



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:15 AM GMT

PDB ID : 3LDW
Title : Crystal Structure of Plasmodium vivax geranylgeranylpyrophosphate synthase PVX_092040 with zoledronate and IPP bound
Authors : Wernimont, A.K.; Lew, J.; Zhao, Y.; Kozieradzki, I.; Cossar, D.; Schapira, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on : 2010-01-13
Resolution : 2.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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

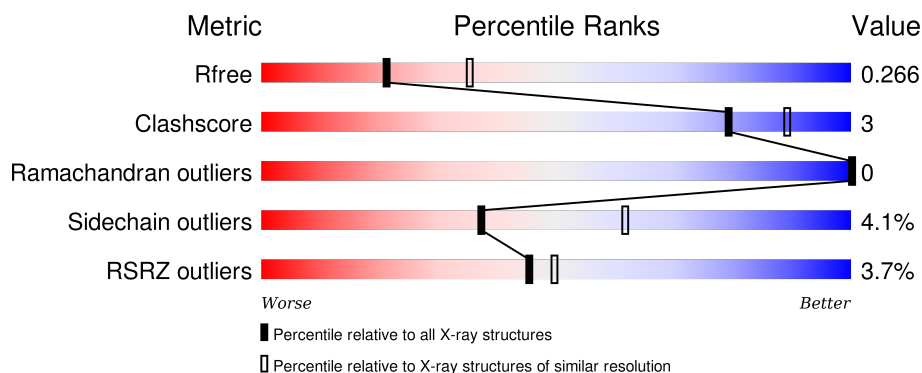
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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 $\leq 5\%$. 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	396	<div> <div>4%</div> <div>82% 8% 10%</div> </div>
1	B	396	<div> <div>4%</div> <div>78% 11% 11%</div> </div>
1	C	396	<div> <div>3%</div> <div>82% 6% 10%</div> </div>
1	D	396	<div> <div>3%</div> <div>78% 11% 11%</div> </div>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1105	-	-	-	X
5	EDO	B	1106	-	-	-	X
6	GOL	A	1106	-	-	-	X
6	GOL	B	1105	-	-	X	X
6	GOL	D	1105	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12338 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 Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	4	0
			2917	1901	462	538	16			
1	B	353	Total	C	N	O	S	0	3	0
			2899	1899	457	528	15			
1	C	357	Total	C	N	O	S	0	5	0
			2919	1908	463	533	15			
1	D	352	Total	C	N	O	S	0	4	0
			2883	1880	456	532	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A5K4U6
A	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	3	SER	-	EXPRESSION TAG	UNP A5K4U6
A	4	SER	-	EXPRESSION TAG	UNP A5K4U6
A	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	11	SER	-	EXPRESSION TAG	UNP A5K4U6
A	12	SER	-	EXPRESSION TAG	UNP A5K4U6
A	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
A	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
A	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
A	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
A	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
A	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
A	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
A	21	GLY	-	EXPRESSION TAG	UNP A5K4U6

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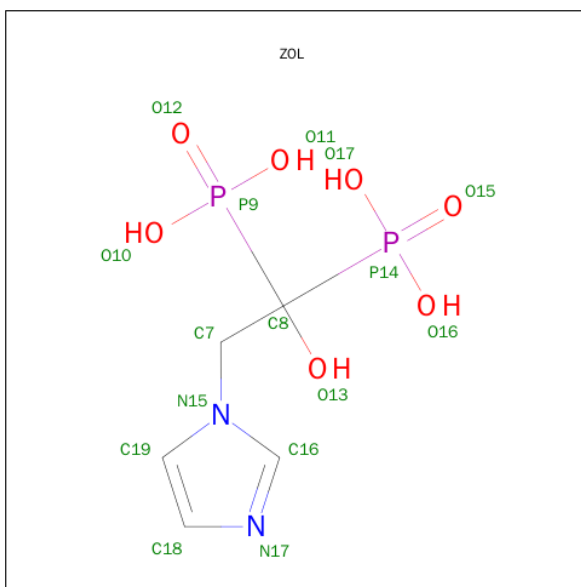
Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	1	MET	-	EXPRESSION TAG	UNP A5K4U6
B	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	3	SER	-	EXPRESSION TAG	UNP A5K4U6
B	4	SER	-	EXPRESSION TAG	UNP A5K4U6
B	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	11	SER	-	EXPRESSION TAG	UNP A5K4U6
B	12	SER	-	EXPRESSION TAG	UNP A5K4U6
B	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
B	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
B	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
B	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
B	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
B	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
B	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
B	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	1	MET	-	EXPRESSION TAG	UNP A5K4U6
C	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	3	SER	-	EXPRESSION TAG	UNP A5K4U6
C	4	SER	-	EXPRESSION TAG	UNP A5K4U6
C	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	11	SER	-	EXPRESSION TAG	UNP A5K4U6
C	12	SER	-	EXPRESSION TAG	UNP A5K4U6
C	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
C	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
C	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
C	17	LEU	-	EXPRESSION TAG	UNP A5K4U6

