



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:22 am GMT

PDB ID : 1LD9
Title : THE THREE-DIMENSIONAL STRUCTURE OF AN H-2LD PEPTIDE COMPLEX EXPLAINS THE UNIQUE INTERACTION OF LD WITH BETA2M AND PEPTIDE
Authors : Balendiran, G.K.; Solheim, J.C.; Young, A.C.M.; Hansen, T.H.; Nathenson, S.G.; Sacchettini, J.C.
Deposited on : 1997-04-24
Resolution : 2.40 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) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

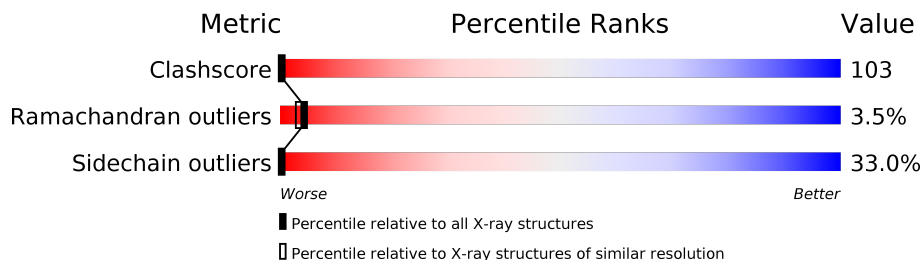
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	268	<div> <div>16%</div> <div>40%</div> <div>25%</div> <div>19%</div> </div>
1	D	268	<div> <div>17%</div> <div>40%</div> <div>25%</div> <div>19%</div> </div>
2	B	99	<div> <div>18%</div> <div>36%</div> <div>30%</div> <div>15%</div> </div>
2	E	99	<div> <div>16%</div> <div>37%</div> <div>31%</div> <div>15%</div> </div>
3	C	9	<div> <div>44%</div> <div>11%</div> <div>44%</div> </div>
3	F	9	<div> <div>44%</div> <div>11%</div> <div>44%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6168 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 MHC CLASS I H-2LD HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2184	1381	381	412	10			
1	D	268	Total	C	N	O	S	0	0	0
			2184	1381	381	412	10			

- Molecule 2 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	E	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

- Molecule 3 is a protein called NANO-PEPTIDE.

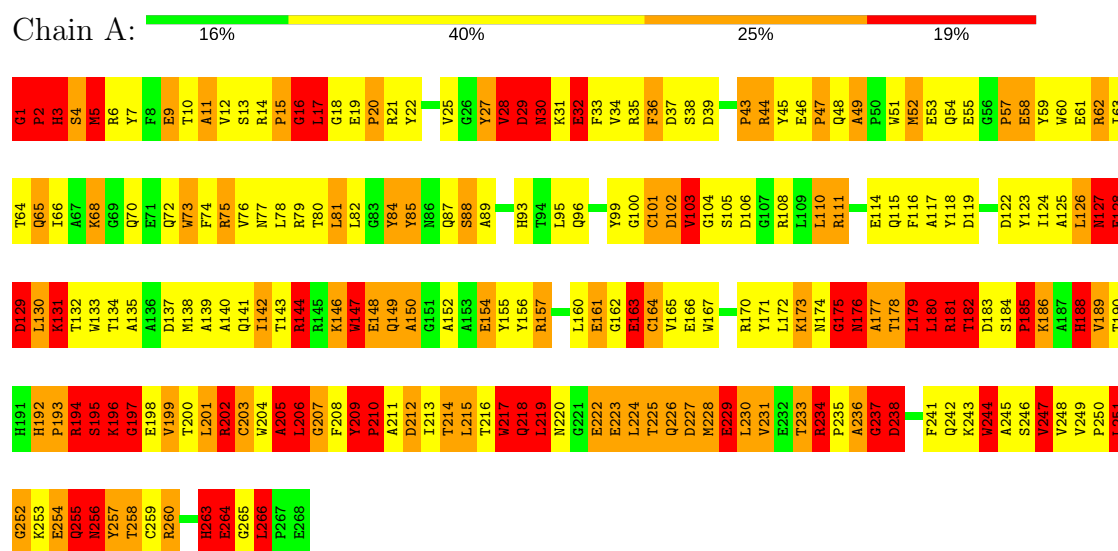
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			80	52	14	14			
3	F	9	Total	C	N	O	0	0	0
			80	52	14	14			

