



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:32 AM GMT

PDB ID : 2R4N
Title : Crystal structure of the long-chain fatty acid transporter FadL mutant N33A
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Deposited on : 2007-08-31
Resolution : 3.20 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

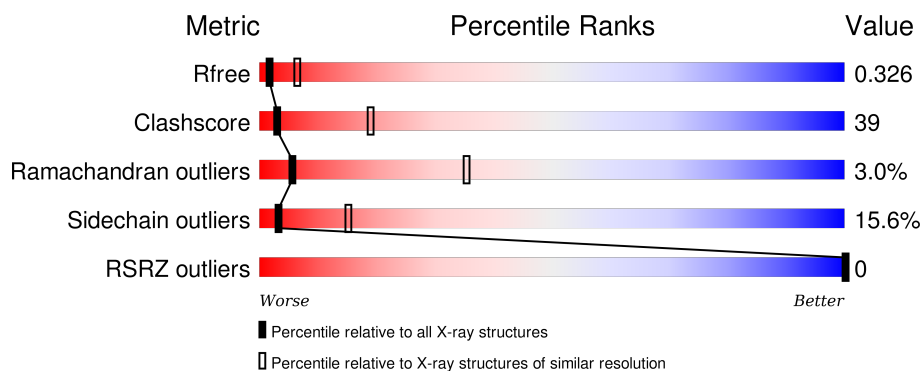
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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.

Mol	Chain	Length	Quality of chain
1	A	427	<div> <div>40%</div> <div>49%</div> <div>9%</div> <div>.</div> </div>
1	B	427	<div> <div>39%</div> <div>49%</div> <div>11%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	501	-	-	-	X
2	LDA	B	502	-	-	X	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6528 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.

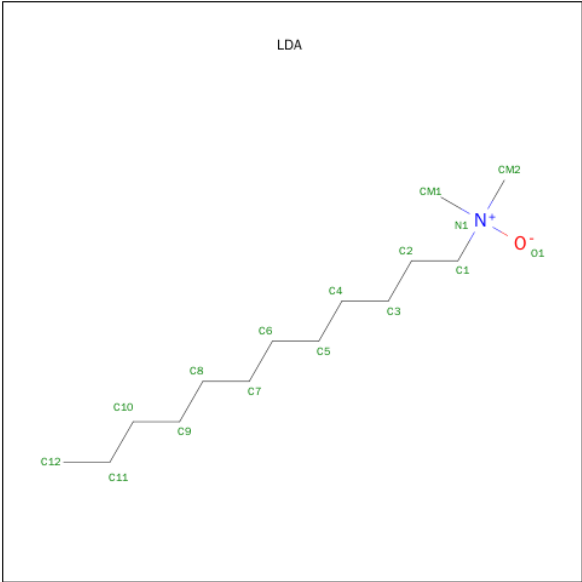
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3248	2054	551	637	6			
1	B	421	Total	C	N	O	S	0	0	0
			3248	2054	551	637	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ALA	ASN	ENGINEERED	UNP P10384
A	197	THR	ILE	CONFLICT	UNP P10384
A	422	HIS	-	EXPRESSION TAG	UNP P10384
A	423	HIS	-	EXPRESSION TAG	UNP P10384
A	424	HIS	-	EXPRESSION TAG	UNP P10384
A	425	HIS	-	EXPRESSION TAG	UNP P10384
A	426	HIS	-	EXPRESSION TAG	UNP P10384
A	427	HIS	-	EXPRESSION TAG	UNP P10384
B	33	ALA	ASN	ENGINEERED	UNP P10384
B	197	THR	ILE	CONFLICT	UNP P10384
B	422	HIS	-	EXPRESSION TAG	UNP P10384
B	423	HIS	-	EXPRESSION TAG	UNP P10384
B	424	HIS	-	EXPRESSION TAG	UNP P10384
B	425	HIS	-	EXPRESSION TAG	UNP P10384
B	426	HIS	-	EXPRESSION TAG	UNP P10384
B	427	HIS	-	EXPRESSION TAG	UNP P10384

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).

