



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 8OZ3 / pdb_00008oz3
Title : Crystal structure of scFv ATOR 1017 bound to human 4-1BB
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Deposited on : 2023-05-08
Resolution : 3.10 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

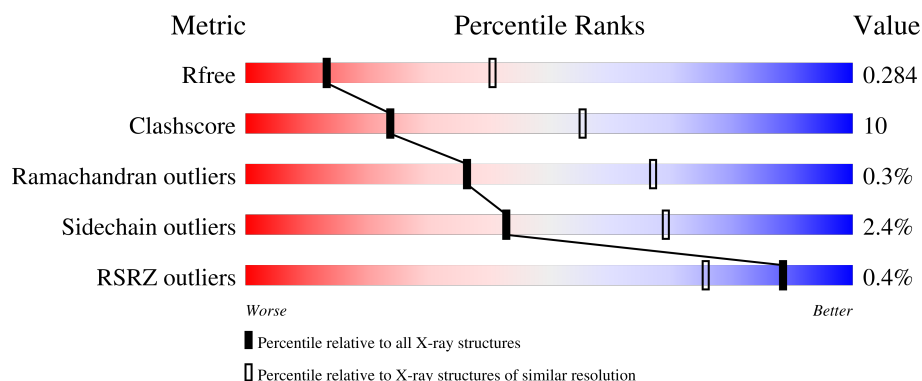
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	230	
1	H	230	
2	B	216	
2	L	216	
3	C	141	

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Mol	Chain	Length	Quality of chain
3	D	141	% 74% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10655 atoms, of which 5182 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 Single chain Fv.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	117	Total	C	H	N	O	S	37	0	0
			1745	561	853	152	175	4			
1	H	118	Total	C	H	N	O	S	37	0	0
			1762	566	861	153	178	4			

- Molecule 2 is a protein called Single chain Fv.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	109	Total	C	H	N	O	S	35	0	0
			1643	527	810	136	167	3			
2	L	109	Total	C	H	N	O	S	35	0	0
			1643	527	810	136	167	3			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	136	Total	C	H	N	O	S	23	0	0
			1926	592	924	187	202	21			
3	D	136	Total	C	H	N	O	S	23	0	0
			1926	592	924	187	202	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	121	SER	CYS	conflict	UNP Q07011
C	138	ASP	ASN	conflict	UNP Q07011
C	149	GLN	ASN	conflict	UNP Q07011
C	161	GLY	-	expression tag	UNP Q07011
C	162	SER	-	expression tag	UNP Q07011
C	163	LEU	-	expression tag	UNP Q07011
C	164	GLY	-	expression tag	UNP Q07011
D	121	SER	CYS	conflict	UNP Q07011

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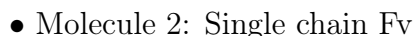
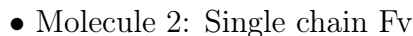
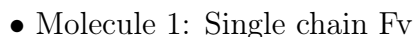
Chain	Residue	Modelled	Actual	Comment	Reference
D	138	ASP	ASN	conflict	UNP Q07011
D	149	GLN	ASN	conflict	UNP Q07011
D	161	GLY	-	expression tag	UNP Q07011
D	162	SER	-	expression tag	UNP Q07011
D	163	LEU	-	expression tag	UNP Q07011
D	164	GLY	-	expression tag	UNP Q07011

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	C	2	Total O 2 2	0	0
4	D	3	Total O 3 3	0	0
4	H	3	Total O 3 3	0	0
4	L	1	Total O 1 1	0	0

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- Molecule 1: Single chain Fv



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.92Å 125.21Å 128.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.78 – 3.10 89.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.78-3.10) 99.9 (89.78-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.205 , 0.271 0.216 , 0.284	Depositor DCC
R_{free} test set	915 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	105.2	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 110.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10655	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

