wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:48 AM GMT

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

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)	:	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 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.
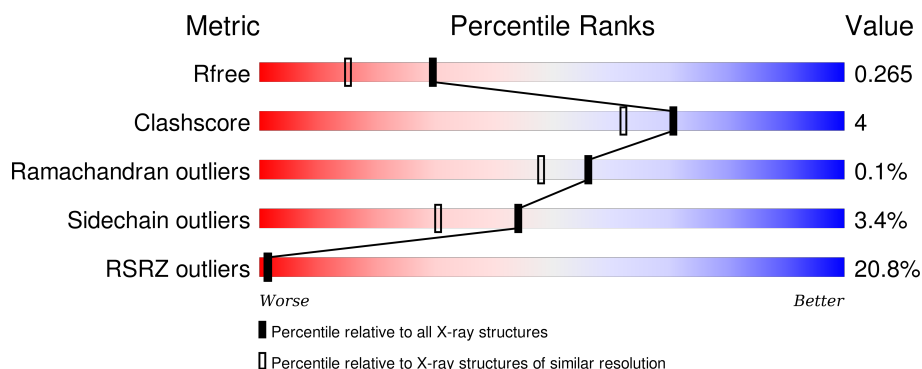
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 >=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.

Mol	Chain	Length	Quality of chain
1	A	584	14% / 85% / 8% · 6%
1	B	584	20% / 82% / 9% · 8%
1	C	584	20% / 83% / 8% · 7%
1	D	584	22% / 82% / 8% · 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 (i)

There are 4 unique types of molecules in this entry. The entry contains 19178 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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE.

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

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: $C_{27}H_{33}N_9O_{15}P_2$).
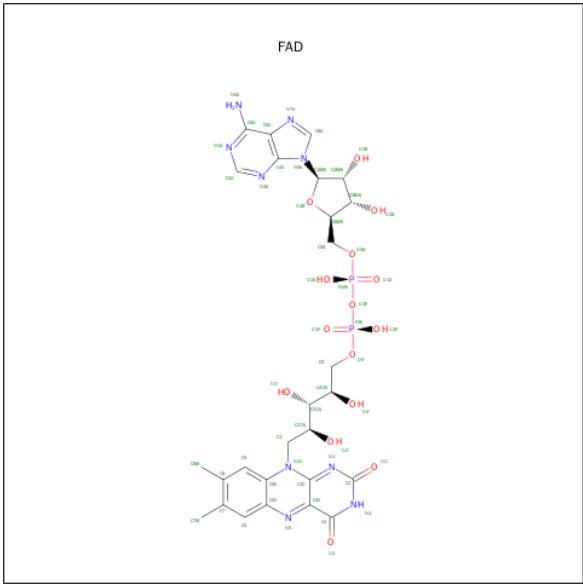
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is HEXADECAN-1-OL (three-letter code: PL3) (formula: $C_{16}H_{34}O$).
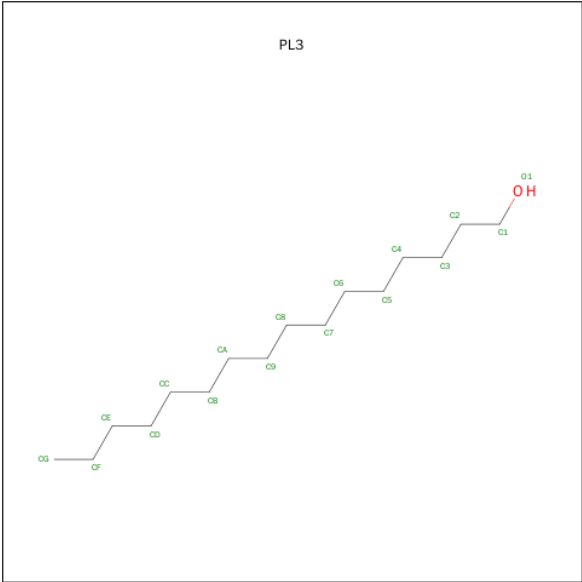
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 17	C 16	O 1	0	0
3	B	1	Total 17	C 16	O 1	0	0
3	C	1	Total 17	C 16	O 1	0	0
3	D	1	Total 17	C 16	O 1	0	0

- Molecule 4 is water.