3 Residue-property plots

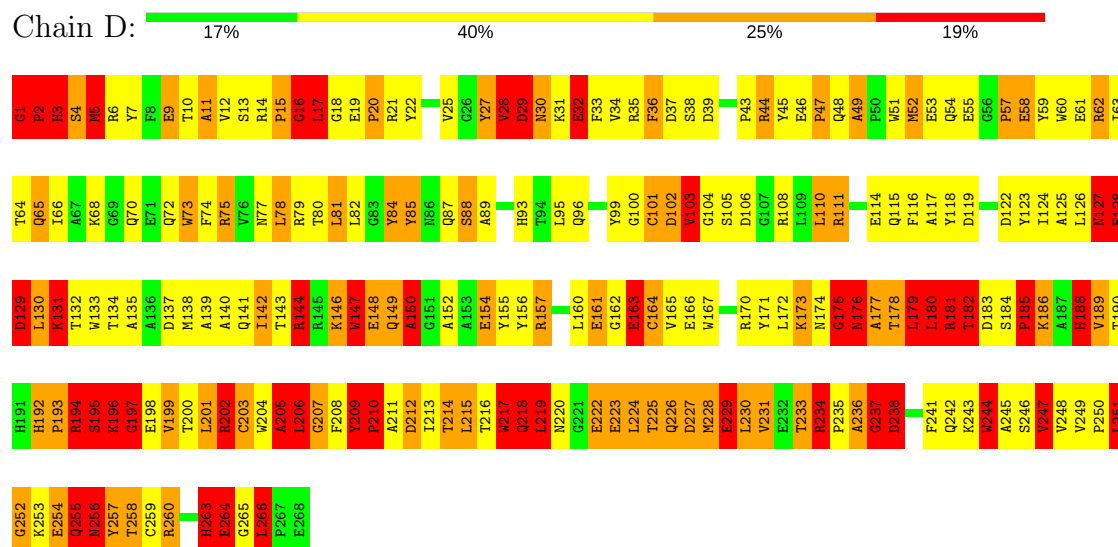
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

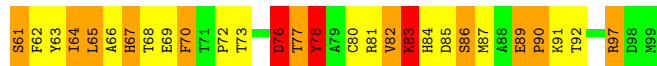
• Molecule 1: MHC CLASS I H-2LD HEAVY CHAIN



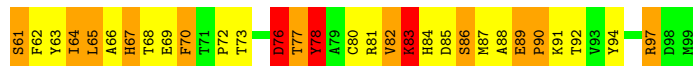
• Molecule 1: MHC CLASS I H-2LD HEAVY CHAIN



● Molecule 2: BETA-2 MICROGLOBULIN

Chain B: 

● Molecule 2: BETA-2 MICROGLOBULIN

Chain E: 

● Molecule 3: NANO-PEPTIDE

Chain C: 

● Molecule 3: NANO-PEPTIDE

Chain F: 

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.10Å 87.20Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	75.0 ((Not available)-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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	1.62	41/2248 (1.8%)	2.94	122/3056 (4.0%)
1	D	1.62	41/2248 (1.8%)	2.94	121/3056 (4.0%)
2	B	1.94	23/846 (2.7%)	2.22	34/1148 (3.0%)
2	E	1.94	22/846 (2.6%)	2.22	35/1148 (3.0%)
3	C	1.26	1/83 (1.2%)	1.74	6/112 (5.4%)
3	F	1.26	1/83 (1.2%)	1.74	6/112 (5.4%)
All	All	1.70	129/6354 (2.0%)	2.74	324/8632 (3.8%)