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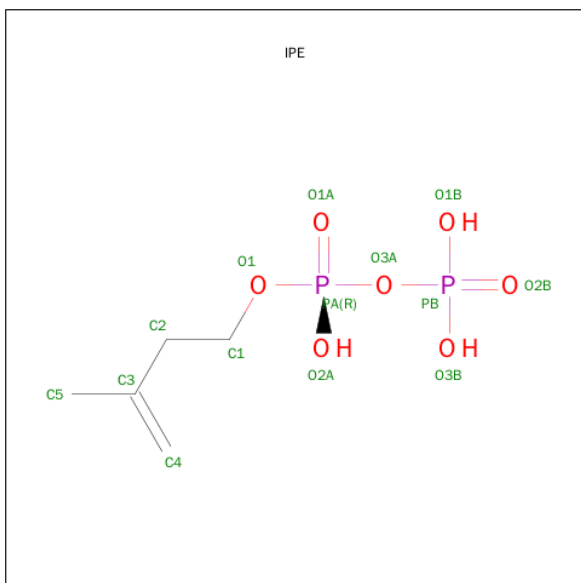
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
C	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
C	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
C	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	1	MET	-	EXPRESSION TAG	UNP A5K4U6
D	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	3	SER	-	EXPRESSION TAG	UNP A5K4U6
D	4	SER	-	EXPRESSION TAG	UNP A5K4U6
D	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	11	SER	-	EXPRESSION TAG	UNP A5K4U6
D	12	SER	-	EXPRESSION TAG	UNP A5K4U6
D	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
D	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
D	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
D	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
D	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
D	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
D	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
D	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- Molecule 2 is ZOLEDRONIC ACID (three-letter code: ZOL) (formula: $C_5H_{10}N_2O_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	B	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	C	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	D	1	Total	C	N	O	P	0	0
			16	5	2	7	2		

- Molecule 3 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: $C_5H_{12}O_7P_2$).

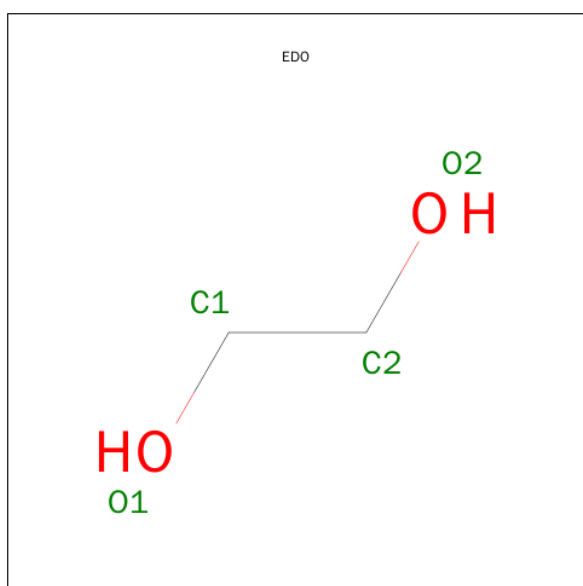


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	7	2		
3	B	1	Total	C	O	P	0	0
			14	5	7	2		
3	C	1	Total	C	O	P	0	0
			14	5	7	2		
3	D	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

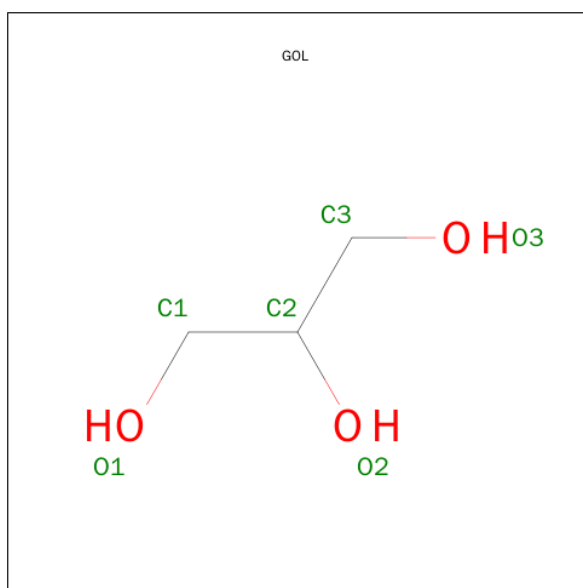
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	A	3	Total	Mg	0	0
			3	3		
4	D	3	Total	Mg	0	0
			3	3		
4	C	3	Total	Mg	0	0
			3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

