



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 04:46 PM BST

PDB ID : 3HZY  
Title : Crystal structure of S73-2 antibody in complex with antigen Kdo(2.4)Kdo(2.4)Kdo  
Authors : Brooks, C.L.; Muller-Loennies, S.; Borisova, S.N.; Brade, L.; Kosma, P.; Hirama, T.; MacKenzie, C.R.; Brade, H.; Evans, S.V.  
Deposited on : 2009-06-24  
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](mailto: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.

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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	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

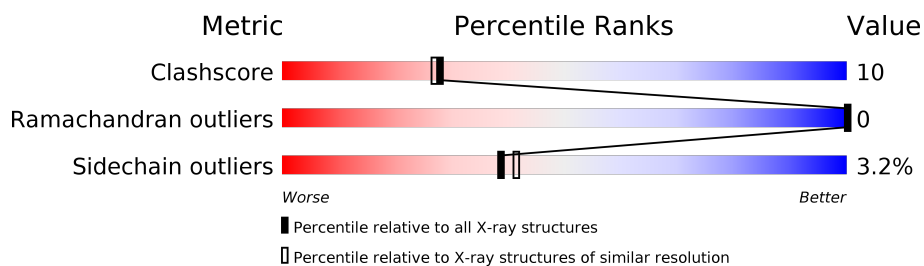
# 1 Overall quality at a glance

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3727 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 S73-2 Fab (IgG1k) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1665	1038	283	337	7			

- Molecule 2 is a protein called S73-2 Fab (IgG1k) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1677	1066	278	326	7			

- Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-prop-2-en-1-yl 3-deoxy-alpha-D-manno-oct-2-ulopyranosidonic acid.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	3	Total	C	O	0	0	0
			49	27	22			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	3	Total	Zn	0	0
			3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	170	Total 170	O 170	0	0
6	B	160	Total 160	O 160	0	0

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.95Å 81.97Å 128.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.10	Depositor
% Data completeness (in resolution range)	96.2 (19.80-2.10)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.56 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.4_4	Depositor
R, $R_{free}$	0.216 , 0.261	Depositor
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.294	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3727	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, KDO, MG, KDA

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	1665	0	1621	31	0
2	B	1677	0	1639	35	0
3	C	49	0	38	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	0	1
5	B	1	0	0	0	1
6	A	170	0	0	2	0
6	B	160	0	0	5	0
All	All	3727	0	3298	66	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 10.

