



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:24 pm BST

PDB ID : 2E90  
Title : S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with magnesium, pyrophosphate and FPP  
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 : 2007-01-24  
Resolution : 2.55 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

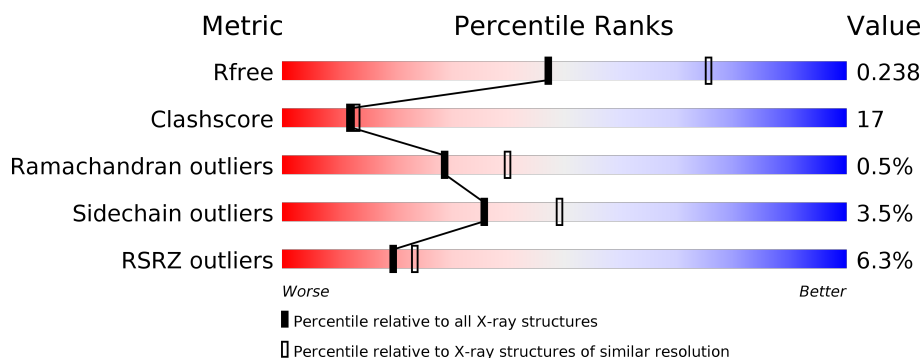
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 respectively. 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>6%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	340	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>11%</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
4	FPP	B	1102	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5313 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	1562	413	455	10			
1	B	304	Total	C	N	O	S	0	0	0
			2485	1595	423	457	10			

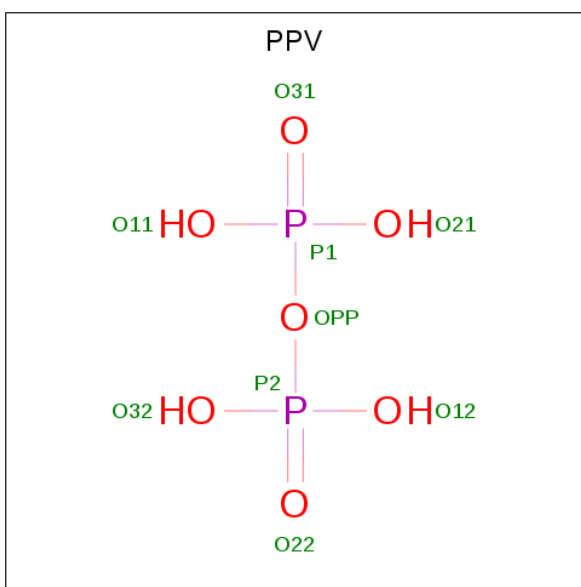
There are 10 discrepancies between the modelled and reference sequences:

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).

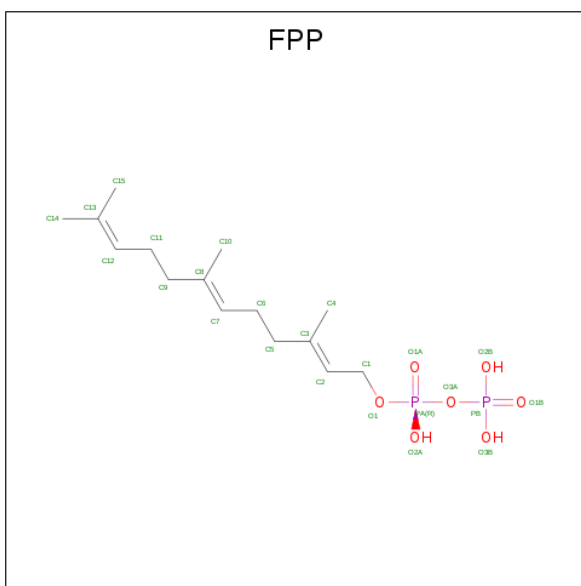
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PYROPHOSPHATE (three-letter code: PPV) (formula: H<sub>4</sub>O<sub>7</sub>P<sub>2</sub>).



