



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:40 PM UTC

PDB ID : 7WKX / pdb_00007wkx
Title : IL-17A in complex with the humanized antibody HB0017
Authors : Xu, J.; Zhu, X.; He, Y.
Deposited on : 2022-01-12
Resolution : 2.81 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

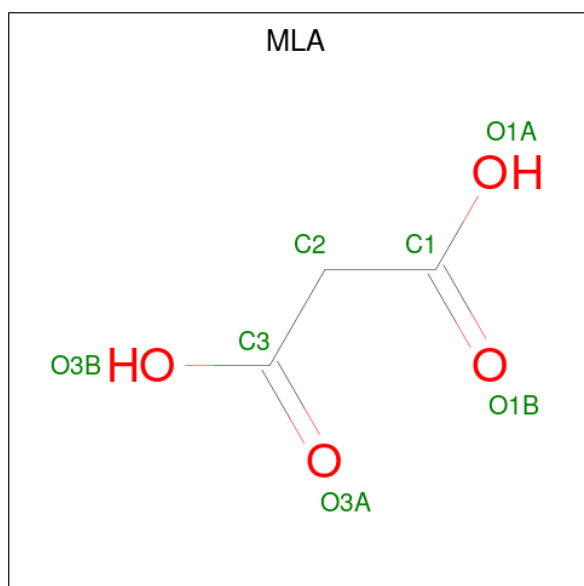
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Mol	Chain	Length	Quality of chain
3	F	151	

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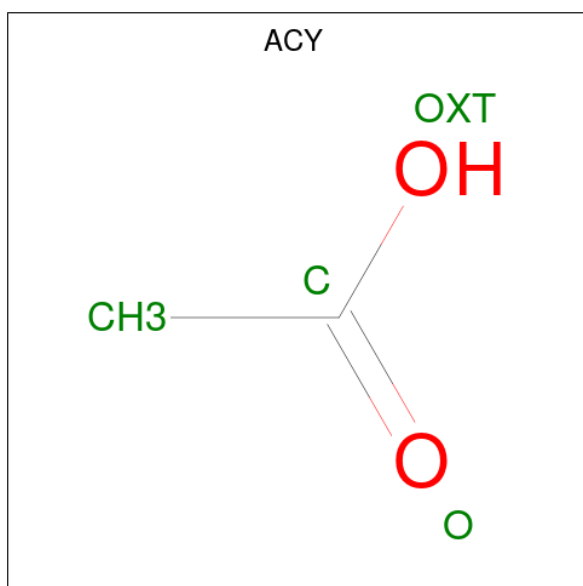
Chain	Residue	Modelled	Actual	Comment	Reference
E	13	GLU	-	expression tag	UNP Q16552
E	14	ASN	-	expression tag	UNP Q16552
E	15	LEU	-	expression tag	UNP Q16552
E	16	TYR	-	expression tag	UNP Q16552
E	17	PHE	-	expression tag	UNP Q16552
E	18	GLN	-	expression tag	UNP Q16552
E	19	GLY	-	expression tag	UNP Q16552
F	5	MET	-	initiating methionine	UNP Q16552
F	6	GLY	-	expression tag	UNP Q16552
F	7	HIS	-	expression tag	UNP Q16552
F	8	HIS	-	expression tag	UNP Q16552
F	9	HIS	-	expression tag	UNP Q16552
F	10	HIS	-	expression tag	UNP Q16552
F	11	HIS	-	expression tag	UNP Q16552
F	12	HIS	-	expression tag	UNP Q16552
F	13	GLU	-	expression tag	UNP Q16552
F	14	ASN	-	expression tag	UNP Q16552
F	15	LEU	-	expression tag	UNP Q16552
F	16	TYR	-	expression tag	UNP Q16552
F	17	PHE	-	expression tag	UNP Q16552
F	18	GLN	-	expression tag	UNP Q16552
F	19	GLY	-	expression tag	UNP Q16552