All (66) 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:B:155:SER:H	2:B:195:ASN:HD21	1.18	0.87
1:A:13:VAL:HG21	1:A:19:VAL:HG22	1.59	0.84
2:B:38:ARG:HE	2:B:46:LYS:HD3	1.44	0.83
1:A:105:LEU:H	1:A:165:GLN:HE22	1.36	0.73
2:B:71:ARG:HE	2:B:73:ASN:HD21	1.38	0.72
2:B:38:ARG:HH21	2:B:46:LYS:HE2	1.57	0.69
2:B:155:SER:H	2:B:195:ASN:ND2	1.92	0.68
2:B:211:PRO:O	2:B:219:ARG:HB2	1.96	0.65
2:B:33:TYR:HB2	2:B:95:ASP:HB3	1.77	0.65
2:B:38:ARG:HH21	2:B:46:LYS:CE	2.11	0.63
1:A:80:ALA:HA	1:A:105:LEU:HD13	1.83	0.61
2:B:186:THR:O	2:B:190:GLU:HB2	2.00	0.61
2:B:46:LYS:NZ	6:B:274:HOH:O	2.32	0.61
1:A:194:GLU:HG2	1:A:205:VAL:HG22	1.82	0.60
2:B:176:LEU:C	2:B:176:LEU:HD12	2.22	0.60
2:B:154:ASN:ND2	2:B:193:THR:H	2.00	0.60
1:A:112:PRO:HG2	1:A:204:ILE:HD12	1.84	0.59
1:A:105:LEU:H	1:A:165:GLN:NE2	2.00	0.58
2:B:146:PRO:O	2:B:198:HIS:HE1	1.87	0.58
2:B:71:ARG:NE	2:B:73:ASN:HD21	2.02	0.57
2:B:113:ARG:HG2	6:B:250:HOH:O	2.04	0.57
1:A:1:ASP:O	1:A:1:ASP:CG	2.42	0.57
2:B:96:ILE:HD12	2:B:98:PRO:HG3	1.87	0.56
2:B:105:GLN:NE2	2:B:105:GLN:H	2.03	0.56
1:A:93:ASN:HD22	1:A:93:ASN:C	2.09	0.55
2:B:82(B):THR:HG22	6:B:325:HOH:O	2.06	0.54
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.89	0.53
2:B:71:ARG:HE	2:B:73:ASN:ND2	2.04	0.53
2:B:33:TYR:CB	2:B:95:ASP:HB3	2.40	0.52
2:B:198:HIS:HD2	2:B:201:SER:OG	1.93	0.52
1:A:80:ALA:O	1:A:105:LEU:HD11	2.11	0.51
1:A:154:ARG:NH1	6:A:281:HOH:O	2.43	0.51
1:A:19:VAL:HG21	1:A:78:VAL:HG21	1.93	0.50
1:A:168:LYS:HG3	1:A:169:ASP:N	2.28	0.49
2:B:154:ASN:HD21	2:B:193:THR:H	1.62	0.47
1:A:135:LEU:N	1:A:135:LEU:HD12	2.30	0.47
2:B:29:PHE:CD2	2:B:76:SER:HA	2.50	0.47
2:B:5:VAL:HA	2:B:105:GLN:HE22	1.80	0.46
1:A:191:TYR:O	1:A:207:SER:HB2	2.15	0.46
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.50	0.46
2:B:19:ARG:NH1	6:B:240:HOH:O	2.48	0.46
2:B:113:ARG:HD3	6:B:261:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HB3	1:A:89:LYS:HE2	1.73	0.45
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.99	0.45
1:A:94:LEU:C	1:A:95:ARG:HD2	2.38	0.44
2:B:83:ARG:HG3	2:B:85:GLU:OE1	2.17	0.44
1:A:27(C):LEU:HD11	1:A:29:ARG:HA	2.00	0.44
2:B:50:PHE:C	2:B:50:PHE:CD1	2.91	0.44
1:A:19:VAL:CG2	1:A:78:VAL:HG21	2.48	0.44
1:A:83:LEU:HD13	1:A:165:GLN:HE21	1.83	0.43
1:A:117:PHE:HA	1:A:118:PRO:HD3	1.81	0.43
1:A:80:ALA:O	1:A:105:LEU:CD1	2.67	0.43
1:A:28:THR:O	1:A:29:ARG:HB2	2.18	0.43
1:A:166:ASP:OD2	1:A:168:LYS:HG2	2.20	0.42
1:A:54:ARG:HD3	1:A:58:VAL:O	2.20	0.42
2:B:34:MET:HB3	2:B:78:LEU:HD22	2.01	0.42
2:B:198:HIS:HB3	2:B:203:THR:HB	2.00	0.42
1:A:188:HIS:O	1:A:210:ARG:NH1	2.53	0.41
2:B:198:HIS:CD2	2:B:201:SER:OG	2.73	0.41
1:A:61:ARG:HB2	1:A:76:SER:O	2.21	0.41
2:B:97:ASN:O	2:B:100(C):TYR:HB2	2.20	0.41
1:A:182:LYS:O	1:A:186:GLU:HG3	2.21	0.41
1:A:102:LYS:HG3	6:A:374:HOH:O	2.21	0.40
1:A:27(F):ARG:HH12	3:C:1:KDA:H7	1.86	0.40
1:A:154:ARG:HE	1:A:154:ARG:HB2	1.65	0.40
2:B:153:TRP:CZ3	2:B:194:CYS:HB3	2.56	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)
5:A:215:ZN:ZN	5:B:215:ZN:ZN[2_454]	1.31	0.89

## 4.3 Torsion angles [i](#)

### 4.3.1 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	211/219 (96%)	206 (98%)	5 (2%)	0	100	100
2	B	215/226 (95%)	212 (99%)	3 (1%)	0	100	100
All	All	426/445 (96%)	418 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 4.3.2 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	190/194 (98%)	183 (96%)	7 (4%)	34	35
2	B	188/192 (98%)	183 (97%)	5 (3%)	44	48
All	All	378/386 (98%)	366 (97%)	12 (3%)	39	41

