



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:04 PM GMT

PDB ID : 1RXT
Title : Crystal structure of human myristoyl-CoA:protein N-myristoyltransferase.
Authors : Yang, J.; Wang, Y.; Frey, G.; Abeles, R.H.; Petsko, G.A.; Ringe, D.
Deposited on : 2003-12-18
Resolution : 3.00 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

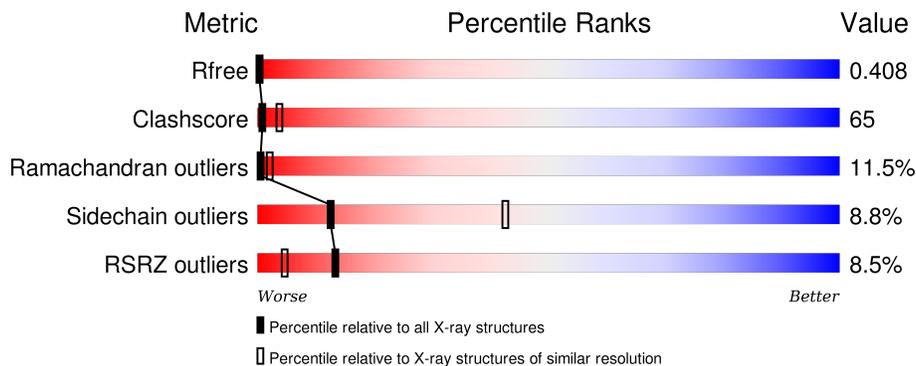
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	496	 4% 20% 40% 8% 31%
1	B	496	 4% 21% 39% 9% 31%
1	C	496	 7% 17% 38% 9% 34%
1	D	496	 8% 17% 39% 8% 34%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10420 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 Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2646	1724	439	471	12	0	0	0
1	B	342	2640	1718	438	472	12	0	0	0
1	C	325	2538	1652	424	450	12	0	0	0
1	D	326	2523	1642	418	451	12	0	0	0

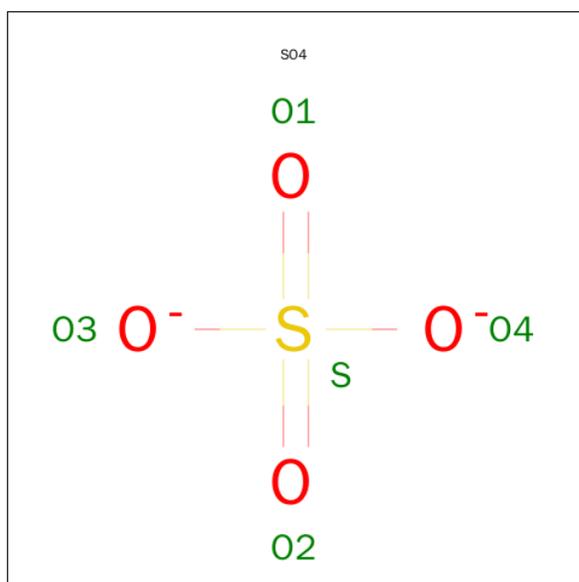
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ILE	LEU	CONFLICT	UNP P30419
B	452	ILE	LEU	CONFLICT	UNP P30419
C	452	ILE	LEU	CONFLICT	UNP P30419
D	452	ILE	LEU	CONFLICT	UNP P30419

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Co	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	13	Total	O	0	0
			13	13		
4	C	10	Total	O	0	0
			10	10		
4	D	16	Total	O	0	0
			16	16		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.63Å 116.42Å 90.36Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 96.5 (29.44-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.283 , 0.391 0.319 , 0.408	Depositor DCC
R_{free} test set	1163 reflections (4.02%)	DCC
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 121.5	EDS
Estimated twinning fraction	0.380 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.43$	Xtriage
Outliers	0 of 28898 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10420	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.63 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7162e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CO, SO4

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	0.76	3/2718 (0.1%)	1.01	8/3715 (0.2%)
1	B	1.04	4/2712 (0.1%)	1.15	8/3709 (0.2%)
1	C	0.74	3/2605 (0.1%)	0.96	6/3551 (0.2%)
1	D	1.10	4/2592 (0.2%)	1.12	9/3542 (0.3%)
All	All	0.92	14/10627 (0.1%)	1.06	31/14517 (0.2%)

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	3
1	B	0	3
1	C	0	4
1	D	0	3
All	All	0	13

