



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:36 pm GMT

PDB ID : 2E8T  
Title : S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with magnesium, FsPP and IPP  
Authors : Guo, R.T.; Ko, T.P.; Chen, C.K.-M.; Jeng, W.Y.; Chang, T.H.; Liang, P.H.; Oldfield, E.; Wang, A.H.-J.  
Deposited on : 2007-01-23  
Resolution : 2.13 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](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

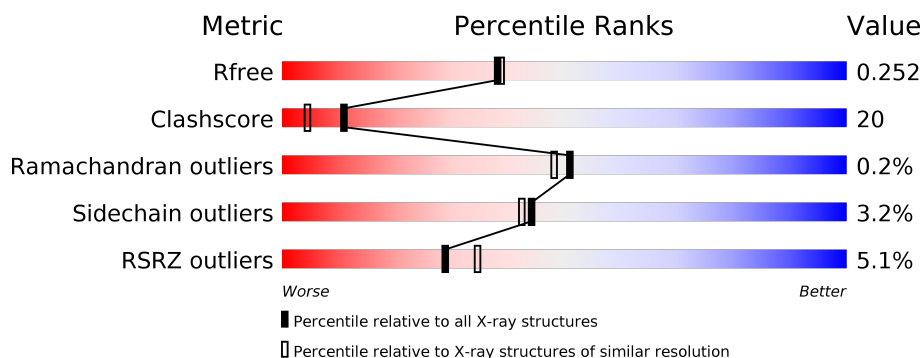
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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	340	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>23%</div> <div>••</div> <div>12%</div> </div> </div>
1	B	340	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>•</div> <div>13%</div> </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
2	MG	B	1304	-	-	-	X
3	IPE	A	1001	-	-	X	-
3	IPE	B	1002	-	-	X	-
4	FPS	A	1201	-	-	X	-
4	FPS	B	1202	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5482 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 Geranylgeranyl pyrophosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2440	1565	415	451	9			
1	B	295	Total	C	N	O	S	0	0	0
			2414	1551	408	446	9			

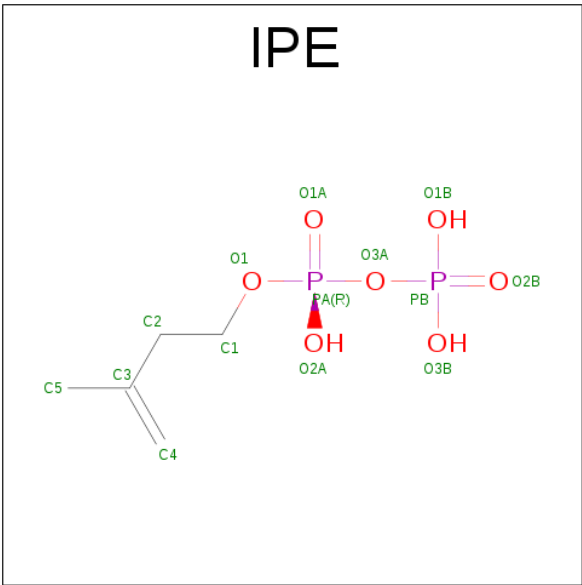
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q12051
A	2	THR	-	CLONING ARTIFACT	UNP Q12051
A	3	LYS	-	CLONING ARTIFACT	UNP Q12051
A	4	ASN	-	CLONING ARTIFACT	UNP Q12051
A	5	LYS	-	CLONING ARTIFACT	UNP Q12051
B	1	MET	-	CLONING ARTIFACT	UNP Q12051
B	2	THR	-	CLONING ARTIFACT	UNP Q12051
B	3	LYS	-	CLONING ARTIFACT	UNP Q12051
B	4	ASN	-	CLONING ARTIFACT	UNP Q12051
B	5	LYS	-	CLONING ARTIFACT	UNP Q12051

