



# wwPDB X-ray Structure Validation Summary Report

Feb 19, 2016 – 06:29 PM GMT

PDB ID : 3DH7  
Title : Structure of T. thermophilus IDI-2 in complex with PPI  
Authors : de Ruyck, J.; Wouters, J.  
Deposited on : 2008-06-17  
Resolution : 2.97 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

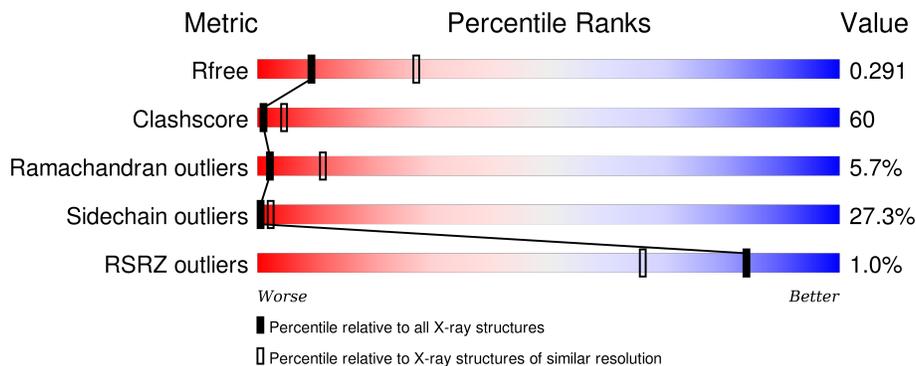
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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. 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	332	 27% 43% 19% 7% .
1	B	332	 20% 51% 19% 5% .
1	C	332	 28% 42% 20% 5% 5%
1	D	332	 25% 45% 19% 5% 6%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	FMN	A	502	-	-	X	X
2	FMN	B	502	-	-	X	X
2	FMN	C	502	-	-	X	X
2	FMN	D	502	-	-	X	X

## 2 Entry composition [i](#)

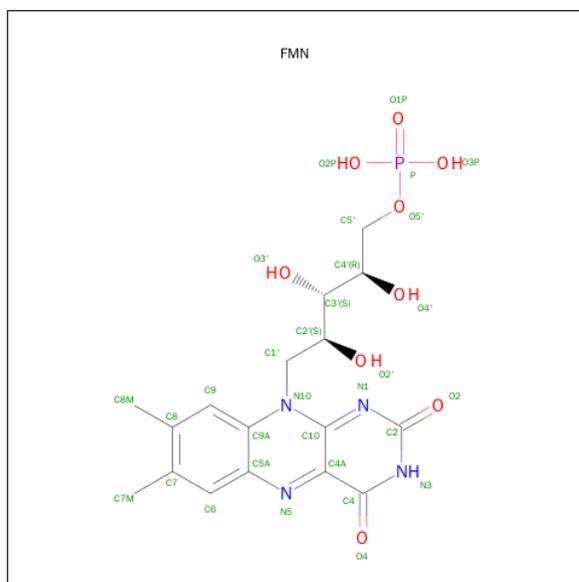
There are 4 unique types of molecules in this entry. The entry contains 9991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	Total 2419	C 1539	N 439	O 434	S 7	0	0	0
1	B	318	Total 2423	C 1543	N 439	O 434	S 7	0	0	0
1	C	316	Total 2406	C 1531	N 437	O 431	S 7	0	0	0
1	D	313	Total 2372	C 1509	N 428	O 428	S 7	0	0	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



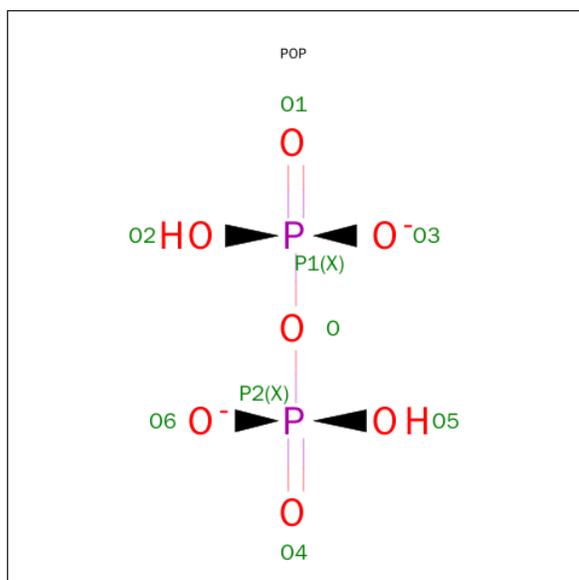
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
2	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	B	1	Total	O	P	0	0
			9	7	2		
3	D	1	Total	O	P	0	0
			9	7	2		

