



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:45 PM UTC

PDB ID : 3C8J / pdb_00003c8j
Title : The crystal structure of natural killer cell receptor Ly49C
Authors : Deng, L.; Mariuzza, R.A.
Deposited on : 2008-02-12
Resolution : 2.60 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
Xtrriage (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

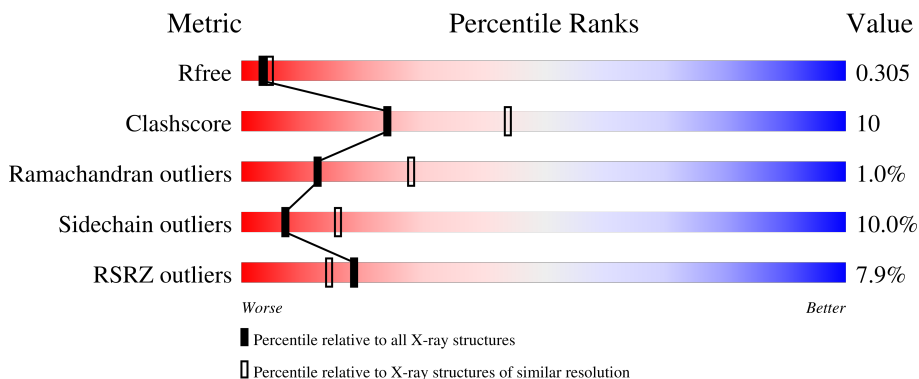
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	203	 5% 47% 12% 37%
1	B	203	 6% 46% 13% 38%
1	C	203	 5% 43% 17% 38%
1	D	203	 3% 41% 19% 36%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4346 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 Natural killer cell receptor Ly49C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	1054	687	175	181	11	0	0	0
1	B	126	1050	684	174	181	11	0	0	0
1	C	126	1050	684	174	181	11	0	0	0
1	D	130	1082	701	181	189	11	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP Q61198
A	62	SER	VAL	SEE REMARK 999	UNP Q61198
A	74	THR	ILE	SEE REMARK 999	UNP Q61198
A	?	-	HIS	SEE REMARK 999	UNP Q61198
A	116	GLY	ARG	engineered mutation	UNP Q61198
A	119	HIS	-	SEE REMARK 999	UNP Q61198
A	171	GLY	SER	engineered mutation	UNP Q61198
A	193	GLY	GLU	engineered mutation	UNP Q61198
A	223	LYS	ARG	engineered mutation	UNP Q61198
B	60	MET	-	initiating methionine	UNP Q61198
B	62	SER	VAL	SEE REMARK 999	UNP Q61198
B	74	THR	ILE	SEE REMARK 999	UNP Q61198
B	?	-	HIS	variant	UNP Q61198
B	116	GLY	ARG	engineered mutation	UNP Q61198
B	119	HIS	-	SEE REMARK 999	UNP Q61198
B	171	GLY	SER	engineered mutation	UNP Q61198
B	193	GLY	GLU	engineered mutation	UNP Q61198
B	223	LYS	ARG	engineered mutation	UNP Q61198
C	60	MET	-	initiating methionine	UNP Q61198
C	62	SER	VAL	SEE REMARK 999	UNP Q61198
C	74	THR	ILE	SEE REMARK 999	UNP Q61198

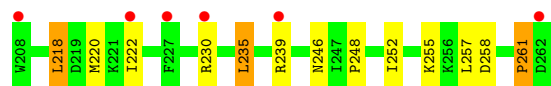
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	HIS	SEE REMARK 999	UNP Q61198
C	116	GLY	ARG	engineered mutation	UNP Q61198
C	119	HIS	-	SEE REMARK 999	UNP Q61198
C	171	GLY	SER	engineered mutation	UNP Q61198
C	193	GLY	GLU	engineered mutation	UNP Q61198
C	223	LYS	ARG	engineered mutation	UNP Q61198
D	60	MET	-	initiating methionine	UNP Q61198
D	62	SER	VAL	SEE REMARK 999	UNP Q61198
D	74	THR	ILE	SEE REMARK 999	UNP Q61198
D	?	-	HIS	SEE REMARK 999	UNP Q61198
D	116	GLY	ARG	engineered mutation	UNP Q61198
D	119	HIS	-	SEE REMARK 999	UNP Q61198
D	171	GLY	SER	engineered mutation	UNP Q61198
D	193	GLY	GLU	engineered mutation	UNP Q61198
D	223	LYS	ARG	engineered mutation	UNP Q61198

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	44	Total O 44 44	0	0
2	C	12	Total O 12 12	0	0
2	D	34	Total O 34 34	0	0

