



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:13 PM EDT

PDB ID : 4AT6 / pdb_00004at6
Title : Fab fragment of antiporphyrin antibody 14H7
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Deposited on : 2012-05-04
Resolution : 2.55 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
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.55 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

There are 3 unique types of molecules in this entry. The entry contains 25238 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 14H7 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1551	980	255	309	7			
1	C	209	Total	C	N	O	S	0	0	0
			1534	971	252	305	6			
1	E	209	Total	C	N	O	S	0	0	0
			1528	965	252	305	6			
1	G	205	Total	C	N	O	S	0	0	0
			1489	939	247	297	6			
1	H	211	Total	C	N	O	S	0	0	0
			1550	981	255	307	7			
1	J	207	Total	C	N	O	S	0	0	0
			1503	951	250	295	7			
1	M	203	Total	C	N	O	S	0	0	0
			1483	938	244	295	6			
1	O	204	Total	C	N	O	S	0	0	0
			1480	933	244	297	6			

- Molecule 2 is a protein called FAB 14H7 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	D	212	Total	C	N	O	S	0	0	0
			1594	995	269	324	6			
2	F	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	I	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	K	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	L	212	Total	C	N	O	S	0	0	0
			1591	993	268	324	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	P	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	31	Total	O	0	0
			31	31		
3	C	25	Total	O	0	0
			25	25		
3	D	26	Total	O	0	0
			26	26		
3	E	24	Total	O	0	0
			24	24		
3	F	23	Total	O	0	0
			23	23		
3	G	16	Total	O	0	0
			16	16		
3	H	15	Total	O	0	0
			15	15		
3	I	23	Total	O	0	0
			23	23		
3	J	22	Total	O	0	0
			22	22		
3	K	27	Total	O	0	0
			27	27		
3	L	21	Total	O	0	0
			21	21		
3	M	12	Total	O	0	0
			12	12		
3	N	24	Total	O	0	0
			24	24		
3	O	16	Total	O	0	0
			16	16		
3	P	35	Total	O	0	0
			35	35		

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.20Å 228.16Å 146.59Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	16.65 – 2.55	Depositor
% Data completeness (in resolution range)	93.5 (16.65-2.55)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.55Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.279 , 0.328	Depositor
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.416	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
Reported twinning fraction	0.499 for h,-k,-l	Depositor
Outliers	3 of 111576 reflections (0.003%)	Xtriage
Total number of atoms	25238	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5837e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

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.