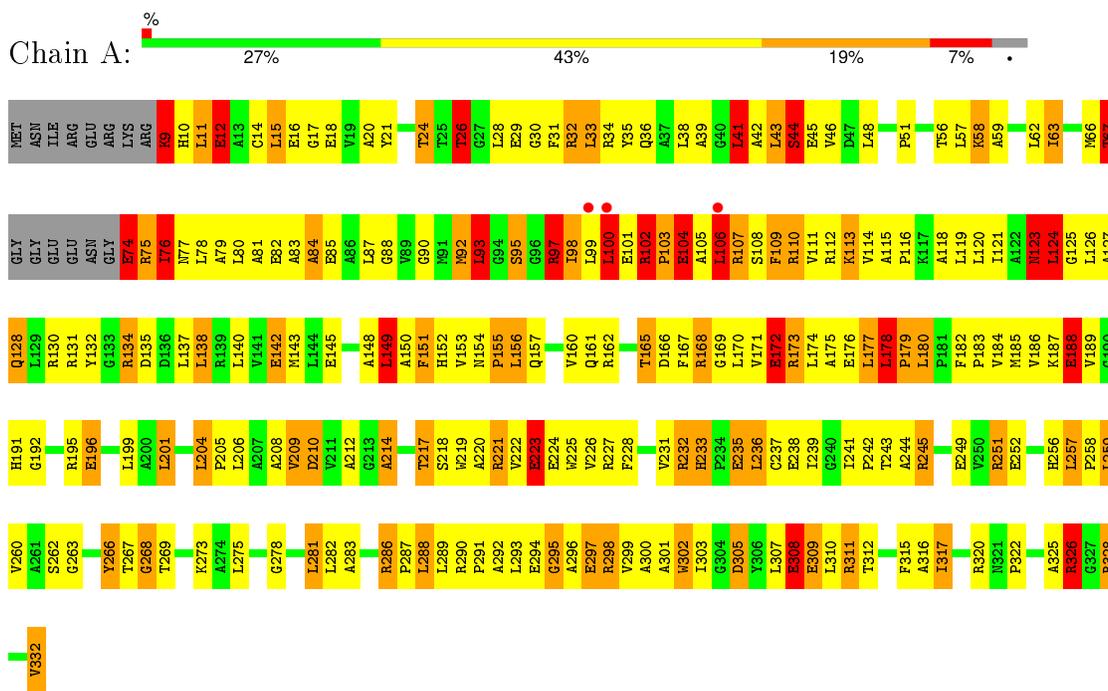
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	48	Total	O	0	0
			48	48		
4	C	59	Total	O	0	0
			59	59		
4	D	68	Total	O	0	0
			68	68		