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

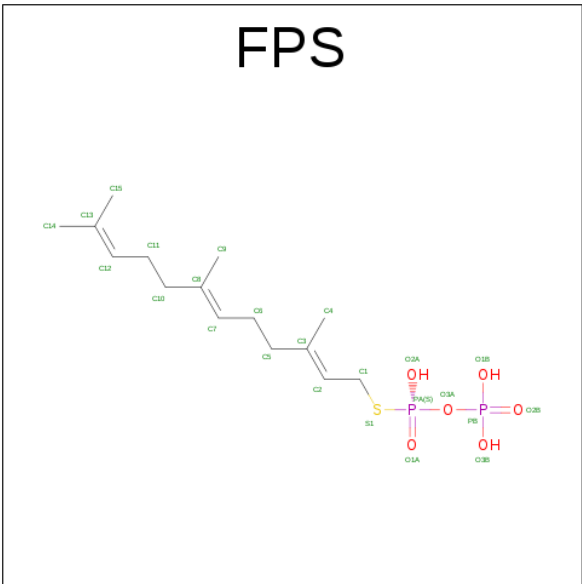
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>7</sub>P<sub>2</sub>).



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		

- Molecule 4 is S-[(2E,6E)-3,7,11-TRIMETHYLDODECA-2,6,10-TRIENYL] TRIHYDRO-GEN THIODIPHOSPHATE (three-letter code: FPS) (formula: C<sub>15</sub>H<sub>28</sub>O<sub>6</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	P	S	0	0
			24	15	6	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	O	P	S	0	0
			24	15	6	2	1		

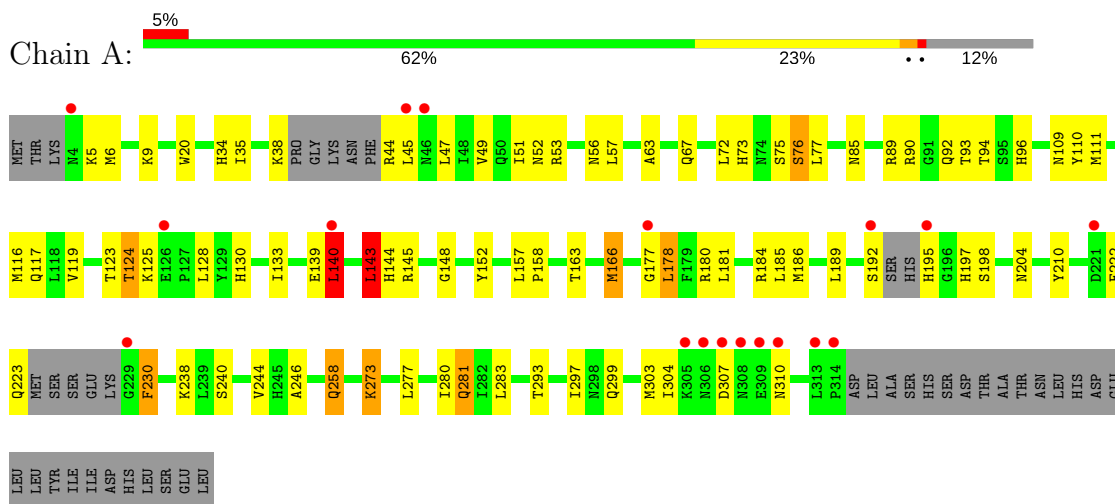
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	276	Total	O	0	0
			276	276		
5	B	272	Total	O	0	0
			272	272		

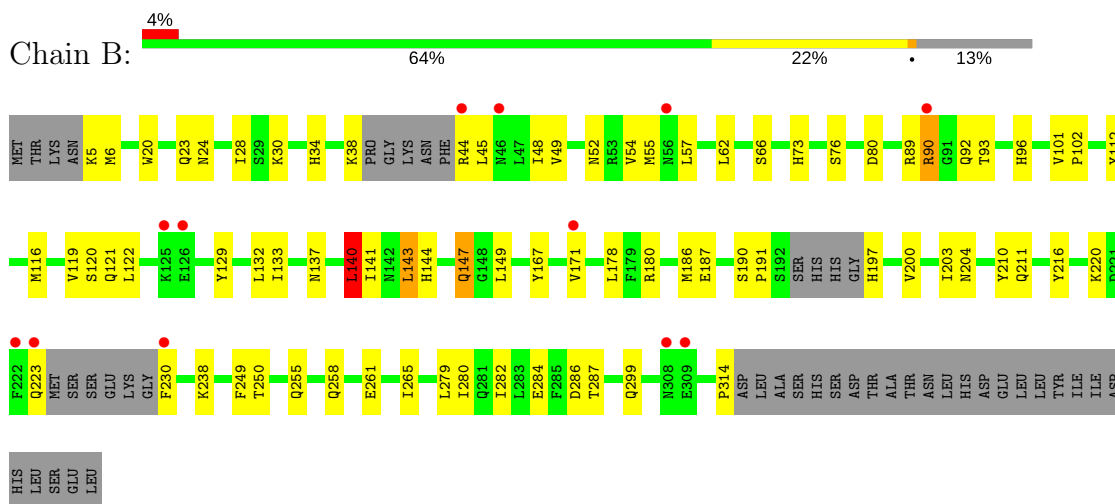
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $RSRZ > 2$ ). 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: Geranylgeranyl pyrophosphate synthetase



