



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:27 AM UTC

PDB ID : 7ZAN / pdb_00007zan
Title : Crystal Structure of human IL-17A in complex with IL-17RA and IL-17RC
Authors : Rondeau, J.M.; Goepfert, A.
Deposited on : 2022-03-22
Resolution : 5.06 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)
Xtrriage (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

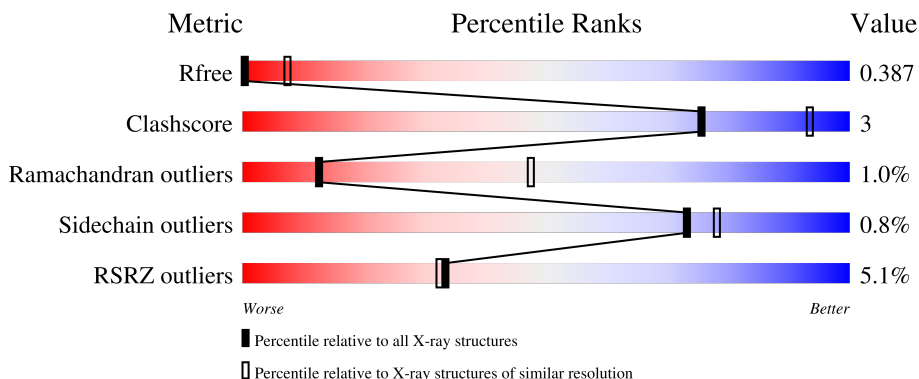
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.06 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	1018 (6.14-3.98)
Clashscore	190562	1050 (6.10-4.00)
Ramachandran outliers	187476	1021 (6.20-3.92)
Sidechain outliers	187428	1139 (6.22-3.90)
RSRZ outliers	180081	1013 (6.14-3.98)

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	123	
1	B	123	
2	C	292	
3	D	453	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14519 atoms, of which 7102 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 Interleukin-17A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	114	1816	576	887	174	173	6	887	0	0
1	B	111	1778	559	873	174	166	6	873	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP Q16552
A	68	ASP	ASN	engineered mutation	UNP Q16552
A	129	SER	CYS	engineered mutation	UNP Q16552
B	33	GLY	-	expression tag	UNP Q16552
B	68	ASP	ASN	engineered mutation	UNP Q16552
B	129	SER	CYS	engineered mutation	UNP Q16552

- Molecule 2 is a protein called Interleukin-17 receptor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	C	274	4362	1406	2127	405	407	17	2127	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	49	ASP	ASN	engineered mutation	UNP Q96F46
C	206	ASP	ASN	engineered mutation	UNP Q96F46
C	265	ASP	ASN	engineered mutation	UNP Q96F46
C	321	GLU	-	expression tag	UNP Q96F46
C	322	PHE	-	expression tag	UNP Q96F46
C	323	ARG	-	expression tag	UNP Q96F46
C	324	HIS	-	expression tag	UNP Q96F46

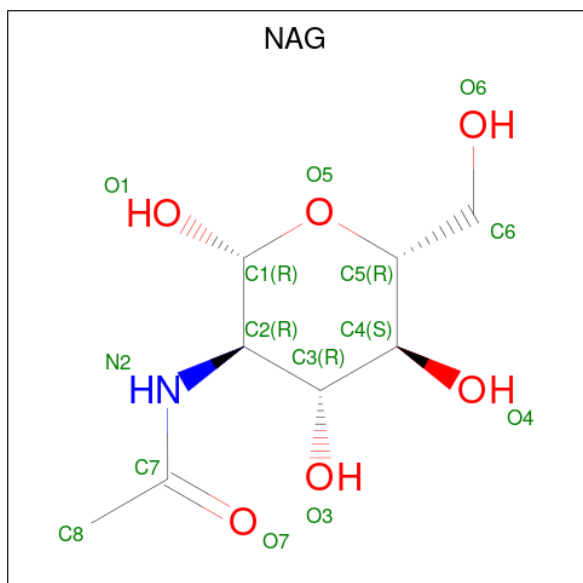
- Molecule 3 is a protein called Isoform 2 of Interleukin-17 receptor C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	D	422	6507	2089	3215	572	608	23	3215	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	307	ARG	GLN	conflict	UNP Q8NAC3
D	468	GLU	-	expression tag	UNP Q8NAC3
D	469	PHE	-	expression tag	UNP Q8NAC3
D	470	ARG	-	expression tag	UNP Q8NAC3
D	471	HIS	-	expression tag	UNP Q8NAC3
D	472	ASP	-	expression tag	UNP Q8NAC3
D	473	SER	-	expression tag	UNP Q8NAC3