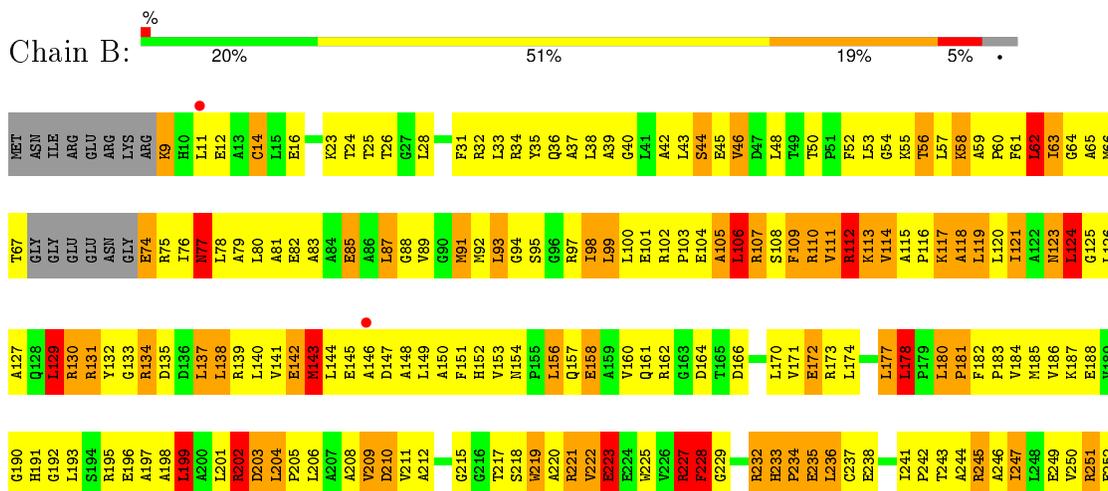
### 3 Residue-property plots

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: Isopentenyl-diphosphate delta-isomerase



- Molecule 1: Isopentenyl-diphosphate delta-isomerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.53Å 142.53Å 109.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 2.97 19.92 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.92-2.97) 98.0 (19.92-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.211 , 0.293 0.210 , 0.291	Depositor DCC
$R_{free}$ test set	2538 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.047 for -h,-k,l 0.457 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 50137 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	9991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.58	32/2457 (1.3%)	1.54	34/3326 (1.0%)
1	B	1.47	22/2462 (0.9%)	1.48	29/3334 (0.9%)
1	C	1.50	17/2443 (0.7%)	1.52	39/3307 (1.2%)
1	D	1.54	26/2408 (1.1%)	1.51	34/3260 (1.0%)
All	All	1.52	97/9770 (1.0%)	1.51	136/13227 (1.0%)

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	8
1	B	1	4
1	C	1	5
1	D	0	4
All	All	2	21

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	35	TYR	C-O	15.71	1.53	1.23
1	A	326	ARG	CG-CD	11.13	1.79	1.51
1	C	326	ARG	CG-CD	10.35	1.77	1.51
1	D	44	SER	CA-CB	8.92	1.66	1.52
1	A	188	GLU	CD-OE2	8.72	1.35	1.25

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	ARG	CG-CD-NE	-10.94	88.83	111.80
1	A	326	ARG	NE-CZ-NH1	10.65	125.63	120.30
1	C	241	ILE	CG1-CB-CG2	-9.74	89.97	111.40
1	A	106	LEU	CA-CB-CG	9.46	137.06	115.30
1	C	326	ARG	NE-CZ-NH1	9.22	124.91	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	178	LEU	CA
1	C	178	LEU	CA

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Peptide
1	A	104	GLU	Peptide
1	A	12	GLU	Peptide
1	A	43	LEU	Peptide
1	A	9	LYS	Peptide

## 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	2419	0	2502	314	1
1	B	2423	0	2515	357	1
1	C	2406	0	2500	283	0
1	D	2372	0	2450	292	0
2	A	31	0	19	13	0
2	B	31	0	19	12	0
2	C	31	0	19	14	0
2	D	31	0	19	10	0
3	B	9	0	0	1	0
3	D	9	0	0	1	0
4	A	54	0	0	2	0
4	B	48	0	0	12	0
4	C	59	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	68	0	0	15	0
All	All	9991	0	10043	1192	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 60.

The worst 5 of 1192 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:326:ARG:CD	1:A:326:ARG:CG	1.79	1.56
1:C:326:ARG:CG	1:C:326:ARG:CD	1.77	1.55
1:C:217:THR:HG22	1:C:286:ARG:NH1	1.16	1.41
1:D:179:PRO:CB	1:D:179:PRO:CG	1.75	1.39
1:C:217:THR:CG2	1:C:286:ARG:NH1	1.87	1.33

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:A:256:HIS:CD2	1:B:101:GLU:OE2[3_655]	2.03	0.17

## 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	314/332 (95%)	257 (82%)	43 (14%)	14 (4%)	<b>3</b> <b>16</b>
1	B	314/332 (95%)	246 (78%)	45 (14%)	23 (7%)	<b>1</b> <b>6</b>
1	C	310/332 (93%)	243 (78%)	50 (16%)	17 (6%)	<b>2</b> <b>12</b>
1	D	307/332 (92%)	249 (81%)	41 (13%)	17 (6%)	<b>2</b> <b>12</b>
All	All	1245/1328 (94%)	995 (80%)	179 (14%)	71 (6%)	<b>2</b> <b>11</b>