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	60
1	D	0	60
2	B	0	12
2	E	0	12
3	C	0	2
3	F	0	2
All	All	0	148

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	20	PRO	N-CD	20.15	1.76	1.47
2	B	20	PRO	N-CD	20.11	1.76	1.47
2	E	47	PRO	N-CD	19.59	1.75	1.47
2	B	47	PRO	N-CD	19.57	1.75	1.47
2	B	19	LYS	C-O	-18.04	0.89	1.23

The worst 5 of 324 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	ALA	O-C-N	-58.63	23.52	123.20
1	A	236	ALA	O-C-N	-58.62	23.55	123.20
1	D	206	LEU	O-C-N	-45.83	45.30	123.20
1	A	206	LEU	O-C-N	-45.81	45.33	123.20
1	D	264	GLU	O-C-N	-42.72	50.57	123.20

There are no chirality outliers.

5 of 148 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	GLY	Mainchain,Peptide
1	A	16	GLY	Mainchain,Peptide
1	A	17	LEU	Mainchain
1	A	2	PRO	Peptide
1	A	3	HIS	Peptide

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	2184	0	2039	503	14
1	D	2184	0	2041	486	17
2	B	820	0	795	141	0
2	E	820	0	795	147	2
3	C	80	0	72	23	2
3	F	80	0	72	23	2
All	All	6168	0	5814	1229	29

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 103.

The worst 5 of 1229 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:2:PRO:HA	1:A:3:HIS:CD2	1.24	1.70
1:D:2:PRO:HA	1:D:3:HIS:CD2	1.25	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:PRO:CG	2:B:20:PRO:CB	1.79	1.61
2:E:47:PRO:CG	2:E:47:PRO:CB	1.76	1.59
2:E:20:PRO:CG	2:E:20:PRO:CB	1.79	1.58

The worst 5 of 29 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:D:105:SER:C	1:D:264:GLU:OE2[2_565]	0.57	1.63
1:D:106:ASP:CA	1:D:264:GLU:OE1[2_565]	0.91	1.29
1:A:106:ASP:CA	1:A:264:GLU:OE1[2_555]	1.04	1.16
1:D:105:SER:O	1:D:264:GLU:OE2[2_565]	1.09	1.11
1:A:76:VAL:CG1	1:D:149:GLN:NE2[3_546]	1.14	1.06

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	266/268 (99%)	204 (77%)	53 (20%)	9 (3%)	4	3
1	D	266/268 (99%)	204 (77%)	53 (20%)	9 (3%)	4	3
2	B	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	3	2
2	E	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	3	2
3	C	7/9 (78%)	3 (43%)	4 (57%)	0	100	100
3	F	7/9 (78%)	3 (43%)	4 (57%)	0	100	100
All	All	740/752 (98%)	572 (77%)	142 (19%)	26 (4%)	4	3

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL

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Mol	Chain	Res	Type
1	A	148	GLU
2	B	41	LYS
1	D	103	VAL
1	D	148	GLU

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	223/223 (100%)	161 (72%)	62 (28%)	0	0
1	D	223/223 (100%)	162 (73%)	61 (27%)	0	0
2	B	94/94 (100%)	54 (57%)	40 (43%)	0	0
2	E	94/94 (100%)	54 (57%)	40 (43%)	0	0
3	C	9/9 (100%)	3 (33%)	6 (67%)	0	0
3	F	9/9 (100%)	3 (33%)	6 (67%)	0	0
All	All	652/652 (100%)	437 (67%)	215 (33%)	0	0

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	85	ASP
1	D	54	GLN
2	E	70	PHE
2	B	90	PRO
1	D	5	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	67	HIS
1	D	70	GLN
2	E	29	GLN
1	D	3	HIS

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Mol	Chain	Res	Type
1	D	72	GLN

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.