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

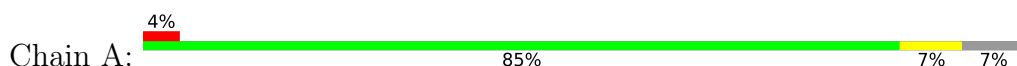


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
4	D	1	14	8	1	5	0	0
4	D	1	14	8	1	5	0	0
4	D	1	14	8	1	5	0	0

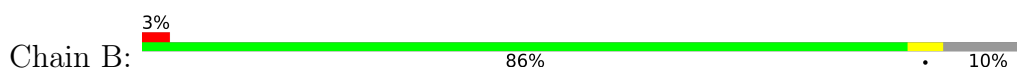
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

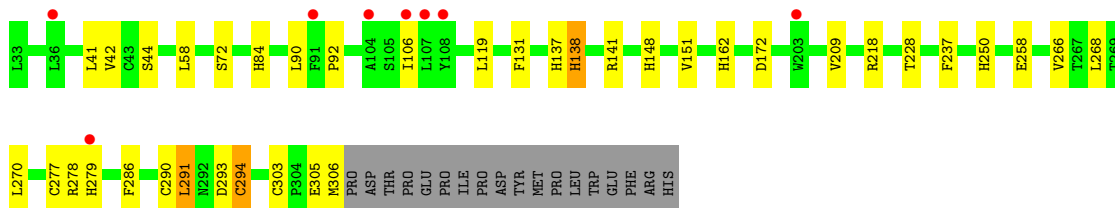
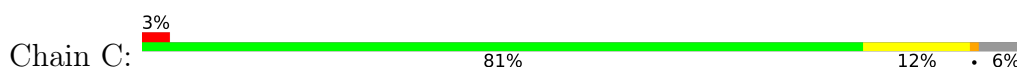
- Molecule 1: Interleukin-17A



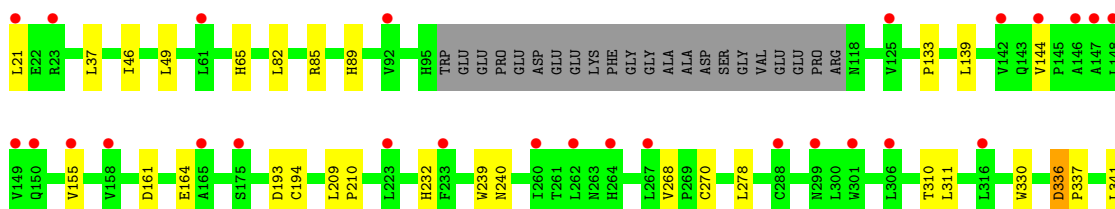
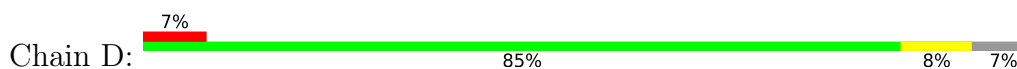
- Molecule 1: Interleukin-17A



- Molecule 2: Interleukin-17 receptor A



- Molecule 3: Isoform 2 of Interleukin-17 receptor C





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	186.31Å 186.31Å 238.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.55 – 5.06 37.55 – 5.06	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.55-5.06) 98.2 (37.55-5.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 5.08Å)	Xtrriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.294 , 0.353 0.317 , 0.387	Depositor DCC
R_{free} test set	530 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	335.2	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 482.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14519	wwPDB-VP
Average B, all atoms (Å ²)	268.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: NAG

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	0.66	0/953	0.98	0/1298
1	B	0.64	0/929	0.95	1/1267 (0.1%)
2	C	0.71	0/2303	0.98	2/3138 (0.1%)
3	D	0.73	0/3381	0.92	2/4637 (0.0%)
All	All	0.71	0/7566	0.95	5/10340 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	349	ASN	CA-CB-CG	7.72	120.32	112.60
1	B	65	ASP	CA-CB-CG	5.40	118.00	112.60
2	C	293	ASP	CA-CB-CG	5.20	117.80	112.60
3	D	194	CYS	N-CA-C	-5.19	102.66	110.70
2	C	131	PHE	CA-CB-CG	5.07	118.87	113.80

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	929	887	887	6	0
1	B	905	873	873	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2235	2127	2128	19	1
3	D	3292	3215	3216	17	0
4	C	14	0	13	0	0
4	D	42	0	39	0	0
All	All	7417	7102	7156	43	1

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 3.