#### • Molecule 1: Geranylgeranyl pyrophosphate synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.38Å 116.10Å 128.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.90 – 2.13 30.91 – 2.13	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.90-2.13) 93.7 (30.91-2.13)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.18 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.196 , 0.250 0.196 , 0.252	Depositor DCC
$R_{free}$ test set	1899 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 68.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5482	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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, FPS, 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	0.72	1/2483 (0.0%)	0.76	2/3360 (0.1%)
1	B	0.68	0/2456	0.76	1/3324 (0.0%)
All	All	0.70	1/4939 (0.0%)	0.76	3/6684 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	MET	SD-CE	-5.20	1.48	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	LEU	CA-CB-CG	-6.34	100.72	115.30
1	B	140	LEU	CA-CB-CG	-5.81	101.94	115.30
1	A	143	LEU	CA-CB-CG	5.33	127.55	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	2440	0	2485	107	0
1	B	2414	0	2466	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	14	0	9	8	0
3	B	14	0	9	10	0
4	A	24	0	25	11	0
4	B	24	0	25	17	0
5	A	276	0	0	10	0
5	B	272	0	0	7	0
All	All	5482	0	5019	201	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 20.

All (201) 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:163:THR:H	1:A:166:MET:HE3	1.12	1.12
1:B:143:LEU:HD22	4:B:1202:FPS:H12	1.31	1.10
3:A:1001:IPE:H53	4:A:1201:FPS:H42	1.34	1.09
1:A:38:LYS:HB3	1:A:90:ARG:HD3	1.41	1.03
1:A:123:THR:HG22	1:A:125:LYS:H	1.27	1.00
3:B:1002:IPE:H42	4:B:1202:FPS:H12A	1.44	0.98
1:A:38:LYS:HD3	1:A:90:ARG:HD2	1.47	0.97
1:A:92:GLN:HG2	5:A:931:HOH:O	1.64	0.96
1:B:52:ASN:HD21	1:B:57:LEU:H	1.12	0.90
1:A:94:THR:HG21	1:A:96:HIS:CD2	2.08	0.88
1:A:258:GLN:HE21	1:A:258:GLN:H	1.21	0.87
1:A:52:ASN:HD21	1:A:57:LEU:H	1.18	0.87
1:B:89:ARG:HH11	1:B:90:ARG:NH2	1.73	0.86
1:A:47:LEU:O	1:A:51:ILE:HD12	1.78	0.83
1:A:281:GLN:HE21	1:A:281:GLN:HA	1.44	0.83
1:A:163:THR:N	1:A:166:MET:HE3	1.92	0.82
1:B:38:LYS:CG	1:B:90:ARG:HG2	2.09	0.82
3:A:1001:IPE:C5	4:A:1201:FPS:H42	2.10	0.82
1:A:94:THR:CG2	1:A:96:HIS:CD2	2.63	0.81
1:B:44:ARG:HH12	3:B:1002:IPE:H11	1.44	0.80
1:B:258:GLN:HG2	1:B:286:ASP:OD2	1.82	0.79
1:A:44:ARG:HA	5:A:924:HOH:O	1.83	0.78
3:A:1001:IPE:O2A	3:A:1001:IPE:H21	1.83	0.78
1:A:38:LYS:HB2	1:A:90:ARG:HH11	1.47	0.78
