



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:29 AM GMT

PDB ID : 3INK
Title : UNRAVELING THE STRUCTURE OF INTERLEUKIN-2: REPLY
Authors : Mckay, D.B.; Brandhuber, B.J.
Deposited on : 1992-12-09
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

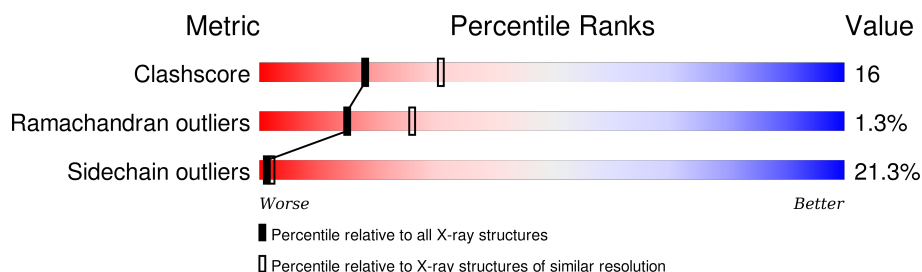
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	133	
1	D	133	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1996 atoms, of which 0 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	122	Total	C	N	O	S	0	0	1
			998	643	167	183	5			
1	D	122	Total	C	N	O	S	0	0	1
			998	643	167	183	5			

There are 2 discrepancies between the modelled and reference sequences:

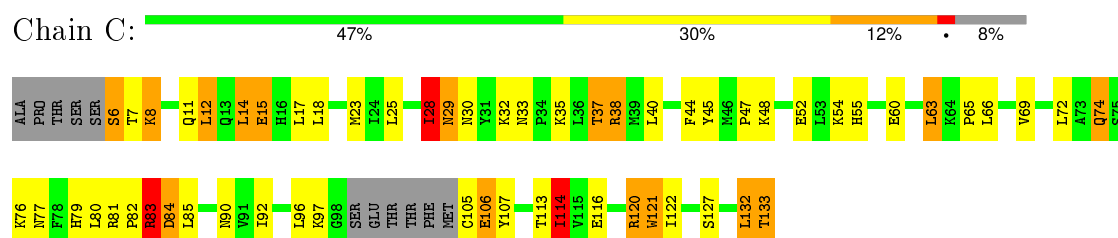
Chain	Residue	Modelled	Actual	Comment	Reference
C	125	ALA	CYS	CONFLICT	UNP P60568
D	125	ALA	CYS	CONFLICT	UNP P60568

3 Residue-property plots

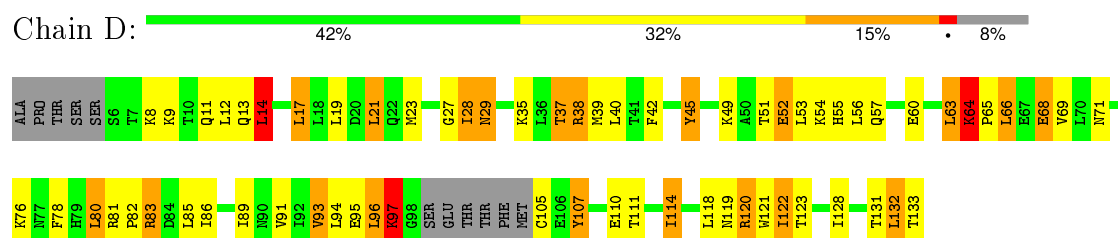
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: INTERLEUKIN-2



