

wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 11:55 PM EDT

PDB ID : 6VRQ

Title : Crystal structure of gl12A21 Fab in complex with anti-idiotypic iv12 Fab

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Deposited on : 2020-02-08

Resolution : 2.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : FAILED

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 (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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 9 unique types of molecules in this entry. The entry contains 12954 atoms, of which 6145 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 iv12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Н	215	Total 3194	C 1029	H 1575	N 267	O 317	S 6	0	1	0

• Molecule 2 is a protein called iv12 Fab Light Chain.

\mathbf{Mol}	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	212	Total 3056	C 987	H 1473	N 268	O 322	S 6	0	2	0

• Molecule 3 is a protein called gl12A21 Fab Heavy Chain.

N	/Iol	Chain	Residues			Atoms	S	ZeroOcc	AltConf	Trace		
	3	A	222	Total 3188	C 1033	H 1547	N 283	O 317	S 8	0	1	0

• Molecule 4 is a protein called gl12A21 Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	В	207	Total 3057	C 985	H 1480	N 259	O 328	S 5	0	4	0

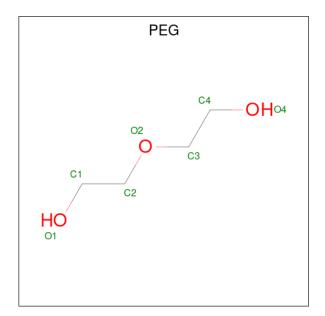
• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
5	Н	1	Total C H O	0	0	
5	11	1	10 2 6 2	U	U	
5	H	1	Total C H O	0	0	
	11	1	10 2 6 2	U		
5	Δ	1	Total C H O	0	0	
	11	1	10 2 6 2	U	U	
5	Δ	1	Total C H O	0	0	
	11	1	10 2 6 2	U	U	
5	В	1	Total C H O	0	0	
	Б	В	10 2 6 2			

 $\bullet \ \ Molecule \ 6 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf	
6	Н	1	Total	С	Н	О	0	0	
	11	1	17	4	10	3	0		
6	Т	1	Total	С	Н	О	0	0	
	П	1	17	4	10	3	0	0	
6	Λ	1	Total	С	Н	О	0	0	
0	A	1	17	4	10	3	0	U	
6	Λ	1	Total	С	Н	О	0	0	
	A		17	4	10	3	U		

• Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total K 1 1	0	0
7	A	2	Total K 2 2	0	0
7	В	2	Total K 2 2	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total Cl 4 4	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
9	Н	79	Total O 79 79	0	0	
9	L	72	Total O 72 72	0	0	
9	A	97	Total O 97 97	0	0	
9	В	84	Total O 84 84	0	0	

 $\operatorname{MolProbity}$ and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	81.17Å 202.86Å 72.34Å	Depositor
a, b, c, α , β , γ	90.00° 93.01° 90.00°	Depositor
Resolution (Å)	36.12 - 2.57	Depositor
% Data completeness	93.0 (36.12-2.57)	Depositor
(in resolution range)	,	•
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.55 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.189 , 0.241	Depositor
Wilson B-factor (\mathring{A}^2)	41.8	Xtriage
Anisotropy	0.038	Xtriage
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12954	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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	Tuno	Chain	Res	Link	В	ond leng	gths	В	ond ang	gles
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	306	-	3,3,3	0.46	0	2,2,2	0.51	0
6	PEG	Н	303	-	6,6,6	0.49	0	5,5,5	0.27	0
6	PEG	L	502	-	6,6,6	0.49	0	5,5,5	0.40	0
6	PEG	A	309	-	6,6,6	0.50	0	5,5,5	0.22	0
5	EDO	В	501	-	3,3,3	0.53	0	2,2,2	0.31	0
5	EDO	Н	302	-	3,3,3	0.54	0	2,2,2	0.25	0
6	PEG	A	310	-	6,6,6	0.47	0	5,5,5	0.31	0
5	EDO	A	305	-	3,3,3	0.48	0	2,2,2	0.41	0
5	EDO	Н	301	-	3,3,3	0.57	0	2,2,2	0.31	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
5	EDO	A	306	-	-	1/1/1/1	-
6	PEG	Н	303	-	-	1/4/4/4	-
6	PEG	L	502	_	-	1/4/4/4	-
6	PEG	A	309	_	-	0/4/4/4	-
5	EDO	В	501	_	-	0/1/1/1	-
5	EDO	Н	302	_	-	0/1/1/1	-
6	PEG	A	310	_	-	0/4/4/4	-
5	EDO	A	305	_	-	1/1/1/1	-
5	EDO	Н	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	305	EDO	O1-C1-C2-O2
6	Н	303	PEG	C4-C3-O2-C2
6	L	502	PEG	C1-C2-O2-C3
5	A	306	EDO	O1-C1-C2-O2



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 (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

