



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:51 AM GMT

PDB ID : 3G9V
Title : Crystal structure of a soluble decoy receptor IL-22BP bound to interleukin-22
Authors : de Moura, P.R.; Watanabe, L.; Bleicher, L.; Colau, D.; Renauld, J.-C.; Polikarpov, I.
Deposited on : 2009-02-14
Resolution : 2.76 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
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

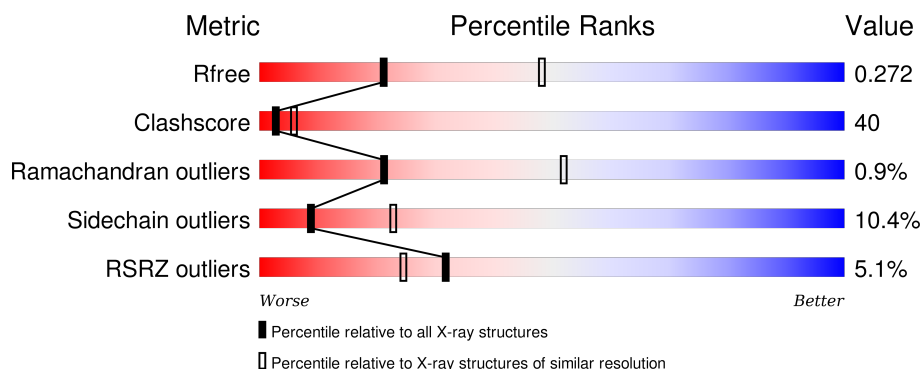
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	211	<div> <div>3%</div> <div>33% 45% 5% 18%</div> </div>
1	C	211	<div> <div>2%</div> <div>33% 43% 7% 17%</div> </div>
2	B	151	<div> <div>6%</div> <div>39% 43% 5% 11%</div> </div>
2	D	151	<div> <div>7%</div> <div>36% 46% 14%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5251 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 22 receptor, alpha 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	8	0	0
			1458	930	253	269	6			
1	C	176	Total	C	N	O	S	13	0	0
			1486	949	259	272	6			

- Molecule 2 is a protein called Interleukin-22.

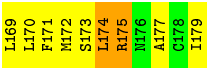
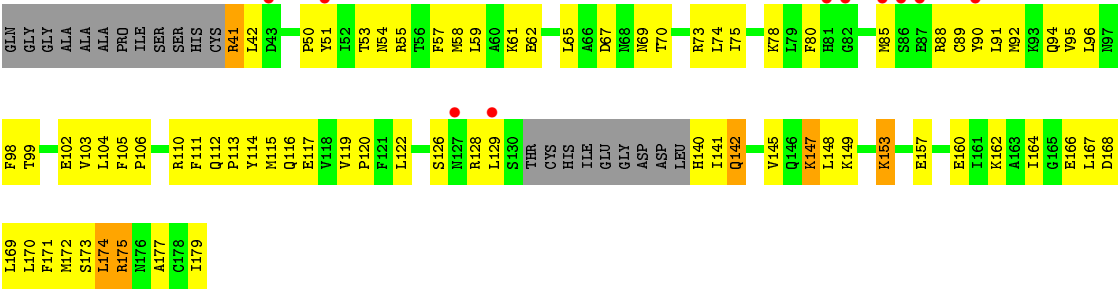
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	24	0	0
			1087	686	194	198	9			
2	D	130	Total	C	N	O	S	28	0	0
			1053	668	186	192	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		
3	B	32	Total	O	0	0
			32	32		
3	C	51	Total	O	0	0
			51	51		
3	D	25	Total	O	0	0
			25	25		



