



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:15 AM GMT

PDB ID : 2UUU  
Title : ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE IN P212121  
Authors : Razeto, A.; Mattioli, F.; Carpanelli, E.; Aliverti, A.; Pandini, V.; Coda, A.;  
Mattevi, A.  
Deposited on : 2007-03-07  
Resolution : 1.95 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

---

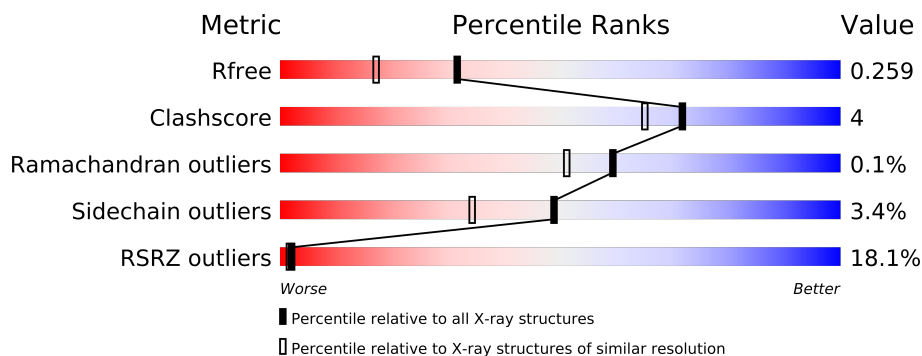
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	
1	C	584	
1	D	584	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PL3	A	1588	-	X
3	PL3	B	1588	-	X
3	PL3	C	1587	-	X
3	PL3	D	1587	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19178 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

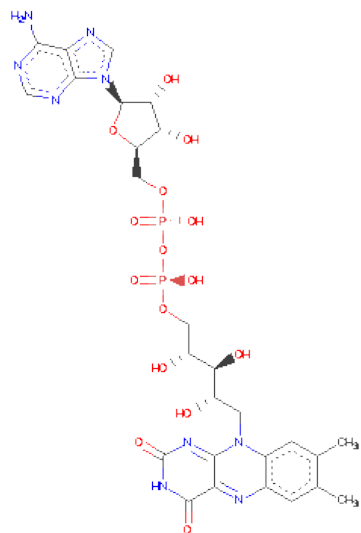
- Molecule 1 is a protein called ALKYLDIHYDROXYACETONEPHOSPHATESYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	3	0
			4408	2839	751	798	20			
1	B	540	Total	C	N	O	S	0	1	0
			4329	2788	739	783	19			
1	C	541	Total	C	N	O	S	0	0	0
			4323	2784	735	786	18			
1	D	537	Total	C	N	O	S	0	0	0
			4288	2763	730	776	19			

There are 20 discrepancies between the modelled and reference sequences:

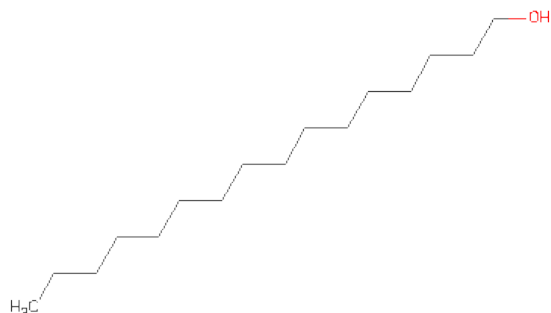
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP O96759
A	-4	ALA	-	EXPRESSION TAG	UNP O96759
A	-3	MET	-	EXPRESSION TAG	UNP O96759
A	-2	GLY	-	EXPRESSION TAG	UNP O96759
A	-1	SER	-	EXPRESSION TAG	UNP O96759
B	-5	GLY	-	EXPRESSION TAG	UNP O96759
B	-4	ALA	-	EXPRESSION TAG	UNP O96759
B	-3	MET	-	EXPRESSION TAG	UNP O96759
B	-2	GLY	-	EXPRESSION TAG	UNP O96759
B	-1	SER	-	EXPRESSION TAG	UNP O96759
C	-5	GLY	-	EXPRESSION TAG	UNP O96759
C	-4	ALA	-	EXPRESSION TAG	UNP O96759
C	-3	MET	-	EXPRESSION TAG	UNP O96759
C	-2	GLY	-	EXPRESSION TAG	UNP O96759
C	-1	SER	-	EXPRESSION TAG	UNP O96759
D	-5	GLY	-	EXPRESSION TAG	UNP O96759
D	-4	ALA	-	EXPRESSION TAG	UNP O96759
D	-3	MET	-	EXPRESSION TAG	UNP O96759
D	-2	GLY	-	EXPRESSION TAG	UNP O96759
D	-1	SER	-	EXPRESSION TAG	UNP O96759

- 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		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is HEXADECAN-1-OL (three-letter code: PL3) (formula:  $C_{16}H_{34}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		
3	C	1	Total	C	O	0	0
			17	16	1		
3	D	1	Total	C	O	0	0
			17	16	1		

- Molecule 4 is water.