- Molecule 4 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	E	1	Total C O 7 3 4	0	0
4	F	1	Total C O 7 3 4	0	0

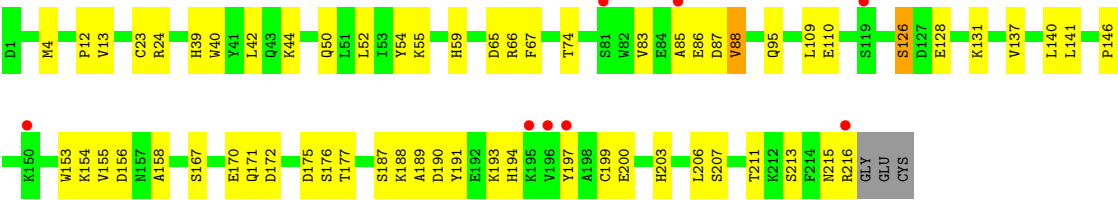
- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



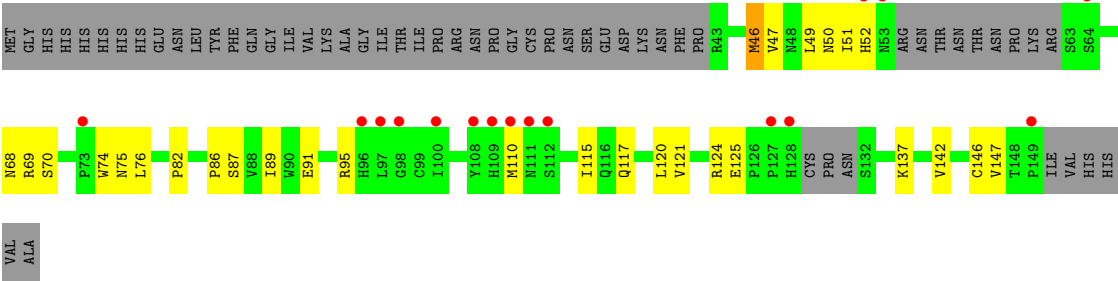
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

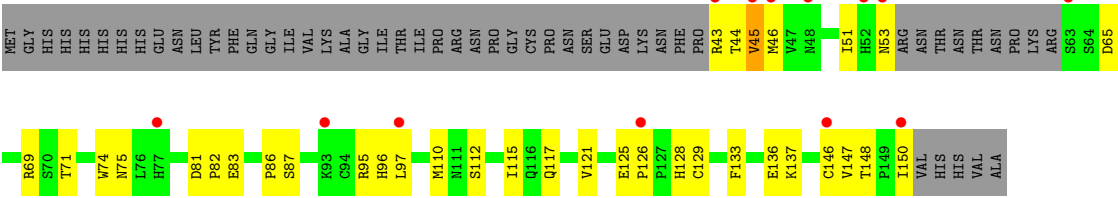
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total 7	O 7	0	0
6	B	3	Total 3	O 3	0	0
6	C	21	Total 21	O 21	0	0
6	D	5	Total 5	O 5	0	0
6	E	1	Total 1	O 1	0	0



● Molecule 3: Interleukin-17A



● Molecule 3: Interleukin-17A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	301.14Å 50.83Å 117.22Å 90.00° 101.27° 90.00°	Depositor
Resolution (Å)	45.20 – 2.81 45.20 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.1 (45.20-2.81) 95.5 (45.20-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.205 , 0.254 0.220 , 0.253	Depositor DCC
R_{free} test set	1997 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	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	0.93	EDS
Total number of atoms	8260	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, MLA