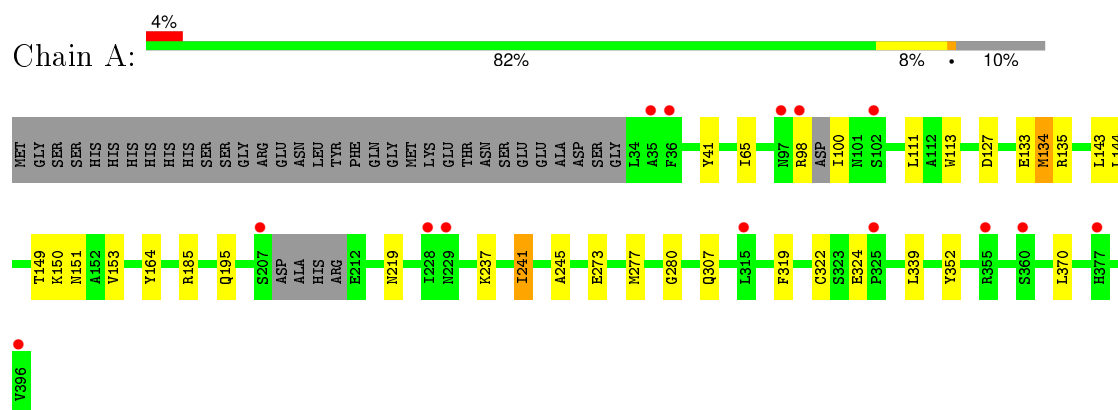
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	144	Total	O	0	0
			144	144		
7	B	144	Total	O	0	0
			144	144		
7	C	143	Total	O	0	0
			143	143		
7	D	131	Total	O	0	0
			131	131		

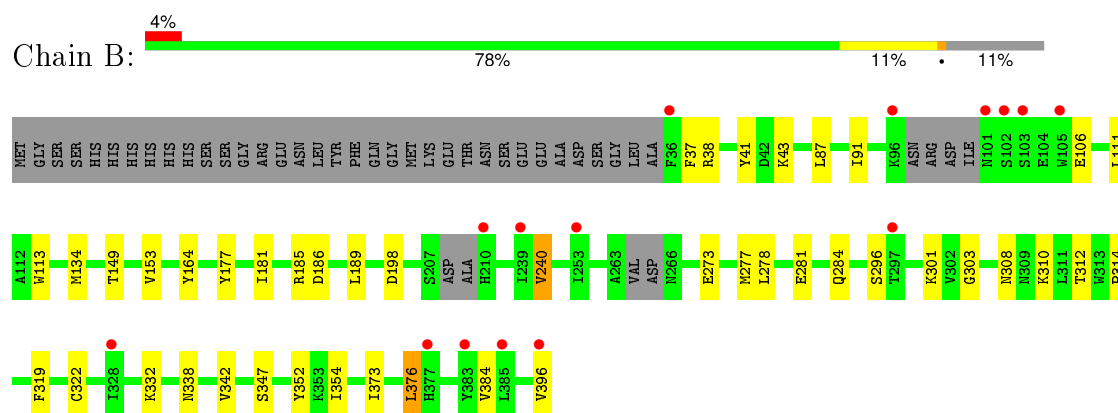
3 Residue-property plots [i](#)

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.

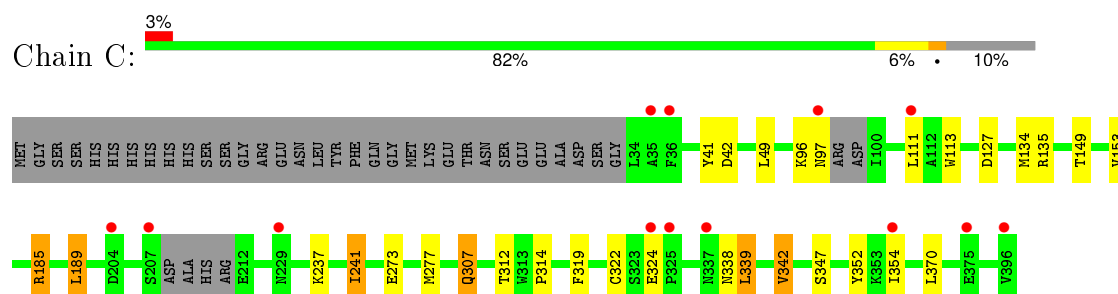
• Molecule 1: Farnesyl pyrophosphate synthase