• Molecule 1: INTERLEUKIN-2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.80 Å 40.10 Å 33.70 Å 90.00° 109.30° 93.20°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1996	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	C	1.06	0/1013	1.87	24/1366 (1.8%)
1	D	1.08	1/1013 (0.1%)	2.00	29/1366 (2.1%)
All	All	1.07	1/2026 (0.0%)	1.94	53/2732 (1.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	LYS	C-N	-5.52	1.23	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	ARG	NE-CZ-NH2	-13.48	113.56	120.30
1	D	83	ARG	NE-CZ-NH1	12.25	126.42	120.30
1	D	120	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	C	120	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	C	37	THR	CA-CB-CG2	-9.15	99.58	112.40
1	D	121	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	D	121	TRP	CG-CD2-CE3	8.22	141.30	133.90
1	C	121	TRP	CD1-CG-CD2	7.73	112.49	106.30
1	C	121	TRP	CG-CD2-CE3	7.58	140.72	133.90
1	C	114	ILE	CB-CA-C	-7.48	96.63	111.60
1	D	45	TYR	CB-CG-CD2	-7.46	116.52	121.00
1	D	114	ILE	CB-CA-C	-7.24	97.12	111.60
1	D	96	LEU	N-CA-C	7.23	130.52	111.00
1	C	132	LEU	CA-CB-CG	7.12	131.68	115.30
1	D	121	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	D	37	THR	CA-CB-CG2	-7.02	102.57	112.40
1	C	121	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	D	93	VAL	CG1-CB-CG2	-6.98	99.73	110.90
1	D	121	TRP	CG-CD1-NE1	-6.74	103.36	110.10
1	C	121	TRP	CB-CG-CD1	-6.53	118.51	127.00
1	C	8	LYS	CA-C-N	6.52	131.53	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	6	SER	N-CA-C	-6.22	94.21	111.00
1	C	132	LEU	N-CA-CB	-6.21	97.98	110.40
1	D	42	PHE	O-C-N	6.20	132.62	122.70
1	C	121	TRP	CG-CD1-NE1	-6.15	103.95	110.10
1	D	81	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	97	LYS	N-CA-CB	-6.12	99.59	110.60
1	D	64	LYS	CD-CE-NZ	6.11	125.74	111.70
1	C	45	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	D	121	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	C	38	ARG	CB-CG-CD	5.86	126.85	111.60
1	C	15	GLU	CA-CB-CG	5.84	126.26	113.40
1	D	9	LYS	CA-CB-CG	-5.78	100.68	113.40
1	D	96	LEU	CA-C-N	5.76	129.88	117.20
1	D	68	GLU	CB-CG-CD	-5.61	99.04	114.20
1	D	80	LEU	CB-CA-C	-5.59	99.59	110.20
1	C	83	ARG	CB-CG-CD	5.58	126.12	111.60
1	D	69	VAL	CG1-CB-CG2	-5.53	102.06	110.90
1	D	9	LYS	CB-CG-CD	5.47	125.82	111.60
1	C	28	ILE	CB-CG1-CD1	-5.45	98.64	113.90
1	C	84	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	17	LEU	CA-CB-CG	5.43	127.79	115.30
1	C	133	THR	CA-CB-CG2	5.43	120.00	112.40
1	D	29	ASN	N-CA-C	5.42	125.62	111.00
1	C	14	LEU	CA-CB-CG	5.33	127.56	115.30
1	D	14	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	68	GLU	CA-CB-CG	5.28	125.01	113.40
1	D	123	THR	CA-CB-CG2	-5.25	105.04	112.40
1	D	114	ILE	N-CA-CB	5.12	122.57	110.80
1	D	28	ILE	CB-CG1-CD1	-5.04	99.77	113.90
1	D	17	LEU	CA-CB-CG	5.02	126.86	115.30
1	C	114	ILE	N-CA-CB	5.01	122.33	110.80

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	C	998	0	1039	30	0
1	D	998	0	1039	35	0
All	All	1996	0	2078	64	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 16.

