



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1QOK
Title : MFE-23 AN ANTI-CARCINOEMBRYONIC ANTIGEN SINGLE-CHAIN
FV ANTIBODY
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Deposited on : 1999-11-11
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	:	2.11
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)	:	2.11

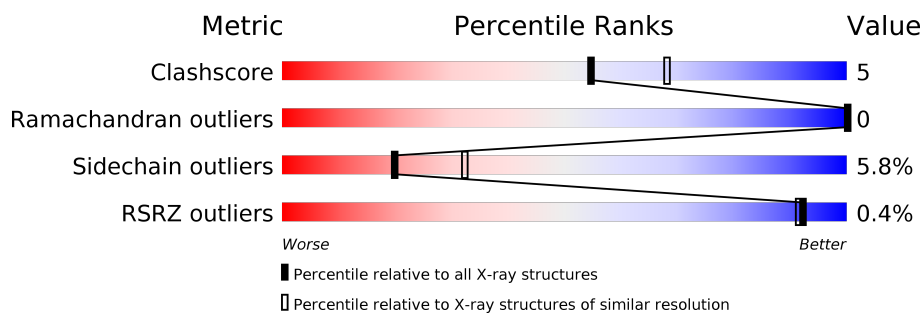
1 Overall quality at a glance

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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1827 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 MFE-23 RECOMBINANT ANTIBODY FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	43	0	1
			1731	1087	281	355	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total	O	0	0
			96	96		

● Molecule 1: MFE-23 RECOMBINANT ANTIBODY FRAGMENT

GLU	GLY	GLU	THR
ASP	GLY	VAL	THR
LEU	GLY	ILE	ILE
ASN	SER	MET	LYS
	GLY	TYR	TYR
	GLY	LEU	LEU
	SER	PRO	PRO
	GLU	THR	THR
	ALA	ALA	ALA
	ALA	ALA	ALA
	GLY	LEU	LEU
	LEU	LEU	LEU
	LEU	LEU	LEU
	ALA	ALA	ALA
	GLN	GLN	GLN
	PRO	PRO	PRO
	ALA	ALA	ALA
	MET	MET	MET
	ALA	ALA	ALA
		Q27	Q27
		L37	L37
		V44	V44
		D57	D57
		H61	H61
		R64	R64
		P67	P67
		E68	E68
		W73	W73
		I74	I74
		G75	G75
		W76	W76
		I77	I77
		D78	D78
		P79	P79
		E80	E80
		L112	L112
		Y121	Y121
		G147	G147
		GLY	GLY
		GLY	GLY
		ILE	ILE
		SER	SER
		GLU	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	61.70 Å 61.70 Å 128.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (8.00-2.40) 100.0 (15.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.98 (at 2.39 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.205 , 0.267 0.169 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1827	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% 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	0.50	0/1775	0.76	0/2416

There are no bond length outliers.

There are no bond angle outliers.

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	1731	0	1632	17	0
2	A	96	0	0	1	0
All	All	1827	0	1632	17	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 5.

All (17) 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)
1:A:44:VAL:HG22	1:A:112:LEU:HD11	1.56	0.85
1:A:61:HIS:HD2	1:A:73:TRP:HE1	1.25	0.78
1:A:61:HIS:CD2	1:A:73:TRP:HE1	2.14	0.60
1:A:176:PRO:HD3	1:A:266:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:SER:O	1:A:237:ARG:HD2	2.09	0.53
1:A:194:HIS:CD2	1:A:210:SER:H	2.27	0.52
1:A:57:ASP:OD2	2:A:2011:HOH:O	2.19	0.52
1:A:194:HIS:HD2	1:A:209:TYR:HA	1.76	0.50
1:A:221:ARG:CZ	1:A:239:GLU:HG3	2.43	0.49
1:A:121:TYR:CE1	1:A:203:SER:HB3	2.47	0.48
1:A:194:HIS:CD2	1:A:209:TYR:HA	2.49	0.46
1:A:180:VAL:O	1:A:234:THR:HA	2.16	0.46
1:A:44:VAL:CG2	1:A:112:LEU:HD11	2.39	0.45
1:A:77:ILE:O	1:A:79:PRO:HD3	2.18	0.44
1:A:226:GLY:HA3	1:A:231:TYR:HA	2.00	0.42
1:A:185:SER:HA	1:A:229:THR:O	2.20	0.41
1:A:73:TRP:CH2	1:A:75:GLY:HA2	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	223/282 (79%)	215 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	191/224 (85%)	180 (94%)	11 (6%)	20	32

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	44	VAL
1	A	64	ARG
1	A	68	GLU
1	A	80	GLU
1	A	173	SER
1	A	188	SER
1	A	191	SER
1	A	203	SER
1	A	237	ARG
1	A	251	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	108	GLN
1	A	194	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 carbohydrates 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/282 (80%)	-0.79	1 (0%) 92 91	9, 22, 41, 62	15 (6%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	PRO	3.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.