



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:01 pm GMT

PDB ID : 1N24  
Title : (+)-Bornyl diphosphate synthase: Complex with Mg and product  
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Deposited on : 2002-10-21  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

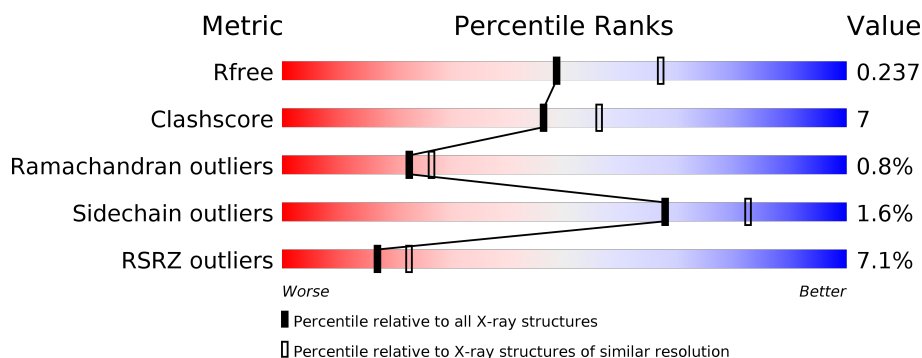
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	549	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	549	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9146 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.

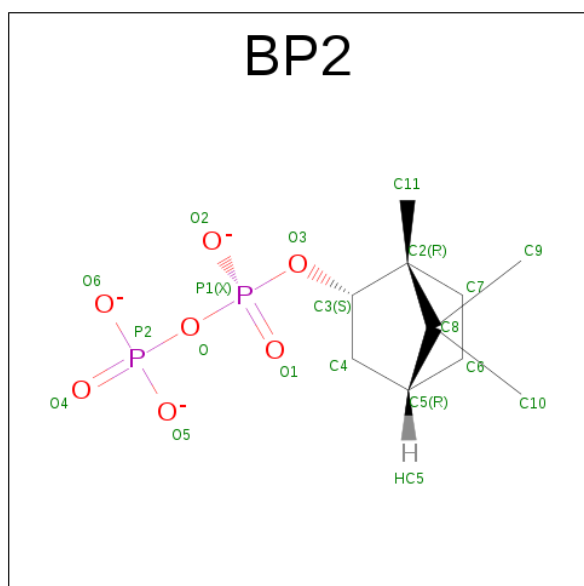
- Molecule 1 is a protein called (+)-bornyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4408	2859	731	801	17			
1	B	527	Total	C	N	O	S	0	0	0
			4346	2817	717	794	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mg	0	0
			3	3		
2	A	3	Total	Mg	0	0
			3	3		

- Molecule 3 is (+)-BORNYL DIPHOSPHATE (three-letter code: BP2) (formula: C<sub>10</sub>H<sub>17</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			19	10	7	2		
3	B	1	Total	C	O	P	0	0
			19	10	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		
4	B	157	Total	O	0	0
			157	157		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 6% 82% 14%
- GLU ALA HIS GLN I54 Q61 P76 Y77 T78 T79 E80 A87 E88 L89 I90 V91 Q92 V93 M101 V104 Q105 E108 Q123 K127 Y134 H137 K138 C139 F140 H141 ASN ASN GLU VAL GLU LYS MET D149 L150 Y151 Q162 Q169 D170 V171 F175 K176 N177 E178 K179 A180 I181 D182 S186 L187 A188 Q189 D190 T191 K192 L203 D209 T210 K224 K225 L226 D227 GLU GLY GLN ASN T232 E233 T234 E235 I236 L237 T241 T253 Q254 L274 L275 F276 K280 R303 L310 V313 A340 T343 T344 V345 L346 A347 T348 V349 I350 D355 V356 T359 E362 W373 D374 T375 L412 E429 V452 A453 S454 P455 A456 I457 I458 S459 P460 S477 L478 Y479 Q480 Y481 L485 L492 R493 L494 P495 T500 E504 L505 A506 V510 Q515 N522 A523 S524 E527 A561 I564 Q565 R566 Y567 A568 Q569 F570 I571 G577 H582 T585 I589 Y597 A598

- Chain B:
- 
- 8% 79% 17%
- GLU  
ALA  
HIS  
GLN  
ILE  
ARG  
SER  
GLY  
ASN  
TYR  
GLN  
P62  
Y77  
E80  
R81  
H82  
R85  
L89  
V93  
L96  
K100  
M101  
V104  
Q105  
E108  
F122  
E125  
I126  
E136  
H137  
K138  
C139  
F140  
H141  
N142  
M143  
E144  
V145  
E146  
K147  
M148  
Y151  
Q162  
S168
- Q169  
D170  
V171  
C174  
F175  
K176  
M177  
E178  
K179  
G180  
I181  
D182  
L187  
Q188  
K192  
L203  
D209  
T210  
K224  
K225  
L226  
D227  
E228  
GLY  
GLY  
N231  
E232  
I233  
D234  
E235  
N236  
L237  
L238  
L241  
R242  
L245  
L263  
Q264  
A266  
M271  
N272  
P273  
L274  
F276  
E277  
V286
- R507  
R503  
K309  
L310  
V313  
W323  
D355  
V356  
T359  
E362  
T367  
K371  
T375  
L412  
K417  
E429  
V452  
A453  
S454  
P455  
L458  
S459  
P460  
Y479  
Q480  
Y481  
H482  
D483  
L484  
L485  
L492  
R493  
L494  
P495  
L498  
G499  
T500  
SER  
TYR  
PHE  
GLU  
L505  
A506