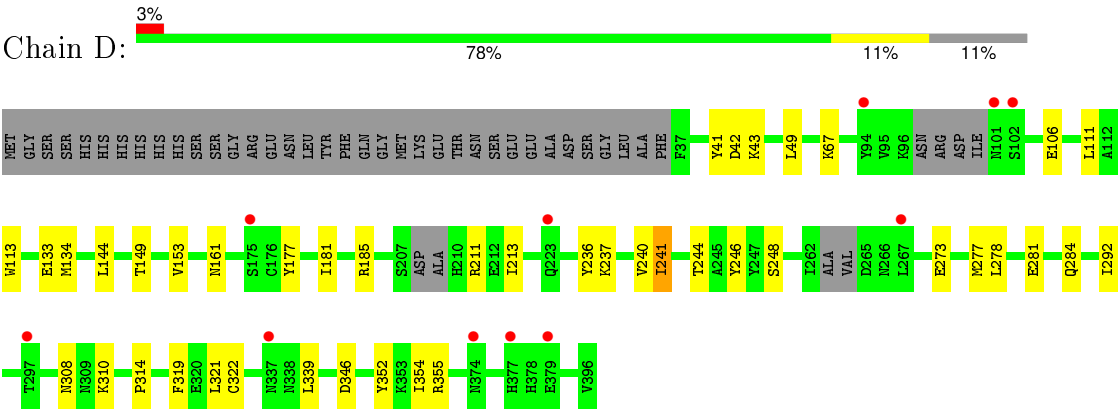
• Molecule 1: Farnesyl pyrophosphate synthase



• Molecule 1: Farnesyl pyrophosphate synthase



● Molecule 1: Farnesyl pyrophosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.26Å 139.54Å 109.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.24 – 2.47 20.07 – 2.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.24-2.47) 98.5 (20.07-2.47)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.47Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.239 , 0.286 0.222 , 0.266	Depositor DCC
R_{free} test set	3026 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.0	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	10 of 60724 reflections (0.016%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12338	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.15 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.7723e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, MG, ZOL, EDO, IPE

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	0.50	0/2986	0.68	0/4036
1	B	0.50	0/2970	0.68	0/4013
1	C	0.50	0/2994	0.67	0/4048
1	D	0.50	0/2953	0.68	0/3990
All	All	0.50	0/11903	0.68	0/16087

There are no bond length outliers.

There are no bond angle outliers.

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	2917	0	2857	17	0
1	B	2899	0	2859	31	0
1	C	2919	0	2889	15	0
1	D	2883	0	2835	22	0
2	A	16	0	6	0	0
2	B	16	0	6	1	0
2	C	16	0	6	0	0
2	D	16	0	6	0	0
3	A	14	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	9	0	0
3	C	14	0	9	0	0
3	D	14	0	9	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	3	0
6	A	6	0	8	2	0
6	B	6	0	8	5	0
6	D	6	0	8	1	0
7	A	144	0	0	2	0
7	B	144	0	0	0	0
7	C	143	0	0	0	0
7	D	131	0	0	2	0
All	All	12338	0	11536	81	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 3.

