wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:27 PM 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 LIGAND H-2Kb
Authors	:	Dimasi, N.; Natarajan, K.; Rangjin, G.; Dam, J.; Margulies, D.H.; Mariuzza, R.A.
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

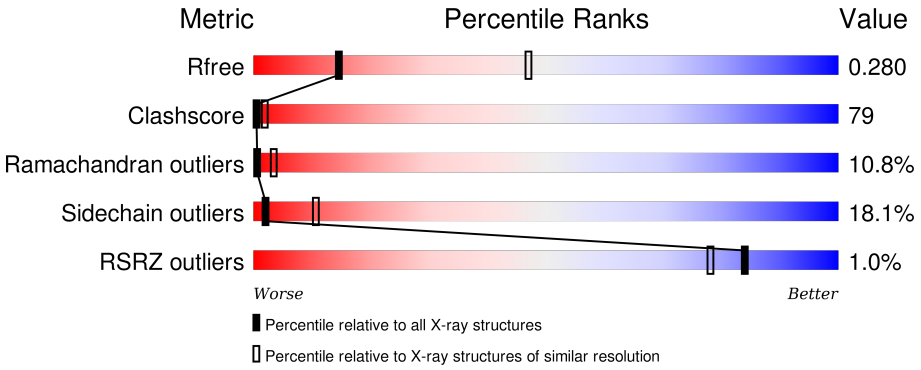
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (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 <=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	19% 56% 15% • 7%
2	B	99	% 25% 57% 15% ••
3	P	8	63% 38%
4	D	120	3% 14% 59% 20% 5% •

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:

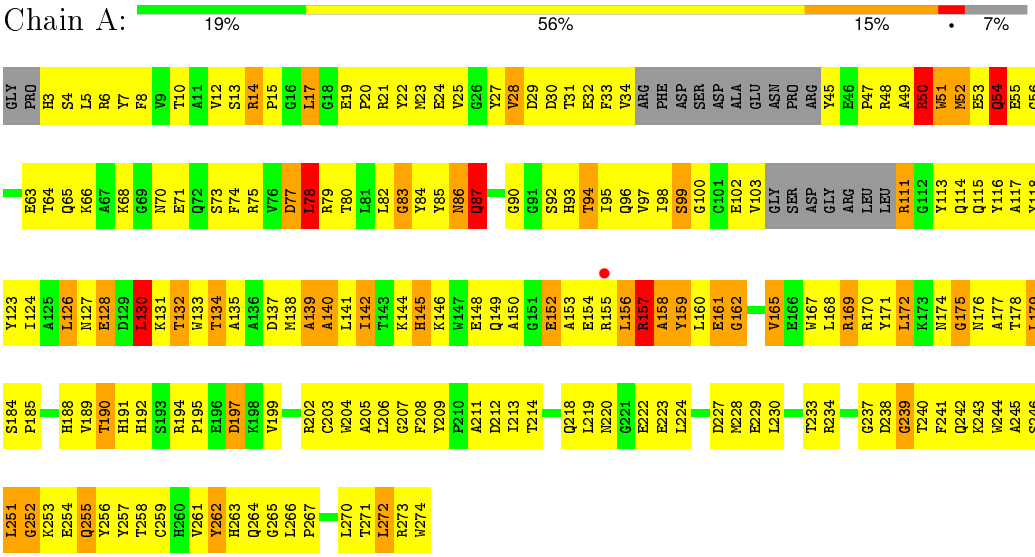
Chain	Residue	Modelled	Actual	Comment	Reference
D	144	VAL	LYS	CONFLICT	UNP Q64329

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 errors 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.

