:A:221:LEU:HD23	1.81	0.60
3:A:307:VAL:HG12	3:A:308:THR:H	1.66	0.59
1:H:64:LEU:O	1:H:68:ILE:HG12	2.02	0.59
3:A:376:ALA:HA	4:A:609:HOH:O	2.04	0.57
1:H:48:ILE:HD12	1:H:64:LEU:HD13	1.85	0.57
3:A:321:MET:HE1	3:A:327:ILE:N	2.22	0.55
3:A:214:TYR:OH	4:A:602:HOH:O	1.99	0.55
2:L:38:LEU:HG	2:L:39:VAL:N	2.22	0.54
2:L:154:LYS:NZ	2:L:200:GLU:OE1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:321:MET:HE1	3:A:327:ILE:H	1.71	0.54
1:H:47:TRP:CD2	2:L:101:PRO:HD2	2.44	0.53
1:H:48:ILE:HD12	1:H:64:LEU:CD1	2.39	0.52
3:A:410:LEU:HD13	3:A:450:LEU:HD22	1.91	0.52
1:H:82:ARG:NH1	4:H:301:HOH:O	2.44	0.51
3:A:335:PHE:CZ	3:A:343:GLN:HG3	2.46	0.51
1:H:222:PRO:HD3	4:H:419:HOH:O	2.11	0.50
3:A:294:GLN:OE1	4:A:605:HOH:O	2.19	0.49
1:H:82:ARG:CZ	4:H:301:HOH:O	2.60	0.49
2:L:196:VAL:HG22	2:L:215:ASN:ND2	2.27	0.49
2:L:150:LYS:HB3	2:L:202:THR:OG1	2.13	0.48
1:H:18:LEU:HD13	1:H:118:VAL:HG11	1.96	0.48
3:A:450:LEU:HD21	3:A:468:LEU:HD13	1.95	0.48
1:H:68:ILE:HD12	1:H:83:VAL:HG22	1.96	0.48
1:H:198:LEU:O	1:H:200:THR:N	2.43	0.47
3:A:277:LEU:HG	3:A:389:SER:HB3	1.96	0.47
1:H:73:ASP:OD2	1:H:76:LYS:HD3	2.14	0.47
2:L:16:GLY:HA2	2:L:82:ARG:HG3	1.97	0.46
3:A:312:TRP:O	3:A:316:LYS:HG3	2.16	0.45
2:L:24:ARG:HG2	2:L:75:ASP:OD2	2.17	0.45
3:A:490:ASN:OD1	3:A:492:HIS:CD2	2.70	0.45
3:A:463:LYS:O	3:A:463:LYS:HG2	2.17	0.45
3:A:467:ASN:HA	3:A:472:GLU:HB2	1.99	0.44
1:H:142:GLY:O	1:H:144:THR:N	2.44	0.44
2:L:150:LYS:HD3	4:L:302:HOH:O	2.17	0.44
3:A:377:PHE:CZ	3:A:382:ILE:HG22	2.53	0.43
2:L:126:SER:OG	2:L:128:GLU:HG2	2.17	0.43
3:A:307:VAL:HG12	3:A:308:THR:N	2.30	0.43
3:A:505:LYS:HE3	3:A:510:GLN:OE1	2.18	0.43
3:A:50:LYS:HG3	3:A:484:PHE:HB3	2.00	0.43
3:A:314:MET:HE2	3:A:314:MET:HB2	1.81	0.43
3:A:3:LEU:N	4:A:641:HOH:O	2.52	0.43
3:A:318:GLU:O	4:A:607:HOH:O	2.21	0.43
1:H:201:GLN:HG2	1:H:203:TYR:CZ	2.55	0.42
2:L:202:THR:HG22	2:L:209:PRO:HG3	2.01	0.42
2:L:145:TYR:CD2	2:L:146:PRO:CD	3.03	0.42
2:L:211:THR:O	2:L:212:LYS:HE2	2.20	0.41
1:H:18:LEU:O	1:H:82:ARG:HA	2.20	0.41
1:H:47:TRP:CG	2:L:101:PRO:HD2	2.55	0.41
1:H:194:PRO:HG2	1:H:197:SER:HB3	2.02	0.41
2:L:100:PRO:HA	2:L:101:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:433:ASP:HA	3:A:436:MET:HG3	2.02	0.41
2:L:42:LEU:HD13	2:L:91:TYR:CZ	2.56	0.40
3:A:492:HIS:CD2	3:A:492:HIS:N	2.89	0.40

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)
4:H:302:HOH:O	4:L:450:HOH:O[2_656]	2.15	0.05

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	H	211/215 (98%)	202 (96%)	5 (2%)	4 (2%)	8	1
2	L	214/216 (99%)	210 (98%)	3 (1%)	1 (0%)	29	15
3	A	535/541 (99%)	520 (97%)	14 (3%)	1 (0%)	47	33
All	All	960/972 (99%)	932 (97%)	22 (2%)	6 (1%)	25	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	156	PRO
1	H	158	PRO
2	L	146	PRO
1	H	143	GLY
3	A	522	PHE
1	H	199	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	H	178/178 (100%)	175 (98%)	3 (2%)	60	51
2	L	191/191 (100%)	189 (99%)	2 (1%)	76	71
3	A	493/495 (100%)	488 (99%)	5 (1%)	76	71
All	All	862/864 (100%)	852 (99%)	10 (1%)	71	65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	63	SER
1	H	157	GLU
1	H	195	SER
2	L	61	SER
2	L	108	LYS
3	A	314	MET
3	A	436	MET
3	A	481	LEU
3	A	518	SER
3	A	522	PHE

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

Mol	Chain	Res	Type
1	H	114	GLN
2	L	47	GLN
2	L	215	ASN
3	A	467	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	135:PRO	C	142:GLY	N	10.73

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	H	215/215 (100%)	0.12	7 (3%) 46 40	16, 27, 51, 65	0
2	L	216/216 (100%)	-0.02	3 (1%) 75 72	17, 27, 39, 46	0
3	A	539/541 (99%)	0.30	28 (5%) 27 22	16, 29, 54, 95	0
All	All	970/972 (99%)	0.19	38 (3%) 39 33	16, 28, 50, 95	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	520	TRP	12.9
1	H	199	GLY	6.9
1	H	142	GLY	5.3
3	A	307	VAL	4.8
3	A	519	LEU	3.7
3	A	338	LEU	3.6
3	A	335	PHE	3.5
3	A	337	MET	3.4
3	A	342	VAL	3.3
3	A	521	SER	3.3
3	A	339	ASP	3.2
3	A	341	GLU	3.1
3	A	165	ARG	3.0
1	H	200	THR	2.9
3	A	309	VAL	2.8
3	A	302	GLU	2.8
3	A	311	PHE	2.8
1	H	1	GLN	2.7
3	A	525	ALA	2.7
3	A	299	GLU	2.6
3	A	524	ASP	2.6
3	A	312	TRP	2.6
3	A	161	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	25	TYR	2.4
3	A	308	THR	2.4
3	A	492	HIS	2.3
3	A	436	MET	2.3
3	A	527	ALA	2.2
3	A	517	ALA	2.2
2	L	195	LYS	2.1
1	H	201	GLN	2.1
3	A	522	PHE	2.1
3	A	503	ILE	2.1
3	A	329	GLU	2.1
2	L	157	ASN	2.1
1	H	198	LEU	2.0
3	A	526	ARG	2.0
2	L	146	PRO	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.