



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:51 PM GMT

PDB ID : 1MFD
Title : THE SOLUTION STRUCTURE OF A TRISACCHARIDE-ANTIBODY COMPLEX: COMPARISON OF NMR MEASUREMENTS WITH A CRYSTAL STRUCTURE
Authors : Zdanov, A.; Cygler, M.
Deposited on : 1993-10-25
Resolution : 2.10 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

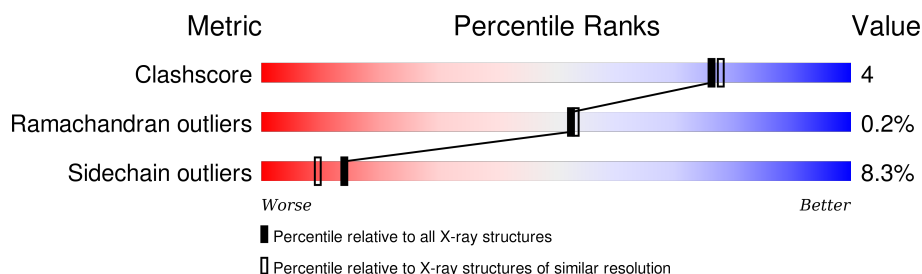
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	 84% 13% ..
2	H	219	 77% 17% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3293 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 IGG1-LAMBDA SE155-4 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1580	985	268	320	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	28	THR	ALA	CONFLICT	GB 387376
L	31	SER	THR	CONFLICT	GB 387376
L	32	GLY	SER	CONFLICT	GB 387376
L	34	HIS	TYR	CONFLICT	GB 387376
L	52	ASP	GLY	CONFLICT	GB 387376
L	82	PRO	THR	CONFLICT	GB 387376
L	94	CYS	TYR	CONFLICT	GB 387376
L	95	ASN	SER	CONFLICT	GB 387376
L	99	ILE	VAL	CONFLICT	GB 387376

- Molecule 2 is a protein called IGG1-LAMBDA SE155-4 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	1
			1595	1018	266	303	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ALA	DELETION	GB 208365
H	468	ARG	ASP	CONFLICT	GB 208365

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	3	Total	C	O	0	0
			33	19	14		

- Molecule 4 is water.

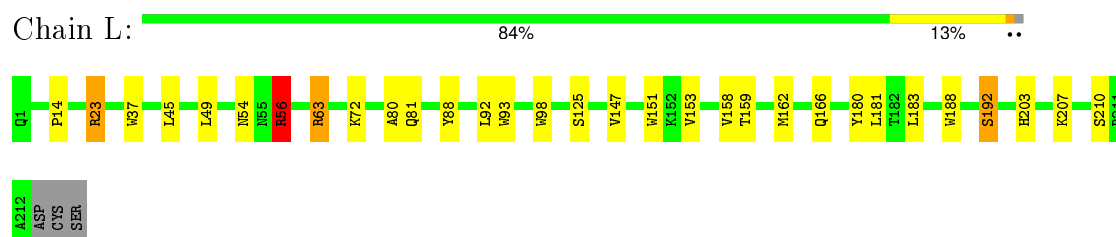
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	34	Total	O	0	0
			34	34		
4	L	51	Total	O	0	0
			51	51		

3 Residue-property plots [i](#)

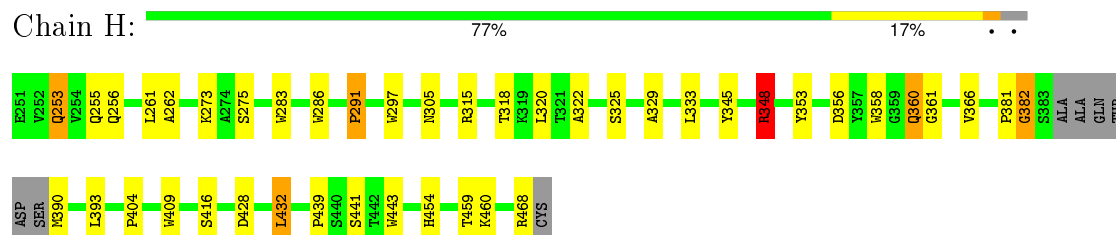
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: IGG1-LAMBDA SE155-4 FAB (LIGHT CHAIN)