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

- Molecule 4 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula:  $C_{15}H_{28}O_7P_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	P	0
			24	15	7	2	
4	B	1	Total	C	O	P	0
			24	15	7	2	

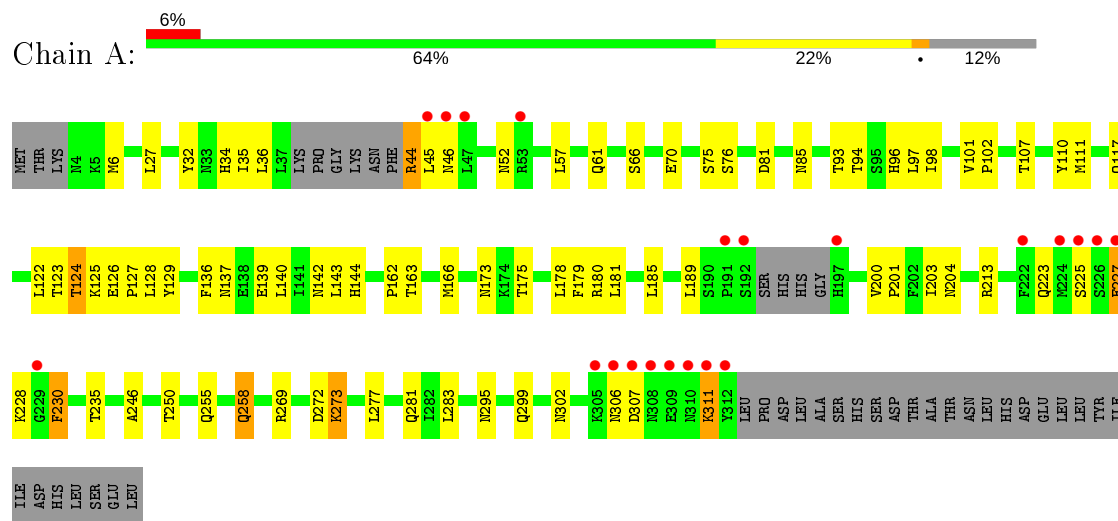
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total 168	O 168	0	0
5	B	150	Total 150	O 150	0	0

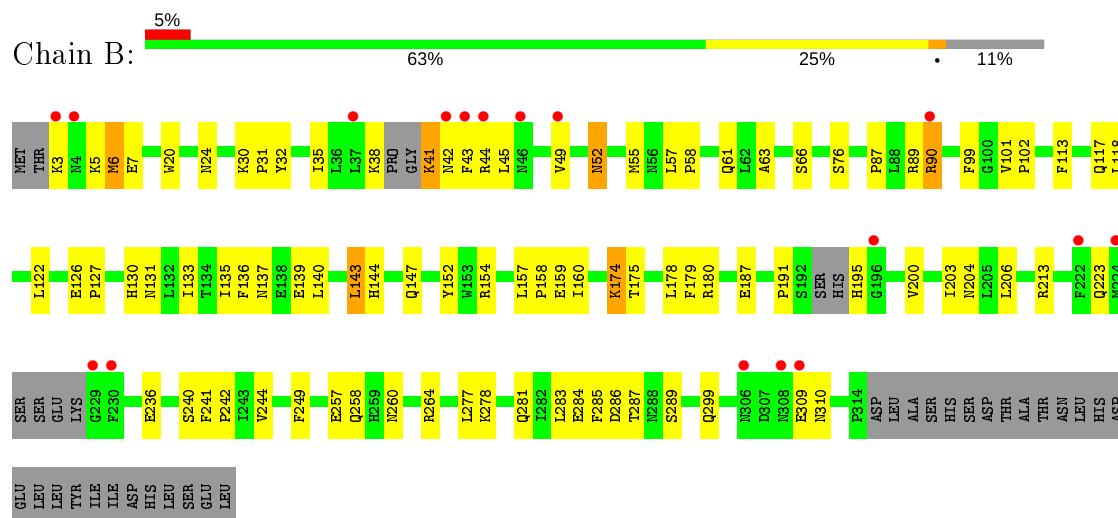
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, $\alpha$ , $\beta$ , $\gamma$	45.77Å 115.94Å 126.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.14 – 2.55 34.14 – 2.56	Depositor EDS
% Data completeness (in resolution range)	93.5 (34.14-2.55) 94.0 (34.14-2.56)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.185 , 0.239 0.181 , 0.238	Depositor DCC
$R_{free}$ test set	1040 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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, FPP, PPV

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	0.53	0/2482	0.67	0/3358
1	B	0.52	0/2529	0.67	0/3419
All	All	0.52	0/5011	0.67	0/6777

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

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	2483	94	0
1	B	2485	0	2535	87	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	1	0
4	A	24	0	25	4	0
4	B	24	0	25	14	0
5	A	168	0	0	5	0
5	B	150	0	0	4	0
All	All	5313	0	5068	173	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 17.

