



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 10:53 am GMT

PDB ID : 1P1Z
Title : X-RAY CRYSTAL STRUCTURE OF THE LECTIN-LIKE NATURAL KILLER CELL RECEPTOR LY-49C BOUND TO ITS MHC CLASS I LIG-AND H-2Kb
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Deposited on : 2003-04-14
Resolution : 3.26 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
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

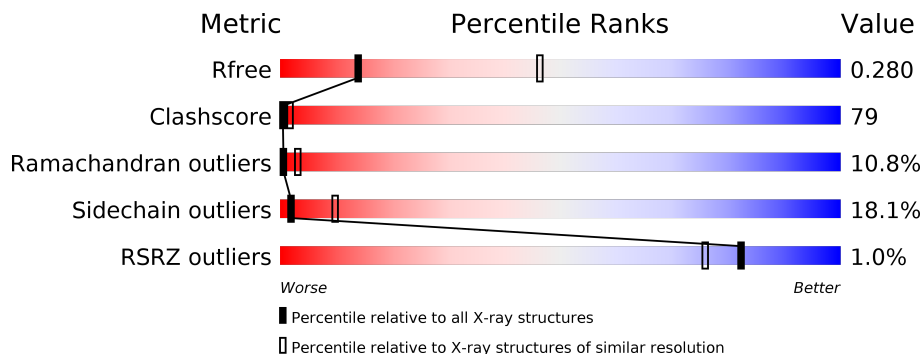
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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	274	
2	B	99	
3	P	8	
4	D	120	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3926 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2072	1312	361	390	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			803	515	136	146	6			

- Molecule 3 is a protein called Ovalbumin peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	8	Total	C	N	O	0	0	0
			68	45	10	13			

- Molecule 4 is a protein called LY49-C antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	118	Total	C	N	O	S	0	0	0
			983	637	161	174	11			

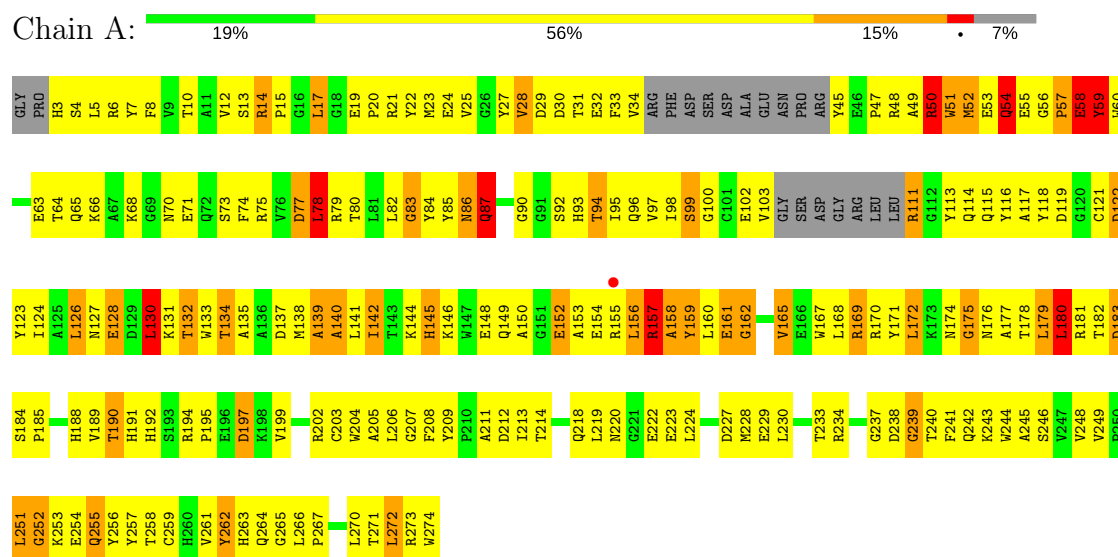
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	144	VAL	LYS	CONFLICT	UNP Q64329

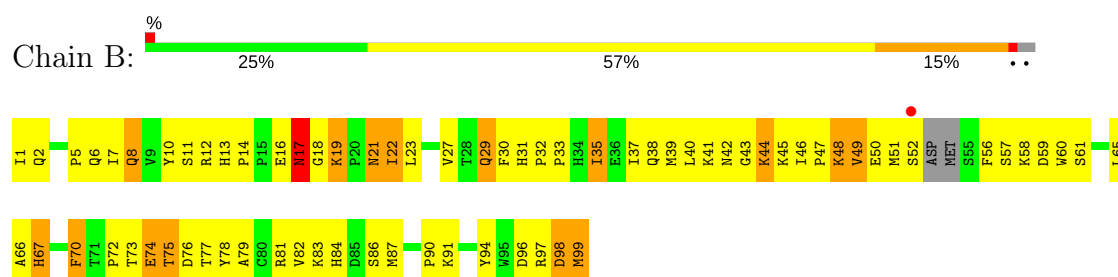
3 Residue-property plots [i](#)

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: H-2 class I histocompatibility antigen, K-B alpha chain