The worst 5 of 43 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:B:74:TRP:CD1	1:B:92:ALA:HB1	2.16	0.81
1:A:74:TRP:CD1	1:A:92:ALA:HB1	2.21	0.76
2:C:250:HIS:ND1	2:C:268:LEU:HD21	2.03	0.73
1:B:90:TRP:NE1	2:C:119:LEU:HD22	2.07	0.69
1:A:151:VAL:HG11	1:A:153:HIS:CE1	2.28	0.68

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:ARG:HH12	2:C:172:ASP:OD1[12_544]	1.51	0.09

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	110/123 (89%)	104 (94%)	6 (6%)	0	100 100
1	B	109/123 (89%)	105 (96%)	4 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	272/292 (93%)	242 (89%)	24 (9%)	6 (2%)	5	28
3	D	418/453 (92%)	376 (90%)	39 (9%)	3 (1%)	18	55
All	All	909/991 (92%)	827 (91%)	73 (8%)	9 (1%)	12	47

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	291	LEU
2	C	294	CYS
2	C	58	LEU
3	D	193	ASP
2	C	277	CYS

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	108/116 (93%)	108 (100%)	0	100	100
1	B	106/116 (91%)	105 (99%)	1 (1%)	70	77
2	C	259/277 (94%)	255 (98%)	4 (2%)	57	71
3	D	370/396 (93%)	368 (100%)	2 (0%)	81	82
All	All	843/905 (93%)	836 (99%)	7 (1%)	73	78

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	237	PHE
2	C	258	GLU
3	D	161	ASP
3	D	37	LEU
2	C	162	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	280	GLN
3	D	89	HIS
3	D	380	GLN
3	D	370	GLN
2	C	95	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	503	3	14,14,15	0.57	0	17,19,21	1.50	3 (17%)
4	NAG	D	501	3	14,14,15	0.53	0	17,19,21	0.69	1 (5%)
4	NAG	C	401	2	14,14,15	0.61	0	17,19,21	1.19	2 (11%)
4	NAG	D	502	3	14,14,15	0.56	0	17,19,21	0.90	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	503	3	-	3/6/23/26	0/1/1/1
4	NAG	D	501	3	-	0/6/23/26	0/1/1/1
4	NAG	C	401	2	-	0/6/23/26	0/1/1/1
4	NAG	D	502	3	-	1/6/23/26	0/1/1/1

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(°)
4	D	503	NAG	C1-C2-N2	3.85	116.49	110.43
4	D	503	NAG	O5-C1-C2	-3.73	105.52	111.29
4	C	401	NAG	O5-C1-C2	-3.42	106.00	111.29
4	C	401	NAG	C1-C2-N2	2.76	114.78	110.43
4	D	503	NAG	C2-N2-C7	2.66	126.46	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	503	NAG	C1-C2-N2-C7
4	D	503	NAG	O5-C5-C6-O6
4	D	502	NAG	O5-C5-C6-O6
4	D	503	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	114/123 (92%)	0.13	5 (4%) 39 36	73, 141, 182, 192	0
1	B	111/123 (90%)	-0.06	4 (3%) 46 40	76, 122, 160, 180	0
2	C	274/292 (93%)	-0.07	8 (2%) 53 44	67, 129, 173, 187	0
3	D	422/453 (93%)	0.28	30 (7%) 22 25	111, 150, 183, 200	0
All	All	921/991 (92%)	0.12	47 (5%) 33 32	67, 140, 180, 200	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	149	VAL	10.6
3	D	148	LEU	8.6
3	D	144	VAL	7.8
1	A	97	LEU	7.5
3	D	61	LEU	7.4

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(\AA^2)	Q<0.9
4	NAG	D	502	14/15	0.54	0.07	300,300,300,300	0
4	NAG	D	503	14/15	0.65	0.08	272,272,273,273	0
4	NAG	D	501	14/15	0.72	0.08	300,300,300,300	0
4	NAG	C	401	14/15	0.85	0.11	223,239,249,250	0

6.5 Other polymers [i](#)

There are no such residues in this entry.