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	44	SER
1	A	97	ARG
1	A	110	ARG
1	A	178	LEU

### 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	239/252 (95%)	171 (72%)	68 (28%)	0	2
1	B	241/252 (96%)	176 (73%)	65 (27%)	0	2
1	C	239/252 (95%)	173 (72%)	66 (28%)	0	2
1	D	234/252 (93%)	173 (74%)	61 (26%)	0	3
All	All	953/1008 (94%)	693 (73%)	260 (27%)	0	2

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	251	ARG
1	C	87	LEU
1	D	182	PHE
1	B	281	LEU
1	B	331	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	77	ASN
1	C	154	ASN
1	C	256	HIS
1	C	10	HIS
1	D	123	ASN

### 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](#)

6 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	FMN	A	502	-	32,33,33	3.08	13 (40%)	34,50,50	2.96	17 (50%)
2	FMN	B	502	-	32,33,33	2.73	9 (28%)	34,50,50	2.77	13 (38%)
3	POP	B	503	-	8,8,8	1.43	1 (12%)	13,13,13	1.62	2 (15%)
2	FMN	C	502	-	32,33,33	3.00	10 (31%)	34,50,50	2.91	15 (44%)
2	FMN	D	502	-	32,33,33	2.82	13 (40%)	34,50,50	3.18	16 (47%)
3	POP	D	503	-	8,8,8	1.98	3 (37%)	13,13,13	1.64	3 (23%)

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	FMN	A	502	-	-	0/18/18/18	0/3/3/3
2	FMN	B	502	-	-	0/18/18/18	0/3/3/3
3	POP	B	503	-	-	0/6/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	C	502	-	-	0/18/18/18	0/3/3/3
2	FMN	D	502	-	-	0/18/18/18	0/3/3/3
3	POP	D	503	-	-	0/6/6/6	0/0/0/0

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	FMN	C6-C5A	-10.44	1.25	1.41
2	A	502	FMN	C6-C5A	-9.94	1.26	1.41
2	B	502	FMN	C6-C5A	-9.55	1.27	1.41
2	D	502	FMN	C6-C5A	-9.06	1.27	1.41
2	C	502	FMN	C9-C9A	-6.23	1.27	1.40

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	FMN	O2P-P-O5'	-6.32	88.29	106.72
2	A	502	FMN	C4A-C4-N3	-4.61	117.49	123.52
2	C	502	FMN	N3-C2-N1	-4.01	120.93	127.69
3	B	503	POP	P2-O-P1	-4.00	121.06	132.51
2	D	502	FMN	C4-C4A-C10	-3.91	117.44	119.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	FMN	13	0
2	B	502	FMN	12	0
3	B	503	POP	1	0
2	C	502	FMN	14	0
2	D	502	FMN	10	0
3	D	503	POP	1	0

## 5.7 Other polymers [\(i\)](#)

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 [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	318/332 (95%)	0.17	3 (0%) 85 69	2, 9, 47, 81	0
1	B	318/332 (95%)	0.15	3 (0%) 85 69	2, 16, 44, 68	0
1	C	316/332 (95%)	0.15	5 (1%) 74 54	2, 9, 42, 85	0
1	D	313/332 (94%)	0.16	2 (0%) 90 77	2, 15, 40, 53	0
All	All	1265/1328 (95%)	0.16	13 (1%) 84 66	2, 12, 42, 85	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	LEU	3.8
1	C	99	LEU	3.7
1	A	100	LEU	3.6
1	C	107	ARG	2.9
1	C	100	LEU	2.7

### 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	FMN	D	502	31/31	0.95	0.40	5.18	17,70,70,70	0
2	FMN	A	502	31/31	0.96	0.39	3.99	8,65,66,66	0
2	FMN	C	502	31/31	0.97	0.36	3.27	9,70,71,71	0
2	FMN	B	502	31/31	0.97	0.35	2.38	2,59,60,60	0
3	POP	D	503	9/9	0.91	0.31	1.87	81,83,93,93	0
3	POP	B	503	9/9	0.91	0.31	1.69	82,84,91,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.