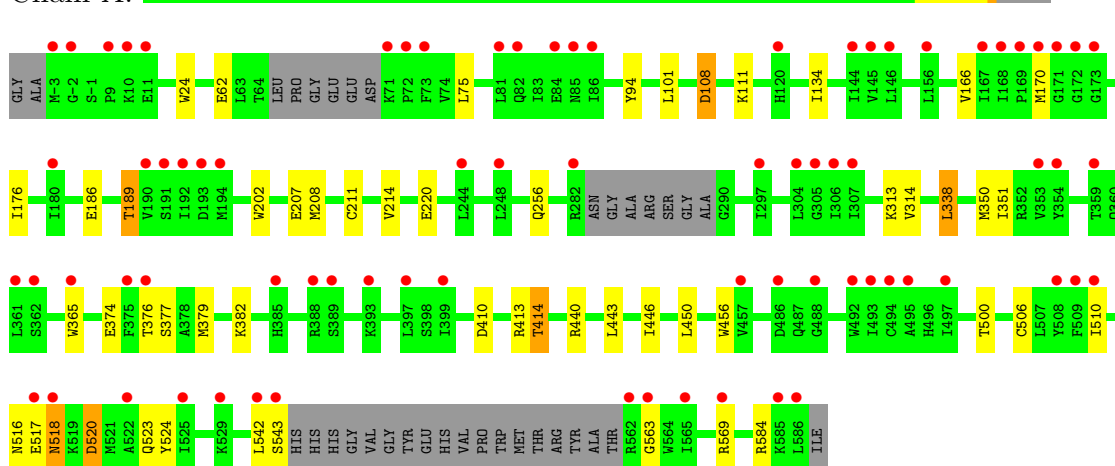
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	484	Total	O	0	0
			484	484		
4	B	385	Total	O	0	0
			385	385		
4	C	333	Total	O	0	0
			333	333		
4	D	348	Total	O	0	0
			348	348		

### 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.

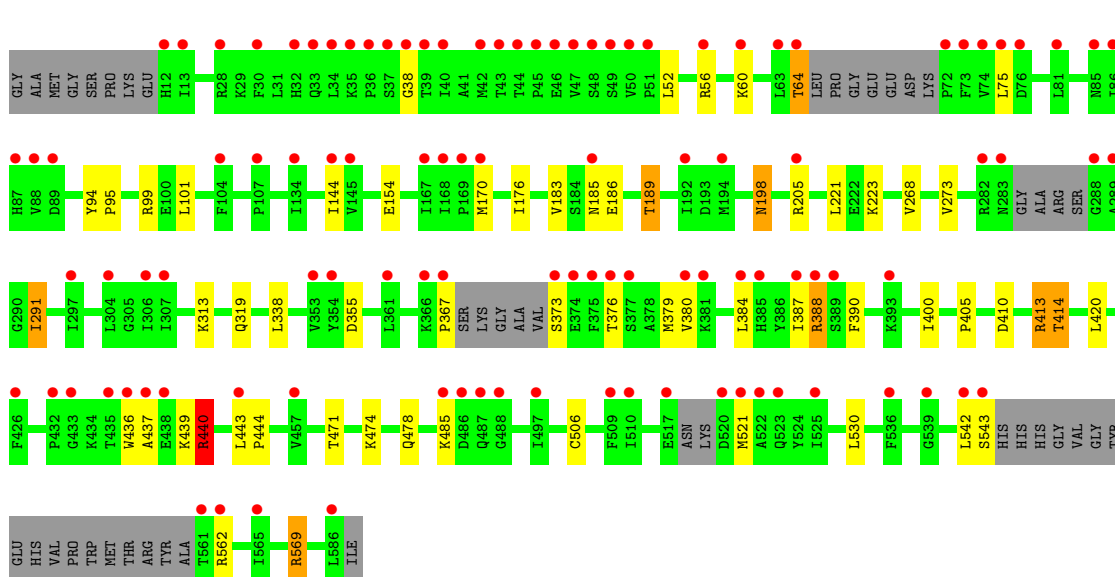
#### • Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTASE

