



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 07:54 AM EDT

PDB ID : 6VL9
Title : Anti-PEG antibody 6-3 Fab fragment in complex with PEG
Authors : Nicely, N.I.; Huckaby, J.T.; Lai, S.K.; Jacobs, T.M.
Deposited on : 2020-01-23
Resolution : 2.63 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
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) : 2.35.1

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 2.63 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6833 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.

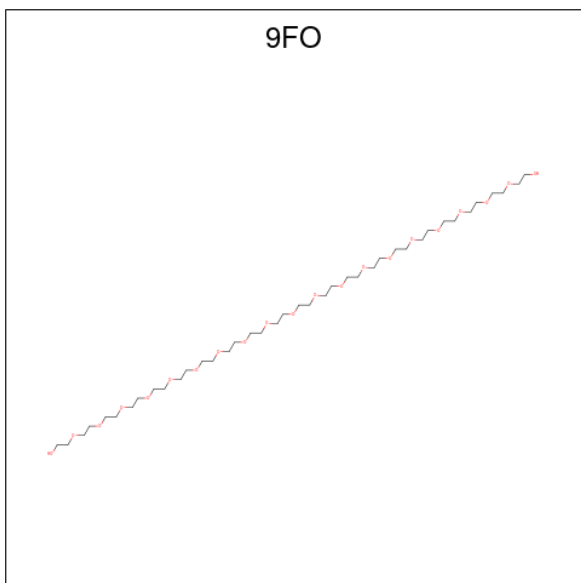
- Molecule 1 is a protein called 6-3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	210	Total 1598	C 1026	N 263	O 303	S 6	0	0	0
1	A	209	Total 1589	C 1020	N 261	O 302	S 6	0	0	0

- Molecule 2 is a protein called 6-3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	218	Total 1683	C 1056	N 278	O 342	S 7	0	0	0
2	B	217	Total 1675	C 1052	N 276	O 340	S 7	0	0	0

- Molecule 3 is 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45,48,51,54,57-nonadecaaxanonapentacontane-1,59-diol (three-letter code: 9FO) (formula: C₄₀H₈₂O₂₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			61	40	21		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	70	Total	O	0	0
			70	70		
4	L	61	Total	O	0	0
			61	61		
4	A	57	Total	O	0	0
			57	57		
4	B	39	Total	O	0	0
			39	39		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.71Å 169.79Å 69.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.82 – 2.63	Depositor
% Data completeness (in resolution range)	97.8 (43.82-2.63)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.178 , 0.250	Depositor
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.581	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6833	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

1 ligand is 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	9FO	H	301	-	60,60,60	0.97	0	59,59,59	0.53	0

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	9FO	H	301	-	-	31/58/58/58	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	301	9FO	CCH-CCG-OCF-CCE
3	H	301	9FO	OAG-CAH-CAI-OAJ
3	H	301	9FO	OBK-CBL-CBM-OBN
3	H	301	9FO	OAV-CAW-CAX-OAY
3	H	301	9FO	OCC-CCD-CCE-OCF
3	H	301	9FO	OBB-CBC-CBD-OBE
3	H	301	9FO	OAJ-CAK-CAL-OAM
3	H	301	9FO	OBZ-CCA-CCB-OCC
3	H	301	9FO	OBH-CBI-CBJ-OBK
3	H	301	9FO	OBW-CBX-CBY-OBZ
3	H	301	9FO	OAY-CAZ-CBA-OBB
3	H	301	9FO	OAA-CAB-CAC-OAD
3	H	301	9FO	CBI-CBJ-OBK-CBL
3	H	301	9FO	CCD-CCE-OCF-CCG
3	H	301	9FO	CBJ-CBI-OBH-CBG
3	H	301	9FO	CBG-CBF-OBE-CBD
3	H	301	9FO	CAB-CAC-OAD-CAE
3	H	301	9FO	CAH-CAI-OAJ-CAK
3	H	301	9FO	OBE-CBF-CBG-OBH
3	H	301	9FO	CAF-CAE-OAD-CAC
3	H	301	9FO	CAO-CAN-OAM-CAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	H	301	9FO	CBP-CBO-OBN-CBM
3	H	301	9FO	CBF-CBG-OBH-CBI
3	H	301	9FO	CAZ-CBA-OB-BCB
3	H	301	9FO	CAT-CAU-OAV-CAW
3	H	301	9FO	CAE-CAF-OAG-CAH
3	H	301	9FO	CCA-CCB-OCC-CCD
3	H	301	9FO	CBL-CBM-OBN-CBO
3	H	301	9FO	OBN-CBO-CBP-OBQ
3	H	301	9FO	CAW-CAX-OAY-CAZ
3	H	301	9FO	OAS-CAT-CAU-OAV

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 9FO H 301	
Bond lengths	Bond angles
Torsions	Rings

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.