



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:07 AM GMT

PDB ID : 2FON  
Title : X-ray crystal structure of LeACX1, an acyl-CoA oxidase from *Lycopersicon esculentum* (tomato)  
Authors : Garavito, R.M.; Powers, R.A.  
Deposited on : 2006-01-13  
Resolution : 2.74 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](mailto: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.

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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

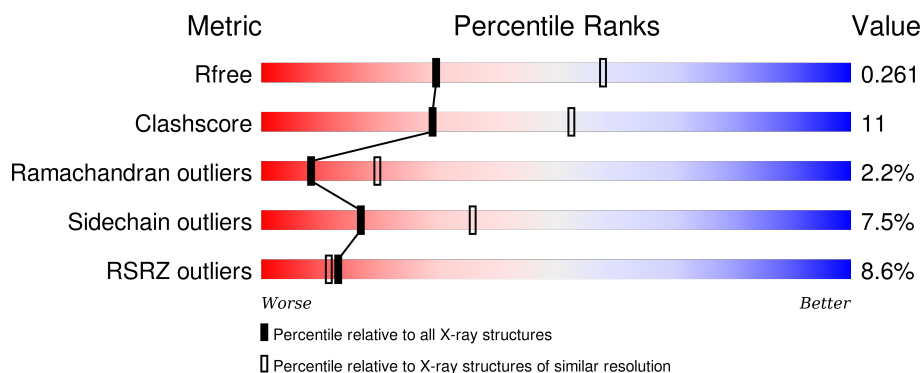
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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  $\geq 3$ , 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	683	<div> <div>4%</div> <div>69%</div> <div>23%</div> <div>• • •</div> </div>
1	B	683	<div> <div>3%</div> <div>71%</div> <div>21%</div> <div>• •</div> </div>
1	C	683	<div> <div>18%</div> <div>70%</div> <div>22%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14949 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 peroxisomal acyl-CoA oxidase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5010	3180	873	932	25			
1	B	656	Total	C	N	O	S	0	0	0
			5040	3198	878	939	25			
1	C	653	Total	C	N	O	S	0	0	0
			4704	2960	828	892	24			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
A	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
A	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
A	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3
A	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
A	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
A	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
A	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
A	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
A	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
A	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
A	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
B	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
B	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
B	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
B	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
B	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
B	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
B	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
B	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
C	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
C	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
C	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3
C	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
C	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
C	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
C	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
C	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
C	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