Chain A:



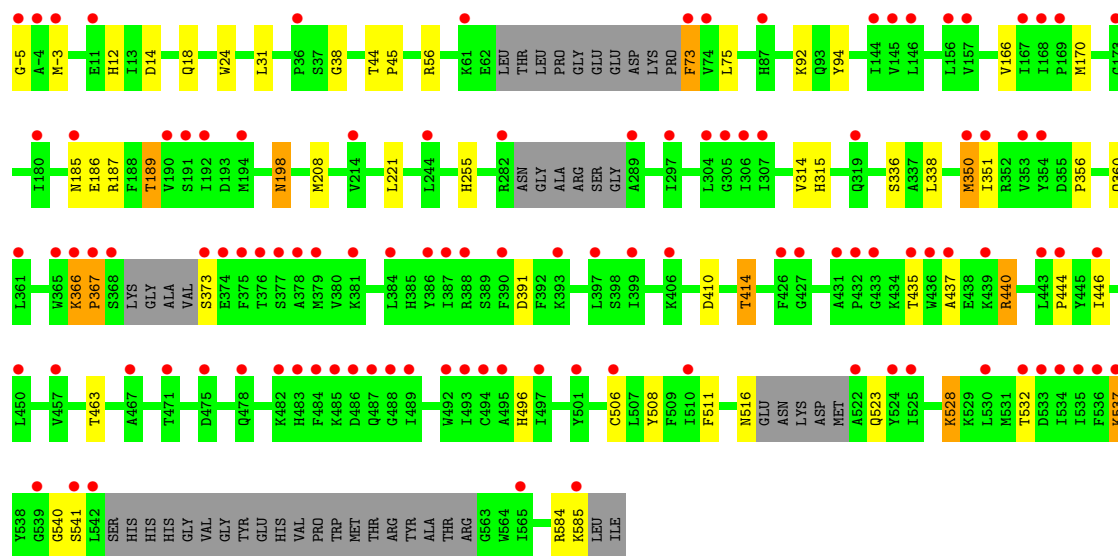
#### • Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTASE

Chain B:



#### • Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATESYNTASE

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.50Å 108.91Å 216.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 1.95 29.93 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.93-1.95) 99.8 (29.93-1.95)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.193 , 0.244 0.220 , 0.259	Depositor DCC
$R_{free}$ test set	8931 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.6	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 177635 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL3, 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	0.80	1/4527 (0.0%)	0.71	2/6127 (0.0%)
1	B	0.72	0/4439	0.71	4/6008 (0.1%)
1	C	0.65	0/4431	0.65	0/6000
1	D	0.69	0/4395	0.67	0/5948
All	All	0.72	1/17792 (0.0%)	0.68	6/24083 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	VAL	CB-CG1	5.50	1.64	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	413	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	413	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	413	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	413	ARG	NE-CZ-NH1	6.06	123.33	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4408	0	4422	40	0
1	B	4329	0	4327	41	0
1	C	4323	0	4311	33	0
1	D	4288	0	4283	40	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	17	0	33	4	0
3	B	17	0	33	2	0
3	C	17	0	33	0	0
3	D	17	0	33	0	0
4	A	484	0	0	9	0
4	B	385	0	0	9	0
4	C	333	0	0	5	0
4	D	348	0	0	11	0
All	All	19178	0	17599	156	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 156 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:GLU:HG2	4:A:2203:HOH:O	1.49	1.13
1:C:92:LYS:HE3	1:C:185:ASN:O	1.48	1.11
1:A:208:MET:CE	1:A:314:VAL:HG23	1.88	1.03
1:B:373:SER:HA	1:B:376:THR:HG22	1.49	0.94
1:B:410:ASP:O	1:B:414:THR:HG23	1.69	0.92

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	545/584 (93%)	538 (99%)	7 (1%)	0	100	100
1	B	529/584 (91%)	518 (98%)	10 (2%)	1 (0%)	56	46
1	C	531/584 (91%)	525 (99%)	6 (1%)	0	100	100
1	D	525/584 (90%)	513 (98%)	10 (2%)	2 (0%)	43	30
All	All	2130/2336 (91%)	2094 (98%)	33 (2%)	3 (0%)	59	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	537	LYS
1	B	562	ARG
1	D	367	PRO

