



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2021 – 01:24 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 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 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	:	2.17.1
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)	:	2.17.1

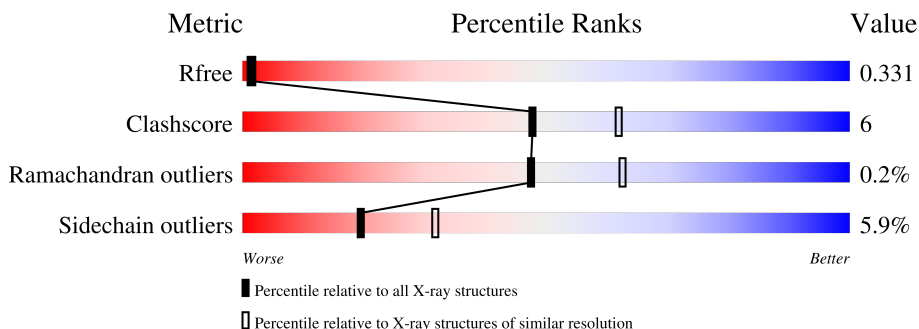
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	
1	C	214	
2	B	229	
2	D	229	

2 Entry composition

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
1	A	213	Total	C	N	O	S	0	0	0
			1657	1038	276	337	6			
1	C	214	Total	C	N	O	S	0	0	0
			1663	1041	277	338	7			

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

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

There are 12 discrepancies between the modelled and reference sequences:

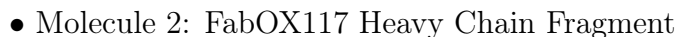
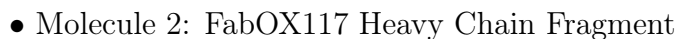
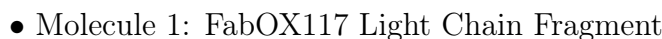
Chain	Residue	Modelled	Actual	Comment	Reference
B	224	HIS	-	expression tag	PDB 3DIF
B	225	HIS	-	expression tag	PDB 3DIF
B	226	HIS	-	expression tag	PDB 3DIF
B	227	HIS	-	expression tag	PDB 3DIF
B	228	HIS	-	expression tag	PDB 3DIF
B	229	HIS	-	expression tag	PDB 3DIF
D	224	HIS	-	expression tag	PDB 3DIF
D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

i

- Molecule 1: FabOX117 Light 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)	Xtriage
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	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.