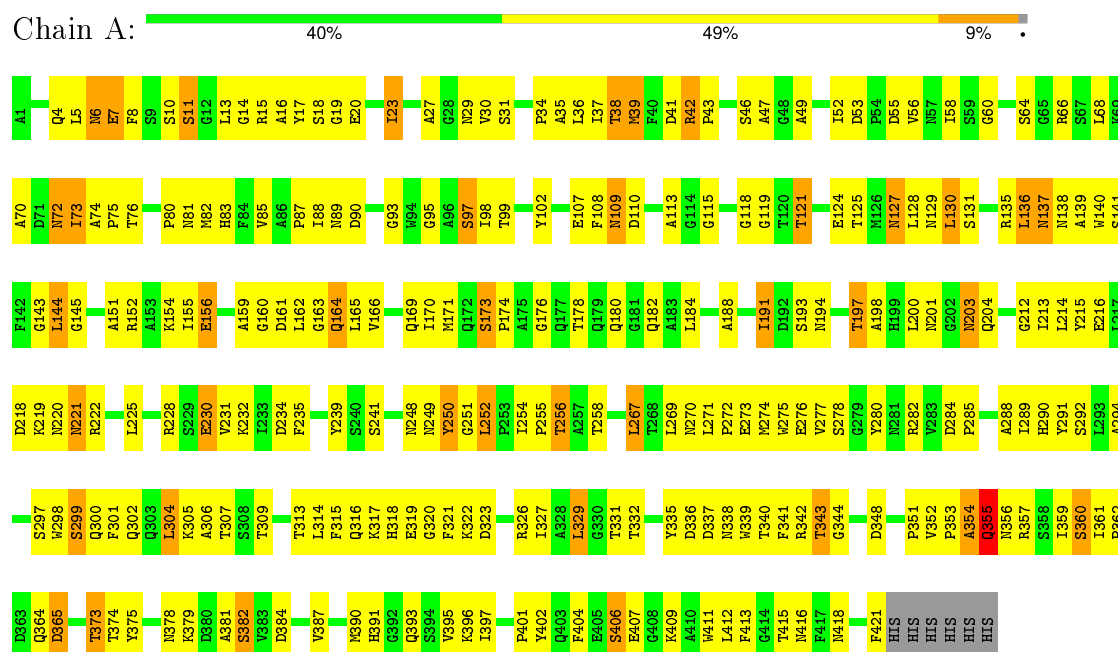


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

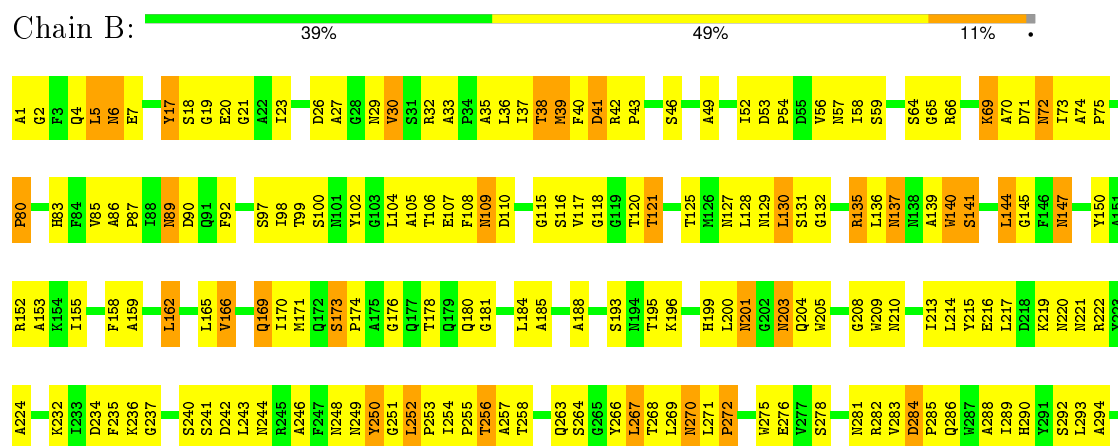
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