All (173) 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:299:GLN:HE21	1:B:3:LYS:HD3	1.17	1.09
1:A:163:THR:H	1:A:166:MET:HE3	1.19	1.08
1:B:143:LEU:HD21	4:B:1102:FPP:H92	1.47	0.96
1:B:143:LEU:HD11	4:B:1102:FPP:H7	1.47	0.96
1:A:123:THR:HG22	1:A:125:LYS:H	1.31	0.93
1:A:52:ASN:HD21	1:A:57:LEU:H	1.09	0.93
1:B:180:ARG:HH11	1:B:204:ASN:HD21	1.17	0.92
1:B:52:ASN:HD21	1:B:57:LEU:H	1.14	0.90
1:A:258:GLN:N	1:A:258:GLN:HE21	1.69	0.90
1:B:213:ARG:HD3	5:B:559:HOH:O	1.75	0.87
1:A:123:THR:HG21	1:A:128:LEU:HD23	1.54	0.87
1:A:258:GLN:NE2	1:A:258:GLN:H	1.73	0.86
1:A:258:GLN:HE21	1:A:258:GLN:H	0.88	0.83
1:B:55:MET:HE1	1:B:187:GLU:HG2	1.61	0.80
1:A:273:LYS:H	1:A:273:LYS:CD	1.92	0.80
1:A:272:ASP:HA	1:A:273:LYS:HE3	1.62	0.80
1:B:38:LYS:HE2	3:B:1002:PPV:O12	1.82	0.79
1:A:52:ASN:ND2	1:A:57:LEU:H	1.81	0.78
1:B:180:ARG:HH11	1:B:204:ASN:ND2	1.82	0.76
1:A:163:THR:N	1:A:166:MET:HE3	1.97	0.76
1:B:143:LEU:HD21	4:B:1102:FPP:C9	2.16	0.75
1:A:44:ARG:O	1:A:46:ASN:N	2.20	0.75
1:A:299:GLN:NE2	1:B:3:LYS:HD3	1.98	0.74
1:B:52:ASN:ND2	1:B:57:LEU:H	1.86	0.72
1:B:147:GLN:HA	1:B:147:GLN:HE21	1.55	0.71
1:A:52:ASN:HD21	1:A:57:LEU:N	1.88	0.71
1:B:89:ARG:HH11	1:B:90:ARG:HH21	1.38	0.71
1:B:159:GLU:HG2	1:B:160:ILE:HG13	1.73	0.70
1:B:157:LEU:HD12	1:B:158:PRO:HA	1.73	0.70
1:A:123:THR:CG2	1:A:128:LEU:HD23	2.22	0.69
1:A:175:THR:HG22	1:A:179:PHE:HE2	1.57	0.69
1:A:225:SER:HB3	1:A:228:LYS:HD3	1.75	0.69
1:B:55:MET:HE2	1:B:187:GLU:HA	1.77	0.67
1:A:6:MET:HE1	1:B:299:GLN:CB	2.25	0.66
1:B:258:GLN:HG2	1:B:286:ASP:OD2	1.95	0.66
1:B:126:GLU:HA	1:B:126:GLU:OE2	1.95	0.66
1:A:6:MET:HE1	1:B:299:GLN:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:H	1:A:273:LYS:CE	2.09	0.65
1:B:41:LYS:HE2	5:B:688:HOH:O	1.96	0.65
1:B:143:LEU:HD11	4:B:1102:FPP:H12	1.79	0.65
1:A:273:LYS:H	1:A:273:LYS:HE3	1.61	0.65
1:B:45:LEU:HD11	5:B:462:HOH:O	1.98	0.64
1:A:180:ARG:HH11	1:A:204:ASN:HD21	1.43	0.64
4:B:1102:FPP:H7	4:B:1102:FPP:H12	1.80	0.64
1:A:299:GLN:CB	1:B:6:MET:HE3	2.28	0.64
1:B:143:LEU:HD13	4:B:1102:FPP:H142	1.79	0.64
1:B:174:LYS:HE3	4:B:1102:FPP:H42	1.80	0.64
1:A:44:ARG:NH1	5:A:424:HOH:O	2.31	0.63
1:B:41:LYS:HD3	1:B:43:PHE:HB2	1.79	0.63
1:A:307:ASP:OD1	1:A:311:LYS:HG2	1.98	0.63
1:B:140:LEU:O	1:B:144:HIS:HD2	1.82	0.62
1:A:225:SER:C	1:A:227:GLU:H	2.02	0.62
1:A:66:SER:O	1:A:70:GLU:HG2	2.01	0.61
1:B:147:GLN:HA	1:B:147:GLN:NE2	2.14	0.61
1:A:123:THR:HG22	1:A:124:THR:H	1.65	0.61
1:A:94:THR:HG23	5:A:515:HOH:O	2.01	0.61
1:B:41:LYS:HG2	1:B:43:PHE:H	1.66	0.60
1:B:52:ASN:HD21	1:B:57:LEU:N	1.93	0.60
1:B:89:ARG:HH11	1:B:90:ARG:NH2	1.97	0.60
1:A:122:LEU:HD13	1:A:189:LEU:HD11	1.82	0.59