### 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	484/507 (96%)	467 (96%)	17 (4%)	48	32
1	B	474/507 (94%)	456 (96%)	18 (4%)	44	29
1	C	472/507 (93%)	459 (97%)	13 (3%)	56	43
1	D	468/507 (92%)	451 (96%)	17 (4%)	47	31
All	All	1898/2028 (94%)	1833 (97%)	65 (3%)	49	34

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	414	THR
1	C	65	LEU
1	D	440	ARG
1	B	440	ARG
1	B	530	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	394	ASN
1	C	12	HIS
1	D	394	ASN
1	B	478	GLN
1	B	499	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 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	1587	-	58,58,58	1.47	7 (12%)	85,89,89	2.01	15 (17%)
3	PL3	A	1588	-	16,16,16	0.87	1 (6%)	15,15,15	0.81	0
2	FAD	B	1587	-	58,58,58	1.46	5 (8%)	85,89,89	2.30	19 (22%)
3	PL3	B	1588	-	16,16,16	0.94	1 (6%)	15,15,15	0.71	0
2	FAD	C	1586	-	58,58,58	1.37	5 (8%)	85,89,89	1.82	10 (11%)
3	PL3	C	1587	-	16,16,16	0.91	1 (6%)	15,15,15	0.84	0
2	FAD	D	1586	-	58,58,58	1.40	7 (12%)	85,89,89	1.98	13 (15%)
3	PL3	D	1587	-	16,16,16	0.90	1 (6%)	15,15,15	0.72	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
2	FAD	A	1587	-	-	0/34/50/50	0/1/6/6
3	PL3	A	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	B	1587	-	-	0/34/50/50	0/1/6/6
3	PL3	B	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	C	1586	-	-	0/34/50/50	0/1/6/6
3	PL3	C	1587	-	-	0/14/14/14	0/0/0/0
2	FAD	D	1586	-	-	0/34/50/50	0/1/6/6
3	PL3	D	1587	-	-	0/14/14/14	0/0/0/0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1587	FAD	C1'-C2'	6.36	1.57	1.51
2	B	1587	FAD	C1'-C2'	6.33	1.57	1.51
2	C	1586	FAD	C1'-N10	5.53	1.54	1.48
2	D	1586	FAD	C1'-N10	4.78	1.53	1.48
2	B	1587	FAD	C2A-N3A	4.62	1.41	1.32

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	FAD	N3A-C2A-N1A	-12.34	118.39	128.71
2	D	1586	FAD	N3A-C2A-N1A	-12.27	118.45	128.71
2	C	1586	FAD	N3A-C2A-N1A	-11.10	119.43	128.71
2	A	1587	FAD	N3A-C2A-N1A	-10.68	119.78	128.71
2	A	1587	FAD	C2'-C1'-N10	6.72	121.36	112.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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	550/584 (94%)	0.81	77 (14%) 3 3	8, 20, 36, 58	0
1	B	540/584 (92%)	1.07	107 (19%) 2 1	8, 21, 43, 66	0
1	C	541/584 (92%)	1.12	101 (18%) 2 1	13, 27, 46, 56	0
1	D	537/584 (91%)	1.18	109 (20%) 1 1	12, 26, 59, 81	0
All	All	2168/2336 (92%)	1.04	394 (18%) 2 1	8, 22, 47, 81	0

The worst 5 of 394 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	377	SER	10.0
1	D	432	PRO	9.9
1	D	375	PHE	9.9
1	D	376	THR	9.5
1	B	522	ALA	8.9

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PL3	D	1587	17/17	0.45	5.01	45,47,49,49	0
3	PL3	C	1587	17/17	0.42	4.09	34,36,42,43	0
3	PL3	B	1588	17/17	0.40	4.07	34,39,42,43	0
3	PL3	A	1588	17/17	0.37	3.59	31,33,37,39	0
2	FAD	C	1586	53/53	0.14	-0.57	6,11,15,16	0
2	FAD	B	1587	53/53	0.12	-0.66	6,12,13,15	0
2	FAD	D	1586	53/53	0.14	-0.81	7,11,15,16	0
2	FAD	A	1587	53/53	0.13	-0.87	3,8,10,11	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.