All (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
1:A:54:ARG:HG3	1:A:58:VAL:HG22	1.68	0.73
2:D:39:GLN:HG2	3:D:328:HOH:O	1.90	0.69
1:A:3:VAL:HG13	1:A:26:SER:HB3	1.74	0.68
2:B:40:ARG:HH11	2:B:40:ARG:HG3	1.60	0.67
2:B:203:VAL:HB	2:B:212:VAL:HG23	1.76	0.66
1:A:17:ASP:O	1:A:78:VAL:HG23	1.96	0.66
3:B:277:HOH:O	2:D:102:ASP:HB3	1.97	0.66
2:D:102:ASP:OD1	3:D:238:HOH:O	2.12	0.65
1:A:83:LEU:HD11	1:A:166:GLN:HB3	1.78	0.65
1:A:27:GLN:OE1	2:D:30:THR:HG21	1.97	0.63
1:C:54:ARG:HH12	1:C:63:THR:HG22	1.63	0.63
1:C:13:THR:HG21	1:C:19:VAL:HG22	1.80	0.62
2:D:76:SER:OG	2:D:78:THR:HG22	2.00	0.60
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.84	0.60
2:B:76:SER:O	2:B:78:THR:HG22	2.03	0.59
2:B:40:ARG:HB2	2:B:43:GLN:HB2	1.85	0.58
1:A:150:ILE:HD11	1:A:189:HIS:CG	2.39	0.58
1:C:3:VAL:HG13	1:C:26:SER:HB3	1.85	0.57
2:D:12:VAL:O	2:D:117:VAL:HA	2.05	0.57
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.85	0.56
1:C:196:ALA:HB3	1:C:205:ILE:HG23	1.87	0.56
1:A:54:ARG:CG	1:A:58:VAL:HG22	2.34	0.55
1:C:145:ASN:HB2	1:C:197:THR:HB	1.89	0.55
1:C:196:ALA:HB3	1:C:205:ILE:CG2	2.38	0.54
1:A:6:GLN:HE21	1:A:21:ILE:HG21	1.73	0.54
2:B:87:THR:O	2:B:117:VAL:HG11	2.08	0.54
2:B:76:SER:OG	2:B:78:THR:HG23	2.08	0.53
1:A:18:ARG:HG3	1:A:76:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:GLN:HE21	2:D:111:GLN:N	1.97	0.53
1:A:4:ILE:HD11	1:A:90:GLN:HB3	1.92	0.52
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.91	0.51
2:B:12:VAL:O	2:B:117:VAL:HA	2.12	0.50
2:B:6:GLN:H	2:B:111:GLN:NE2	1.99	0.50
1:C:159:VAL:HG22	1:C:179:LEU:HD13	1.93	0.49
2:B:103:ARG:HD3	2:B:105:TRP:CH2	2.47	0.49
1:C:54:ARG:NH1	1:C:63:THR:HG22	2.26	0.49
2:B:40:ARG:HH11	2:B:40:ARG:CG	2.25	0.49
2:B:11:LEU:HB2	2:B:153:PRO:HG3	1.94	0.49
2:B:161:ASN:HD21	2:B:199:VAL:HA	1.78	0.49
1:C:115:VAL:HG23	1:C:205:ILE:HD13	1.95	0.48
2:B:39:GLN:HG2	3:B:285:HOH:O	2.14	0.48
2:B:161:ASN:ND2	2:B:200:THR:H	2.11	0.48
1:A:1:ASP:N	2:D:53:PRO:O	2.46	0.48
1:A:55:TYR:O	1:A:58:VAL:HG13	2.13	0.48
2:D:40:ARG:HB2	2:D:43:GLN:HB2	1.94	0.48
1:C:164:THR:HG22	1:C:174:SER:H	1.79	0.47
2:D:111:GLN:H	2:D:111:GLN:NE2	2.00	0.47
1:A:35:TRP:CE2	1:A:73:PHE:HB2	2.49	0.47
2:B:103:ARG:HD3	2:B:105:TRP:CZ3	2.49	0.47
2:D:11:LEU:HB2	2:D:153:PRO:HG3	1.96	0.47
1:A:1:ASP:HB2	2:D:52:PHE:CE2	2.50	0.46
1:C:35:TRP:CE2	1:C:73:PHE:HB2	2.51	0.46
2:B:157:THR:CG2	2:B:204:ALA:HB3	2.46	0.45
1:C:11:MET:CE	1:C:12:SER:H	2.29	0.45
1:A:54:ARG:HG3	1:A:58:VAL:CG2	2.43	0.45
1:A:136:LEU:HD12	1:A:136:LEU:N	2.32	0.44
1:A:183:LYS:O	1:A:187:GLU:HG2	2.17	0.44
2:D:62:GLU:HA	2:D:65:LYS:HD3	2.01	0.43
2:D:160:TRP:CZ3	2:D:201:CYS:HB3	2.53	0.43
2:B:29:PHE:CE2	2:B:53:PRO:HB3	2.53	0.43
2:B:103:ARG:HB2	3:B:296:HOH:O	2.19	0.43
1:C:13:THR:HG21	1:C:19:VAL:CG2	2.46	0.43
2:B:91:SER:OG	2:B:117:VAL:HG13	2.19	0.42
1:C:183:LYS:O	1:C:187:GLU:HG2	2.20	0.42
2:B:174:ALA:HB2	2:B:183:LEU:HD23	2.02	0.41
1:A:108:ARG:HH21	1:A:111:ALA:HB2	1.85	0.41
2:B:58:THR:HG23	2:B:60:TYR:CE2	2.55	0.41
1:A:91:HIS:HA	1:A:96:TRP:CD1	2.56	0.41
1:A:135:PHE:C	1:A:136:LEU:HD12	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:CZ	1:C:74:THR:HG21	2.52	0.40
2:B:36:TRP:CD1	2:B:70:LEU:HD22	2.57	0.40
1:A:150:ILE:HD11	1:A:189:HIS:HB3	2.04	0.40
2:B:67:LYS:HE2	2:B:84:SER:O	2.22	0.40
2:D:120:ALA:HB3	2:D:152:PHE:CE2	2.57	0.40

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

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	58	VAL
1	A	79	GLN
1	A	125	LEU
1	A	150	ILE
1	A	151	ASP
1	A	164	THR
1	A	181	LEU
1	A	207	LYS
2	B	13	LYS
2	B	28	SER
2	B	39	GLN
2	B	40	ARG
2	B	52	PHE
2	B	58	THR
2	B	67	LYS
2	B	78	THR
2	B	111	GLN
2	B	117	VAL
1	C	3	VAL
1	C	24	LYS
1	C	58	VAL
1	C	69	THR
1	C	81	GLU
1	C	83	LEU
1	C	103	LYS
1	C	125	LEU
1	C	143	ASP
1	C	164	THR
1	C	175	MET
1	C	181	LEU

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Mol	Chain	Res	Type
1	C	184	ASP
1	C	198	HIS
1	C	207	LYS
2	D	39	GLN
2	D	52	PHE
2	D	67	LYS
2	D	82	GLN
2	D	102	ASP
2	D	103	ARG
2	D	111	GLN
2	D	117	VAL
2	D	126	SER
2	D	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
2	B	111	GLN
2	B	161	ASN
1	C	137	ASN
1	C	161	ASN
1	C	198	HIS
2	D	5	GLN
2	D	82	GLN
2	D	111	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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