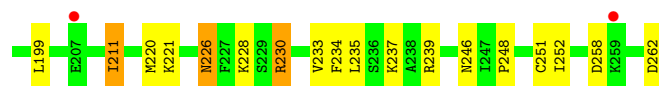


- Molecule 1: Natural killer cell receptor Ly49C



MET ALA SER TRP ASP ILE PHE GLN TYR ASN GLN HIS LYS GLN THR ASN THR GLU THR LEU ASN HIS HIS ASN CYS SER ASN MET GLN ARG ALA PHE ASN LEU LYS GLU MET LEU THR ASN LYS SER ILE ASP CYS ARG PRO SER ASN GLU THR LEU GLU TYR ILE LYS GLY GLN HIS

ASP ARG TRP ASP SER LYS THR LYS THR VAL LEU ASP SER S153 R134 D135 T136 G137 R138 G139 V140 K141 C145 T148 K149 C150 Y151 Y152 F153 I154 M155 M156 K157 T158 S161 G162 C163 M166 C167 Q168 H169 V172 P173 I174 K184 F195 L186 Q187 R188 H189 V190 M194 Y195



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.10Å 94.89Å 104.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.00-2.60) 93.4 (30.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.198 , 0.263 0.259 , 0.305	Depositor DCC
R_{free} test set	1276 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4346	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.66	0/1085	0.90	1/1457 (0.1%)
1	B	0.83	0/1081	1.08	1/1450 (0.1%)
1	C	0.74	2/1081 (0.2%)	0.89	2/1450 (0.1%)
1	D	0.66	0/1113	0.98	4/1493 (0.3%)
All	All	0.72	2/4360 (0.0%)	0.97	8/5850 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	GLU	CD-OE2	11.30	1.46	1.25
1	C	207	GLU	CD-OE1	9.86	1.44	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	THR	CA-C-O	8.63	130.13	119.95
1	D	148	THR	O-C-N	-7.79	112.68	122.26
1	C	148	THR	CA-C-O	7.67	130.04	120.15
1	C	148	THR	O-C-N	-6.47	113.84	122.19
1	B	148	THR	CA-C-O	6.24	128.10	120.55

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	1054	0	1038	14	0
1	B	1050	0	1036	22	0
1	C	1050	0	1036	23	1
1	D	1082	0	1065	29	1
2	A	20	0	0	1	0
2	B	44	0	0	2	0
2	C	12	0	0	1	0
2	D	34	0	0	6	0
All	All	4346	0	4175	84	1

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 10.

The worst 5 of 84 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:135:ASP:HA	2:D:297:HOH:O	1.48	1.14
1:D:138:ARG:HB3	1:D:156:ASN:HD21	1.24	1.01
1:D:136:THR:OG1	1:D:137:GLY:N	1.96	0.91
1:C:155:MET:HE1	1:C:195:TYR:HE2	1.37	0.88
1:D:190:VAL:O	1:D:237:LYS:HE2	1.74	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:NH2	1:D:228:LYS:O[2_875]	1.85	0.35

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	125/203 (62%)	114 (91%)	10 (8%)	1 (1%)	16	34
1	B	124/203 (61%)	117 (94%)	5 (4%)	2 (2%)	7	16
1	C	124/203 (61%)	111 (90%)	12 (10%)	1 (1%)	16	34
1	D	128/203 (63%)	116 (91%)	11 (9%)	1 (1%)	16	34
All	All	501/812 (62%)	458 (91%)	38 (8%)	5 (1%)	12	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	B	229	SER
1	B	230	ARG
1	D	134	ARG
1	C	261	PRO

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	114/188 (61%)	104 (91%)	10 (9%)	9	21
1	B	114/188 (61%)	104 (91%)	10 (9%)	9	21
1	C	114/188 (61%)	103 (90%)	11 (10%)	8	17
1	D	118/188 (63%)	103 (87%)	15 (13%)	4	9
All	All	460/752 (61%)	414 (90%)	46 (10%)	7	16

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	246	ASN
1	D	168	GLN
1	C	257	LEU
1	D	141	LYS
1	D	190	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	156	ASN
1	D	246	ASN
1	D	194	ASN
1	C	166	ASN
1	C	246	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 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(Å ²)	Q < 0.9
1	A	127/203 (62%)	0.82	11 (8%) 16 12	50, 59, 72, 74	0
1	B	126/203 (62%)	0.91	12 (9%) 14 10	45, 56, 69, 81	0
1	C	126/203 (62%)	1.05	10 (7%) 18 14	53, 61, 71, 73	0
1	D	130/203 (64%)	0.85	7 (5%) 31 26	54, 61, 71, 85	0
All	All	509/812 (62%)	0.90	40 (7%) 18 14	45, 60, 71, 85	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	SER	6.6
1	C	137	GLY	4.9
1	D	136	THR	4.7
1	A	136	THR	4.3
1	D	134	ARG	3.8

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.