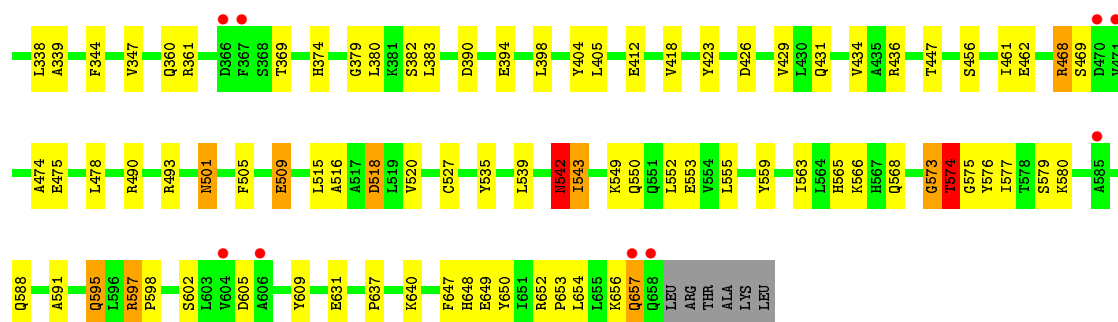


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

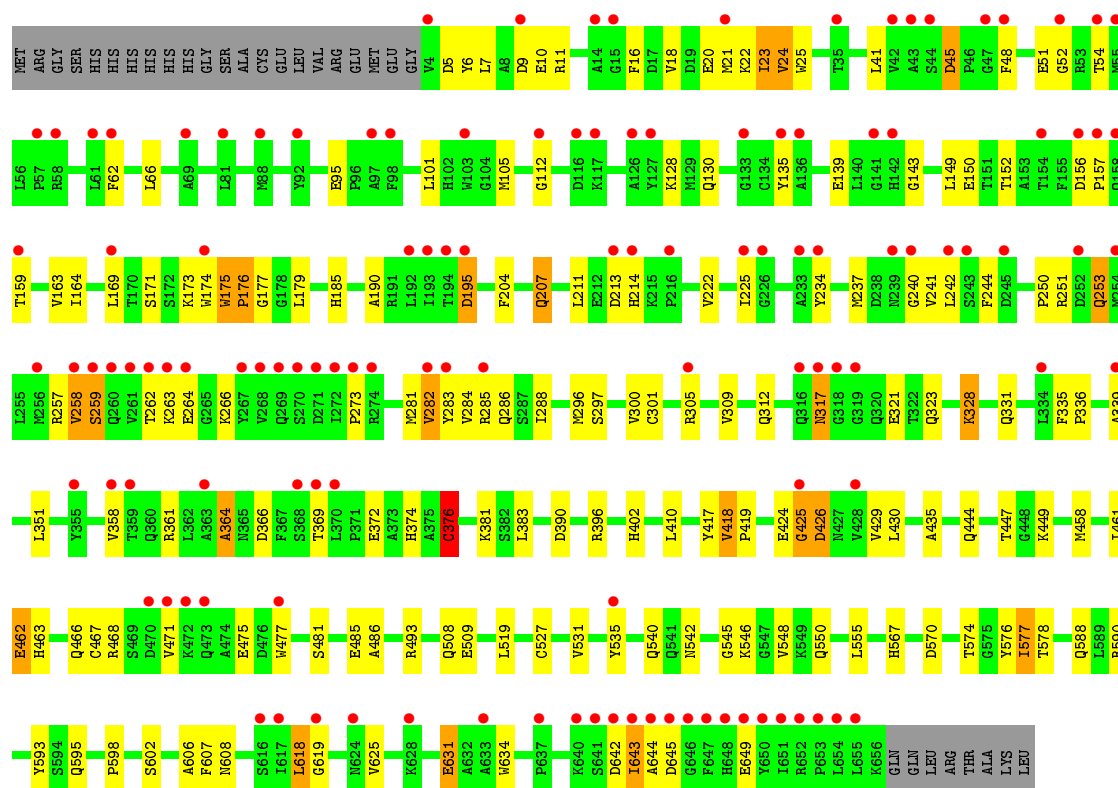
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	22	Total	O	0	0
			22	22		





- Molecule 1: peroxisomal acyl-CoA oxidase 1A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.20 Å   240.33 Å   89.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.74 29.82 – 2.74	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.74) 92.8 (29.82-2.74)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.72 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.212   ,   0.267 0.205   ,   0.261	Depositor DCC
$R_{free}$ test set	3221 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 63840 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.99	2/5120 (0.0%)	1.00	18/6948 (0.3%)
1	B	0.94	4/5150 (0.1%)	0.96	12/6988 (0.2%)
1	C	0.61	1/4803 (0.0%)	0.70	2/6552 (0.0%)
All	All	0.87	7/15073 (0.0%)	0.90	32/20488 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	VAL	CB-CG1	-6.60	1.39	1.52
1	B	243	SER	CA-CB	6.01	1.61	1.52
1	B	404	TYR	CD2-CE2	-5.64	1.30	1.39
1	C	376	CYS	CB-SG	-5.43	1.73	1.81
1	A	100	ASP	CB-CG	5.28	1.62	1.51

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	B	53	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	53	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	101	LEU	CA-CB-CG	-7.94	97.04	115.30
1	A	345	ARG	NE-CZ-NH1	-7.71	116.44	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	5010	0	4838	122	0
1	B	5040	0	4884	112	0
1	C	4704	0	4258	98	0
2	A	53	0	31	7	0
2	B	53	0	31	6	0
2	C	53	0	31	5	0
3	A	14	0	0	0	0
3	B	22	0	0	2	0
All	All	14949	0	14073	329	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 11.