All (64) 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:D:13:GLN:NE2	1:D:95:GLU:OE1	1.75	1.18
1:D:64:LYS:HG3	1:D:65:PRO:HD3	1.41	1.00
1:C:44:PHE:CE2	1:C:114:ILE:HD13	2.08	0.89
1:C:35:LYS:NZ	1:C:74:GLN:OE1	2.08	0.86
1:C:44:PHE:HE2	1:C:114:ILE:HD13	1.41	0.85
1:D:128:ILE:O	1:D:131:THR:OG1	1.96	0.81
1:D:52:GLU:H	1:D:55:HIS:CD2	2.08	0.71
1:D:51:THR:H	1:D:55:HIS:CD2	2.10	0.70
1:D:105:CYS:SG	1:D:107:TYR:CE1	2.86	0.68
1:D:13:GLN:HE21	1:D:95:GLU:CD	1.95	0.66
1:D:56:LEU:HB3	1:D:93:VAL:HG13	1.79	0.64
1:C:18:LEU:HD11	1:C:122:ILE:HG23	1.81	0.63
1:D:35:LYS:HA	1:D:38:ARG:HE	1.65	0.62
1:C:11:GLN:HB2	1:C:132:LEU:HD23	1.81	0.62
1:D:52:GLU:H	1:D:55:HIS:HD2	1.46	0.61
1:D:35:LYS:O	1:D:38:ARG:HG2	2.01	0.60
1:C:8:LYS:O	1:C:12:LEU:HB2	2.01	0.60
1:C:105:CYS:SG	1:C:107:TYR:CE1	2.95	0.60
1:C:82:PRO:HG2	1:C:83:ARG:HH11	1.68	0.59
1:C:81:ARG:HB3	1:C:83:ARG:HG2	1.85	0.58
1:D:64:LYS:HG3	1:D:65:PRO:CD	2.27	0.57
1:D:28:ILE:HG12	1:D:39:MET:HE1	1.88	0.56
1:D:68:GLU:HA	1:D:71:ASN:ND2	2.20	0.56
1:C:23:MET:SD	1:C:79:HIS:HD2	2.31	0.54
1:D:52:GLU:OE1	1:D:54:LYS:HG2	2.10	0.51
1:C:47:PRO:HG3	1:C:121:TRP:CZ2	2.46	0.51
1:C:92:ILE:HG22	1:C:96:LEU:HD12	1.93	0.50
1:C:32:LYS:HE2	1:C:76:LYS:HD3	1.93	0.49
1:D:132:LEU:HD13	1:D:132:LEU:N	2.26	0.49
1:C:69:VAL:HG11	1:C:114:ILE:HD11	1.95	0.49
1:C:83:ARG:H	1:C:83:ARG:HD3	1.78	0.49
1:D:23:MET:SD	1:D:80:LEU:HD13	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:GLU:HA	1:D:63:LEU:HD22	1.95	0.47
1:D:14:LEU:HD13	1:D:96:LEU:HD21	1.95	0.47
1:D:51:THR:N	1:D:55:HIS:CD2	2.81	0.47
1:D:51:THR:N	1:D:55:HIS:HD2	2.12	0.47
1:D:66:LEU:HD13	1:D:86:ILE:HD11	1.96	0.47
1:D:132:LEU:O	1:D:133:THR:HB	2.16	0.46
1:C:25:LEU:O	1:C:29:ASN:HB2	2.16	0.46
1:D:51:THR:H	1:D:55:HIS:HD2	1.60	0.46
1:C:52:GLU:O	1:C:55:HIS:HB2	2.16	0.46
1:D:53:LEU:O	1:D:97:LYS:HB3	2.17	0.45
1:C:18:LEU:CD1	1:C:122:ILE:HG23	2.44	0.44
1:D:13:GLN:HG2	1:D:95:GLU:OE1	2.18	0.44
1:D:89:ILE:O	1:D:93:VAL:HG23	2.17	0.44
1:C:114:ILE:H	1:C:114:ILE:HG12	1.69	0.44
1:C:28:ILE:HA	1:C:33:ASN:ND2	2.33	0.43
1:C:80:LEU:HB3	1:C:85:LEU:HG	2.01	0.43
1:C:83:ARG:H	1:C:83:ARG:CD	2.29	0.43
1:C:60:GLU:HA	1:C:63:LEU:HD22	2.00	0.43
1:D:17:LEU:HG	1:D:21:LEU:HD22	2.00	0.42
1:C:48:LYS:HB2	1:C:106:GLU:O	2.19	0.42
1:D:118:LEU:O	1:D:122:ILE:HD12	2.20	0.42
1:C:11:GLN:O	1:C:15:GLU:HG3	2.20	0.42
1:C:28:ILE:C	1:C:33:ASN:HD22	2.16	0.42
1:C:113:THR:CG2	1:C:116:GLU:H	2.33	0.42
1:D:23:MET:SD	1:D:80:LEU:CD1	3.08	0.41
1:D:27:GLY:HA3	1:D:78:PHE:CE1	2.55	0.41
1:C:80:LEU:HD12	1:C:80:LEU:HA	1.82	0.41
1:D:13:GLN:CG	1:D:95:GLU:OE1	2.68	0.41
1:C:35:LYS:HD3	1:C:72:LEU:O	2.20	0.41
1:D:78:PHE:CD2	1:D:82:PRO:HG3	2.55	0.41
1:D:8:LYS:O	1:D:12:LEU:HD13	2.21	0.40
1:C:83:ARG:HG3	1:D:45:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	118/133 (89%)	111 (94%)	6 (5%)	1 (1%)	24	41
1	D	118/133 (89%)	111 (94%)	5 (4%)	2 (2%)	11	19
All	All	236/266 (89%)	222 (94%)	11 (5%)	3 (1%)	15	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	29	ASN
1	C	29	ASN
1	D	107	TYR

5.3.2 Protein sidechains ⓘ

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	C	115/125 (92%)	92 (80%)	23 (20%)	1	3
1	D	115/125 (92%)	89 (77%)	26 (23%)	1	1
All	All	230/250 (92%)	181 (79%)	49 (21%)	1	2

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	SER
1	C	7	THR
1	C	12	LEU
1	C	14	LEU
1	C	28	ILE
1	C	30	ASN
1	C	37	THR
1	C	38	ARG
1	C	40	LEU

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Mol	Chain	Res	Type
1	C	54	LYS
1	C	63	LEU
1	C	65	PRO
1	C	66	LEU
1	C	74	GLN
1	C	77	ASN
1	C	83	ARG
1	C	84	ASP
1	C	90	ASN
1	C	106	GLU
1	C	114	ILE
1	C	120	ARG
1	C	127	SER
1	C	133	THR
1	D	11	GLN
1	D	14	LEU
1	D	19	LEU
1	D	21	LEU
1	D	37	THR
1	D	38	ARG
1	D	40	LEU
1	D	49	LYS
1	D	52	GLU
1	D	57	GLN
1	D	63	LEU
1	D	64	LYS
1	D	66	LEU
1	D	76	LYS
1	D	83	ARG
1	D	85	LEU
1	D	91	VAL
1	D	94	LEU
1	D	97	LYS
1	D	110	GLU
1	D	111	THR
1	D	114	ILE
1	D	119	ASN
1	D	120	ARG
1	D	122	ILE
1	D	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	79	HIS
1	D	57	GLN
1	D	71	ASN
1	D	90	ASN
1	D	119	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.