



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 02:33 PM EDT

PDB ID : 3DIF
Title : Crystal structure of FabOX117
Authors : Nettleship, J.E.; Ren, J.; Owens, R.J.; Oxford Protein Production Facility (OPPF)
Deposited on : 2008-06-20
Resolution : 2.40 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 ⓘ 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

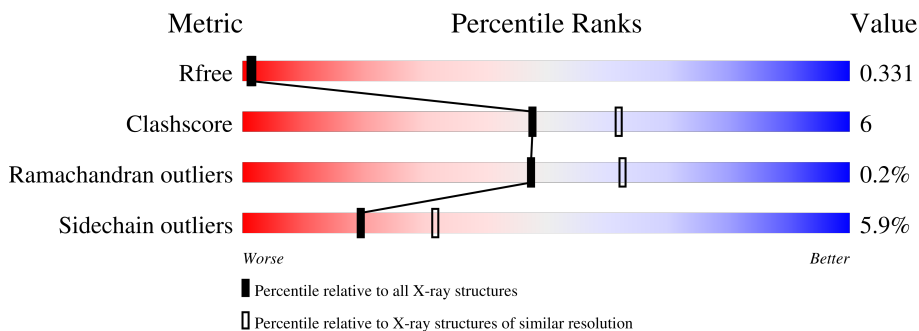
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	214	82% 16% .
1	C	214	83% 16% .
2	B	229	75% 14% . 8%
2	D	229	82% 9% . 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6854 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 FabOX117 Light Chain Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	Total 1657	C 1038	N 276	O 337	S 6	0	0	0
1	C	214	Total 1663	C 1041	N 277	O 338	S 7	0	0	0

- Molecule 2 is a protein called FabOX117 Heavy Chain Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	211	Total 1604	C 1030	N 259	O 309	S 6	0	0	0
2	D	213	Total 1619	C 1038	N 264	O 311	S 6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	224	HIS	-	expression tag	PDB 3DIF
B	225	HIS	-	expression tag	PDB 3DIF
B	226	HIS	-	expression tag	PDB 3DIF
B	227	HIS	-	expression tag	PDB 3DIF
B	228	HIS	-	expression tag	PDB 3DIF
B	229	HIS	-	expression tag	PDB 3DIF
D	224	HIS	-	expression tag	PDB 3DIF
D	225	HIS	-	expression tag	PDB 3DIF
D	226	HIS	-	expression tag	PDB 3DIF
D	227	HIS	-	expression tag	PDB 3DIF
D	228	HIS	-	expression tag	PDB 3DIF
D	229	HIS	-	expression tag	PDB 3DIF

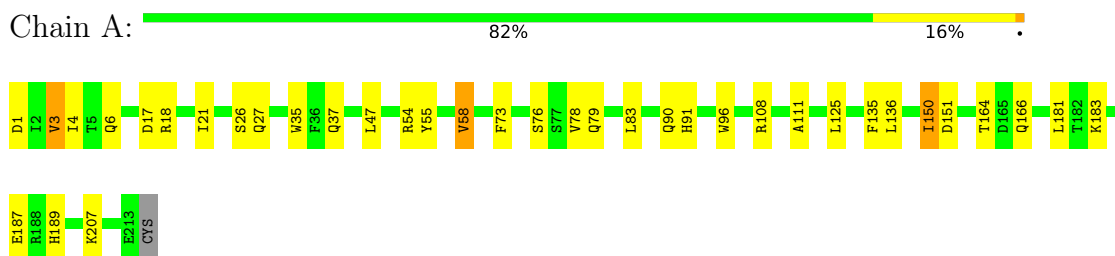
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	83	Total 83	O 83	0	0
3	C	74	Total 74	O 74	0	0
3	D	115	Total 115	O 115	0	0

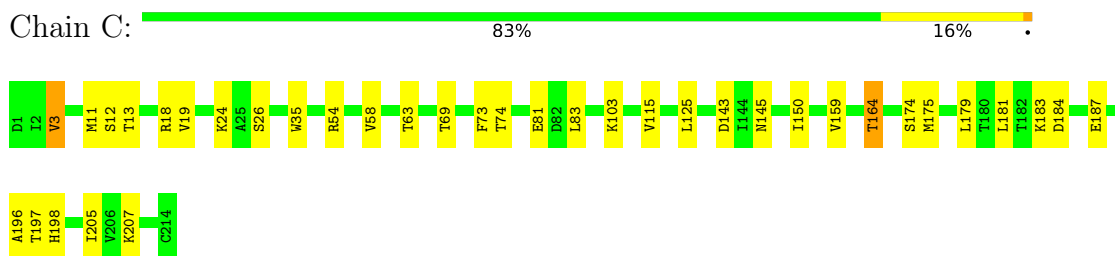
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