1:B:89:ARG:HH11	1:B:90:ARG:HH22	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:NZ	4:A:1201:FPS:O2A	2.18	0.77
1:A:38:LYS:CB	1:A:90:ARG:HD3	2.15	0.76
1:A:35:ILE:HG13	1:A:38:LYS:HD2	1.70	0.74
1:B:143:LEU:HD13	4:B:1202:FPS:H142	1.71	0.73
1:B:249:PHE:CD2	1:B:287:THR:HG22	2.25	0.71
1:B:23:GLN:NE2	5:B:879:HOH:O	2.22	0.70
1:B:38:LYS:HG3	1:B:90:ARG:HG2	1.72	0.70
3:B:1002:IPE:H51	4:B:1202:FPS:O1A	1.93	0.69
1:B:120:SER:HA	1:B:129:TYR:HE1	1.59	0.68
1:B:52:ASN:ND2	1:B:57:LEU:H	1.90	0.68
1:A:143:LEU:HD13	1:A:177:GLY:HA3	1.75	0.68
1:B:120:SER:HA	1:B:129:TYR:CE1	2.29	0.68
1:B:89:ARG:NH1	1:B:90:ARG:HH22	1.91	0.67
1:A:140:LEU:O	1:A:144:HIS:HD2	1.77	0.67
1:A:96:HIS:HE1	5:A:404:HOH:O	1.77	0.67
1:A:148:GLY:HA3	1:B:28:ILE:CD1	2.25	0.67
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.40	0.66
1:A:210:TYR:OH	3:A:1001:IPE:H12	1.94	0.66
1:A:140:LEU:HD21	4:A:1201:FPS:H153	1.78	0.66
1:B:143:LEU:CD2	4:B:1202:FPS:H7	2.26	0.66
1:B:38:LYS:HG3	1:B:90:ARG:CB	2.28	0.64
1:A:143:LEU:HG	4:A:1201:FPS:C12	2.28	0.63
1:B:284:GLU:OE1	1:B:284:GLU:HA	1.99	0.62
1:B:230:PHE:N	5:B:860:HOH:O	2.32	0.62
1:A:180:ARG:HH11	1:A:204:ASN:ND2	1.98	0.61
1:A:148:GLY:HA3	1:B:28:ILE:HD12	1.82	0.61
1:A:47:LEU:HG	1:A:51:ILE:HD11	1.83	0.61
1:B:143:LEU:HD23	4:B:1202:FPS:H7	1.83	0.60
1:B:197:HIS:HE1	1:B:314:PRO:HA	1.65	0.60
1:A:281:GLN:HE21	1:A:281:GLN:CA	2.14	0.60
1:A:223:GLN:HB2	1:A:280:ILE:HG21	1.83	0.60
1:A:94:THR:HG22	1:A:96:HIS:CD2	2.38	0.59
1:A:123:THR:HG22	1:A:124:THR:H	1.68	0.59
1:B:38:LYS:HG3	1:B:90:ARG:CG	2.32	0.59
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.14	0.59
1:A:238:LYS:HZ1	4:A:1201:FPS:PA	2.26	0.58
1:B:180:ARG:HH11	1:B:204:ASN:ND2	2.01	0.58
1:B:55:MET:HE2	1:B:190:SER:HB2	1.85	0.58
1:A:5:LYS:O	1:A:9:LYS:HG3	2.03	0.58
1:A:117:GLN:HA	1:B:137:ASN:HD21	1.68	0.58
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:HG23	1:A:166:MET:CE	2.33	0.57
1:A:94:THR:HG21	1:A:96:HIS:NE2	2.20	0.57
1:B:171:VAL:HG22	1:B:211:GLN:HG2	1.86	0.57
1:A:52:ASN:ND2	1:A:57:LEU:HG	2.18	0.57
1:B:112:TYR:CE2	4:B:1202:FPS:H152	2.40	0.56
1:B:55:MET:CE	1:B:190:SER:HB2	2.35	0.56
1:A:38:LYS:HE3	1:A:89:ARG:O	2.05	0.56
1:B:55:MET:CE	1:B:187:GLU:HA	2.36	0.56
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.53	0.55
1:B:143:LEU:CD1	4:B:1202:FPS:H142	2.36	0.55
1:A:34:HIS:HE1	1:A:93:THR:O	1.89	0.55
1:B:90:ARG:NH1	5:B:631:HOH:O	2.39	0.55
1:B:45:LEU:HD13	1:B:66:SER:OG	2.07	0.54
1:A:273:LYS:HB3	5:A:798:HOH:O	2.08	0.54
1:A:53:ARG:NH1	5:A:728:HOH:O	2.40	0.54
1:B:5:LYS:N	5:B:852:HOH:O	2.40	0.54
1:B:210:TYR:HE2	3:B:1002:IPE:H22	1.73	0.54
