Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 11:36 AM EDT

PDB ID	:	1OR3 / pdb_00001or3
Title	:	APOLIPOPROTEIN E3 (APOE3), TRIGONAL TRUNCATION MUTANT 165
Authors	:	Rupp, B.; Segelke, B.W.
Deposited on	:	1998-12-01
Resolution	:	1.73 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

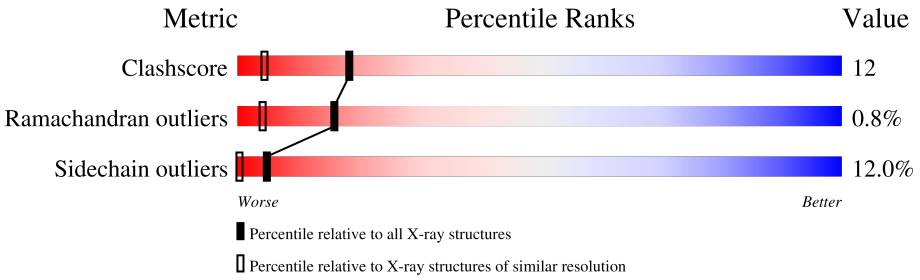
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.73 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	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)

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 of 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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	165	56% 20% 6% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1306 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 PROTEIN (APOLIPOPROTEIN E).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	6	0
			1148	712	219	212	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		

3 Residue-property plots (i)

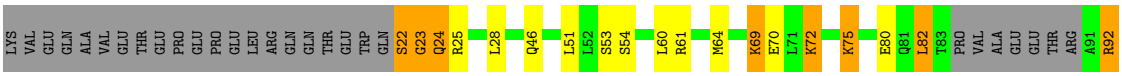
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

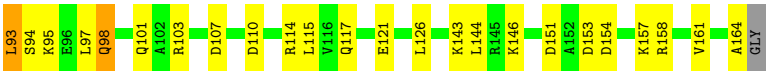
Note EDS failed to run properly.

- Molecule 1: PROTEIN (APOLIPOPROTEIN E)

Chain A:







4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	47.37Å 47.37Å 104.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.73	Depositor
% Data completeness (in resolution range)	89.9 (10.00-1.73)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	6.80	Depositor
$< I/\sigma(I) >$ [1]	5.31 (at 1.73Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.229 , 0.238	Depositor
Wilson B-factor (Å^2)	5.5	Xtriage
Anisotropy	0.675	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.198 for -h,-k,l	Xtriage
Total number of atoms	1306	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.42	0/1184	0.88	0/1581

There are no bond length outliers.

There are no bond angle outliers.

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	1148	0	1178	28	0
2	A	158	0	0	0	0
All	All	1306	0	1178	28	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 (28) 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:22:SER:N	1:A:25:ARG:HB2	2.10	0.66
1:A:53:SER:O	1:A:54:SER:HB2	1.98	0.63
1:A:93:LEU:HD11	1:A:161:VAL:HG12	1.80	0.63
1:A:75:LYS:HE3	1:A:97:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD21	1:A:115:LEU:HD22	1.84	0.59
1:A:22:SER:O	1:A:23:GLY:C	2.48	0.57
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.69	0.56
1:A:153:ASP:O	1:A:157:LYS:HG3	2.06	0.56
1:A:107:ASP:OD2	1:A:151:ASP:OD2	2.26	0.54
1:A:69:LYS:HG3	1:A:70:GLU:N	2.24	0.53
1:A:114[B]:ARG:CZ	1:A:117:GLN:OE1	2.57	0.52
1:A:24:GLN:HG3	1:A:28:LEU:HG	1.94	0.50
1:A:24:GLN:O	1:A:28:LEU:HG	2.12	0.49
1:A:110:ASP:HB3	1:A:144:LEU:HD21	1.95	0.47
1:A:98:GLN:O	1:A:101:GLN:HB3	2.15	0.47
1:A:82:LEU:HB2	1:A:164:ALA:HB2	1.96	0.47
1:A:61:ARG:HH11	1:A:64:MET:HE1	1.78	0.46
1:A:103:ARG:NH2	1:A:154:ASP:OD2	2.49	0.45
1:A:117:GLN:O	1:A:121:GLU:HG3	2.17	0.44
1:A:117:GLN:NE2	1:A:121:GLU:OE2	2.52	0.43
1:A:75:LYS:HE3	1:A:97:LEU:CG	2.49	0.42
1:A:92:ARG:O	1:A:93:LEU:C	2.62	0.41
1:A:158:ARG:HG2	1:A:158:ARG:NH1	2.33	0.41
1:A:110:ASP:O	1:A:114[A]:ARG:HG2	2.21	0.41
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.92	0.41
1:A:72:LYS:HE3	1:A:72:LYS:HB2	1.79	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	138/165 (84%)	137 (99%)	0	1 (1%)	18 6

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	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	123/143 (86%)	108 (88%)	15 (12%)	5 0

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	24	GLN
1	A	46[A]	GLN
1	A	46[B]	GLN
1	A	69	LYS
1	A	72	LYS
1	A	75	LYS
1	A	80	GLU
1	A	82	LEU
1	A	92	ARG
1	A	93	LEU
1	A	94	SER
1	A	95	LYS
1	A	98	GLN
1	A	126	LEU

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	58	GLN
1	A	123	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 oligosaccharides 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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.