



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:01 PM UTC

PDB ID : 3G8L / pdb_00003g8l
Title : Crystal structure of murine natural killer cell receptor, Ly49L4
Authors : Cho, S.
Deposited on : 2009-02-12
Resolution : 2.50 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

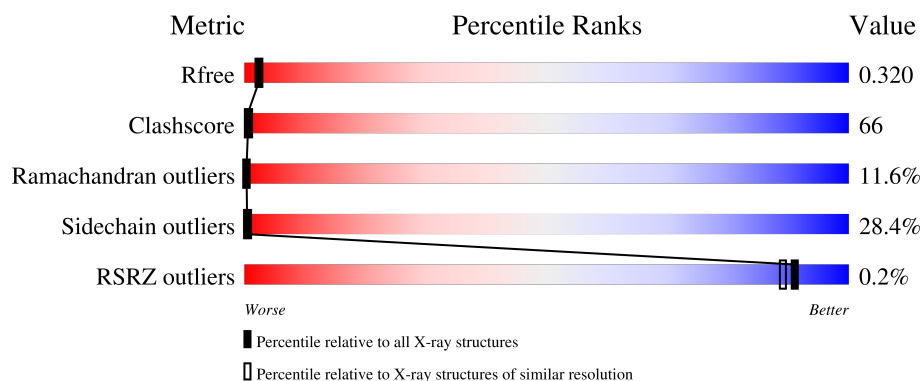
1 Overall quality at a glance

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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	190	
1	B	190	
1	C	190	
1	D	190	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5162 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 Lectin-related NK cell receptor LY49L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1293	823	219	240	11			
1	B	161	Total	C	N	O	S	0	0	0
			1327	843	226	246	12			
1	C	154	Total	C	N	O	S	0	0	0
			1267	808	213	235	11			
1	D	152	Total	C	N	O	S	0	0	0
			1258	804	211	231	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	expression tag	UNP Q9JIP9
A	77	ALA	-	expression tag	UNP Q9JIP9
A	78	SER	-	expression tag	UNP Q9JIP9
A	198	TYR	CYS	engineered mutation	UNP Q9JIP9
B	76	MET	-	expression tag	UNP Q9JIP9
B	77	ALA	-	expression tag	UNP Q9JIP9
B	78	SER	-	expression tag	UNP Q9JIP9
B	198	TYR	CYS	engineered mutation	UNP Q9JIP9
C	76	MET	-	expression tag	UNP Q9JIP9
C	77	ALA	-	expression tag	UNP Q9JIP9
C	78	SER	-	expression tag	UNP Q9JIP9
C	198	TYR	CYS	engineered mutation	UNP Q9JIP9
D	76	MET	-	expression tag	UNP Q9JIP9
D	77	ALA	-	expression tag	UNP Q9JIP9
D	78	SER	-	expression tag	UNP Q9JIP9
D	198	TYR	CYS	engineered mutation	UNP Q9JIP9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	6	Total 6	O 6	0	0
2	C	2	Total 2	O 2	0	0
2	D	2	Total 2	O 2	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	78.05Å 78.05Å 216.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.50) 90.1 (30.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.287 0.221 , 0.320	Depositor DCC
R_{free} test set	1229 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5162	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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

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	2.57	69/1326 (5.2%)	2.27	65/1781 (3.6%)
1	B	2.49	77/1360 (5.7%)	2.24	83/1827 (4.5%)
1	C	2.49	66/1298 (5.1%)	2.33	80/1741 (4.6%)
1	D	2.42	66/1289 (5.1%)	2.27	75/1730 (4.3%)
All	All	2.49	278/5273 (5.3%)	2.28	303/7079 (4.3%)

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	5
1	B	0	2
1	C	0	4
1	D	0	9
All	All	0	20

The worst 5 of 278 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	CYS	CA-C	14.54	1.71	1.52
1	A	180	ILE	CA-CB	-13.19	1.38	1.54
1	B	180	ILE	CA-CB	-13.02	1.37	1.54
1	C	255	ILE	C-O	12.15	1.38	1.24
1	A	253	ILE	CA-CB	-11.86	1.42	1.54

The worst 5 of 303 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	VAL	CA-C-N	-16.24	103.95	120.03
1	C	193	VAL	C-N-CA	-16.24	103.95	120.03
1	C	217	GLY	CA-C-N	-14.50	101.71	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	GLY	C-N-CA	-14.50	101.71	119.84
1	A	181	ASP	N-CA-C	13.47	127.44	111.82

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	SER	Peptide
1	A	136	GLN	Peptide
1	A	205	ASP	Peptide
1	A	215	ASN	Peptide
1	A	256	CYS	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	1293	0	1252	195	0
1	B	1327	0	1285	149	0
1	C	1267	0	1229	173	0
1	D	1258	0	1221	176	0
2	A	7	0	0	2	0
2	B	6	0	0	1	0
2	C	2	0	0	2	0
2	D	2	0	0	1	0
All	All	5162	0	4987	665	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 66.

The worst 5 of 665 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:A:253:ILE:CD1	1:A:253:ILE:CG1	1.74	1.61
1:A:255:ILE:CB	1:A:255:ILE:CG2	1.74	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ILE:CG1	1:C:151:ILE:CD1	1.75	1.59
1:A:152:LYS:CE	1:A:152:LYS:NZ	1.72	1.51
1:A:151:ILE:CD1	1:A:151:ILE:CG1	1.90	1.50

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	155/190 (82%)	119 (77%)	22 (14%)	14 (9%)	0	0
1	B	159/190 (84%)	114 (72%)	24 (15%)	21 (13%)	0	0
1	C	150/190 (79%)	108 (72%)	23 (15%)	19 (13%)	0	0
1	D	148/190 (78%)	108 (73%)	23 (16%)	17 (12%)	0	0
All	All	612/760 (80%)	449 (73%)	92 (15%)	71 (12%)	0	0

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLU
1	A	138	THR
1	A	214	ILE
1	A	226	MET
1	A	231	ARG

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	145/177 (82%)	102 (70%)	43 (30%)	0	0
1	B	149/177 (84%)	117 (78%)	32 (22%)	1	2
1	C	142/177 (80%)	98 (69%)	44 (31%)	0	0
1	D	141/177 (80%)	96 (68%)	45 (32%)	0	0
All	All	577/708 (82%)	413 (72%)	164 (28%)	0	0

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	250	LYS
1	D	208	LYS
1	D	106	GLU
1	D	159	ASP
1	D	226	MET

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

Mol	Chain	Res	Type
1	C	171	GLN
1	C	229	ASN
1	C	216	ASN
1	C	265	HIS
1	B	111	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 oligosaccharides 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(Å²)	Q<0.9	
1	A	157/190 (82%)	-1.16	0	100	100	37, 55, 79, 85	0
1	B	161/190 (84%)	-1.14	0	100	100	37, 56, 86, 119	0
1	C	154/190 (81%)	-1.15	0	100	100	36, 58, 88, 99	0
1	D	152/190 (80%)	-1.09	1 (0%)	84	81	36, 56, 89, 116	0
All	All	624/760 (82%)	-1.14	1 (0%)	91	89	36, 56, 86, 119	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	GLY	3.9

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 oligosaccharides 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.