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27(F)	ARG
1	A	78	VAL
1	A	93	ASN
1	A	154	ARG
1	A	168	LYS
1	A	174	MET
1	A	180	LEU
2	B	50	PHE
2	B	83	ARG
2	B	105	GLN
2	B	176	LEU
2	B	207	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	A	42	GLN
1	A	79	GLN
1	A	93	ASN
1	A	165	GLN
2	B	73	ASN
2	B	105	GLN
2	B	154	ASN
2	B	195	ASN
2	B	198	HIS

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

#### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates [i](#)

3 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

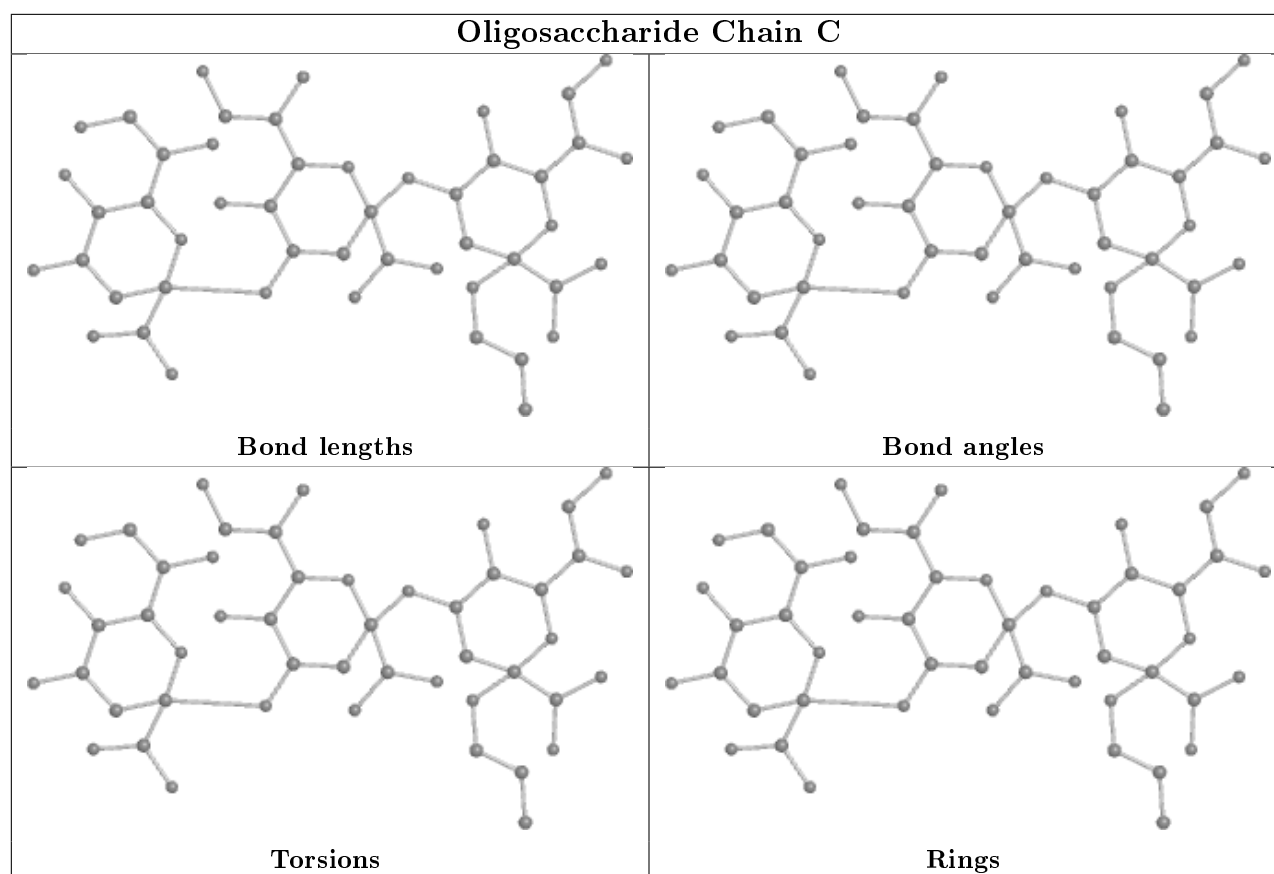
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



#### 4.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.