1:A:225:SER:HB3	1:A:228:LYS:CG	2.33	0.59
1:A:123:THR:HG22	1:A:124:THR:N	2.18	0.59
4:B:1102:FPP:H12	4:B:1102:FPP:C7	2.32	0.58
1:A:81:ASP:HB3	1:A:94:THR:HG21	1.86	0.57
1:B:143:LEU:HD21	4:B:1102:FPP:C11	2.35	0.57
1:A:162:PRO:HA	1:A:166:MET:HE1	1.86	0.57
1:B:55:MET:CE	1:B:187:GLU:HA	2.34	0.56
1:A:139:GLU:OE2	1:A:139:GLU:HA	2.05	0.56
1:A:27:LEU:HD22	1:B:152:TYR:CZ	2.41	0.56
1:B:45:LEU:O	1:B:49:VAL:HG23	2.06	0.56
1:A:175:THR:O	1:A:179:PHE:HD2	1.89	0.56
1:B:38:LYS:HB3	1:B:38:LYS:NZ	2.20	0.55
1:A:180:ARG:HD3	1:A:204:ASN:HD21	1.72	0.55
1:B:240:SER:O	1:B:244:VAL:HG23	2.07	0.55
1:B:147:GLN:CA	1:B:147:GLN:HE21	2.16	0.55
1:B:3:LYS:O	1:B:7:GLU:HG3	2.07	0.55
1:A:180:ARG:HH11	1:A:204:ASN:ND2	2.05	0.54
1:A:225:SER:HB3	1:A:228:LYS:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASN:O	1:A:306:ASN:HB2	2.09	0.53
1:B:41:LYS:HG2	1:B:42:ASN:N	2.24	0.53
1:A:250:THR:HG22	1:A:255:GLN:NE2	2.23	0.53
1:B:101:VAL:HB	1:B:102:PRO:HD3	1.91	0.53
1:A:227:GLU:HG3	5:A:563:HOH:O	2.09	0.52
1:B:203:ILE:HD12	1:B:206:LEU:HD23	1.92	0.52
1:A:299:GLN:HB3	1:B:6:MET:HE3	1.91	0.52
1:B:249:PHE:CD2	1:B:287:THR:HG22	2.45	0.52
1:B:139:GLU:HA	1:B:139:GLU:OE2	2.10	0.51
1:A:94:THR:CG2	1:A:96:HIS:CD2	2.94	0.51
1:A:140:LEU:HD13	1:B:113:PHE:CE2	2.46	0.51
1:A:299:GLN:HB2	1:B:6:MET:HE3	1.93	0.51
1:B:87:PRO:HD2	5:B:710:HOH:O	2.11	0.51
1:A:75:SER:OG	1:A:111:MET:HB2	2.11	0.50
1:A:162:PRO:HA	1:A:166:MET:CE	2.41	0.50
1:B:20:TRP:CH2	1:B:24:ASN:HB3	2.47	0.50
1:A:140:LEU:HA	1:A:143:LEU:HD12	1.92	0.50
1:B:131:ASN:O	1:B:135:ILE:HG13	2.12	0.50
1:A:273:LYS:N	1:A:273:LYS:CD	2.70	0.50
1:A:273:LYS:H	1:A:273:LYS:HD3	1.73	0.49
1:B:200:VAL:O	1:B:203:ILE:HG22	2.12	0.49
1:A:101:VAL:N	1:A:102:PRO:CD	2.75	0.49
1:B:143:LEU:HD23	1:B:144:HIS:CD2	2.48	0.49
1:A:230:PHE:CD2	1:A:230:PHE:N	2.81	0.48
1:A:225:SER:CB	1:A:228:LYS:HD3	2.41	0.48
1:B:32:TYR:O	1:B:35:ILE:HG22	2.14	0.48
1:B:55:MET:O	1:B:191:PRO:HD2	2.13	0.48
1:B:143:LEU:HD11	4:B:1102:FPP:C12	2.43	0.48
1:B:61:GLN:NE2	1:B:122:LEU:O	2.46	0.47
1:A:295:ASN:HD21	1:B:3:LYS:NZ	2.12	0.47
1:A:213:ARG:NH1	5:A:698:HOH:O	2.47	0.47
1:A:93:THR:HB	1:A:98:ILE:HD11	1.95	0.47
1:B:30:LYS:HB3	1:B:99:PHE:CE2	2.48	0.47
1:A:126:GLU:HB2	1:A:127:PRO:HD3	1.96	0.47
1:A:277:LEU:O	1:A:281:GLN:HG2	2.13	0.47
1:A:94:THR:HG21	1:A:96:HIS:CD2	2.49	0.47
1:A:163:THR:HG23	1:A:166:MET:CE	2.45	0.47
1:A:175:THR:HG22	1:A:179:PHE:CE2	2.43	0.47
1:A:200:VAL:HB	1:A:201:PRO:HD3	1.96	0.47
1:B:278:LYS:O	1:B:281:GLN:HG2	2.14	0.47
1:B:63:ALA:O	1:B:66:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:H	1:A:166:MET:CE	2.07	0.46