All (81) 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:D:292:ILE:HD11	7:D:1164:HOH:O	1.54	1.08
1:B:91:ILE:HD12	1:B:384:VAL:HG11	1.48	0.94
1:A:133:GLU:HG2	6:A:1106:GOL:H2	1.55	0.88
1:B:240:VAL:HG22	1:B:284:GLN:HG2	1.65	0.78
1:B:342:VAL:HG23	1:D:339:LEU:HD13	1.65	0.76
1:B:303:GLY:H	6:B:1105:GOL:H31	1.50	0.74
1:D:240:VAL:HG22	1:D:284:GLN:HG2	1.69	0.73
1:B:87:LEU:HD12	1:B:91:ILE:HD13	1.74	0.69
1:B:43:LYS:HE2	1:B:106:GLU:HG3	1.78	0.66
1:B:301:LYS:HG3	5:B:1106:EDO:H22	1.77	0.65
1:D:43:LYS:HE2	1:D:106:GLU:HG3	1.79	0.64
1:D:241:ILE:HG23	1:D:277:MET:HE1	1.80	0.64
1:D:241:ILE:HG23	1:D:277:MET:CE	2.32	0.60
1:A:134:MET:HG2	7:A:1232:HOH:O	2.01	0.59
1:B:338:ASN:HD21	1:D:133:GLU:CD	2.06	0.58
1:B:87:LEU:HD12	1:B:91:ILE:CD1	2.35	0.57
1:D:185[A]:ARG:NH2	7:D:1199:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ILE:O	1:B:376:LEU:HB2	2.07	0.55
1:A:164:TYR:OH	1:A:185[A]:ARG:HG3	2.07	0.55
1:A:195:GLN:NE2	7:A:1161:HOH:O	2.40	0.54
1:B:303:GLY:N	6:B:1105:GOL:H12	2.25	0.52
1:B:303:GLY:H	6:B:1105:GOL:C3	2.19	0.52
1:B:87:LEU:CD1	1:B:91:ILE:HD13	2.41	0.51
1:C:189[A]:LEU:HD13	1:D:161:ASN:HB3	1.92	0.51
1:B:296:SER:HB3	6:B:1105:GOL:H32	1.94	0.49
1:D:273:GLU:O	1:D:277:MET:HG2	2.14	0.48
1:B:177:TYR:CZ	1:B:181:ILE:HD11	2.49	0.47
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.49	0.47
1:C:273:GLU:O	1:C:277:MET:HG2	2.14	0.47
1:B:273:GLU:O	1:B:277:MET:HG2	2.14	0.47
1:A:273:GLU:O	1:A:277:MET:HG2	2.15	0.47
1:D:177:TYR:CZ	1:D:181:ILE:HD11	2.50	0.47
1:C:322:CYS:HA	1:C:352:TYR:CE2	2.50	0.47
1:B:41:TYR:HB2	1:B:113:TRP:CZ2	2.50	0.46
1:C:127:ASP:OD2	1:C:135:ARG:HD2	2.14	0.46
1:A:98:ARG:O	1:A:100:ILE:N	2.48	0.46
1:C:185[A]:ARG:HB2	1:C:185[A]:ARG:HH11	1.80	0.46
1:B:303:GLY:HA2	5:B:1106:EDO:H21	1.96	0.46
1:A:185[A]:ARG:HD2	1:B:164:TYR:HB2	1.97	0.46
1:A:127:ASP:OD2	1:A:135:ARG:HD2	2.16	0.45
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.51	0.45
1:A:150[B]:LYS:HG2	1:A:151:ASN:N	2.32	0.45
1:C:338:ASN:O	1:C:342:VAL:HG13	2.16	0.45
1:A:143:LEU:HD13	6:A:1106:GOL:H32	1.98	0.45
1:D:322:CYS:HA	1:D:352:TYR:CE1	2.51	0.45
1:D:346:ASP:OD1	6:D:1105:GOL:H11	2.16	0.45
1:C:41:TYR:HB2	1:C:113:TRP:CZ2	2.51	0.45
1:C:237:LYS:O	1:C:241:ILE:HB	2.16	0.45
1:B:312:THR:HB	1:B:314:PRO:HD2	1.99	0.45
1:B:91:ILE:HD12	1:B:384:VAL:CG1	2.33	0.45
1:D:246:TYR:CE1	1:D:277:MET:HE1	2.52	0.45
1:A:322:CYS:HA	1:A:352:TYR:CE2	2.51	0.45
1:C:149:THR:O	1:C:153[A]:VAL:HG23	2.16	0.45
1:D:237:LYS:O	1:D:241:ILE:HB	2.17	0.44
1:D:240:VAL:CG1	1:D:281:GLU:HA	2.47	0.44
1:C:307:GLN:HE21	1:C:307:GLN:H	1.66	0.44
1:B:314:PRO:HB3	1:B:354:ILE:HG21	1.98	0.44
1:B:322:CYS:HA	1:B:352:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:PRO:HB3	1:D:354:ILE:HG21	2.00	0.44
1:B:303:GLY:H	6:B:1105:GOL:H12	1.83	0.43
1:B:240:VAL:HG22	1:B:284:GLN:CG	2.43	0.43
1:A:237:LYS:O	1:A:241:ILE:HB	2.17	0.43
1:B:87:LEU:CD1	1:B:91:ILE:CD1	2.96	0.43
1:D:149:THR:O	1:D:153:VAL:HG23	2.18	0.43
1:A:149:THR:O	1:A:153:VAL:HG23	2.18	0.43
1:C:314:PRO:HB3	1:C:354:ILE:HG21	2.01	0.42
1:A:245:ALA:HB2	1:A:280:GLY:HA3	2.01	0.42
1:D:308:ASN:HB3	1:D:310:LYS:HE2	2.01	0.42
1:C:189[A]:LEU:HA	1:C:189[A]:LEU:HD12	1.93	0.42
1:B:91:ILE:CD1	1:B:384:VAL:HG11	2.34	0.42
1:D:236:TYR:CZ	1:D:240:VAL:HG21	2.55	0.42
2:B:397:ZOL:O16	5:B:1106:EDO:H11	2.20	0.41
1:B:149:THR:O	1:B:153:VAL:HG23	2.20	0.41
1:C:96:LYS:HA	1:C:96:LYS:HE2	2.01	0.41
1:B:240:VAL:CG1	1:B:281:GLU:HA	2.51	0.41
1:B:185[A]:ARG:NH2	1:B:186:ASP:OD1	2.53	0.41
1:C:312:THR:HB	1:C:314:PRO:HD2	2.03	0.41
1:D:244:THR:O	1:D:248:SER:HB2	2.21	0.41
1:B:308:ASN:HB3	1:B:310:LYS:HE2	2.02	0.40
1:A:307:GLN:OE1	1:C:339:LEU:HD22	2.21	0.40
1:A:219[B]:ASN:H	1:A:219[B]:ASN:HD22	1.70	0.40

