



Full wwPDB X-ray Structure Validation Report ⓘ

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
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Deposited on : 2020-10-05
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
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

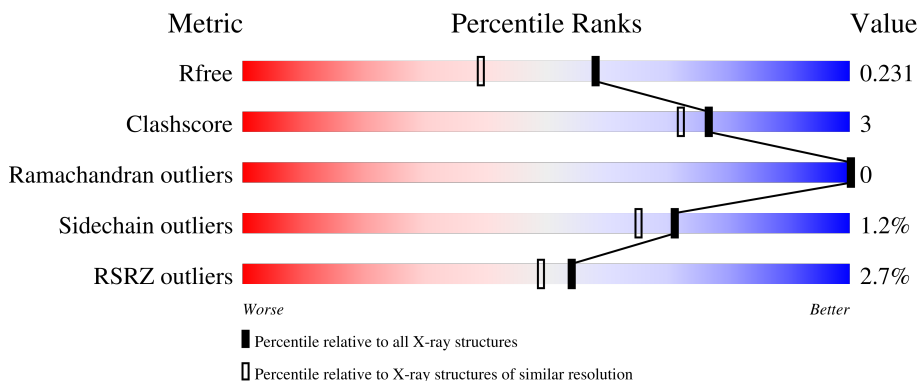
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 $\leq 5\%$. 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	172	 2%
2	B	390	 2%

2 Entry composition

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	
			Total	C	H	N	O				S
1	A	108	1662	539	818	144	156	5	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	157	2527	801	1252	212	252	10	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	A	1	28	8	14	1	5	0	0
3	A	1	28	8	14	1	5	0	0
3	A	1	28	8	14	1	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	77	Total	O	0	0
			77	77		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.81Å 44.52Å 60.28Å 90.00° 99.86° 90.00°	Depositor
Resolution (Å)	59.39 – 1.80 59.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (59.39-1.80) 98.8 (59.39-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.209 , 0.232 0.209 , 0.231	Depositor 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 ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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.*

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

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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	0/859	0.68	0/1178
2	B	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

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	844	818	823	6	0
2	B	1275	1252	1255	7	0
3	A	42	42	39	1	0
4	A	53	0	0	0	0
4	B	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.

All (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
2:B:51:LEU:H	2:B:51:LEU:HD23	1.78	0.48
1:A:84:LEU:HD12	1:A:134:LEU:HD23	1.99	0.45
1:A:154:ASP:HB2	1:A:155:PRO:CD	2.47	0.45
1:A:162:HIS:CE1	3:A:303:NAG:H5	2.52	0.44
1:A:147:ASN:HA	1:A:164:VAL:HG22	2.02	0.42
1:A:71:TRP:CE2	1:A:168:LEU:HD22	2.56	0.41
2:B:117:ILE:HD11	2:B:174:LEU:HB2	2.03	0.41
2:B:71:ASP:O	4:B:201:HOH:O	2.22	0.41

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	Percentiles	
1	A	107/172 (62%)	104 (97%)	3 (3%)	0	100	100
2	B	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 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	95/145 (66%)	94 (99%)	1 (1%)	73	68
2	B	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	A	64	CYS
2	B	59	ASP
2	B	62	ASN

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

Mol	Chain	Res	Type
2	B	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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CSO	B	104	2	3,6,7	2.14	1 (33%)	0,6,8	-	-
1	PCA	A	63	1	7,8,9	2.34	2 (28%)	9,10,12	1.95	5 (55%)

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	B	104	2	-	0/1/5/7	-
1	PCA	A	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)	Ideal(Å)
1	A	63	PCA	CD-N	4.70	1.47	1.34
1	A	63	PCA	CA-N	3.92	1.51	1.46
2	B	104	CSO	O-C	3.69	1.34	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	PCA	CA-N-CD	-3.01	103.28	113.58
1	A	63	PCA	OE-CD-CG	-2.75	121.96	126.76
1	A	63	PCA	O-C-CA	-2.67	117.78	124.78
1	A	63	PCA	CG-CD-N	2.23	114.16	108.39
1	A	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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	302	1	14,14,15	0.42	0	17,19,21	0.49	0
3	NAG	A	301	1	14,14,15	0.53	0	17,19,21	0.49	0
3	NAG	A	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	A	302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	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)	Ideal(Å)
3	A	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(°)	Ideal(°)
3	A	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	A	303	NAG	O5-C5-C6-O6
3	A	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	A	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, 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	107/172 (62%)	0.27	1 (0%) 84 82	17, 28, 59, 99	0
2	B	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

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	192	GLU	4.3
2	B	75	ARG	3.1
1	A	125	SER	2.5
2	B	193	ASP	2.4
2	B	143	PRO	2.2
2	B	145	HIS	2.2
2	B	72	SER	2.1

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, 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
1	PCA	A	63	8/9	0.81	0.17	50,75,97,97	0
2	CSO	B	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, 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
3	NAG	A	302	14/15	0.81	0.22	71,94,105,115	0
3	NAG	A	303	14/15	0.87	0.20	63,79,90,96	0
3	NAG	A	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.