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

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: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

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Chain C:

20%

83%

8%

7%

GLY ALA MET GLY SER PRO LYS GLU H12 I13 W24 F30 L31 L34 K35 P36 T39 M42 T43 T44 P45 E46 V47 S48 S49 V50 P51 L52 P53 R56 I59 T64 L65 P66 G67 E68 K71 P72 F73 V74 L75 H87 K92 Q93 Y94 P95 E96 I134

N139 V145 V153 L156 V166 I167 I168 P169 M170 G171 G172 I180 V183 S184 N185 T189 V190 S191 I192 D193 M194 M208 V214 L221 L225 L244 I248 A249 R282 N283 GLY ALA ARG SER G288 A289 Y293 I296 L304 G305 I306 I307

H315 A316 P329 A332 H333 L338 M350 I351 L361 S362 F363 A364 W365 K366 P367 S368 LYS GLY ALA VAL SER E374 F375 T376 S377 A378 M379 V380 K381 K382 Y383 L384 H385 Y386 I387 R388 S389 F390 D391 F392 I399 E403 D410 T414 A424 A425 F426 G427

S430 A431 P432 G433 K434 T435 W436 A437 E438 K439 R440 L443 W456 V457 D458 V459 A467 A476 F480 V481 K482 K485 D486 I489 W492 A495 H496 I497 T500 Y501 Y509 F509 I510 F511 N516 E517 ASN LYS ASP MET ALA GLN Y524 I525 E526 D533 I534

I535 F536 K537 L542 S543 HIS HIS HIS GLY VAL GLY TYR GLU HIS VAL PRO TRP MET THR ARG ALA THR R562 G563 W564 I565 R569 D579 P583 K584 K585 LEU ILE

• **Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE**

Chain D:

22%

82%

8%

8%

G-5 A-4 M-3 E11 H12 I13 D14 Q18 W24 L31 P36 S37 G38 T44 P45 E46 V47 R56 K61 E62 LEU THR LEU PRO GLY GLU GLU ASP LYS PRO F73 V74 L75 H87 K92 Q93 Y94 I144 V145 L146 L156 V157 V166 I167 I168 P169 M170

G173 I180 N185 E186 R187 F188 T189 V190 S191 I192 D193 M194 R195 N198 M208 V214 L221 L244 W247 H255 R282 ASN GLY ALA ARG SER GLY A289 G290 I297 L304 G305 I306 I307 A310 V314 H315 Q319 S336 A337 L338 M350

I351 R352 V353 Y354 D355 P356 T359 Q360 L361 W365 K366 P367 S368 LYS GLY ALA VAL S373 E374 F375 T376 S377 A378 M379 V380 K381 K382 Y383 L384 H385 Y386 I387 R388 S389 F390 D391 F392 K393 N394 L397 S398 I399 K406 D410 T414 I419 L420 S421 A425 F426 G427

S430 A431 P432 G433 K434 T435 W436 A437 E438 K439 R440 L443 P444 Y445 I446 L450 V457 T463 A467 T471 D475 Q478 T479 K482 H483 F484 K485 D486 Q487 G488 I489 W492 I493 C494 A495 H496 I497 Y501 C506 L507 Y508 F509 I510 F511 N516 GLU ASN

LYS ASP MET A522 Q523 Y524 I525 K528 K529 L530 M531 T532 D533 I534 I535 F536 K537 Y538 G539 G540 S541 L542 SER HIS HIS HIS GLY VAL GLY TYR GLU HIS VAL PRO TRP MET THR ARG ALA THR ARG G563 W564 I565 R569 R584 K585 LEU ILE

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.56 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.244 0.223 , 0.265	Depositor DCC
R_{free} test set	8930 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 59.9	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	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^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 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	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

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 4.