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	356/396 (90%)	347 (98%)	9 (2%)	0	100	100
1	B	348/396 (88%)	341 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	356/396 (90%)	348 (98%)	8 (2%)	0	100	100
1	D	348/396 (88%)	341 (98%)	7 (2%)	0	100	100
All	All	1408/1584 (89%)	1377 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	310/357 (87%)	301 (97%)	9 (3%)	50	75
1	B	307/357 (86%)	294 (96%)	13 (4%)	36	60
1	C	310/357 (87%)	293 (94%)	17 (6%)	27	46
1	D	308/357 (86%)	295 (96%)	13 (4%)	36	60
All	All	1235/1428 (86%)	1183 (96%)	52 (4%)	37	60

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	111	LEU
1	A	134	MET
1	A	144	LEU
1	A	241	ILE
1	A	319	PHE
1	A	324	GLU
1	A	339	LEU
1	A	370	LEU
1	B	37	PHE
1	B	38	ARG
1	B	111	LEU
1	B	134	MET
1	B	189	LEU

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Mol	Chain	Res	Type
1	B	198	ASP
1	B	240	VAL
1	B	278	LEU
1	B	319	PHE
1	B	332	LYS
1	B	347	SER
1	B	376	LEU
1	B	396	VAL
1	C	42	ASP
1	C	49	LEU
1	C	97	ASN
1	C	111	LEU
1	C	134	MET
1	C	185[A]	ARG
1	C	185[B]	ARG
1	C	189[A]	LEU
1	C	189[B]	LEU
1	C	241	ILE
1	C	307	GLN
1	C	319	PHE
1	C	324	GLU
1	C	339	LEU
1	C	342	VAL
1	C	347	SER
1	C	370	LEU
1	D	42	ASP
1	D	49	LEU
1	D	67	LYS
1	D	111	LEU
1	D	134	MET
1	D	144	LEU
1	D	211	ARG
1	D	213	ILE
1	D	241	ILE
1	D	278	LEU
1	D	319	PHE
1	D	321	LEU
1	D	355	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	B	307	GLN
1	C	82	ASN
1	C	307	GLN
1	D	82	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](#)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	IPE	A	1101	-	10,13,13	2.20	2 (20%)	14,19,19	0.98	1 (7%)
5	EDO	A	1105	-	3,3,3	0.54	0	2,2,2	0.21	0
6	GOL	A	1106	-	5,5,5	0.87	0	5,5,5	1.02	0
2	ZOL	A	397	4	15,16,16	3.09	8 (53%)	19,26,26	1.96	6 (31%)
3	IPE	B	1101	-	10,13,13	2.14	2 (20%)	14,19,19	0.97	1 (7%)
6	GOL	B	1105	-	5,5,5	0.36	0	5,5,5	1.23	0
5	EDO	B	1106	-	3,3,3	0.68	0	2,2,2	0.37	0
2	ZOL	B	397	4	15,16,16	3.10	8 (53%)	19,26,26	2.14	7 (36%)
3	IPE	C	1101	-	10,13,13	2.09	2 (20%)	14,19,19	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ZOL	C	397	4	15,16,16	3.21	8 (53%)	19,26,26	2.27	7 (36%)
3	IPE	D	1101	-	10,13,13	2.18	2 (20%)	14,19,19	0.96	1 (7%)
6	GOL	D	1105	-	5,5,5	0.83	0	5,5,5	1.52	2 (40%)
2	ZOL	D	397	4	15,16,16	3.76	9 (60%)	19,26,26	2.12	6 (31%)