• Molecule 2: Interleukin-22



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	67.95Å 67.95Å 172.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 2.76 29.25 – 2.76	Depositor EDS
% Data completeness (in resolution range)	96.5 (24.84-2.76) 96.5 (29.25-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.213 , 0.282 0.213 , 0.272	Depositor DCC
R_{free} test set	993 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	EDS
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19452 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	A	0.55	0/1496	0.66	0/2025
1	C	1.06	11/1526 (0.7%)	0.70	1/2066 (0.0%)
2	B	0.90	11/1104 (1.0%)	0.75	3/1481 (0.2%)
2	D	0.40	0/1068	0.63	2/1431 (0.1%)
All	All	0.79	22/5194 (0.4%)	0.69	6/7003 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
2	B	0	2
All	All	0	5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	PHE	CE2-CZ	-15.57	1.07	1.37
1	C	174	PHE	CD1-CE1	-14.18	1.10	1.39
1	C	174	PHE	CD2-CE2	-12.61	1.14	1.39
1	C	174	PHE	CE1-CZ	-11.92	1.14	1.37
1	C	174	PHE	CG-CD1	-10.82	1.22	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	ARG	NE-CZ-NH1	-10.24	115.18	120.30
2	D	175	ARG	NE-CZ-NH2	-10.15	115.22	120.30
2	D	175	ARG	NE-CZ-NH1	9.67	125.14	120.30
2	B	175	ARG	NE-CZ-NH2	9.19	124.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	ILE	CB-CA-C	-7.57	96.46	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ARG	Peptide
2	B	130	SER	Peptide
2	B	131	THR	Peptide
1	C	175	ILE	Peptide
1	C	192	ARG	Peptide

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	1458	0	1393	108	0
1	C	1486	0	1416	117	0
2	B	1087	0	1096	100	0
2	D	1053	0	1073	87	0
3	A	59	0	0	4	0
3	B	32	0	0	1	0
3	C	51	0	0	6	0
3	D	25	0	0	1	0
All	All	5251	0	4978	395	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 40.

The worst 5 of 395 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:130:SER:O	2:B:131:THR:CG2	1.66	1.40
2:B:40:CYS:O	2:B:41:ARG:CD	1.81	1.29
2:B:130:SER:C	2:B:131:THR:HG23	1.49	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:SER:O	2:B:131:THR:HG23	0.98	1.14
1:C:170:LEU:HD22	1:C:214:PRO:HG3	1.27	1.13

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	163/211 (77%)	152 (93%)	10 (6%)	1 (1%)	30	62
1	C	166/211 (79%)	154 (93%)	10 (6%)	2 (1%)	16	43
2	B	130/151 (86%)	118 (91%)	10 (8%)	2 (2%)	13	36
2	D	126/151 (83%)	120 (95%)	6 (5%)	0	100	100
All	All	585/724 (81%)	544 (93%)	36 (6%)	5 (1%)	21	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	CYS
1	A	51	ARG
2	B	128	ARG
1	C	51	ARG
1	C	185	LYS

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	158/193 (82%)	141 (89%)	17 (11%)	8	21
1	C	161/193 (83%)	141 (88%)	20 (12%)	6	15
2	B	123/134 (92%)	112 (91%)	11 (9%)	12	31
2	D	118/134 (88%)	108 (92%)	10 (8%)	13	34
All	All	560/654 (86%)	502 (90%)	58 (10%)	9	23

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	157	GLU
1	C	70	ARG
2	D	147	LYS
2	B	174	LEU
1	C	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	142	GLN
1	C	69	GLN
2	D	140	HIS
1	C	26	HIS
1	C	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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](#)

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	173/211 (81%)	0.07	7 (4%)	42	35	18, 32, 65, 94	3 (1%)
1	C	176/211 (83%)	0.02	5 (2%)	56	50	18, 32, 64, 90	4 (2%)
2	B	134/151 (88%)	0.12	9 (6%)	21	15	20, 39, 76, 86	9 (6%)
2	D	130/151 (86%)	0.29	10 (7%)	16	11	21, 41, 73, 87	8 (6%)
All	All	613/724 (84%)	0.11	31 (5%)	32	24	18, 35, 69, 94	24 (3%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	133	HIS	5.7
2	D	81	HIS	4.7
2	D	85	MET	4.1
1	C	176	ILE	3.8
2	B	82	GLY	3.4

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

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.