Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:29 PM GMT

PDB ID	:	1FW3
Title	:	OUTER MEMBRANE PHOSPHOLIPASE A FROM ESCHERICHIA COLI
Authors	:	Snijder, H.J.; Kingma, R.L.; Kalk, K.H.; Dekker, N.; Egmond, M.R.; Dijkstra, B.W.
Deposited on	:	2000-09-21
Resolution	:	2.80 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 (i) symbol.

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

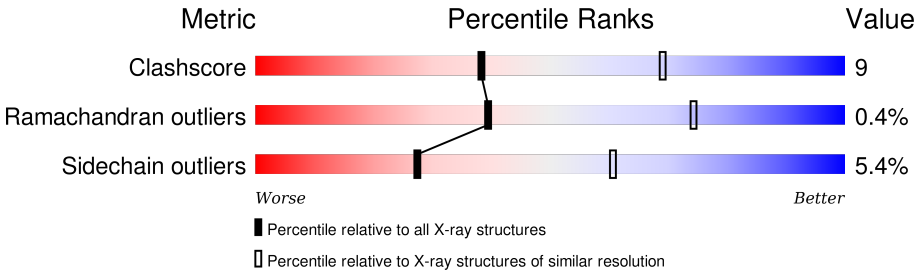
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	67% 23% • 9%
1	B	275	69% 21% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4102 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 OUTER MEMBRANE PHOSPHOLIPASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2051	1317	338	390	6			
1	B	250	Total	C	N	O	S	0	0	0
			2051	1317	338	390	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	N-TERMINAL EXTENSION	UNP P0A921
A	-4	ARG	-	N-TERMINAL EXTENSION	UNP P0A921
A	-3	ILE	-	N-TERMINAL EXTENSION	UNP P0A921
A	-2	ARG	-	N-TERMINAL EXTENSION	UNP P0A921
A	-1	ALA	-	N-TERMINAL EXTENSION	UNP P0A921
A	0	PRO	-	N-TERMINAL EXTENSION	UNP P0A921
A	144	S1H	SER	modified residue	UNP P0A921
B	-5	ALA	-	N-TERMINAL EXTENSION	UNP P0A921
B	-4	ARG	-	N-TERMINAL EXTENSION	UNP P0A921
B	-3	ILE	-	N-TERMINAL EXTENSION	UNP P0A921
B	-2	ARG	-	N-TERMINAL EXTENSION	UNP P0A921
B	-1	ALA	-	N-TERMINAL EXTENSION	UNP P0A921
B	0	PRO	-	N-TERMINAL EXTENSION	UNP P0A921
B	144	S1H	SER	modified residue	UNP P0A921

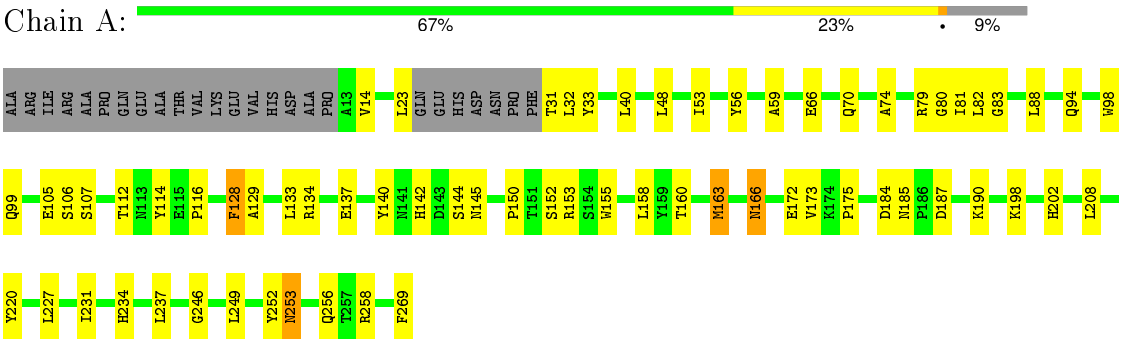
3 Residue-property plots (i)

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.

Note EDS was not executed.

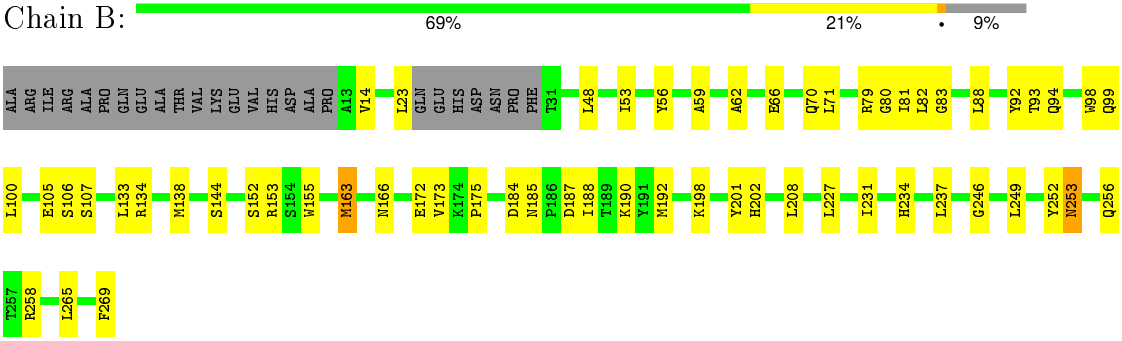
- Molecule 1: OUTER MEMBRANE PHOSPHOLIPASE A

