WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:50 AM GMT

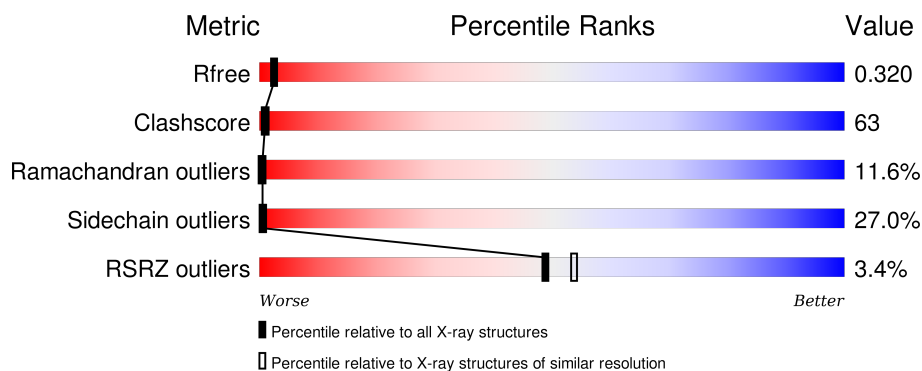|		
PDB ID	:	3G8L
Title	:	Crystal structure of murine natural killer cell receptor, Ly49L4
Authors	:	Cho, S.
Deposited on	:	2009-02-12
Resolution	:	2.50 Å(reported)

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1   Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.320
Clashscore		63
Ramachandran outliers		11.6%
Sidechain outliers		27.0%
RSRZ outliers		3.4%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 <=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	% — 13% / 29% / 28% / 12% / 17%
1	B	190	4% — 17% / 37% / 21% / 9% / 15%
1	C	190	4% — 14% / 31% / 26% / 11% / 19%
1	D	190	2% — 16% / 29% / 19% / 16% / 20%

2 Entry composition (i)

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	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	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	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	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

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 di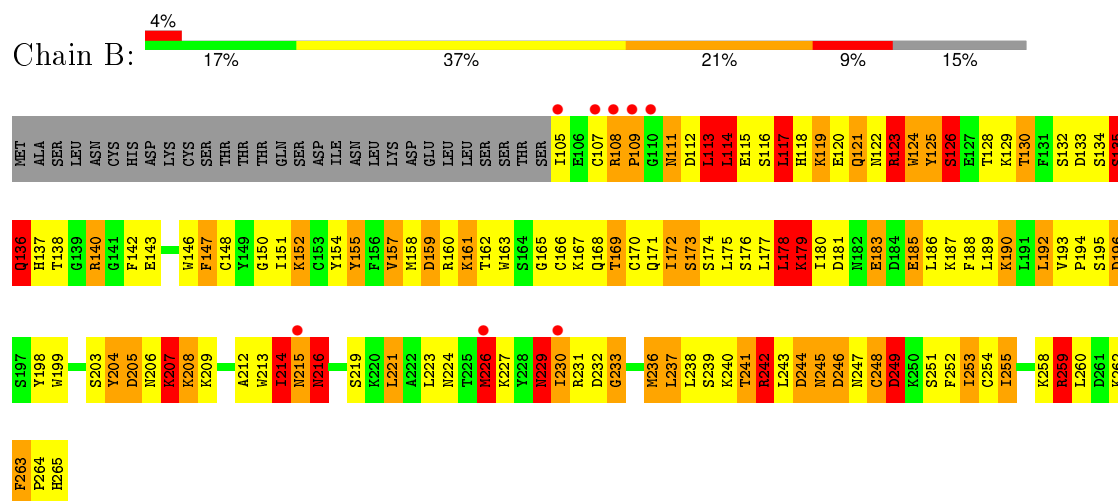splayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or 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.

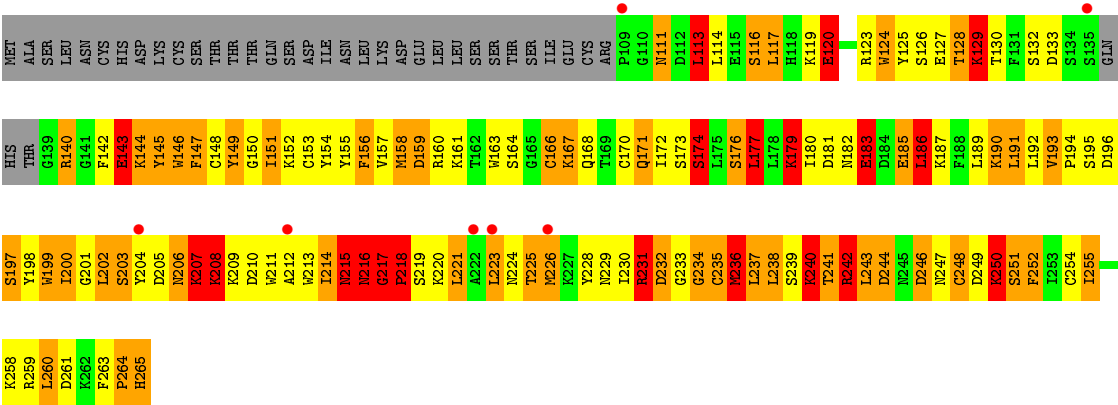• Molecule 1: Lectin-related NK cell receptor LY49L1

