



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 05:47 am BST

PDB ID : 1LMK
Title : THE STRUCTURE OF A BIVALENT DIABODY
Authors : Williams, R.L.
Deposited on : 1994-08-29
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

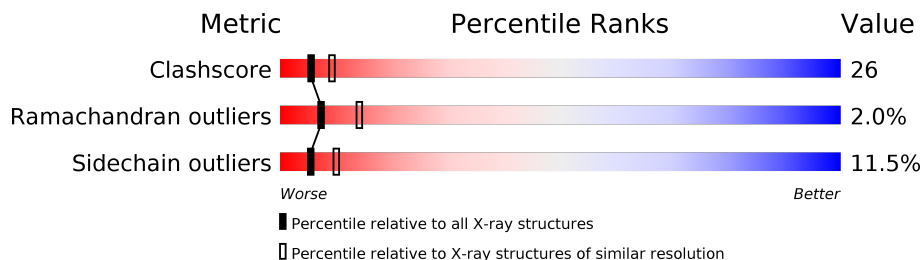
1 Overall quality at a glance

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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 on 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	
1	C	238	
1	E	238	
1	G	238	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7613 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 ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	238	Total 1838	C 1167	N 305	O 360	S 6	61	0	0
1	C	238	Total 1838	C 1167	N 305	O 360	S 6	30	0	0
1	E	238	Total 1838	C 1167	N 305	O 360	S 6	64	0	0
1	G	238	Total 1838	C 1167	N 305	O 360	S 6	37	0	0

- Molecule 2 is water.

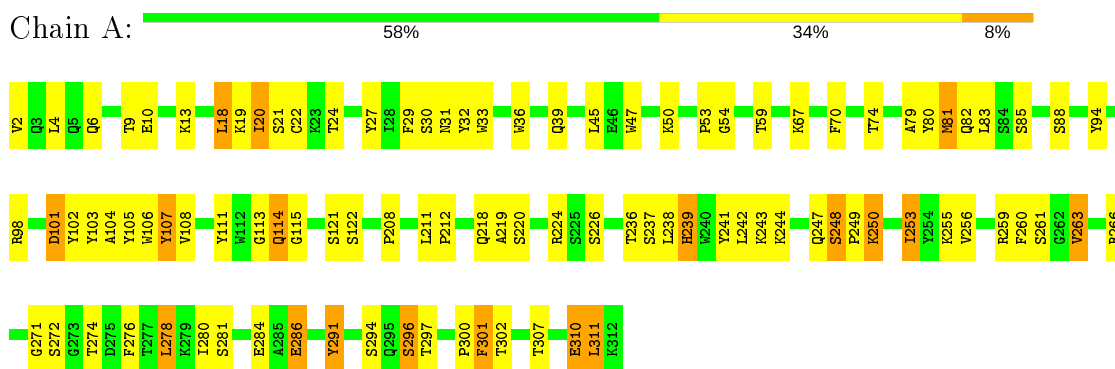
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total 72	O 72	0	0
2	C	65	Total 65	O 65	0	0
2	E	66	Total 66	O 66	0	0
2	G	58	Total 58	O 58	0	0

3 Residue-property plots [i](#)

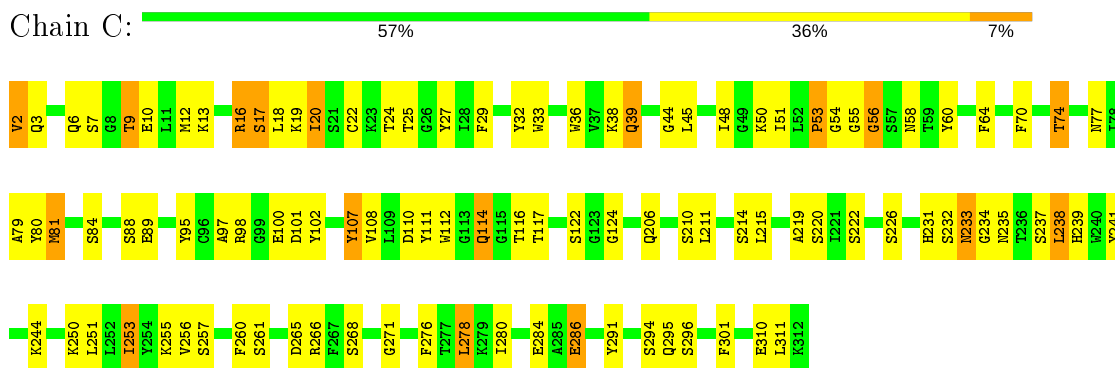
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

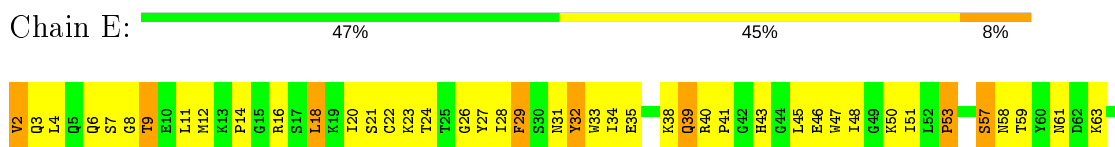
- Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY

