

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2022 – 10:58 am BST

PDB ID : 7ZAN

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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.31.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

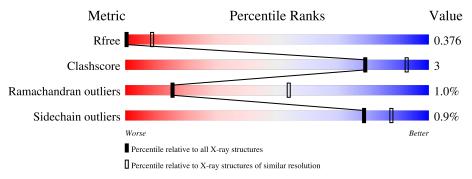
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.31.2 \end{tabular}$

1 Overall quality at a glance (i)

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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
R_{free}	130704	1143 (6.32-3.80)		
Clashscore	141614	1004 (6.30-3.82)		
Ramachandran outliers	138981	1149 (6.32-3.80)		
Sidechain outliers	138945	1125 (6.32-3.80)		

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 <=5%

Mol	Chain	Length	Quality of chain		
1	A	123	85%	7%	7%
1	В	123	87%	•	10%
2	С	292	81%	12%	• 6%
3	D	453	86%	7%	7%



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	\mathbf{Atoms}				ZeroOcc	AltConf	Trace		
1	Λ	114	Total	С	Н	N	О	S	887	0	0
1	Λ	114	1816	576	887	174	173	6	001		
1	R	111	Total	С	Н	N	О	S	873	0	0
1	Ъ	111	1778	559	873	174	166	6	019	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
В	33	GLY	-	expression tag	UNP Q16552
В	68	ASP	ASN	engineered mutation	UNP Q16552
В	129	SER	CYS	engineered mutation	UNP Q16552

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

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

There are 7 discrepancies between the modelled and reference sequences:

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



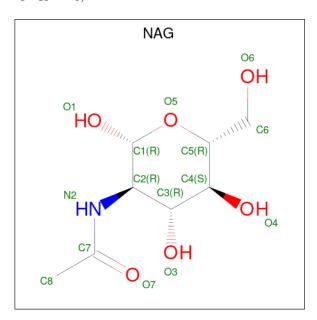
• Molecule 3 is a protein called Isoform 2 of Interleukin-17 receptor C.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
3	D	422	Total 6507	C 2089	H 3215	N 572	O 608	S 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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



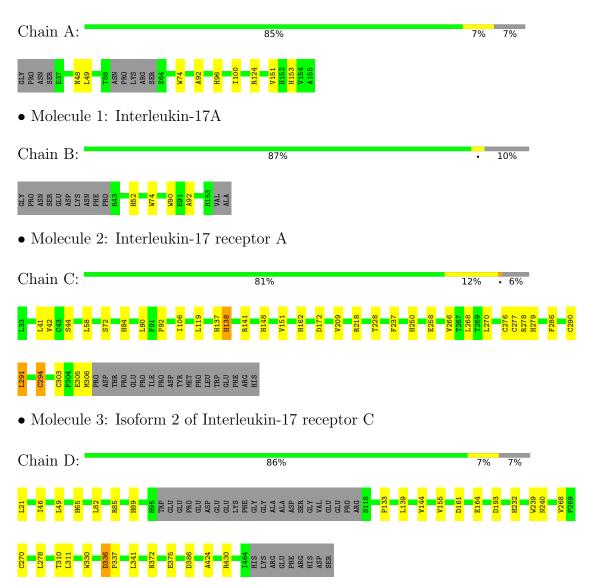
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0



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. 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. 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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	186.31Å 186.31Å 238.31Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.55 - 5.06	Depositor
Resolution (A)	37.55 - 5.06	EDS
% Data completeness	98.6 (37.55-5.06)	Depositor
(in resolution range)	98.6 (37.55-5.06)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.40 (at 5.08Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
D D.	0.294 , 0.353	Depositor
R, R_{free}	0.317 , 0.376	DCC
R_{free} test set	530 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	335.2	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L > = 0.38, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	14519	wwPDB-VP
Average B, all atoms (Å ²)	268.0	wwPDB-VP

Xtriage'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.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.33	0/953	0.55	0/1298	
1	В	0.31	0/929	0.51	0/1267	
2	С	0.35	0/2303	0.51	0/3138	
3	D	0.36	0/3381	0.51	0/4637	
All	All	0.34	0/7566	0.51	0/10340	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	929	887	887	6	0
1	В	905	873	873	4	0
2	С	2235	2127	2128	19	1
3	D	3292	3215	3216	15	0
4	С	14	0	13	0	0
4	D	42	0	39	0	0
All	All	7417	7102	7156	41	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 41 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	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	Perce	entiles
1	A	110/123 (89%)	104 (94%)	6 (6%)	0	100	100
1	В	109/123 (89%)	105 (96%)	4 (4%)	0	100	100
2	С	$272/292 \ (93\%)$	242 (89%)	24 (9%)	6 (2%)	6	37
3	D	418/453 (92%)	376 (90%)	39 (9%)	3 (1%)	22	62
All	All	909/991 (92%)	827 (91%)	73 (8%)	9 (1%)	15	54

5 of 9 Ramachandran outliers are listed below:

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

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
2	С	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	Percei	ntiles
1	A	108/116 (93%)	108 (100%)	0	100	100
1	В	106/116 (91%)	105 (99%)	1 (1%)	78	87
2	С	259/277~(94%)	254 (98%)	5 (2%)	57	75
3	D	370/396 (93%)	368 (100%)	2 (0%)	88	93
All	All	843/905 (93%)	835 (99%)	8 (1%)	78	87

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	386	ASP
3	D	161	ASP
2	С	258	GLU
2	С	237	PHE
2	С	276	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	С	101	GLN
2	С	148	HIS
3	D	89	HIS
3	D	65	HIS
2	С	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 monosaccharides 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	Trino	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	cles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	С	401	2	14,14,15	0.60	0	17,19,21	1.14	2 (11%)
4	NAG	D	501	3	14,14,15	0.52	0	17,19,21	0.67	1 (5%)
4	NAG	D	503	3	14,14,15	0.55	0	17,19,21	1.42	3 (17%)
4	NAG	D	502	3	14,14,15	0.55	0	17,19,21	0.87	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	С	401	2	-	0/6/23/26	0/1/1/1
4	NAG	D	501	3	-	0/6/23/26	0/1/1/1
4	NAG	D	503	3	-	3/6/23/26	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	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
4	D	503	NAG	O5-C1-C2	-3.65	105.52	111.29
4	D	503	NAG	C1-C2-N2	3.52	116.49	110.49
4	С	401	NAG	O5-C1-C2	-3.35	106.00	111.29
4	С	401	NAG	C1-C2-N2	2.51	114.78	110.49
4	D	502	NAG	O5-C1-C2	-2.51	107.33	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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.