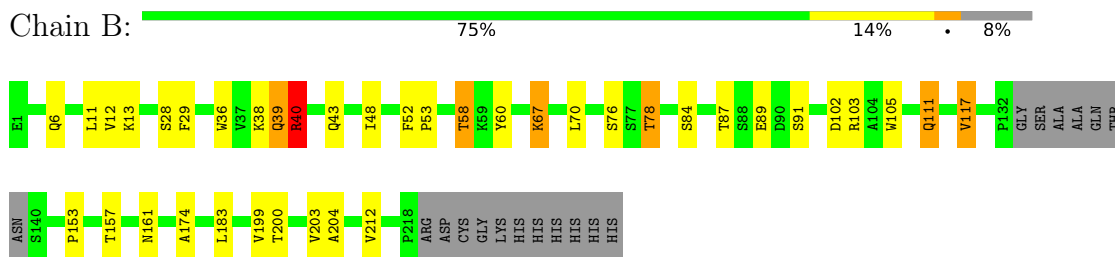
- Molecule 1: FabOX117 Light Chain Fragment



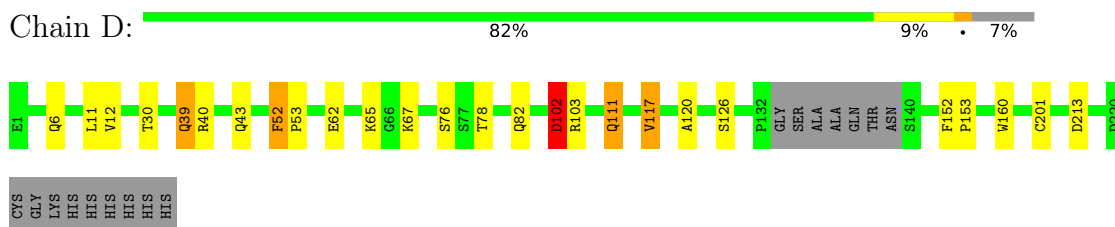
- Molecule 1: FabOX117 Light Chain Fragment



- Molecule 2: FabOX117 Heavy Chain Fragment



- Molecule 2: FabOX117 Heavy Chain Fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.21Å 70.60Å 87.85Å 101.50° 102.94° 98.32°	Depositor
Resolution (Å)	30.00 – 2.40 33.91 – 2.37	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.40) 95.6 (33.91-2.37)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.36Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.286 0.285 , 0.331	Depositor DCC
R_{free} test set	1797 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.354	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.33% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.35	0/1697	0.55	0/2307
1	C	0.36	0/1703	0.53	0/2315
2	B	0.41	0/1652	0.58	1/2259 (0.0%)
2	D	0.38	0/1667	0.54	0/2278
All	All	0.38	0/6719	0.55	1/9159 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	40	ARG	NE-CZ-NH1	6.79	123.69	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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	1657	0	1583	22	0
1	C	1663	0	1588	16	0
2	B	1604	0	1569	27	0
2	D	1619	0	1583	17	0
3	A	39	0	0	0	0
3	B	83	0	0	3	0
3	C	74	0	0	0	0
3	D	115	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6854	0	6323	79	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 6.

The worst 5 of 79 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:D:111:GLN:HE21	2:D:111:GLN:H	1.19	0.86
2:B:87:THR:HG22	2:B:89:GLU:H	1.39	0.86
2:B:6:GLN:H	2:B:111:GLN:HE22	1.19	0.84
2:D:6:GLN:H	2:D:111:GLN:HE22	1.25	0.84
2:B:111:GLN:HE21	2:B:111:GLN:H	1.34	0.74

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	A	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
1	C	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	207/229 (90%)	202 (98%)	4 (2%)	1 (0%)	29	41
2	D	209/229 (91%)	205 (98%)	3 (1%)	1 (0%)	29	41
All	All	839/886 (95%)	817 (97%)	20 (2%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	102	ASP
2	B	102	ASP

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	A	189/190 (100%)	180 (95%)	9 (5%)	25	41
1	C	190/190 (100%)	175 (92%)	15 (8%)	12	19
2	B	180/194 (93%)	170 (94%)	10 (6%)	21	34
2	D	181/194 (93%)	171 (94%)	10 (6%)	21	35
All	All	740/768 (96%)	696 (94%)	44 (6%)	19	32

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	164	THR
2	D	52	PHE
1	C	175	MET
1	C	198	HIS
2	D	82	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	82	GLN
2	D	111	GLN
1	C	137	ASN
1	C	161	ASN
1	C	198	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.