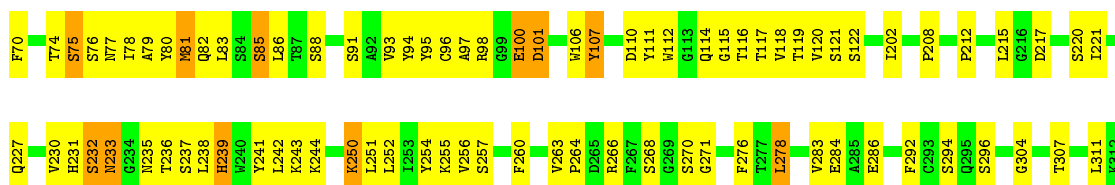


- Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY



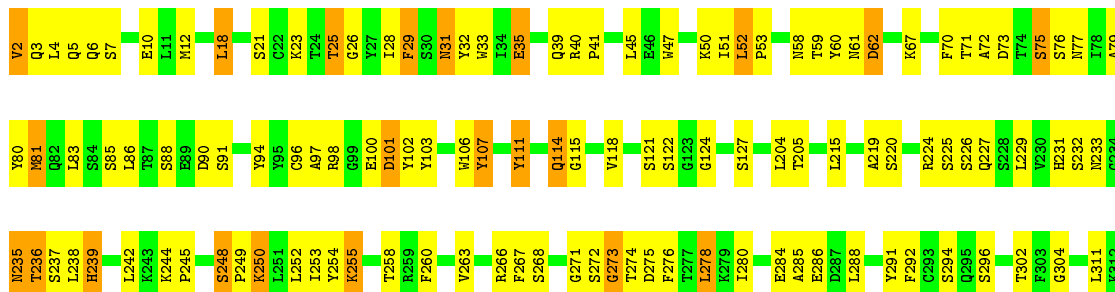
- Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY





• Molecule 1: ANTI-PHOSPHATIDYLINOSITOL SPECIFIC PHOSPHOLIPASE C DIABODY

Chain G: 49% 42% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.14Å 80.71Å 88.01Å 90.00° 99.81° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7613	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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	0.89	0/1885	1.04	1/2554 (0.0%)
1	C	0.93	0/1885	1.04	1/2554 (0.0%)
1	E	0.91	0/1885	1.06	4/2554 (0.2%)
1	G	0.83	0/1885	1.01	0/2554
All	All	0.89	0/7540	1.03	6/10216 (0.1%)

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	1
1	C	0	1
1	E	0	1
1	G	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	238	LEU	CA-CB-CG	-6.42	100.53	115.30
1	A	238	LEU	CA-CB-CG	-5.83	101.89	115.30
1	E	101	ASP	CB-CG-OD1	5.74	123.47	118.30
1	E	38	LYS	CD-CE-NZ	-5.42	99.23	111.70
1	C	253	ILE	CG1-CB-CG2	-5.30	99.74	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	TYR	Sidechain
1	C	291	TYR	Sidechain
1	E	32	TYR	Sidechain
1	G	103	TYR	Sidechain
1	G	111	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	1838	0	1777	87	0
1	C	1838	0	1777	92	0
1	E	1838	0	1777	100	0
1	G	1838	0	1777	99	0
2	A	72	0	0	4	0
2	C	65	0	0	4	0
2	E	66	0	0	3	0
2	G	58	0	0	5	0
All	All	7613	0	7108	364	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 26.

The worst 5 of 364 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:C:39:GLN:HG3	1:C:45:LEU:HD23	1.41	1.01
1:A:39:GLN:HG2	1:A:45:LEU:HD23	1.47	0.95
1:C:20:ILE:HG21	1:C:116:THR:HG21	1.50	0.93
1:E:2:VAL:HG11	1:E:98:ARG:HH21	1.35	0.91
1:A:114:GLN:H	1:A:114:GLN:HE21	1.19	0.90

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	236/238 (99%)	216 (92%)	18 (8%)	2 (1%)	19	39
1	C	236/238 (99%)	215 (91%)	16 (7%)	5 (2%)	7	13
1	E	236/238 (99%)	215 (91%)	16 (7%)	5 (2%)	7	13
1	G	236/238 (99%)	209 (89%)	20 (8%)	7 (3%)	4	7
All	All	944/952 (99%)	855 (91%)	70 (7%)	19 (2%)	7	14

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	124	GLY
1	E	85	SER
1	E	256	VAL
1	A	85	SER
1	C	55	GLY

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	203/203 (100%)	182 (90%)	21 (10%)	7	13
1	C	203/203 (100%)	182 (90%)	21 (10%)	7	13
1	E	203/203 (100%)	179 (88%)	24 (12%)	5	9
1	G	203/203 (100%)	176 (87%)	27 (13%)	4	7
All	All	812/812 (100%)	719 (88%)	93 (12%)	5	10

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	VAL
1	E	85	SER
1	G	238	LEU
1	E	7	SER
1	E	39	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	239	HIS
1	E	218	GLN
1	G	114	GLN
1	C	233	ASN
1	E	239	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

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.