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	LEU	C-N	-32.53	0.59	1.34
1	D	401	LEU	C-N	-32.37	0.59	1.34
1	B	401	LEU	C-N	-31.27	0.62	1.34
1	B	402	MET	C-N	28.57	1.99	1.34
1	D	302	GLU	C-N	-27.80	0.70	1.34

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	GLN	O-C-N	-47.53	46.66	122.70
1	B	301	GLN	O-C-N	-44.79	51.04	122.70
1	C	301	GLN	O-C-N	-37.26	63.09	122.70
1	A	301	GLN	O-C-N	-29.43	75.62	122.70
1	B	401	LEU	O-C-N	-24.32	83.78	122.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	GLN	Mainchain
1	A	401	LEU	Mainchain,Peptide
1	B	301	GLN	Mainchain
1	B	401	LEU	Mainchain,Peptide
1	C	301	GLN	Mainchain

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	2646	0	2523	316	0
1	B	2640	0	2514	336	0
1	C	2538	0	2434	338	1
1	D	2523	0	2395	332	1
2	C	1	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	13	0	0	3	0
4	B	13	0	0	3	0
4	C	10	0	0	4	0
4	D	16	0	0	2	0
All	All	10420	0	9866	1322	1

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 65.

The worst 5 of 1322 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:302:GLU:CA	1:B:303:ASN:N	1.95	1.29
1:D:302:GLU:CA	1:D:303:ASN:N	1.94	1.29
1:D:302:GLU:C	1:D:303:ASN:CA	2.03	1.26
1:C:302:GLU:O	1:C:303:ASN:N	1.61	1.26
1:D:302:GLU:O	1:D:303:ASN:N	1.68	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:O	1:D:196:LEU:O[1_655]	2.17	0.03

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	338/496 (68%)	224 (66%)	80 (24%)	34 (10%)	1	3
1	B	340/496 (68%)	226 (66%)	73 (22%)	41 (12%)	0	2
1	C	317/496 (64%)	212 (67%)	65 (20%)	40 (13%)	0	1
1	D	322/496 (65%)	213 (66%)	73 (23%)	36 (11%)	0	2
All	All	1317/1984 (66%)	875 (66%)	291 (22%)	151 (12%)	0	2

5 of 151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	A	151	ALA
1	A	232	VAL
1	A	238	SER
1	A	239	ARG

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	272/443 (61%)	247 (91%)	25 (9%)	11	40
1	B	271/443 (61%)	247 (91%)	24 (9%)	12	42
1	C	263/443 (59%)	240 (91%)	23 (9%)	13	43
1	D	259/443 (58%)	237 (92%)	22 (8%)	13	45
All	All	1065/1772 (60%)	971 (91%)	94 (9%)	12	42

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	325	ASP
1	C	134	HIS
1	D	267	LYS
1	B	327	LEU
1	B	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	426	ASN
1	C	236	HIS
1	D	397	ASN
1	B	455	GLN
1	C	132	GLN

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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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
3	SO4	A	902	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	A	903	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SO4	B	901	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	C	904	-	4,4,4	0.22	0	6,6,6	0.08	0

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
3	SO4	A	902	-	-	0/0/0/0	0/0/0/0
3	SO4	A	903	-	-	0/0/0/0	0/0/0/0
3	SO4	B	901	-	-	0/0/0/0	0/0/0/0
3	SO4	C	904	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	342/496 (68%)	0.28	21 (6%) 25 9	0, 32, 106, 190	0
1	B	342/496 (68%)	0.26	18 (5%) 30 12	0, 30, 100, 197	0
1	C	325/496 (65%)	0.83	36 (11%) 7 3	3, 47, 131, 191	0
1	D	326/496 (65%)	0.81	39 (11%) 6 2	1, 50, 129, 197	0
All	All	1335/1984 (67%)	0.54	114 (8%) 13 5	0, 39, 122, 197	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	ASP	10.5
1	A	341	THR	8.2
1	C	236	HIS	7.9
1	A	107	ASP	7.8
1	D	340	PRO	7.6

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
3	SO4	B	901	5/5	0.77	0.24	0.58	69,72,75,77	0
2	CO	C	990	1/1	0.88	0.29	-0.32	61,61,61,61	0
3	SO4	A	902	5/5	0.81	0.30	-	106,108,111,112	0
3	SO4	A	903	5/5	0.87	0.19	-	80,84,86,86	0
3	SO4	C	904	5/5	0.56	0.32	-	104,105,109,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.