Chain A:



- Molecule 1: OUTER MEMBRANE PHOSPHOLIPASE A

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.54Å 84.97Å 95.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.90 – 2.80	Depositor
% Data completeness (in resolution range)	81.0 (37.90-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.224 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4102	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S1H

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	0.51	0/2083	0.66	0/2833
1	B	0.47	0/2083	0.65	0/2833
All	All	0.49	0/4166	0.65	0/5666

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	201	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	2051	0	1948	45	0
1	B	2051	0	1948	37	0
All	All	4102	0	3896	73	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 9.

All (73) 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:231:ILE:HD11	1:A:237:LEU:HG	1.46	0.97
1:B:231:ILE:HD11	1:B:237:LEU:HG	1.47	0.96
1:B:173:VAL:HG12	1:B:175:PRO:HD3	1.78	0.66
1:A:173:VAL:HG12	1:A:175:PRO:HD3	1.78	0.64
1:B:187:ASP:O	1:B:190:LYS:HB3	1.97	0.64
1:A:187:ASP:O	1:A:190:LYS:HB3	1.97	0.63
1:B:246:GLY:HA2	1:B:252:TYR:HA	1.82	0.61
1:A:246:GLY:HA2	1:A:252:TYR:HA	1.82	0.61
1:B:153:ARG:HB3	1:B:249:LEU:HB3	1.83	0.60
1:A:153:ARG:HB3	1:A:249:LEU:HB3	1.84	0.59
1:B:92:TYR:CD1	1:B:144:S1H:H72	2.41	0.56
1:A:98:TRP:CZ3	1:B:144:S1H:H42	2.41	0.55
1:A:134:ARG:HB2	1:A:163:MET:HE2	1.89	0.55
1:A:114:TYR:HB2	1:A:144:S1H:H11	1.89	0.54
1:A:40:LEU:HD13	1:B:144:S1H:H82	1.90	0.54
1:A:172:GLU:HB3	1:A:198:LYS:HB2	1.91	0.52
1:A:98:TRP:CH2	1:B:144:S1H:H22	2.46	0.51
1:B:172:GLU:HB3	1:B:198:LYS:HB2	1.92	0.51
1:B:70:GLN:HA	1:B:94:GLN:O	2.12	0.49
1:B:152:SER:O	1:B:184:ASP:HB3	2.12	0.49
1:B:134:ARG:HB2	1:B:163:MET:HE2	1.95	0.49
1:A:140:TYR:CE2	1:A:158:LEU:CD2	2.96	0.49
1:A:70:GLN:HA	1:A:94:GLN:O	2.14	0.48
1:A:99:GLN:O	1:A:107:SER:HA	2.13	0.48
1:A:128:PHE:HD2	1:A:129:ALA:N	2.12	0.48
1:A:98:TRP:CZ2	1:B:144:S1H:H22	2.48	0.48
1:A:33:TYR:HB2	1:A:74:ALA:O	2.14	0.48
1:B:99:GLN:O	1:B:107:SER:HA	2.14	0.47
1:A:66:GLU:OE1	1:A:258:ARG:NH2	2.47	0.47
1:A:152:SER:O	1:A:184:ASP:HB3	2.14	0.46
1:A:253:ASN:HD22	1:A:253:ASN:C	2.18	0.46
1:B:105:GLU:O	1:B:106:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HD11	1:A:237:LEU:CG	2.31	0.46
1:B:23:LEU:HA	1:B:79:ARG:HE	1.81	0.45
1:A:234:HIS:CE1	1:B:79:ARG:HH12	2.34	0.45
1:B:66:GLU:OE1	1:B:258:ARG:NH2	2.49	0.45
1:B:208:LEU:HD23	1:B:227:LEU:HD13	1.99	0.45
1:B:253:ASN:HD22	1:B:253:ASN:C	2.19	0.45
1:A:23:LEU:HA	1:A:79:ARG:HE	1.82	0.45
1:A:53:ILE:O	1:A:59:ALA:HB2	2.17	0.44
1:A:32:LEU:HD22	1:B:265:LEU:HD13	1.98	0.44
1:A:105:GLU:O	1:A:106:SER:HB2	2.18	0.44
1:A:134:ARG:HB2	1:A:163:MET:CE	2.47	0.44
1:B:253:ASN:ND2	1:B:253:ASN:H	2.15	0.44
1:B:53:ILE:O	1:B:59:ALA:HB2	2.18	0.44
1:B:134:ARG:HB2	1:B:163:MET:CE	2.47	0.43
1:A:208:LEU:HD23	1:A:227:LEU:HD13	2.00	0.43
1:A:80:GLY:HA2	1:A:83:GLY:O	2.17	0.43
1:A:144:S1H:H11	1:A:144:S1H:HB3	1.73	0.43
1:B:53:ILE:HB	1:B:56:TYR:CD2	2.54	0.43
1:A:253:ASN:H	1:A:253:ASN:ND2	2.16	0.43
1:B:80:GLY:HA2	1:B:83:GLY:O	2.18	0.43
1:A:116:PRO:HD2	1:A:142:HIS:O	2.19	0.42
1:A:79:ARG:HH12	1:B:234:HIS:CE1	2.38	0.42
1:B:81:ILE:O	1:B:82:LEU:HD23	2.19	0.42
1:A:140:TYR:CD2	1:A:158:LEU:CD2	3.03	0.42
1:B:48:LEU:CD2	1:B:62:ALA:HB1	2.50	0.42
1:A:81:ILE:O	1:A:82:LEU:HD23	2.20	0.42
1:A:53:ILE:HB	1:A:56:TYR:CD2	2.55	0.41
1:A:128:PHE:C	1:A:128:PHE:HD2	2.24	0.41
1:A:166:ASN:C	1:A:166:ASN:HD22	2.24	0.41
1:A:190:LYS:HE2	1:A:220:TYR:HE2	1.85	0.41
1:A:40:LEU:HB2	1:B:144:S1H:H102	2.01	0.41
1:A:137:GLU:O	1:A:160:THR:HA	2.20	0.41
1:B:133:LEU:HD12	1:B:163:MET:O	2.21	0.41
1:A:128:PHE:CD2	1:A:128:PHE:C	2.93	0.41
1:B:188:ILE:HG12	1:B:192:MET:HG3	2.02	0.41
1:A:144:S1H:H22	1:B:98:TRP:CZ2	2.55	0.41
1:B:98:TRP:CH2	1:B:100:LEU:HD13	2.56	0.40
1:A:112:THR:O	1:A:145:ASN:HA	2.21	0.40
1:B:208:LEU:CD2	1:B:227:LEU:HD13	2.52	0.40
1:B:71:LEU:O	1:B:93:THR:HA	2.21	0.40
1:A:133:LEU:HD12	1:A:163:MET:O	2.21	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	245/275 (89%)	229 (94%)	15 (6%)	1 (0%)	39	74
1	B	245/275 (89%)	232 (95%)	12 (5%)	1 (0%)	39	74
All	All	490/550 (89%)	461 (94%)	27 (6%)	2 (0%)	39	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	B	14	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	213/234 (91%)	200 (94%)	13 (6%)	23	55
1	B	213/234 (91%)	203 (95%)	10 (5%)	32	67
All	All	426/468 (91%)	403 (95%)	23 (5%)	27	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR