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.20Å 117.53Å 120.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (30.00-2.30) 94.8 (30.00-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.19 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.210 , 0.238 0.210 , 0.237	Depositor DCC
$R_{free}$ test set	2465 reflections (4.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, BP2

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	0.41	1/4527 (0.0%)	0.58	3/6135 (0.0%)
1	B	0.38	0/4460	0.54	1/6042 (0.0%)
All	All	0.40	1/8987 (0.0%)	0.56	4/12177 (0.0%)

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	PRO	CA-C	-8.17	1.36	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	PRO	CA-N-CD	-10.30	97.08	111.50
1	A	76	PRO	CB-CA-C	-5.25	98.88	112.00
1	B	480	GLN	N-CA-C	-5.17	97.05	111.00
1	A	76	PRO	O-C-N	-5.07	114.58	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	481	TYR	Sidechain
1	B	481	TYR	Sidechain

## 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	4293	62	0
1	B	4346	0	4236	65	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	19	0	17	0	0
3	B	19	0	17	0	0
4	A	191	0	0	5	0
4	B	157	0	0	3	0
All	All	9146	0	8563	125	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 7.

The worst 5 of 125 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:429:GLU:HB3	1:A:510:VAL:HG21	1.28	1.13
1:B:429:GLU:HB3	1:B:510:VAL:HG21	1.28	1.13
1:B:146:GLU:HG2	1:B:147:LYS:H	1.22	1.05
1:B:141:HIS:O	1:B:142:ASN:OD1	1.86	0.93
1:B:143:ASN:OD1	1:B:171:VAL:HG22	1.73	0.88

There are no symmetry-related clashes.

## 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	528/549 (96%)	507 (96%)	17 (3%)	4 (1%)	22	26
1	B	519/549 (94%)	489 (94%)	26 (5%)	4 (1%)	22	26
All	All	1047/1098 (95%)	996 (95%)	43 (4%)	8 (1%)	22	26

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	TYR
1	A	77	TYR
1	A	177	ASN
1	B	136	GLU
1	B	142	ASN

### 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	468/480 (98%)	460 (98%)	8 (2%)	66	81
1	B	463/480 (96%)	456 (98%)	7 (2%)	70	83
All	All	931/960 (97%)	916 (98%)	15 (2%)	68	82

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	571	ILE
1	A	582	HIS
1	B	323	TRP
1	A	492	LEU
1	B	254	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	HIS
1	B	531	HIS
1	B	173	ASN
1	A	282	ASN
1	B	169	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	BP2	A	801	2	19,20,20	1.26	2 (10%)	27,35,35	2.16	6 (22%)
3	BP2	B	802	2	19,20,20	1.33	2 (10%)	27,35,35	2.23	6 (22%)

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	BP2	A	801	2	-	0/11/42/42	0/0/2/2
3	BP2	B	802	2	-	0/11/42/42	0/0/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	BP2	P1-O3	-3.26	1.52	1.60
3	A	801	BP2	P1-O3	-2.98	1.53	1.60
3	B	802	BP2	P2-O4	2.69	1.59	1.50
3	A	801	BP2	P2-O4	2.95	1.60	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	BP2	C2-C8-C5	-2.61	88.06	93.78
3	A	801	BP2	C2-C8-C5	-2.56	88.17	93.78
3	A	801	BP2	C6-C7-C2	-2.17	100.44	104.22
3	B	802	BP2	C6-C7-C2	-2.09	100.57	104.22
3	A	801	BP2	C7-C2-C8	2.28	104.72	101.48

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, 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	534/549 (97%)	0.18	33 (6%) 21 28	21, 38, 71, 93	0
1	B	527/549 (95%)	0.31	42 (7%) 13 17	20, 41, 89, 114	0
All	All	1061/1098 (96%)	0.24	75 (7%) 17 22	20, 40, 81, 114	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	GLU	7.4
1	B	143	ASN	6.8
1	B	147	LYS	6.4
1	B	142	ASN	6.3
1	B	506	ALA	6.3

### 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
3	BP2	A	801	19/19	0.98	0.17	-0.15	26,33,35,37	0
3	BP2	B	802	19/19	0.97	0.13	-0.55	36,44,49,49	0
2	MG	A	701	1/1	0.98	0.11	-1.11	29,29,29,29	0
2	MG	B	705	1/1	0.97	0.06	-1.13	38,38,38,38	0
2	MG	A	702	1/1	0.97	0.10	-1.36	28,28,28,28	0
2	MG	A	703	1/1	0.97	0.11	-1.48	37,37,37,37	0
2	MG	B	704	1/1	0.96	0.04	-3.99	25,25,25,25	0
2	MG	B	706	1/1	0.73	0.08	-	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.