



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:51 pm GMT

PDB ID : 2IRT
Title : INITIAL CRYSTALLOGRAPHIC ANALYSES OF A RECOMBINANT
INTERLEUKIN-1 RECEPTOR ANTAGONIST PROTEIN
Authors : Finzel, B.C.; Clancy, L.L.; Einspahr, H.M.
Deposited on : 1994-07-13
Resolution : 3.20 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

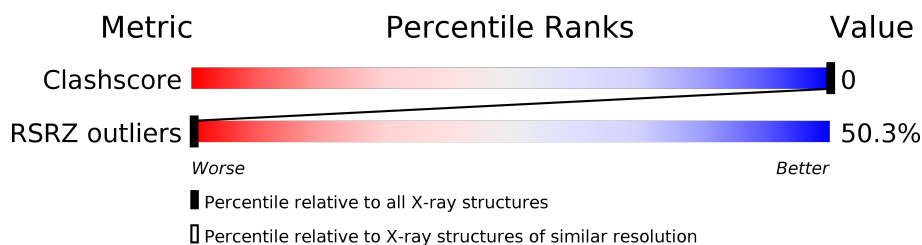
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	112137	1009 (3.20-3.20)
RSRZ outliers	101464	1020 (3.22-3.18)

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.

Mol	Chain	Length	Quality of chain
1	A	152	<div> <div>44%</div> <div>95%</div> <div>5%</div> </div>
1	B	152	<div> <div>52%</div> <div>95%</div> <div>5%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 290 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.

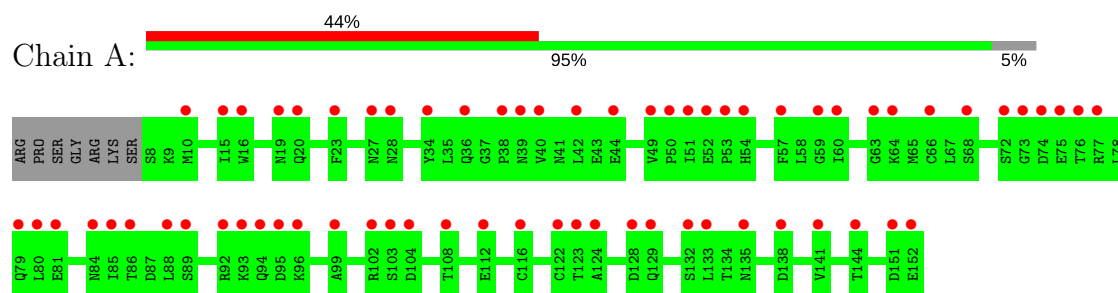
- Molecule 1 is a protein called INTERLEUKIN-1 RECEPTOR ANTAGONIST.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	145	Total 145	C 145	0	0	145
1	B	145	Total 145	C 145	0	0	145

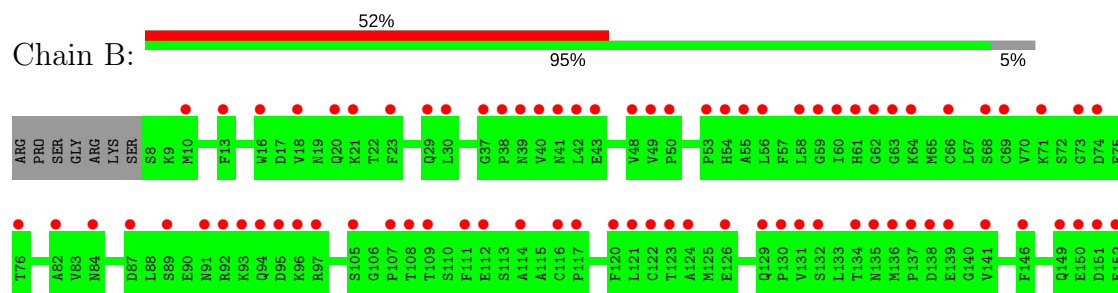
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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-1 RECEPTOR ANTAGONIST



• Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.35Å 72.35Å 114.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.00-3.20) 98.9 (19.77-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	54.64 (at 3.22Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.440 , (Not available) 0.439 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.36	EDS
Total number of atoms	290	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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](#)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	145	0	0	0	0
1	B	145	0	0	0	0
All	All	290	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