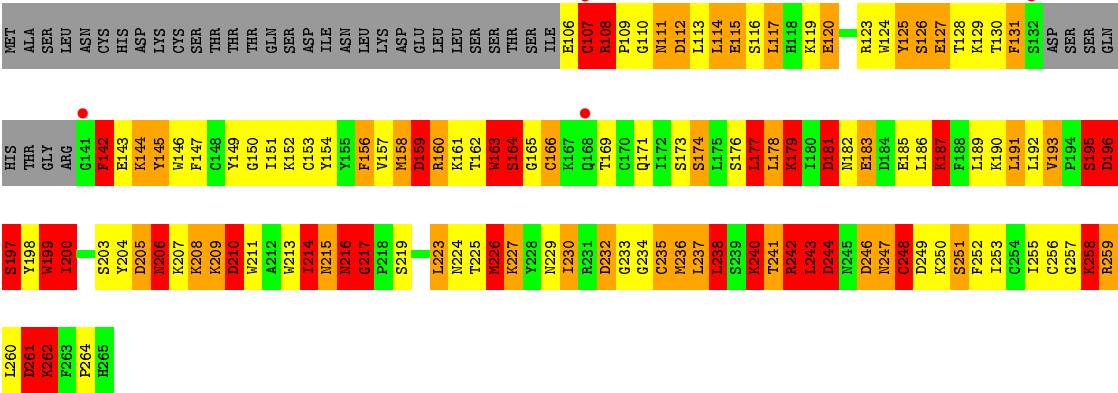• Molecule 1: Lectin-related NK cell receptor LY49L1

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• Molecule 1: Lectin-related NK cell receptor LY49L1

Chain D:

4   Data and refinement statistics (i)

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 29.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.50) 90.1 (29.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [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 (5.41%)	DCC
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.2	EDS
Estimated twinning fraction	0.487 for -h,-k,l	Xtriage
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 23934 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	2.19	48/1326 (3.6%)	1.84	36/1781 (2.0%)
1	B	2.11	43/1360 (3.2%)	1.77	29/1827 (1.6%)
1	C	2.09	32/1298 (2.5%)	1.81	33/1741 (1.9%)
1	D	2.02	31/1289 (2.4%)	1.83	37/1730 (2.1%)
All	All	2.10	154/5273 (2.9%)	1.81	135/7079 (1.9%)

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 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	146	TRP	CE3-CZ3	12.77	1.60	1.38
1	A	198	TYR	CD2-CE2	11.69	1.56	1.39
1	A	155	TYR	CE2-CZ	10.74	1.52	1.38
1	C	254	CYS	CB-SG	10.60	2.00	1.82
1	B	185	GLU	CD-OE1	9.39	1.35	1.25

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	246	ASP	CB-CG-OD1	-13.10	106.51	118.30
1	D	117	LEU	CB-CG-CD1	-11.95	90.69	111.00
1	C	231	ARG	NE-CZ-NH1	10.51	125.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	196	ASP	CB-CG-OD2	-10.03	109.27	118.30
1	C	236	MET	CA-CB-CG	-9.20	97.66	113.30

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	191	0
1	B	1327	0	1285	144	0
1	C	1267	0	1229	169	0
1	D	1258	0	1221	166	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	642	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 63.

The worst 5 of 642 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:CG1	1:A:253:ILE:CD1	1.74	1.61
1:A:255:ILE:CG2	1:A:255:ILE:CB	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:NZ	1:A:152:LYS:CE	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%)	1	1	
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%)	105 (72%)	40 (28%)	0	0	
1	B	149/177 (84%)	118 (79%)	31 (21%)	1	2	
1	C	142/177 (80%)	100 (70%)	42 (30%)	0	0	
1	D	141/177 (80%)	98 (70%)	43 (30%)	0	0	
All	All	577/708 (82%)	421 (73%)	156 (27%)	0	0	

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	265	HIS
1	C	176	SER
1	D	237	LEU
1	C	116	SER
1	C	142	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	ASN
1	B	224	ASN
1	C	215	ASN
1	B	111	ASN
1	B	118	HIS

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)

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	157/190 (82%)	0.08	2 (1%)	79	82	37, 55, 79, 85	0
1	B	161/190 (84%)	0.31	8 (4%)	32	37	37, 56, 86, 119	0
1	C	154/190 (81%)	0.14	7 (4%)	37	42	36, 58, 88, 99	0
1	D	152/190 (80%)	0.22	4 (2%)	59	63	36, 56, 89, 116	0
All	All	624/760 (82%)	0.19	21 (3%)	49	54	36, 56, 86, 119	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	ILE	8.2
1	D	141	GLY	7.2
1	B	110	GLY	6.8
1	B	226	MET	5.2
1	B	108	ARG	5.0

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.