The worst 5 of 156 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: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%)	52	43
1	C	531/584 (91%)	525 (99%)	6 (1%)	0	100	100
1	D	525/584 (90%)	513 (98%)	10 (2%)	2 (0%)	39	27
All	All	2130/2336 (91%)	2094 (98%)	33 (2%)	3 (0%)	56	48

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 (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	484/507 (96%)	467 (96%)	17 (4%)	43	29
1	B	474/507 (94%)	456 (96%)	18 (4%)	40	25
1	C	472/507 (93%)	459 (97%)	13 (3%)	51	39
1	D	468/507 (92%)	451 (96%)	17 (4%)	42	28
All	All	1898/2028 (94%)	1833 (97%)	65 (3%)	44	30

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 (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)

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	-	48,58,58	1.52	8 (16%)	54,89,89	2.29	11 (20%)
3	PL3	A	1588	-	16,16,16	0.87	1 (6%)	15,15,15	0.84	0
2	FAD	B	1587	-	48,58,58	1.47	6 (12%)	54,89,89	2.66	14 (25%)
3	PL3	B	1588	-	16,16,16	0.93	1 (6%)	15,15,15	0.73	0
2	FAD	C	1586	-	48,58,58	1.49	6 (12%)	54,89,89	2.19	8 (14%)
3	PL3	C	1587	-	16,16,16	0.90	1 (6%)	15,15,15	0.87	0
2	FAD	D	1586	-	48,58,58	1.50	8 (16%)	54,89,89	2.58	10 (18%)
3	PL3	D	1587	-	16,16,16	0.89	1 (6%)	15,15,15	0.74	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	-	-	0/30/50/50	0/6/6/6
3	PL3	A	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	B	1587	-	-	0/30/50/50	0/6/6/6
3	PL3	B	1588	-	-	0/14/14/14	0/0/0/0
2	FAD	C	1586	-	-	0/30/50/50	0/6/6/6
3	PL3	C	1587	-	-	0/14/14/14	0/0/0/0
2	FAD	D	1586	-	-	0/30/50/50	0/6/6/6
3	PL3	D	1587	-	-	0/14/14/14	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1588	PL3	O1-C1	-3.61	1.22	1.42
3	C	1587	PL3	O1-C1	-3.47	1.23	1.42
3	D	1587	PL3	O1-C1	-3.46	1.23	1.42
3	A	1588	PL3	O1-C1	-3.43	1.23	1.42
2	C	1586	FAD	C6-C5X	-2.28	1.38	1.41

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	FAD	N3A-C2A-N1A	-13.72	118.39	128.89
2	D	1586	FAD	N3A-C2A-N1A	-13.64	118.45	128.89
2	C	1586	FAD	N3A-C2A-N1A	-12.36	119.43	128.89
2	A	1587	FAD	N3A-C2A-N1A	-11.90	119.78	128.89
2	B	1587	FAD	C4X-C4-N3	-3.99	118.13	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1587	FAD	1	0
3	A	1588	PL3	4	0
3	B	1588	PL3	2	0
2	C	1586	FAD	1	0

Continued on next page...

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1586	FAD	2	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	550/584 (94%)	0.88	84 (15%)	3	4	8, 20, 36, 58	0
1	B	540/584 (92%)	1.14	117 (21%)	1	1	8, 21, 43, 66	0
1	C	541/584 (92%)	1.21	118 (21%)	1	1	13, 27, 46, 56	0
1	D	537/584 (91%)	1.31	131 (24%)	1	1	12, 26, 59, 81	0
All	All	2168/2336 (92%)	1.13	450 (20%)	1	1	8, 22, 47, 81	0

The worst 5 of 450 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	375	PHE	11.8
1	D	377	SER	10.1
1	D	376	THR	10.0
1	B	522	ALA	9.4
1	D	432	PRO	9.1

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, 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	PL3	D	1587	17/17	0.81	0.48	5.67	45,47,49,49	0
3	PL3	C	1587	17/17	0.78	0.41	4.17	34,36,42,43	0
3	PL3	B	1588	17/17	0.83	0.38	4.02	34,39,42,43	0
3	PL3	A	1588	17/17	0.77	0.37	3.44	31,33,37,39	0
2	FAD	B	1587	53/53	0.97	0.12	-0.54	6,12,13,15	0
2	FAD	C	1586	53/53	0.96	0.14	-0.66	6,11,15,16	0
2	FAD	A	1587	53/53	0.96	0.12	-0.90	3,8,10,11	0
2	FAD	D	1586	53/53	0.96	0.13	-1.04	7,11,15,16	0

6.5 Other polymers (i)

There are no such residues in this entry.