



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:54 pm GMT

PDB ID : 1LE4
Title : STRUCTURAL BASIS FOR ALTERED FUNCTION IN THE COMMON
MUTANTS OF HUMAN APOLIPOPROTEIN-E
Authors : Wilson, C.; Agard, D.A.
Deposited on : 1991-08-22
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

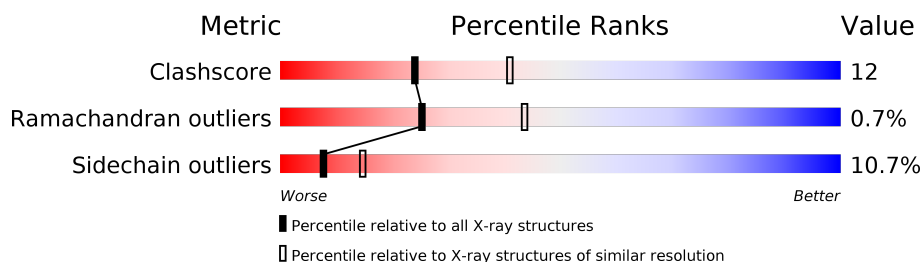
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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	144	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1251 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 APOLIPOPROTEIN E4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1150	714	215	217	4			

- Molecule 2 is water.

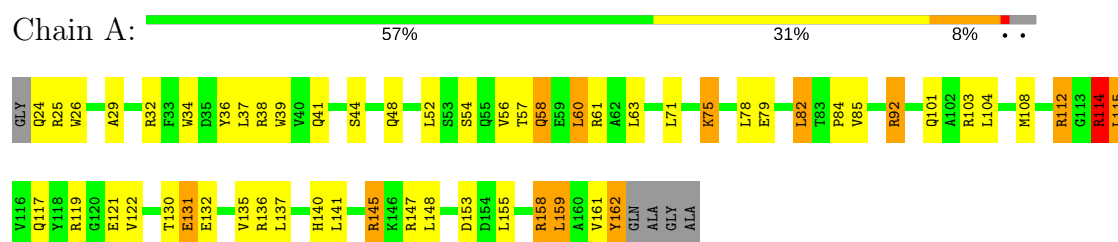
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	101	Total	O	0	0
			101	101		

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.

Note EDS was not executed.

• Molecule 1: APOLIPOPROTEIN E4



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 21	Depositor
Cell constants a, b, c, α , β , γ	40.71Å 53.33Å 85.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1251	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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	0.92	0/1162	1.78	29/1559 (1.9%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-14.97	112.82	120.30
1	A	114	ARG	NE-CZ-NH1	11.45	126.02	120.30
1	A	38	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	112	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	A	34	TRP	CD1-CG-CD2	9.29	113.73	106.30
1	A	34	TRP	CE2-CD2-CG	-8.77	100.28	107.30
1	A	26	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	39	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	39	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	A	103	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	39	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	A	34	TRP	CG-CD2-CE3	7.45	140.60	133.90
1	A	158	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	34	TRP	CB-CG-CD1	-7.28	117.54	127.00
1	A	26	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	158	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	39	TRP	CB-CG-CD1	-6.70	118.29	127.00
1	A	145	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	147	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	82	LEU	N-CA-C	6.07	127.38	111.00
1	A	38	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	60	LEU	CA-CB-CG	5.62	128.24	115.30
1	A	26	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	92	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	34	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	25	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	39	TRP	CG-CD1-NE1	-5.11	104.99	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	136	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1150	0	1172	29	0
2	A	101	0	0	0	0
All	All	1251	0	1172	29	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 12.

All (29) 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:78:LEU:HD13	1:A:162:TYR:HB3	1.70	0.73
1:A:57:THR:HA	1:A:60:LEU:HD12	1.73	0.69
1:A:114:ARG:HD3	1:A:140:HIS:ND1	2.12	0.64
1:A:44:SER:O	1:A:48:GLN:HG3	2.02	0.60
1:A:60:LEU:HD11	1:A:115:LEU:HD23	1.86	0.58
1:A:29:ALA:HA	1:A:32:ARG:HH11	1.68	0.57
1:A:131:GLU:O	1:A:135:VAL:HG23	2.04	0.56
1:A:37:LEU:HG	1:A:145:ARG:HD3	1.89	0.55
1:A:108:MET:HG2	1:A:148:LEU:HD11	1.89	0.54
1:A:79:GLU:HA	1:A:82:LEU:HD12	1.90	0.54
1:A:41:GLN:HE21	1:A:145:ARG:HE	1.57	0.52
1:A:117:GLN:O	1:A:121:GLU:HG3	2.10	0.51
1:A:41:GLN:HE21	1:A:145:ARG:HH21	1.59	0.50
1:A:54:SER:O	1:A:58:GLN:HB2	2.12	0.49
1:A:52:LEU:HA	1:A:119:ARG:HG3	1.94	0.49
1:A:58:GLN:HE21	1:A:61:ARG:HE	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD21	1:A:101:GLN:HG2	1.98	0.46
1:A:37:LEU:HG	1:A:145:ARG:CD	2.45	0.46
1:A:141:LEU:O	1:A:145:ARG:HG3	2.16	0.45
1:A:36:TYR:OH	1:A:56:VAL:HG12	2.18	0.43
1:A:104:LEU:HD22	1:A:155:LEU:CD2	2.48	0.43
1:A:75:LYS:HE3	1:A:75:LYS:HB3	1.84	0.43
1:A:41:GLN:HE21	1:A:145:ARG:NH2	2.17	0.42
1:A:122:VAL:HG13	1:A:130:THR:HG21	2.02	0.42
1:A:29:ALA:HA	1:A:32:ARG:NH1	2.34	0.41
1:A:158:ARG:O	1:A:161:VAL:HG12	2.21	0.41
1:A:159:LEU:HA	1:A:159:LEU:HD12	1.81	0.40
1:A:36:TYR:OH	1:A:56:VAL:HA	2.21	0.40
1:A:82:LEU:O	1:A:84:PRO:HD3	2.22	0.40

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	137/144 (95%)	127 (93%)	9 (7%)	1 (1%)	25	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	VAL

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	121/122 (99%)	108 (89%)	13 (11%)	8 15

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	58	GLN
1	A	63	LEU
1	A	75	LYS
1	A	92	ARG
1	A	112	ARG
1	A	114	ARG
1	A	115	LEU
1	A	131	GLU
1	A	132	GLU
1	A	137	LEU
1	A	153	ASP
1	A	159	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	58	GLN
1	A	117	GLN

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

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.