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	0.91	0/1678	1.25	3/2290 (0.1%)
1	B	0.92	0/1639	1.24	1/2237 (0.0%)
2	C	0.97	0/1741	1.23	1/2370 (0.0%)
2	D	0.93	0/1706	1.21	0/2325
3	E	0.91	0/791	1.21	0/1075
3	F	0.90	0/822	1.22	3/1120 (0.3%)
All	All	0.93	0/8377	1.23	8/11417 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASN	N-CA-C	-6.42	105.44	113.20
1	A	46	GLU	CB-CA-C	5.92	119.99	110.16
1	A	178	GLY	N-CA-C	-5.56	107.65	115.32
2	C	17	GLU	CB-CA-C	5.20	117.64	109.37
3	F	71	THR	N-CA-C	-5.17	105.77	111.71

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	1633	0	1569	36	0
1	B	1595	0	1522	61	0
2	C	1692	0	1635	21	0
2	D	1663	0	1603	42	0
3	E	773	0	743	33	0
3	F	802	0	773	33	0
4	A	7	0	2	0	0
4	B	7	0	2	0	0
4	C	21	0	6	1	0
4	E	7	0	2	0	0
4	F	7	0	2	1	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	A	7	0	0	0	0
6	B	3	0	0	0	0
6	C	21	0	0	0	0
6	D	5	0	0	0	0
6	E	1	0	0	0	0
All	All	8260	0	7871	197	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 12.

The worst 5 of 197 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)
3:E:115:ILE:HD12	3:F:115:ILE:HD12	1.50	0.94
3:E:52:HIS:HB3	3:F:136:GLU:HG2	1.58	0.84
1:B:76:VAL:HG13	1:B:78:THR:HG22	1.67	0.77
2:D:4:MET:HE3	2:D:23:CYS:SG	2.27	0.74
1:A:154:VAL:CG2	1:A:182:LEU:HD21	2.17	0.74

There are no symmetry-related clashes.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	192/195 (98%)	190 (99%)	2 (1%)	68	88
3	E	90/140 (64%)	89 (99%)	1 (1%)	65	86
3	F	94/140 (67%)	92 (98%)	2 (2%)	47	78
All	All	928/1032 (90%)	906 (98%)	22 (2%)	43	75

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	113	ARG
2	D	88	VAL
2	C	210	VAL
2	D	126	SER
1	B	26	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	59	HIS
3	E	111	ASN
2	D	215	ASN
2	C	47	GLN
2	D	14	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	217/217 (100%)	0.12	0 100 100	35, 55, 82, 123	0
1	B	212/217 (97%)	0.78	16 (7%) 20 14	47, 77, 106, 125	0
2	C	218/219 (99%)	-0.04	6 (2%) 55 44	34, 47, 73, 100	2 (0%)
2	D	216/219 (98%)	0.61	8 (3%) 45 36	47, 72, 108, 134	0
3	E	95/151 (62%)	1.16	16 (16%) 4 3	53, 80, 121, 136	0
3	F	99/151 (65%)	0.88	13 (13%) 7 5	47, 75, 112, 128	0
All	All	1057/1174 (90%)	0.49	59 (5%) 30 23	34, 65, 106, 136	2 (0%)

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	150	ILE	5.5
3	E	149	PRO	5.3
3	E	97	LEU	5.0
2	C	148[A]	GLU	4.4
3	F	53	ASN	3.7

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACY	A	302	4/4	0.51	0.26	69,75,82,93	0
5	ACY	D	301	4/4	0.60	0.26	86,91,91,97	0
4	MLA	F	201	7/7	0.65	0.11	95,100,106,106	0
5	ACY	C	301	4/4	0.77	0.20	68,74,75,81	0
5	ACY	B	302	4/4	0.77	0.20	75,77,77,79	0
4	MLA	E	201	7/7	0.85	0.12	85,95,99,102	0
4	MLA	C	304	7/7	0.87	0.16	63,69,78,84	0
4	MLA	C	303	7/7	0.91	0.14	68,80,90,96	0
4	MLA	C	302	7/7	0.91	0.15	61,70,87,91	0
4	MLA	B	301	7/7	0.92	0.16	63,68,80,83	0
4	MLA	A	301	7/7	0.95	0.09	46,53,65,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.