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	IPE	A	1101	-	-	0/13/13/13	0/0/0/0
5	EDO	A	1105	-	-	0/1/1/1	0/0/0/0
6	GOL	A	1106	-	-	0/4/4/4	0/0/0/0
2	ZOL	A	397	4	-	0/23/23/23	0/1/1/1
3	IPE	B	1101	-	-	0/13/13/13	0/0/0/0
6	GOL	B	1105	-	-	0/4/4/4	0/0/0/0
5	EDO	B	1106	-	-	0/1/1/1	0/0/0/0
2	ZOL	B	397	4	-	0/23/23/23	0/1/1/1
3	IPE	C	1101	-	-	0/13/13/13	0/0/0/0
2	ZOL	C	397	4	-	0/23/23/23	0/1/1/1
3	IPE	D	1101	-	-	0/13/13/13	0/0/0/0
6	GOL	D	1105	-	-	0/4/4/4	0/0/0/0
2	ZOL	D	397	4	-	0/23/23/23	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	397	ZOL	P14-O17	-4.13	1.46	1.54
2	A	397	ZOL	P9-O10	-3.91	1.47	1.54
2	A	397	ZOL	P14-O17	-3.65	1.47	1.54
2	C	397	ZOL	P9-O10	-3.40	1.48	1.54
3	B	1101	IPE	C5-C3	-3.38	1.33	1.48
3	D	1101	IPE	C5-C3	-3.37	1.33	1.48
3	A	1101	IPE	C5-C3	-3.36	1.33	1.48
3	C	1101	IPE	C5-C3	-3.27	1.33	1.48
2	B	397	ZOL	P9-O10	-3.17	1.48	1.54
2	C	397	ZOL	P14-O17	-3.12	1.48	1.54
2	D	397	ZOL	P9-O10	-3.03	1.49	1.54
2	B	397	ZOL	P14-O17	-2.51	1.50	1.54
2	A	397	ZOL	C19-N15	-2.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	397	ZOL	C19-N15	-2.37	1.33	1.37
2	C	397	ZOL	C19-N15	-2.11	1.33	1.37
2	B	397	ZOL	C19-N15	-2.07	1.33	1.37
2	B	397	ZOL	P9-O11	2.08	1.58	1.54
2	A	397	ZOL	P14-C8	2.23	1.86	1.85
2	C	397	ZOL	P14-C8	3.30	1.87	1.85
2	D	397	ZOL	P14-O16	3.67	1.61	1.54
2	D	397	ZOL	P14-C8	3.73	1.87	1.85
2	C	397	ZOL	P9-O11	3.74	1.61	1.54
2	A	397	ZOL	P14-O16	4.08	1.62	1.54
2	B	397	ZOL	P14-O16	4.10	1.62	1.54
2	C	397	ZOL	P14-O16	4.31	1.63	1.54
2	A	397	ZOL	P14-O15	4.35	1.57	1.50
2	B	397	ZOL	P9-C8	4.46	1.88	1.85
2	D	397	ZOL	P9-O11	4.50	1.63	1.54
2	A	397	ZOL	P9-O11	4.54	1.63	1.54
3	C	1101	IPE	C4-C3	5.38	1.50	1.33
3	B	1101	IPE	C4-C3	5.59	1.51	1.33
3	A	1101	IPE	C4-C3	5.70	1.51	1.33
3	D	1101	IPE	C4-C3	5.74	1.51	1.33
2	D	397	ZOL	P9-O12	5.77	1.59	1.50
2	B	397	ZOL	P14-O15	5.82	1.59	1.50
2	C	397	ZOL	P14-O15	5.84	1.59	1.50
2	A	397	ZOL	P9-O12	6.41	1.60	1.50
2	D	397	ZOL	P9-C8	6.55	1.89	1.85
2	B	397	ZOL	P9-O12	6.69	1.61	1.50
2	C	397	ZOL	P9-O12	6.93	1.61	1.50
2	D	397	ZOL	P14-O15	7.29	1.62	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	397	ZOL	P9-C8-P14	-5.15	104.97	112.84
2	D	397	ZOL	O16-P14-O15	-4.66	102.00	113.04
2	B	397	ZOL	P9-C8-P14	-3.65	107.27	112.84
2	C	397	ZOL	O16-P14-O15	-3.45	104.86	113.04
2	A	397	ZOL	P9-C8-P14	-3.43	107.59	112.84
2	D	397	ZOL	O11-P9-O12	-3.38	105.04	113.04
2	D	397	ZOL	O15-P14-C8	-3.32	101.02	109.95
2	A	397	ZOL	O15-P14-C8	-3.11	101.58	109.95
2	A	397	ZOL	O16-P14-O15	-2.79	106.44	113.04
2	C	397	ZOL	O11-P9-O12	-2.63	106.81	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	ZOL	O16-P14-C8	-2.57	100.16	105.90
2	A	397	ZOL	O11-P9-O12	-2.56	106.97	113.04
2	B	397	ZOL	O11-P9-O12	-2.49	107.13	113.04
6	D	1105	GOL	O1-C1-C2	2.03	120.05	110.18
3	B	1101	IPE	O3B-PB-O1B	2.05	115.18	107.38
3	D	1101	IPE	O3B-PB-O1B	2.06	115.22	107.38
3	A	1101	IPE	O3B-PB-O1B	2.09	115.32	107.38
2	B	397	ZOL	O11-P9-O10	2.14	114.30	108.24
2	A	397	ZOL	O10-P9-C8	2.16	110.71	105.90
2	B	397	ZOL	C19-N15-C16	2.16	110.29	108.20
2	D	397	ZOL	O11-P9-O10	2.25	114.60	108.24
6	D	1105	GOL	O2-C2-C1	2.42	119.77	108.65
2	C	397	ZOL	O16-P14-O17	2.58	115.54	108.24
2	C	397	ZOL	O11-P9-O10	2.60	115.59	108.24
2	D	397	ZOL	O16-P14-C8	2.86	112.29	105.90
2	C	397	ZOL	O10-P9-C8	3.14	112.90	105.90
2	D	397	ZOL	O17-P14-C8	3.54	113.80	105.90
2	B	397	ZOL	O10-P9-C8	3.78	114.33	105.90
2	C	397	ZOL	O17-P14-C8	3.97	114.75	105.90
2	B	397	ZOL	O17-P14-C8	4.49	115.92	105.90
2	A	397	ZOL	O17-P14-C8	4.71	116.40	105.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1106	GOL	2	0
6	B	1105	GOL	5	0
5	B	1106	EDO	3	0
2	B	397	ZOL	1	0
6	D	1105	GOL	1	0