1:A:123:THR:HG22	1:A:124:THR:N	2.23	0.53
1:A:117:GLN:CA	1:B:137:ASN:HD21	2.22	0.53
1:B:96:HIS:HE1	5:B:452:HOH:O	1.90	0.53
1:A:143:LEU:HB3	4:A:1201:FPS:H102	1.90	0.53
1:A:143:LEU:HG	4:A:1201:FPS:H12	1.89	0.53
1:A:139:GLU:O	1:A:143:LEU:HD22	2.09	0.52
1:A:166:MET:HE1	5:A:641:HOH:O	2.09	0.52
1:B:119:VAL:HG11	1:B:133:ILE:HD13	1.91	0.51
1:A:148:GLY:HA3	1:B:28:ILE:HD11	1.92	0.51
1:B:44:ARG:HH12	3:B:1002:IPE:C1	2.18	0.51
1:A:180:ARG:O	1:A:184:ARG:HG3	2.10	0.51
1:A:73:HIS:O	1:A:77:LEU:HG	2.10	0.51
1:B:89:ARG:NH1	1:B:90:ARG:NH2	2.47	0.51
1:B:48:ILE:HG22	1:B:62:LEU:HD11	1.93	0.50
1:A:210:TYR:OH	3:A:1001:IPE:C1	2.58	0.50
1:A:246:ALA:HB2	1:A:283:LEU:HD22	1.94	0.50
1:A:140:LEU:CD2	4:A:1201:FPS:H153	2.42	0.50
1:B:73:HIS:HE1	3:B:1002:IPE:H12	1.77	0.50
1:A:222:PHE:CD1	1:A:230:PHE:HA	2.47	0.49
1:B:76:SER:HB2	4:B:1202:FPS:H52	1.93	0.49
3:A:1001:IPE:H53	4:A:1201:FPS:C4	2.24	0.49
1:A:38:LYS:HB3	1:A:90:ARG:CD	2.27	0.49
1:A:52:ASN:ND2	1:A:57:LEU:H	1.98	0.49
1:B:55:MET:HE1	1:B:187:GLU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:MET:CE	1:B:299:GLN:NE2	2.76	0.49
1:B:116:MET:O	1:B:119:VAL:HB	2.13	0.49
1:B:180:ARG:HD3	1:B:204:ASN:HD21	1.76	0.49
1:B:122:LEU:HD12	1:B:132:LEU:HD13	1.96	0.48
1:A:145:ARG:HD3	1:B:20:TRP:CD2	2.49	0.48
4:B:1202:FPS:O1A	4:B:1202:FPS:O2B	2.31	0.48
1:A:210:TYR:CE2	3:A:1001:IPE:H12	2.47	0.48
1:A:178:LEU:HB2	5:A:437:HOH:O	2.14	0.48
1:B:249:PHE:HD2	1:B:287:THR:HG22	1.78	0.48
1:B:52:ASN:ND2	1:B:57:LEU:HG	2.29	0.48
1:B:34:HIS:HE1	1:B:93:THR:O	1.97	0.47
1:B:143:LEU:HD22	4:B:1202:FPS:H7	1.95	0.47
1:B:143:LEU:HD22	4:B:1202:FPS:C12	2.23	0.47
1:B:261:GLU:OE1	1:B:261:GLU:HA	2.14	0.47
1:A:293:THR:O	1:A:297:ILE:HG13	2.14	0.47
1:A:109:ASN:HB3	1:B:144:HIS:CE1	2.49	0.47
1:A:38:LYS:HE2	1:A:89:ARG:CG	2.44	0.47
1:A:72:LEU:O	1:A:76:SER:HB2	2.14	0.47
1:B:250:THR:HG22	1:B:255:GLN:HE21	1.79	0.47
1:A:152:TYR:OH	1:B:30:LYS:NZ	2.46	0.47
1:B:89:ARG:HD2	1:B:90:ARG:NH2	2.30	0.47
1:A:240:SER:O	1:A:244:VAL:HG23	2.16	0.46
1:B:52:ASN:HD21	1:B:57:LEU:HG	1.80	0.46
1:B:250:THR:HG22	1:B:255:GLN:NE2	2.30	0.46
1:A:52:ASN:HD21	1:A:57:LEU:HG	1.78	0.46
1:A:20:TRP:HZ3	1:B:149:LEU:HD22	1.81	0.46
4:B:1202:FPS:H12	4:B:1202:FPS:C7	2.46	0.46
1:A:116:MET:CE	1:B:116:MET:SD	3.04	0.46
1:A:130:HIS:CD2	1:B:129:TYR:CD2	3.04	0.46
1:A:258:GLN:N	1:A:258:GLN:HE21	2.01	0.46
1:A:38:LYS:HE2	1:A:89:ARG:HG3	1.98	0.46
1:B:101:VAL:N	1:B:102:PRO:CD	2.79	0.46
1:A:117:GLN:HA	1:B:137:ASN:ND2	2.31	0.45
1:A:63:ALA:O	1:A:67:GLN:HG3	2.16	0.45
1:A:143:LEU:HD11	5:A:437:HOH:O	2.16	0.45