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Mol	Chain	Res	Type
1	A	48	LEU
1	A	88	LEU
1	A	128	PHE
1	A	150	PRO
1	A	155	TRP
1	A	163	MET
1	A	166	ASN
1	A	185	ASN
1	A	202	HIS
1	A	253	ASN
1	A	256	GLN
1	A	269	PHE
1	B	88	LEU
1	B	138	MET
1	B	155	TRP
1	B	163	MET
1	B	166	ASN
1	B	185	ASN
1	B	202	HIS
1	B	253	ASN
1	B	256	GLN
1	B	269	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	253	ASN
1	B	166	ASN
1	B	253	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	S1H	A	144	1	23,24,25	0.61	1 (4%)	23,27,29	1.10	2 (8%)
1	S1H	B	144	1	23,24,25	0.44	0	23,27,29	1.09	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	S1H	A	144	1	-	0/22/25/27	0/0/0/0
1	S1H	B	144	1	-	0/22/25/27	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	S1H	OG-CB	-2.26	1.36	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	144	S1H	C2-C1-S1	-2.24	109.47	113.11
1	A	144	S1H	O-C-CA	-2.21	119.74	125.49
1	B	144	S1H	O-C-CA	-2.12	119.98	125.49
1	A	144	S1H	O1S-S1-C1	2.07	109.69	106.83
1	B	144	S1H	O2S-S1-C1	2.41	110.16	106.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	144	S1H	3	0
1	B	144	S1H	6	0

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.