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, 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	358/396 (90%)	0.16	14 (3%)	43 47	20, 34, 54, 76	12 (3%)
1	B	353/396 (89%)	0.16	15 (4%)	40 44	19, 32, 50, 72	10 (2%)
1	C	357/396 (90%)	0.13	13 (3%)	46 51	19, 33, 52, 83	8 (2%)
1	D	352/396 (88%)	0.17	11 (3%)	52 56	19, 33, 53, 76	4 (1%)
All	All	1420/1584 (89%)	0.15	53 (3%)	45 50	19, 33, 53, 83	34 (2%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	VAL	4.8
1	B	105[A]	TRP	4.5
1	D	267	LEU	4.2
1	D	102	SER	4.0
1	A	315	LEU	3.9
1	B	36	PHE	3.9
1	A	325	PRO	3.8
1	D	101	ASN	3.6
1	A	97	ASN	3.5
1	C	35	ALA	3.4
1	A	35	ALA	3.3
1	D	374	ASN	3.2
1	C	325	PRO	3.1
1	A	377	HIS	3.1
1	D	297	THR	3.1
1	C	207	SER	3.1
1	B	297	THR	3.1
1	D	377	HIS	2.9
1	B	377	HIS	2.8
1	A	396	VAL	2.8
1	D	337	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	355	ARG	2.7
1	B	96	LYS	2.7
1	D	94	TYR	2.6
1	A	102	SER	2.5
1	D	223	GLN	2.5
1	A	98	ARG	2.5
1	C	229	ASN	2.5
1	C	97	ASN	2.3
1	B	103	SER	2.3
1	A	360	SER	2.3
1	B	383	TYR	2.3
1	B	328	ILE	2.2
1	C	354	ILE	2.2
1	A	36	PHE	2.2
1	A	228	ILE	2.2
1	B	239	ILE	2.2
1	D	175	SER	2.2
1	C	337	ASN	2.2
1	A	207	SER	2.2
1	B	210	HIS	2.2
1	D	379	GLU	2.2
1	C	111	LEU	2.2
1	B	101	ASN	2.2
1	C	36	PHE	2.1
1	A	229	ASN	2.1
1	C	396	VAL	2.1
1	C	324	GLU	2.1
1	B	385	LEU	2.1
1	C	204	ASP	2.1
1	C	375	GLU	2.0
1	B	253	ILE	2.0
1	B	102	SER	2.0

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
5	EDO	B	1106	4/4	0.71	0.46	16.36	37,38,38,39	0
6	GOL	D	1105	6/6	0.86	0.36	14.25	49,51,51,52	0
6	GOL	A	1106	6/6	0.74	0.33	5.35	60,63,64,66	0
5	EDO	A	1105	4/4	0.36	0.33	3.83	72,72,73,76	0
6	GOL	B	1105	6/6	0.92	0.24	3.01	45,47,48,48	0
3	IPE	C	1101	14/14	0.97	0.13	-0.64	3,25,39,41	3
3	IPE	A	1101	14/14	0.98	0.11	-1.02	17,28,38,38	0
3	IPE	B	1101	14/14	0.98	0.11	-1.35	11,28,47,59	0
2	ZOL	B	397	16/16	0.98	0.10	-1.57	11,23,31,50	0
3	IPE	D	1101	14/14	0.98	0.09	-1.57	15,27,53,57	0
4	MG	C	1104	1/1	0.99	0.10	-1.58	27,27,27,27	0
4	MG	B	1103	1/1	0.98	0.11	-1.90	16,16,16,16	0
2	ZOL	C	397	16/16	0.98	0.09	-2.08	7,23,38,45	0
4	MG	B	1102	1/1	0.96	0.06	-2.31	21,21,21,21	0
2	ZOL	A	397	16/16	0.99	0.08	-2.50	15,21,37,43	0
2	ZOL	D	397	16/16	0.99	0.08	-2.62	10,24,29,31	0
4	MG	D	1104	1/1	0.98	0.06	-5.15	16,16,16,16	0
4	MG	C	1103	1/1	0.95	0.05	-5.18	27,27,27,27	0
4	MG	D	1102	1/1	0.98	0.03	-5.94	17,17,17,17	0
4	MG	A	1104	1/1	0.99	0.08	-6.17	23,23,23,23	0
4	MG	A	1103	1/1	0.96	0.05	-	22,22,22,22	0
4	MG	A	1102	1/1	0.97	0.04	-	21,21,21,21	0
4	MG	C	1102	1/1	0.97	0.07	-	23,23,23,23	0
4	MG	D	1103	1/1	1.00	0.07	-	18,18,18,18	0
4	MG	B	1104	1/1	0.97	0.08	-	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.