1:A:44:ARG:HD3	1:A:73:HIS:CD2	2.52	0.45
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.98	0.45
1:B:48:ILE:HG23	1:B:186:MET:SD	2.57	0.45
1:A:123:THR:HG21	1:A:125:LYS:HB2	1.99	0.45
1:A:94:THR:CG2	1:A:96:HIS:HD2	2.24	0.45
1:B:167:TYR:C	1:B:167:TYR:CD2	2.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:CD	1:B:90:ARG:HG2	2.47	0.45
1:A:110:TYR:HE1	1:B:141:ILE:HG23	1.81	0.44
1:A:34:HIS:CE1	1:A:93:THR:O	2.70	0.44
1:A:197:HIS:HD2	1:A:198:SER:O	1.99	0.44
1:B:120:SER:CA	1:B:129:TYR:HE1	2.29	0.44
1:B:55:MET:HE2	1:B:187:GLU:HA	1.99	0.44
1:A:38:LYS:CB	1:A:90:ARG:CD	2.93	0.44
1:A:57:LEU:HD11	1:A:186:MET:HG2	1.99	0.44
1:A:85:ASN:ND2	5:A:404:HOH:O	2.50	0.44
1:B:220:LYS:HD2	1:B:220:LYS:HA	1.76	0.43
1:B:282:ILE:O	1:B:286:ASP:HB3	2.18	0.43
1:A:148:GLY:C	1:B:28:ILE:HD11	2.39	0.43
1:B:200:VAL:O	1:B:203:ILE:HG22	2.17	0.43
1:B:265:ILE:HG21	1:B:279:LEU:HB2	2.00	0.43
1:B:38:LYS:HG2	1:B:90:ARG:HG2	1.98	0.43
1:A:144:HIS:HE1	5:A:408:HOH:O	2.02	0.43
1:B:140:LEU:O	1:B:144:HIS:HD2	2.01	0.43
1:A:304:ILE:O	1:A:307:ASP:HB3	2.19	0.43
1:B:52:ASN:HD22	1:B:55:MET:HB2	1.83	0.43
4:A:1201:FPS:O2B	4:A:1201:FPS:H11	2.19	0.43
1:B:238:LYS:NZ	4:B:1202:FPS:O2A	2.45	0.43
1:B:44:ARG:NH1	3:B:1002:IPE:H11	2.24	0.42
1:A:47:LEU:O	1:A:51:ILE:CD1	2.59	0.42
1:A:56:ASN:HD22	1:A:192:SER:HB2	1.83	0.42
1:A:6:MET:HE1	1:B:299:GLN:NE2	2.35	0.42
1:B:133:ILE:HD13	1:B:133:ILE:HA	1.96	0.42
1:A:45:LEU:O	1:A:49:VAL:HG23	2.20	0.42
1:B:44:ARG:NH1	3:B:1002:IPE:C1	2.83	0.42
1:A:119:VAL:HG11	1:A:133:ILE:HD13	2.01	0.42
1:B:52:ASN:C	1:B:54:VAL:N	2.73	0.42
1:A:157:LEU:HD12	1:A:158:PRO:HA	2.01	0.42
1:B:20:TRP:CH2	1:B:24:ASN:HB3	2.55	0.42
1:A:307:ASP:OD2	1:A:310:ASN:HA	2.20	0.42
1:A:185:LEU:O	1:A:189:LEU:HG	2.20	0.41
1:B:147:GLN:HA	1:B:147:GLN:HE21	1.85	0.41
1:A:47:LEU:HG	1:A:51:ILE:CD1	2.49	0.41
1:B:55:MET:O	1:B:191:PRO:HD2	2.19	0.41
1:A:38:LYS:HD3	1:A:90:ARG:CD	2.34	0.41
1:B:140:LEU:HD21	4:B:1202:FPS:H153	2.02	0.41
3:B:1002:IPE:C4	4:B:1202:FPS:H42	2.51	0.41
1:B:144:HIS:HE1	5:B:414:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:O	1:A:281:GLN:HG2	2.21	0.41
1:B:28:ILE:HG23	1:B:28:ILE:HD12	1.78	0.41
1:A:210:TYR:CZ	3:A:1001:IPE:H12	2.55	0.41
1:A:299:GLN:O	1:A:303:MET:HG3	2.21	0.41
1:B:80:ASP:OD2	4:B:1202:FPS:S1	2.79	0.41
1:A:222:PHE:CE1	1:A:230:PHE:HA	2.56	0.41
1:B:121:GLN:NE2	5:B:686:HOH:O	2.54	0.41
1:A:75:SER:OG	1:A:111:MET:HB2	2.21	0.40
1:B:223:GLN:HB2	1:B:280:ILE:HG21	2.03	0.40
3:B:1002:IPE:O1B	3:B:1002:IPE:O1A	2.39	0.40
1:B:216:TYR:CE2	1:B:220:LYS:HG2	2.56	0.40
1:A:116:MET:HE2	1:B:116:MET:SD	2.62	0.40