The worst 5 of 329 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:29:ARG:HH11	1:A:29:ARG:HG3	1.15	1.07
1:C:361:ARG:HD2	1:C:369:THR:HG21	1.47	0.97
1:A:29:ARG:HH11	1:A:29:ARG:CG	1.77	0.96
1:B:361:ARG:HD3	1:B:369:THR:HG21	1.45	0.94
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.35	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	652/683 (96%)	591 (91%)	47 (7%)	14 (2%)	9	21
1	B	654/683 (96%)	617 (94%)	27 (4%)	10 (2%)	13	30
1	C	651/683 (95%)	560 (86%)	71 (11%)	20 (3%)	5	11
All	All	1957/2049 (96%)	1768 (90%)	145 (7%)	44 (2%)	8	20

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	175	TRP
1	A	317	ASN
1	A	318	GLY
1	B	175	TRP

### 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	509/571 (89%)	470 (92%)	39 (8%)	16	34
1	B	516/571 (90%)	482 (93%)	34 (7%)	21	43
1	C	434/571 (76%)	397 (92%)	37 (8%)	13	28
All	All	1459/1713 (85%)	1349 (92%)	110 (8%)	17	36

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	228	LYS
1	B	501	ASN
1	C	535	TYR
1	B	257	ARG
1	B	338	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	202	ASN
1	B	444	GLN
1	C	550	GLN
1	B	260	GLN
1	B	374	HIS

### 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](#)

3 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	FAD	A	1000	-	48,58,58	1.52	8 (16%)	54,89,89	2.72	14 (25%)
2	FAD	B	2000	-	48,58,58	1.46	7 (14%)	54,89,89	2.26	12 (22%)
2	FAD	C	3000	-	48,58,58	1.37	6 (12%)	54,89,89	2.08	8 (14%)

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	FAD	A	1000	-	-	0/30/50/50	0/6/6/6
2	FAD	B	2000	-	-	0/30/50/50	0/6/6/6
2	FAD	C	3000	-	-	0/30/50/50	0/6/6/6

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	FAD	C6-C5X	-3.26	1.36	1.41
2	B	2000	FAD	C10-N10	-2.98	1.35	1.39
2	B	2000	FAD	C6-C5X	-2.97	1.37	1.41
2	A	1000	FAD	O2'-C2'	-2.29	1.38	1.43
2	B	2000	FAD	O3B-C3B	-2.10	1.37	1.43

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	N3A-C2A-N1A	-13.20	118.79	128.89
2	B	2000	FAD	N3A-C2A-N1A	-11.72	119.92	128.89
2	C	3000	FAD	N3A-C2A-N1A	-10.32	120.99	128.89
2	C	3000	FAD	P-O3P-PA	-5.17	118.22	132.73
2	A	1000	FAD	C2B-C1B-N9A	-4.59	107.28	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	FAD	7	0
2	B	2000	FAD	6	0
2	C	3000	FAD	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	654/683 (95%)	0.16	25 (3%)	44	46	49, 67, 78, 91	0
1	B	656/683 (96%)	0.19	19 (2%)	55	57	53, 67, 78, 85	0
1	C	653/683 (95%)	0.98	124 (18%)	2	1	55, 70, 89, 112	0
All	All	1963/2049 (95%)	0.44	168 (8%)	13	11	49, 68, 81, 112	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	GLY	8.3
1	C	646	GLY	6.8
1	C	273	PRO	6.4
1	C	159	THR	6.3
1	C	644	ALA	6.1

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	FAD	C	3000	53/53	0.79	0.35	1.65	87,99,107,107	0
2	FAD	A	1000	53/53	0.93	0.21	0.32	43,55,59,63	0
2	FAD	B	2000	53/53	0.94	0.18	-0.52	45,49,55,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.