

# wwPDB X-ray Structure Validation Summary Report (i)

#### Apr 11, 2022 – 10:10 am BST

PDB ID	:	7AL7
Title	:	The Crystal Structure of Human IL-18 in Complex With Human IL-18 Binding
		Protein
Authors	:	Detry, S.; Andries, J.; Bloch, Y.; Clancy, D.; Savvides, S.N.
Deposited on		
Resolution	:	1.80  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 following versions of software and data (see references (1)) were used in the production of this report:

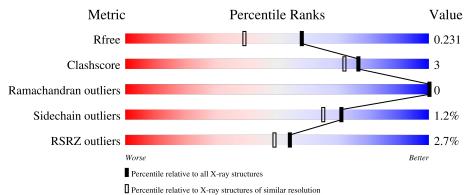
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793(1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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% 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	А	172	.% •	55%		8%	37%		
2	В	390	<u>2%</u> 36%		•		60%		



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4403 atoms, of which 2112 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-18-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	108	Total 1662	C 539	Н 818	N 144	0 156	${ m S}{ m 5}$	0	1	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	61	THR	-	expression tag	UNP O95998
А	62	GLY	-	expression tag	UNP O95998
А	195	GLY	-	expression tag	UNP 095998
А	196	THR	-	expression tag	UNP O95998
А	197	SER	-	expression tag	UNP O95998
А	198	ASP	-	expression tag	UNP O95998
А	199	GLU	-	expression tag	UNP O95998
А	200	VAL	-	expression tag	UNP O95998
A	201	ASP	-	expression tag	UNP O95998
А	202	GLY	-	expression tag	UNP O95998
А	203	GLY	-	expression tag	UNP O95998
A	204	SER	-	expression tag	UNP O95998
А	205	GLY	-	expression tag	UNP O95998
А	206	GLY	-	expression tag	UNP O95998
А	207	SER	-	expression tag	UNP O95998
А	208	GLY	-	expression tag	UNP O95998
A	209	LEU	-	expression tag	UNP O95998
А	210	ASN	-	expression tag	UNP O95998
A	211	ASP	-	expression tag	UNP O95998
A	212	ILE	-	expression tag	UNP O95998
А	213	PHE	-	expression tag	UNP O95998
А	214	GLU	-	expression tag	UNP O95998
А	215	ALA	-	expression tag	UNP O95998
А	216	GLN	-	expression tag	UNP O95998
А	217	LYS	-	expression tag	UNP O95998
А	218	ILE	-	expression tag	UNP O95998
А	219	GLU	-	expression tag	UNP O95998

There are 40 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference
А	220	TRP	-	expression tag	UNP O95998
А	221	HIS	-	expression tag	UNP O95998
A	222	GLU	-	expression tag	UNP O95998
А	223	GLY	-	expression tag	UNP O95998
А	224	ARG	-	expression tag	UNP O95998
А	225	THR	-	expression tag	UNP O95998
А	226	LYS	-	expression tag	UNP O95998
А	227	HIS	-	expression tag	UNP O95998
А	228	HIS	-	expression tag	UNP O95998
А	229	HIS	-	expression tag	UNP O95998
А	230	HIS	-	expression tag	UNP O95998
А	231	HIS	-	expression tag	UNP O95998
А	232	HIS	-	expression tag	UNP O95998

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• Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Interleuki n-18.

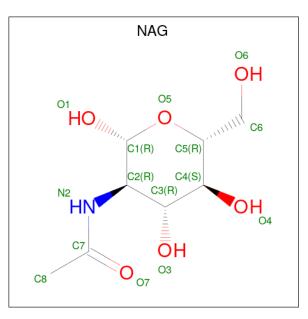
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	В	157	$\begin{array}{c} \text{Total} \\ 2527 \end{array}$	C 801	Н 1252	N 212	O 252	S 10	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-196	MET	-	initiating methionine	UNP P08515
В	-195	HIS	-	expression tag	UNP P08515
В	-194	HIS	-	expression tag	UNP P08515
В	-193	HIS	-	expression tag	UNP P08515
В	-192	HIS	-	expression tag	UNP P08515
В	-191	HIS	-	expression tag	UNP P08515
В	-190	HIS	-	expression tag	UNP P08515
В	28	SER	-	linker	UNP P08515
В	29	ASP	-	linker	UNP P08515
В	30	ARG	-	linker	UNP P08515
В	31	GLU	-	linker	UNP P08515
В	32	PHE	-	linker	UNP P08515
В	33	ASP	-	linker	UNP P08515
В	34	GLU	-	linker	UNP P08515
В	35	VAL	-	linker	UNP P08515

• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Δ	1	Total	С	Η	Ν	0	0	0
0	11	T	28	8	14	1	5	0	0
3	Δ	1	Total	С	Η	Ν	Ο	0	0
0	11	I	28	8	14	1	5	0	0
3	Δ	1	Total	Ċ	Η	N	0	0	0
5	11	1	28	8	14	1	5		0

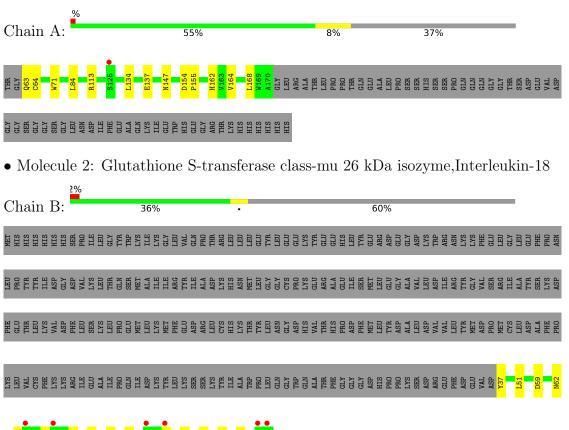
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	53	Total         O           53         53	0	0
4	В	77	Total O 77 77	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-18-binding protein