6.1 Protein, DNA and RNA chains

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	145/152 (95%)	2.59	67 (46%) 0 0	0, 0, 0, 0	0
1	B	145/152 (95%)	3.01	79 (54%) 0 0	0, 0, 0, 0	0
All	All	290/304 (95%)	2.80	146 (50%) 0 0	0, 0, 0, 0	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	TRP	16.7
1	B	74	ASP	16.3
1	B	138	ASP	15.0
1	A	63	GLY	14.3
1	B	63	GLY	13.3
1	A	151	ASP	13.0
1	B	116	CYS	12.5
1	A	92	ARG	11.9
1	A	138	ASP	11.0
1	B	96	LYS	10.7
1	B	61	HIS	9.9
1	B	108	THR	9.9
1	A	68	SER	9.0
1	B	117	PRO	8.8
1	B	94	GLN	8.6
1	B	152	GLU	8.6
1	A	20	GLN	8.5
1	A	103	SER	8.2
1	B	129	GLN	8.2
1	A	44	GLU	7.7
1	B	37	GLY	7.5
1	B	50	PRO	7.5
1	B	139	GLU	7.5
1	B	13	PHE	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	71	LYS	7.2
1	B	21	LYS	6.8
1	B	10	MET	6.8
1	A	36	GLN	6.6
1	A	93	LYS	6.6
1	A	89	SER	6.5
1	A	94	GLN	6.5
1	A	108	THR	6.5
1	A	40	VAL	6.4
1	A	74	ASP	6.3
1	B	55	ALA	6.1
1	A	85	ILE	6.1
1	B	109	THR	6.1
1	B	132	SER	6.0
1	B	84	ASN	6.0
1	A	15	ILE	5.9
1	B	87	ASP	5.8
1	A	38	PRO	5.7
1	B	124	ALA	5.3
1	B	92	ARG	5.2
1	A	135	ASN	5.2
1	A	19	ASN	5.1
1	A	128	ASP	5.1
1	B	122	CYS	4.9
1	A	124	ALA	4.7
1	A	95	ASP	4.7
1	B	150	GLU	4.7
1	A	76	THR	4.7
1	B	93	LYS	4.7
1	B	105	SER	4.5
1	B	20	GLN	4.5
1	B	89	SER	4.5
1	A	28	ASN	4.5
1	A	52	GLU	4.4
1	A	51	ILE	4.2
1	A	144	THR	4.2
1	B	62	GLY	4.2
1	B	48	VAL	4.1
1	B	126	GLU	4.0
1	A	34	TYR	4.0
1	B	64	LYS	3.9
1	B	66	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	91	ASN	3.9
1	B	114	ALA	3.8
1	B	121	LEU	3.7
1	B	82	ALA	3.7
1	B	38	PRO	3.7
1	B	53	PRO	3.7
1	A	73	GLY	3.6
1	B	73	GLY	3.5
1	A	53	PRO	3.5
1	B	41	ASN	3.5
1	B	107	PRO	3.5
1	B	40	VAL	3.4
1	A	102	ARG	3.4
1	B	95	ASP	3.4
1	B	137	PRO	3.3
1	B	54	HIS	3.3
1	A	123	THR	3.3
1	B	135	ASN	3.3
1	A	129	GLN	3.3
1	A	27	ASN	3.2
1	A	80	LEU	3.1
1	A	54	HIS	3.1
1	B	69	CYS	3.1
1	B	16	TRP	3.1
1	B	29	GLN	3.1
1	A	81	GLU	3.0
1	A	99	ALA	3.0
1	B	59	GLY	3.0
1	A	152	GLU	3.0
1	B	141	VAL	3.0
1	B	112	GLU	3.0
1	B	39	ASN	2.9
1	A	75	GLU	2.8
1	A	59	GLY	2.8
1	A	133	LEU	2.7
1	A	39	ASN	2.7
1	A	96	LYS	2.7
1	B	18	VAL	2.7
1	B	76	THR	2.7
1	A	132	SER	2.7
1	A	49	VAL	2.7
1	B	120	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	42	LEU	2.6
1	B	42	LEU	2.6
1	A	64	LYS	2.5
1	B	56	LEU	2.5
1	A	112	GLU	2.5
1	B	68	SER	2.5
1	A	10	MET	2.4
1	B	134	THR	2.4
1	A	84	ASN	2.4
1	B	146	PHE	2.4
1	B	111	PHE	2.3
1	B	30	LEU	2.3
1	B	149	GLN	2.3
1	B	151	ASP	2.3
1	A	141	VAL	2.3
1	B	49	VAL	2.3
1	A	104	ASP	2.3
1	A	116	CYS	2.2
1	A	122	CYS	2.2
1	B	97	ARG	2.2
1	B	60	ILE	2.2
1	B	23	PHE	2.1
1	A	72	SER	2.1
1	B	130	PRO	2.1
1	B	136	MET	2.1
1	B	131	VAL	2.1
1	A	77	ARG	2.1
1	A	57	PHE	2.1
1	A	88	LEU	2.1
1	A	66	CYS	2.1
1	B	43	GLU	2.1
1	A	79	GLN	2.0
1	A	60	ILE	2.0
1	A	86	THR	2.0
1	B	58	LEU	2.0
1	A	50	PRO	2.0
1	A	23	PHE	2.0
1	B	123	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.