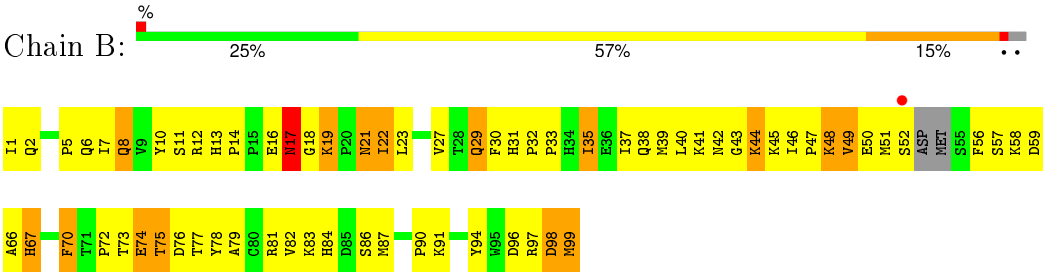
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain A:



- Molecule 2: Beta-2-microglobulin

Chain B:

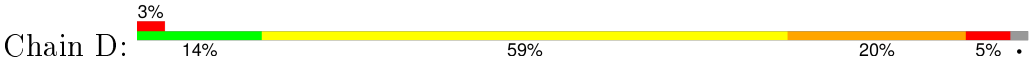


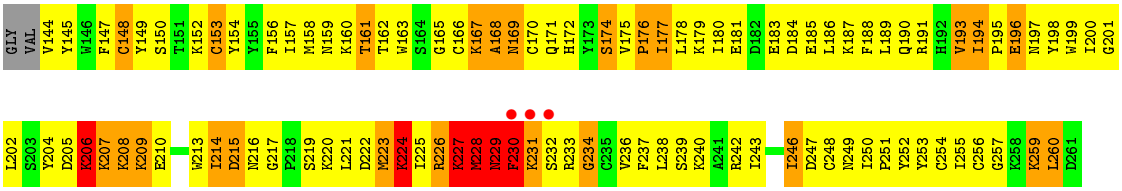
- Molecule 3: Ovalbumin peptide

Chain P:

- Molecule 4: LY49-C antigen

Chain D:




GLY
VAL
V144
Y145
W146
F147
C148
Y149
S150
T151
K152
C153
Y154
Y155
F156
I157
M158
N159
K160
T161
T162
W163
S164
G165
C166
K167
A168
N169
C170
Q171
H172
Y173
S174
V175
P176
I177
L178
K179
I180
E181
D182
E183
D184
E185
L186
K187
F188
L189
Q190
R191
H192
V193
I194
P195
E196
N197
Y198
W199
I200
G201
L202
S203
Y204
D205
K206
K207
K208
K209
E210
W213
I214
D215
M216
G217
P218
S219
K220
L221
D222
M223
K224
I225
R226
K227
M228
M229
F230
K231
S232
R233
G234
C235
V236
F237
L238
S239
K240
A241
R242
I243
I246
D247
C248
N249
I250
P251
Y252
Y253
C254
I255
C256
G257
K258
K259
L260
D261

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 11741 reflections	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.*

[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

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	0.54	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(^{o})	Ideal(^{o})
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

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

5.3.1 Protein backbone

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%)	1 4
2	B	93/99 (94%)	77 (83%)	11 (12%)	5 (5%)	2 18
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 (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	214/232 (92%)	179 (84%)	35 (16%)	3 14
2	B	90/94 (96%)	74 (82%)	16 (18%)	2 11
3	P	8/8 (100%)	6 (75%)	2 (25%)	1 3
4	D	107/111 (96%)	84 (78%)	23 (22%)	1 6
All	All	419/445 (94%)	343 (82%)	76 (18%)	2 11

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

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.31	1 (0%)	93	91	18, 50, 84, 128	0
2	B	97/99 (97%)	-0.22	1 (1%)	84	78	16, 46, 81, 110	0
3	P	8/8 (100%)	-0.01	0	100	100	52, 54, 67, 74	0
4	D	118/120 (98%)	-0.22	3 (2%)	61	51	22, 48, 94, 142	0
All	All	478/501 (95%)	-0.26	5 (1%)	84	78	16, 49, 86, 142	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	230	PHE	4.2
4	D	231	LYS	2.9
2	B	52	SER	2.5
1	A	155	ARG	2.4
4	D	232	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.