- Molecule 2: IGG1-LAMBDA SE155-4 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.30Å 129.30Å 79.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3293	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, MMA, ABE

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	L	0.79	0/1618	1.47	19/2211 (0.9%)
2	H	0.80	0/1642	1.53	25/2246 (1.1%)
All	All	0.80	0/3260	1.50	44/4457 (1.0%)

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
2	H	1	0

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56	ARG	NE-CZ-NH1	11.03	125.81	120.30
2	H	297	TRP	CD1-CG-CD2	9.47	113.88	106.30
2	H	291	PRO	CB-CA-C	8.89	134.22	112.00
2	H	348	ARG	NE-CZ-NH1	8.72	124.66	120.30
2	H	348	ARG	NE-CZ-NH2	-8.53	116.03	120.30
2	H	286	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	L	93	TRP	CG-CD2-CE3	8.40	141.46	133.90
1	L	93	TRP	CE2-CD2-CG	-8.29	100.67	107.30
1	L	188	TRP	CD1-CG-CD2	8.26	112.91	106.30
2	H	358	TRP	CD1-CG-CD2	8.25	112.90	106.30
2	H	443	TRP	CD1-CG-CD2	8.19	112.86	106.30
2	H	358	TRP	CE2-CD2-CG	-8.06	100.85	107.30
1	L	93	TRP	CD1-CG-CD2	7.95	112.66	106.30
2	H	409	TRP	CD1-CG-CD2	7.71	112.46	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	151	TRP	CD1-CG-CD2	7.67	112.44	106.30
2	H	283	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	L	188	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	L	88	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	L	98	TRP	CD1-CG-CD2	7.37	112.20	106.30
1	L	93	TRP	CB-CG-CD1	-7.37	117.42	127.00
2	H	297	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	H	286	TRP	CE2-CD2-CG	-7.29	101.47	107.30
2	H	315	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	H	283	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	L	151	TRP	CE2-CD2-CG	-7.12	101.60	107.30
2	H	409	TRP	CE2-CD2-CG	-6.87	101.80	107.30
2	H	443	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	L	98	TRP	CE2-CD2-CG	-6.51	102.09	107.30
2	H	353	TYR	CB-CG-CD2	-6.49	117.10	121.00
1	L	37	TRP	CD1-CG-CD2	6.28	111.32	106.30
2	H	286	TRP	CG-CD1-NE1	-6.10	104.00	110.10
2	H	382	GLY	N-CA-C	-6.04	97.99	113.10
2	H	358	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	L	37	TRP	CE2-CD2-CG	-5.91	102.57	107.30
2	H	297	TRP	CG-CD1-NE1	-5.75	104.35	110.10
2	H	432	LEU	CA-CB-CG	5.74	128.50	115.30
1	L	23	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	L	180	TYR	CB-CG-CD1	-5.52	117.69	121.00
2	H	291	PRO	CA-N-CD	-5.47	103.85	111.50
1	L	63	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	H	381	PRO	CA-C-N	-5.26	105.67	116.20
1	L	56	ARG	CD-NE-CZ	5.20	130.88	123.60
2	H	443	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	L	56	ARG	CG-CD-NE	5.08	122.47	111.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	291	PRO	CA

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	L	1580	0	1511	9	0
2	H	1595	0	1547	15	0
3	H	33	0	32	0	0
4	H	34	0	0	0	0
4	L	51	0	0	0	0
All	All	3293	0	3090	24	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 4.