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	109.81Å 44.52Å 60.28Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $99.86^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	59.39 - 1.80	Depositor
Resolution (A)	59.39 - 1.80	EDS
% Data completeness	98.3 (59.39-1.80)	Depositor
(in resolution range)	98.8(59.39-1.80)	EDS
R <sub>merge</sub>	0.05	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.02 (at 1.80 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D.	0.209 , $0.232$	Depositor
$R, R_{free}$	0.209 , $0.231$	DCC
$R_{free}$ test set	2651  reflections  (10.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	35.0	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4403	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.65% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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, CSO, PCA

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		
	Moi Chain		# Z  > 5	RMSZ	# Z  > 5	
1	А	0.56	0/859	0.68	0/1178	
2	В	0.47	0/1288	0.67	0/1725	
All	All	0.51	0/2147	0.67	0/2903	

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	А	844	818	823	6	0
2	В	1275	1252	1255	7	0
3	А	42	42	39	1	0
4	А	53	0	0	0	0
4	В	77	0	0	1	0
All	All	2291	2112	2117	13	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 3.

The worst 5 of 13 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:B:74:CYS:HA	2:B:77:ASN:OD1	1.88	0.74
1:A:113:ARG:HB3	1:A:137:GLU:HB2	1.75	0.68
2:B:162:ALA:HB2	2:B:185:ILE:HG22	1.84	0.60
2:B:37:TYR:N	2:B:91:SER:HG	2.01	0.58
2:B:145:HIS:HB3	2:B:148:LYS:HD2	1.93	0.51

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	Perce	ntiles
1	А	107/172~(62%)	104 (97%)	3~(3%)	0	100	100
2	В	154/390~(40%)	152 (99%)	2(1%)	0	100	100
All	All	261/562~(46%)	256~(98%)	5(2%)	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 side chain 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	Analysed Rotameric Outliers		Percentiles		
1	А	95/145~(66%)	94 (99%)	1 (1%)	73	68	
2	В	147/356~(41%)	145 (99%)	2(1%)	67	59	
All	All	242/501~(48%)	239~(99%)	3 (1%)	71	65	



All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	64	CYS
2	В	59	ASP
2	В	62	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type	
2	В	62	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)

2 non-standard protein/DNA/RNA residues 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).

Mal	Mol Type Chain H	Type	Chain	Res	Ros	Doc	Dec	Dec	Link	B	ond leng	gths	B	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2					
2	CSO	В	104	2	3,6,7	2.14	1 (33%)	0,6,8	-	-					
1	PCA	А	63	1	7,8,9	2.34	2 (28%)	9,10,12	1.95	<mark>5 (55%)</mark>					

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
2	CSO	В	104	2	-	0/1/5/7	-
1	PCA	А	63	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	63	PCA	CD-N	4.70	1.47	1.34
1	А	63	PCA	CA-N	3.92	1.51	1.46
2	В	104	CSO	O-C	3.69	1.34	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	А	63	PCA	CA-N-CD	-3.01	103.28	113.58
1	А	63	PCA	OE-CD-CG	-2.75	121.96	126.76
1	А	63	PCA	O-C-CA	-2.67	117.78	124.78
1	А	63	PCA	CG-CD-N	2.23	114.16	108.39
1	А	63	PCA	CB-CA-N	2.11	109.35	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

3 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	Turne	Chain	Res	Link	Bo	Bond lengths			Bond angles		
	Type	Ullalli		LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
3	NAG	А	302	1	14,14,15	0.42	0	17,19,21	0.49	0	
3	NAG	А	301	1	14,14,15	0.53	0	17,19,21	0.49	0	
3	NAG	А	303	1	14,14,15	0.72	1 (7%)	17,19,21	1.06	1 (5%)	

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
3	NAG	А	302	1	-	0/6/23/26	0/1/1/1
3	NAG	А	301	1	-	0/6/23/26	0/1/1/1
3	NAG	А	303	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	303	NAG	O5-C1	2.12	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	
3	А	303	NAG	C1-O5-C5	3.69	117.19	112.19	

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	303	NAG	O5-C5-C6-O6
3	А	303	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	303	NAG	1	0

## 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	107/172~(62%)	0.27	1 (0%) 84 82	17, 28, 59, 99	0
2	В	156/390~(40%)	0.24	6 (3%) 40 35	13, 27, 75, 94	0
All	All	263/562~(46%)	0.25	7 (2%) 54 49	13, 28, 67, 99	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	192	GLU	4.3
2	В	75	ARG	3.1
1	А	125	SER	2.5
2	В	193	ASP	2.4
2	В	143	PRO	2.2

## 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
1	PCA	А	63	8/9	0.81	0.17	50,75,97,97	0
2	CSO	В	104	7/8	0.92	0.16	37,48,52,63	0

## 6.3 Carbohydrates (i)

There are no monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	NAG	А	302	14/15	0.81	0.22	71,94,105,115	0
3	NAG	А	303	14/15	0.87	0.20	63,79,90,96	0
3	NAG	А	301	14/15	0.91	0.09	32,44,64,65	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