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	291/340 (86%)	285 (98%)	6 (2%)	0	100	100
1	B	287/340 (84%)	277 (96%)	9 (3%)	1 (0%)	44	39
All	All	578/680 (85%)	562 (97%)	15 (3%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	VAL

### 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	279/317 (88%)	268 (96%)	11 (4%)	37	34
1	B	277/317 (87%)	270 (98%)	7 (2%)	53	53
All	All	556/634 (88%)	538 (97%)	18 (3%)	44	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	A	124	THR
1	A	140	LEU
1	A	143	LEU
1	A	178	LEU
1	A	181	LEU
1	A	195	HIS
1	A	230	PHE
1	A	258	GLN
1	A	273	LYS
1	A	281	GLN
1	B	6	MET
1	B	90	ARG
1	B	92	GLN
1	B	140	LEU
1	B	143	LEU
1	B	147	GLN
1	B	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	52	ASN
1	A	56	ASN
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	85	ASN
1	A	96	HIS
1	A	130	HIS
1	A	137	ASN
1	A	144	HIS
1	A	197	HIS
1	A	204	ASN
1	A	211	GLN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	A	298	ASN
1	B	52	ASN
1	B	56	ASN
1	B	73	HIS
1	B	74	ASN
1	B	96	HIS
1	B	121	GLN
1	B	131	ASN
1	B	137	ASN
1	B	144	HIS
1	B	147	GLN
1	B	204	ASN
1	B	281	GLN
1	B	288	ASN
1	B	298	ASN
1	B	299	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1001	-	12,13,13	2.66	4 (33%)	12,19,19	0.79	0
4	FPS	A	1201	2	20,23,23	1.96	8 (40%)	23,31,31	1.35	4 (17%)
3	IPE	B	1002	-	12,13,13	2.64	4 (33%)	12,19,19	0.85	0
4	FPS	B	1202	2	20,23,23	1.97	8 (40%)	23,31,31	1.70	4 (17%)