All (24) 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:L:23:ARG:HH11	1:L:72:LYS:HD3	1.52	0.74
2:H:256:GLN:HE22	2:H:345:TYR:HA	1.60	0.67
2:H:360:GLN:NE2	2:H:360:GLN:H	1.98	0.61
2:H:255:GLN:OE1	2:H:275:SER:HB2	2.04	0.58
2:H:360:GLN:H	2:H:360:GLN:HE21	1.52	0.58
2:H:382:GLY:HA2	2:H:468:ARG:HB2	1.86	0.57
1:L:56:ARG:HG3	1:L:56:ARG:HH11	1.69	0.57
1:L:192:SER:O	1:L:210:SER:HA	2.07	0.55
2:H:318:THR:HG22	2:H:333:LEU:HD23	1.89	0.54
2:H:256:GLN:NE2	2:H:361:GLY:H	2.05	0.53
1:L:158:VAL:HG11	1:L:181:LEU:HD11	1.93	0.50
2:H:390:MET:HG2	2:H:439:PRO:HA	1.95	0.48
1:L:63:ARG:CZ	1:L:81:GLN:HG3	2.43	0.47
1:L:14:PRO:HA	1:L:80:ALA:O	2.15	0.47
2:H:253:GLN:CG	2:H:275:SER:HB3	2.45	0.46
2:H:318:THR:HG22	2:H:333:LEU:CD2	2.45	0.46
1:L:23:ARG:HB3	1:L:72:LYS:HG2	1.99	0.45
2:H:360:GLN:HE21	2:H:360:GLN:N	2.15	0.44
1:L:23:ARG:NH1	1:L:72:LYS:HD3	2.25	0.44
1:L:153:VAL:HG23	1:L:158:VAL:HG21	2.01	0.43
2:H:348:ARG:HD2	2:H:356:ASP:OD1	2.19	0.43
2:H:454:HIS:HB3	2:H:459:THR:HB	2.01	0.43
2:H:322:ALA:HA	2:H:329:ALA:HA	2.01	0.42
2:H:262:ALA:O	2:H:366:VAL:HA	2.20	0.41

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	L	210/215 (98%)	204 (97%)	6 (3%)	0	100	100
2	H	208/219 (95%)	195 (94%)	12 (6%)	1 (0%)	34	30
All	All	418/434 (96%)	399 (96%)	18 (4%)	1 (0%)	52	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	291	PRO

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	L	176/183 (96%)	162 (92%)	14 (8%)	15	11
2	H	175/184 (95%)	160 (91%)	15 (9%)	13	9
All	All	351/367 (96%)	322 (92%)	29 (8%)	14	9

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	45	LEU
1	L	49	LEU
1	L	54	ASN
1	L	56	ARG
1	L	92	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	125	SER
1	L	147	VAL
1	L	159	THR
1	L	162	MET
1	L	166	GLN
1	L	183	LEU
1	L	192	SER
1	L	203	HIS
1	L	207	LYS
2	H	253	GLN
2	H	261	LEU
2	H	273	LYS
2	H	305	ASN
2	H	320	LEU
2	H	325	SER
2	H	348	ARG
2	H	360	GLN
2	H	393	LEU
2	H	404	PRO
2	H	416	SER
2	H	428	ASP
2	H	432	LEU
2	H	441	SER
2	H	460	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	36	ASN
1	L	54	ASN
2	H	253	GLN
2	H	256	GLN
2	H	289	GLN
2	H	305	ASN
2	H	312	HIS
2	H	419	HIS
2	H	426	GLN

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 ⓘ

3 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GLA	H	501	3	11,11,12	1.21	2 (18%)	14,15,17	1.92	5 (35%)
3	MMA	H	502	3	13,13,13	0.93	0	18,18,18	1.38	3 (16%)
3	ABE	H	503	3	8,9,10	0.89	0	9,12,14	1.29	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLA	H	501	3	-	0/2/19/22	0/1/1/1
3	MMA	H	502	3	-	0/4/24/24	0/1/1/1
3	ABE	H	503	3	-	0/0/13/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	GLA	C2-C3	2.09	1.55	1.52
3	H	501	GLA	C1-C2	2.71	1.58	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	501	GLA	O4-C4-C3	-2.50	104.70	110.34
3	H	502	MMA	O2-C2-C1	-2.15	105.30	110.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	502	MMA	C3-C4-C5	-2.09	106.55	110.20
3	H	501	GLA	O3-C3-C2	-2.02	106.35	110.00
3	H	501	GLA	C1-C2-C3	2.03	111.94	109.54
3	H	503	ABE	C1-O5-C5	2.51	116.25	112.38
3	H	503	ABE	O5-C1-C2	2.59	113.77	110.85
3	H	502	MMA	C7-O1-C1	3.32	118.73	113.29
3	H	501	GLA	C6-C5-C4	3.72	122.20	113.02
3	H	501	GLA	O2-C2-C1	3.78	116.78	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.