1:A:136:PHE:CE2	1:A:140:LEU:HD12	2.50	0.46
1:B:58:PRO:HG2	1:B:61:GLN:HB2	1.97	0.46
4:B:1102:FPP:O2B	4:B:1102:FPP:C1	2.64	0.46
1:B:241:PHE:HB3	1:B:242:PRO:HD3	1.96	0.46
1:A:181:LEU:O	1:A:181:LEU:HD12	2.16	0.46
1:A:137:ASN:HD21	1:B:117:GLN:CA	2.29	0.46
1:A:143:LEU:HD13	4:A:1101:FPP:H142	1.98	0.45
1:A:140:LEU:O	1:A:144:HIS:HD2	1.99	0.45
1:B:260:ASN:O	1:B:264:ARG:HG3	2.16	0.45
1:A:101:VAL:HB	1:A:102:PRO:HD3	1.99	0.45
1:A:129:TYR:CE2	1:B:130:HIS:CD2	3.05	0.45
1:A:142:ASN:O	1:A:173:ASN:HB3	2.17	0.45
1:A:225:SER:C	1:A:227:GLU:N	2.69	0.45
1:B:175:THR:O	1:B:179:PHE:HD2	2.00	0.45
1:B:154:ARG:HD2	1:B:236:GLU:O	2.16	0.45
1:B:76:SER:CB	4:B:1102:FPP:C12	2.95	0.45
1:A:223:GLN:HE21	1:A:281:GLN:HE22	1.65	0.44
1:A:94:THR:CG2	1:A:96:HIS:HD2	2.29	0.44
1:B:133:ILE:HD13	1:B:133:ILE:HA	1.85	0.44
1:B:5:LYS:HA	1:B:5:LYS:HD2	1.67	0.44
1:A:32:TYR:O	1:A:35:ILE:HG22	2.17	0.44
1:A:117:GLN:N	1:B:137:ASN:HD21	2.16	0.44
1:B:38:LYS:HB3	1:B:38:LYS:HZ2	1.81	0.44
1:A:225:SER:HB3	1:A:228:LYS:HG3	1.98	0.43
1:B:30:LYS:HB2	1:B:31:PRO:HD3	2.00	0.43
1:B:76:SER:HB3	4:B:1102:FPP:C12	2.48	0.43
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.80	0.43
1:A:181:LEU:HD12	1:A:185:LEU:HG	2.00	0.43
1:A:235:THR:O	1:A:269:ARG:HA	2.19	0.43
1:B:41:LYS:HD2	1:B:44:ARG:N	2.34	0.43
1:B:136:PHE:CE2	1:B:140:LEU:HD12	2.53	0.43
1:B:283:LEU:HG	1:B:289:SER:HB2	2.01	0.43
1:A:140:LEU:HD21	4:A:1101:FPP:H153	2.01	0.42
4:A:1101:FPP:H12	4:A:1101:FPP:C7	2.50	0.42
1:A:246:ALA:HB2	1:A:283:LEU:HD22	2.02	0.42
1:B:309:GLU:O	1:B:310:ASN:HB2	2.19	0.42
1:A:203:ILE:HD12	1:A:203:ILE:HA	1.88	0.42
1:A:94:THR:HG22	5:A:701:HOH:O	2.19	0.42
1:B:140:LEU:O	1:B:144:HIS:CD2	2.67	0.42
1:B:204:ASN:HA	1:B:204:ASN:HD22	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:HE1	1:A:93:THR:O	2.03	0.41
4:B:1102:FPP:H11	4:B:1102:FPP:O2B	2.19	0.41
1:A:302:ASN:HB3	1:A:306:ASN:HD22	1.85	0.41
1:B:52:ASN:HA	1:B:52:ASN:HD22	1.63	0.41
1:B:180:ARG:NH1	1:B:204:ASN:ND2	2.58	0.41
1:A:36:LEU:HA	1:A:36:LEU:HD23	1.87	0.41
1:B:223:GLN:HE22	1:B:284:GLU:CG	2.34	0.41
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.93	0.40
1:A:107:THR:O	1:A:110:TYR:HB3	2.21	0.40
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.37	0.40
1:A:273:LYS:N	1:A:273:LYS:HD3	2.35	0.40
1:A:140:LEU:CD2	4:A:1101:FPP:H153	2.51	0.40
1:B:285:PHE:N	1:B:285:PHE:CD2	2.87	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	293/340 (86%)	279 (95%)	13 (4%)	1 (0%)	41	51
1	B	296/340 (87%)	286 (97%)	8 (3%)	2 (1%)	22	30
All	All	589/680 (87%)	565 (96%)	21 (4%)	3 (0%)	29	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	B	174	LYS
1	B	127	PRO