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	1001	-	-	0/13/13/13	0/0/0/0
4	FPS	A	1201	2	-	0/19/25/25	0/0/0/0
3	IPE	B	1002	-	-	0/13/13/13	0/0/0/0
4	FPS	B	1202	2	-	0/19/25/25	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1202	FPS	PA-O2A	-3.29	1.48	1.56
4	B	1202	FPS	C11-C12	-3.27	1.39	1.50
4	B	1202	FPS	C6-C7	-3.24	1.39	1.50
4	A	1201	FPS	C11-C12	-3.23	1.39	1.50
4	A	1201	FPS	PA-O2A	-3.17	1.48	1.56
4	A	1201	FPS	C6-C7	-3.17	1.39	1.50
3	B	1002	IPE	C5-C3	-2.17	1.39	1.48
4	B	1202	FPS	C1-C2	-2.16	1.39	1.48
3	A	1001	IPE	C5-C3	-2.16	1.39	1.48
4	A	1201	FPS	C1-C2	-2.12	1.39	1.48
4	A	1201	FPS	C7-C8	2.44	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1202	FPS	C7-C8	2.47	1.39	1.33
4	B	1202	FPS	C2-C3	2.49	1.39	1.33
4	A	1201	FPS	C12-C13	2.55	1.39	1.32
4	B	1202	FPS	C12-C13	2.55	1.39	1.32
4	A	1201	FPS	C2-C3	2.68	1.39	1.33
3	B	1002	IPE	PA-O1A	2.80	1.61	1.50
3	A	1001	IPE	PA-O1A	2.81	1.61	1.50
4	A	1201	FPS	PB-O2B	2.98	1.60	1.50
4	B	1202	FPS	PB-O2B	3.03	1.61	1.50
3	B	1002	IPE	PB-O2B	3.13	1.61	1.50
3	A	1001	IPE	PB-O2B	3.15	1.61	1.50
3	B	1002	IPE	C4-C3	7.17	1.53	1.33
3	A	1001	IPE	C4-C3	7.24	1.53	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1202	FPS	PB-O3A-PA	-3.92	119.34	132.29
4	A	1201	FPS	PB-O3A-PA	-2.92	122.66	132.29
4	B	1202	FPS	C15-C13-C14	2.19	119.70	114.60
4	A	1201	FPS	C15-C13-C14	2.21	119.75	114.60
4	A	1201	FPS	C4-C3-C5	2.32	119.31	115.29
4	A	1201	FPS	C9-C8-C10	3.13	120.72	115.29
4	B	1202	FPS	C4-C3-C5	3.49	121.34	115.29
4	B	1202	FPS	C9-C8-C10	3.60	121.54	115.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	IPE	8	0
4	A	1201	FPS	11	0
3	B	1002	IPE	10	0
4	B	1202	FPS	17	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, 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	299/340 (87%)	0.10	18 (6%) 23 27	21, 36, 77, 98	0
1	B	295/340 (86%)	0.13	12 (4%) 38 44	23, 39, 65, 85	0
All	All	594/680 (87%)	0.11	30 (5%) 29 34	21, 37, 69, 98	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	HIS	5.1
1	A	310	ASN	4.6
1	B	230	PHE	4.5
1	A	45	LEU	4.3
1	A	314	PRO	4.2
1	A	307	ASP	4.1
1	A	308	ASN	4.1
1	A	309	GLU	3.9
1	A	46	ASN	3.7
1	B	222	PHE	3.7
1	B	90	ARG	3.4
1	A	313	LEU	3.3
1	A	229	GLY	3.1
1	A	4	ASN	3.0
1	B	223	GLN	3.0
1	B	308	ASN	2.9
1	B	309	GLU	2.8
1	A	192	SER	2.6
1	A	306	ASN	2.4
1	B	126	GLU	2.4
1	A	140	LEU	2.4
1	B	171	VAL	2.3
1	B	125	LYS	2.3
1	A	305	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLY	2.2
1	A	126	GLU	2.1
1	B	46	ASN	2.1
1	B	44	ARG	2.1
1	B	56	ASN	2.1
1	A	221	ASP	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, 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	MG	B	1304	1/1	0.91	0.25	3.75	23,23,23,23	0
4	FPS	B	1202	24/24	0.90	0.24	2.32	47,63,69,69	0
3	IPE	A	1001	14/14	0.88	0.21	1.29	75,79,81,81	0
2	MG	A	1301	1/1	0.95	0.19	1.07	14,14,14,14	0
4	FPS	A	1201	24/24	0.92	0.19	0.91	40,48,59,61	0
2	MG	B	1303	1/1	0.89	0.11	0.32	32,32,32,32	0
2	MG	A	1302	1/1	0.97	0.11	0.00	29,29,29,29	0
3	IPE	B	1002	14/14	0.90	0.17	-0.09	86,87,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.