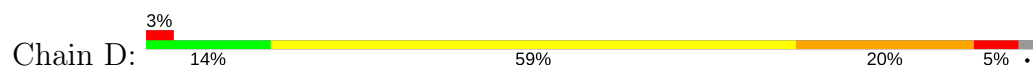
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Ovalbumin peptide



- Molecule 4: LY49-C antigen



L202	GLY	GLY
S203	VAL	VAL
Y204	Y144	Y144
D205	Y145	Y145
K206	W146	W146
K207	F147	F147
K208	C148	C148
K209	Y149	Y149
E210	S150	S150
	T151	T151
W213	K152	K152
I214	C153	C153
D215	Y154	Y154
N216	Y155	Y155
G217	F156	F156
P218	I157	I157
S219	M158	M158
K220	N159	N159
L221	K160	K160
D222	T161	T161
M223	T162	T162
K224	W163	W163
I225	S164	S164
R226	G165	G165
K227	C166	C166
K228	K167	K167
N229	A168	A168
F230	N169	N169
K231	C170	C170
S232	Q171	Q171
R233	H172	H172
G234	Y173	Y173
C235	S174	S174
V236	V175	V175
F237	P176	P176
L238	I177	I177
S239	L178	L178
K240	K179	K179
A241	I180	I180
R242	E181	E181
I243	D182	D182
	E183	E183
I246	D184	D184
D247	E185	E185
C248	L186	L186
N249	K187	K187
I250	F188	F188
P251	L189	L189
Y252	Q190	Q190
Y253	R191	R191
C254	H192	H192
I255	V193	V193
C256	I194	I194
G257	P195	P195
K258	E196	E196
K259	N197	N197
L260	Y198	Y198
D261	W199	W199
	I200	I200
	G201	G201

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.05Å 149.05Å 64.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.26 48.72 – 3.26	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.26) 99.5 (48.72-3.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.25Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.263 , 0.316 0.260 , 0.280	Depositor DCC
R_{free} test set	558 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3926	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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	0.54	0/2126	0.93	4/2885 (0.1%)
2	B	0.57	0/828	0.86	0/1122
3	P	0.63	0/68	0.90	0/88
4	D	0.67	1/1011 (0.1%)	1.09	5/1362 (0.4%)
All	All	0.58	1/4033 (0.0%)	0.96	9/5457 (0.2%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	147	PHE	CB-CG	-5.15	1.42	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	TYR	N-CA-C	-8.61	87.75	111.00
1	A	28	VAL	N-CA-C	-7.01	92.07	111.00
4	D	234	GLY	N-CA-C	6.79	130.08	113.10
4	D	148	CYS	CA-CB-SG	6.48	125.66	114.00
4	D	230	PHE	N-CA-C	-6.17	94.35	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	TYR	Sidechain
1	A	59	TYR	Sidechain

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	2072	0	1968	330	0
2	B	803	0	776	118	0
3	P	68	0	74	26	0
4	D	983	0	949	180	0
All	All	3926	0	3767	610	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 79.

The worst 5 of 610 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)
3:P:7:LYS:H	3:P:7:LYS:HD2	1.03	1.16
1:A:29:ASP:HA	4:D:230:PHE:CZ	1.81	1.13
4:D:157:ILE:HB	4:D:254:CYS:HB2	1.24	1.12
2:B:38:GLN:HB2	2:B:81:ARG:HB3	1.29	1.12
2:B:2:GLN:NE2	2:B:86:SER:HA	1.65	1.10

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	249/274 (91%)	167 (67%)	56 (22%)	26 (10%)	0	3
2	B	93/99 (94%)	77 (83%)	11 (12%)	5 (5%)	2	16
3	P	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	1
4	D	116/120 (97%)	75 (65%)	23 (20%)	18 (16%)	0	1
All	All	464/501 (93%)	322 (69%)	92 (20%)	50 (11%)	0	3

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	87	GLN
1	A	130	LEU
1	A	139	ALA
1	A	145	HIS

5.3.2 Protein sidechains ⓘ

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	214/232 (92%)	179 (84%)	35 (16%)	2	13
2	B	90/94 (96%)	74 (82%)	16 (18%)	2	10
3	P	8/8 (100%)	6 (75%)	2 (25%)	1	2
4	D	107/111 (96%)	84 (78%)	23 (22%)	1	6
All	All	419/445 (94%)	343 (82%)	76 (18%)	2	10

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	LEU
2	B	44	LYS
4	D	227	LYS
2	B	6	GLN
2	B	19	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
2	B	2	GLN
2	B	67	HIS
1	A	192	HIS
4	D	169	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 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	255/274 (93%)	-0.32	1 (0%) 92 90	18, 50, 84, 128	0
2	B	97/99 (97%)	-0.24	1 (1%) 82 76	16, 46, 81, 110	0
3	P	8/8 (100%)	-0.03	0 100 100	52, 54, 67, 74	0
4	D	118/120 (98%)	-0.23	3 (2%) 58 48	22, 48, 94, 142	0
All	All	478/501 (95%)	-0.28	5 (1%) 82 76	16, 49, 86, 142	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	230	PHE	4.0
4	D	231	LYS	2.8
2	B	52	SER	2.4
1	A	155	ARG	2.3
4	D	232	SER	2.1

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.