5.1 Standard geometry

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	0.58	0/913	0.89	0/1238
1	H	0.57	0/922	0.97	0/1250
2	B	0.59	0/853	0.97	1/1158 (0.1%)
2	L	0.58	0/853	0.98	1/1158 (0.1%)
3	C	0.59	0/1018	1.06	2/1367 (0.1%)
3	D	0.58	0/1018	0.99	0/1367
All	All	0.58	0/5577	0.98	4/7538 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
2	B	0	1
3	C	0	3
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	99	PHE	CA-CB-CG	5.98	119.78	113.80
2	B	99	PHE	CA-CB-CG	5.96	119.76	113.80
3	C	42	ASN	N-CA-C	-5.49	106.53	113.23
3	C	42	ASN	CA-CB-CG	5.46	118.06	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	20	ARG	Sidechain
3	C	41	ARG	Sidechain
3	C	60	ARG	Sidechain
3	C	66	ARG	Sidechain
1	H	98	ARG	Sidechain

5.2 Too-close contacts

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	892	853	851	12	0
1	H	901	861	860	13	0
2	B	833	810	807	15	0
2	L	833	810	807	30	0
3	C	1002	924	922	20	0
3	D	1002	924	922	24	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	H	3	0	0	0	0
4	L	1	0	0	0	0
All	All	5473	5182	5169	107	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 10.

The worst 5 of 107 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:L:80:LEU:HD13	2:L:81:GLN:N	1.79	0.95
1:A:97:ALA:HB1	1:A:105:ILE:HG21	1.60	0.81
3:D:113:THR:OG1	3:D:116:GLY:O	1.99	0.80
2:L:17:VAL:HA	2:L:80:LEU:HD12	1.61	0.80
1:H:97:ALA:HB1	1:H:105:ILE:HG21	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	115/230 (50%)	110 (96%)	5 (4%)	0	100	100
1	H	116/230 (50%)	112 (97%)	4 (3%)	0	100	100
2	B	107/216 (50%)	100 (94%)	7 (6%)	0	100	100
2	L	107/216 (50%)	97 (91%)	8 (8%)	2 (2%)	6	27
3	C	134/141 (95%)	125 (93%)	9 (7%)	0	100	100
3	D	134/141 (95%)	123 (92%)	11 (8%)	0	100	100
All	All	713/1174 (61%)	667 (94%)	44 (6%)	2 (0%)	36	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	79	SER
2	L	42	PRO

5.3.2 Protein sidechains

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	96/195 (49%)	94 (98%)	2 (2%)	47	71
1	H	97/195 (50%)	97 (100%)	0	100	100
2	B	94/190 (50%)	90 (96%)	4 (4%)	26	57
2	L	94/190 (50%)	91 (97%)	3 (3%)	34	64
3	C	117/121 (97%)	113 (97%)	4 (3%)	32	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	117/121 (97%)	115 (98%)	2 (2%)	53	74
All	All	615/1012 (61%)	600 (98%)	15 (2%)	43	69

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	45	CYS
2	L	41	LYS
3	C	86	CYS
2	L	80	LEU
3	D	86	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	40	ASN
3	D	51	ASN
2	L	39	GLN
1	H	82	GLN
1	H	84	ASN

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 oligosaccharides 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	117/230 (50%)	-0.61	1 (0%) 81 63	94, 139, 175, 208	0
1	H	118/230 (51%)	-0.73	0 100 100	87, 117, 147, 172	0
2	B	109/216 (50%)	-0.58	0 100 100	91, 137, 179, 188	0
2	L	109/216 (50%)	-0.62	0 100 100	90, 126, 168, 182	0
3	C	136/141 (96%)	-0.73	0 100 100	88, 122, 163, 181	0
3	D	136/141 (96%)	-0.66	2 (1%) 72 52	88, 124, 170, 202	0
All	All	725/1174 (61%)	-0.66	3 (0%) 88 76	87, 127, 171, 208	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	161	GLY	3.0
1	A	102	SER	2.5
3	D	143	GLY	2.3

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 oligosaccharides 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.