• Molecule 1: Long-chain fatty acid transport protein



• Molecule 1: Long-chain fatty acid transport protein



S297	S298	S299	F300	F301	Q302	Q303	L304	K305	A306		T309		L314	F315		E319	Q320	F321	K322	D323	A324	G325	K326	I327		T331	T332	G333	Y334	Y335		W339	T340	F341		W411	I412	T413	G414	T415	N416	F417	N418		F421	HIS	HIS	HIS	HIS	HIS	HIS
M368	L369		G372	T373	T374	Y375	A376	F377	N378	K379	D380	A381	S382	V383	D384		V387		M390	H391	G392	Q393	S394		I397	N398		Y402	Q403	F404		E407		W411	I412	T413	G414	T415	N416	F417	N418		F421	HIS	HIS	HIS	HIS	HIS	HIS		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.21Å 39.99Å 175.00Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 37.12 – 3.11	Depositor EDS
% Data completeness (in resolution range)	85.2 (10.00-3.20) 84.6 (37.12-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.332 0.235 , 0.326	Depositor DCC
R_{free} test set	1050 reflections (7.68%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.943	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 6.9	EDS
Estimated twinning fraction	0.460 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 15292 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6528	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/3337	0.74	0/4544
1	B	0.48	0/3337	0.76	0/4544
All	All	0.48	0/6674	0.75	0/9088

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	335	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	3248	0	3028	254	0
1	B	3248	0	3028	237	0
2	A	16	0	31	5	0
2	B	16	0	31	10	0
All	All	6528	0	6118	489	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 39.

The worst 5 of 489 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:B:178:THR:HG22	1:B:180:GLN:H	1.10	1.12
1:A:178:THR:HG22	1:A:180:GLN:H	1.21	0.99
1:A:58:ILE:HB	1:A:70:ALA:HB3	1.45	0.97
1:B:152:ARG:HG2	1:B:203:ASN:HB3	1.43	0.97
1:A:164:GLN:HE21	1:A:164:GLN:N	1.66	0.94

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	419/427 (98%)	353 (84%)	55 (13%)	11 (3%)	7	40
1	B	419/427 (98%)	355 (85%)	50 (12%)	14 (3%)	5	32
All	All	838/854 (98%)	708 (84%)	105 (12%)	25 (3%)	5	35

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	THR

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Mol	Chain	Res	Type
1	B	354	ALA
1	B	355	GLN
1	A	39	MET
1	A	119	GLY

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	330/336 (98%)	280 (85%)	50 (15%)	3	17
1	B	330/336 (98%)	277 (84%)	53 (16%)	3	14
All	All	660/672 (98%)	557 (84%)	103 (16%)	3	15

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	HIS
1	B	69	LYS
1	B	379	LYS
1	A	396	LYS
1	B	7	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	B	83	HIS
1	B	356	ASN
1	A	418	ASN
1	B	57	ASN

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 ⓘ

2 ligands 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	$\# Z > 2$
2	LDA	A	501	-	15,15,15	3.85	2 (13%)	16,17,17	1.78	2 (12%)
2	LDA	B	502	-	15,15,15	3.93	2 (13%)	16,17,17	1.97	5 (31%)

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
2	LDA	A	501	-	-	0/13/13/13	0/0/0/0
2	LDA	B	502	-	-	0/13/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	LDA	O1-N1	-14.53	1.25	1.39
2	A	501	LDA	O1-N1	-14.26	1.26	1.39
2	A	501	LDA	CM2-N1	-4.10	1.43	1.49
2	B	502	LDA	CM2-N1	-3.54	1.44	1.49

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	502	LDA	CM2-N1-CM1	-5.09	103.08	108.83
2	A	501	LDA	CM2-N1-CM1	-4.86	103.35	108.83
2	B	502	LDA	C6-C5-C4	-2.69	100.64	114.53
2	B	502	LDA	O1-N1-CM1	-2.05	106.31	109.05
2	B	502	LDA	O1-N1-CM2	2.46	112.34	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LDA	5	0
2	B	502	LDA	10	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/427 (98%)	-0.52	0 100 100	4, 20, 44, 84	0
1	B	421/427 (98%)	-0.45	0 100 100	4, 19, 44, 82	0
All	All	842/854 (98%)	-0.49	0 100 100	4, 20, 44, 84	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	LDA	A	501	16/16	0.92	0.42	4.09	21,21,21,21	0
2	LDA	B	502	16/16	0.93	0.33	2.62	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.