### 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	280/317 (88%)	269 (96%)	11 (4%)	32	44
1	B	284/317 (90%)	275 (97%)	9 (3%)	39	53
All	All	564/634 (89%)	544 (96%)	20 (4%)	36	49

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	61	GLN
1	A	76	SER
1	A	85	ASN
1	A	124	THR
1	A	178	LEU
1	A	227	GLU
1	A	230	PHE
1	A	258	GLN
1	A	273	LYS
1	A	311	LYS
1	B	6	MET
1	B	41	LYS
1	B	52	ASN
1	B	90	ARG
1	B	143	LEU
1	B	178	LEU
1	B	195	HIS
1	B	257	GLU
1	B	277	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	52	ASN

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Mol	Chain	Res	Type
1	A	61	GLN
1	A	85	ASN
1	A	92	GLN
1	A	96	HIS
1	A	109	ASN
1	A	137	ASN
1	A	144	HIS
1	A	204	ASN
1	A	211	GLN
1	A	223	GLN
1	A	255	GLN
1	A	258	GLN
1	A	260	ASN
1	A	281	GLN
1	A	295	ASN
1	A	298	ASN
1	A	299	GLN
1	A	306	ASN
1	B	33	ASN
1	B	52	ASN
1	B	67	GLN
1	B	92	GLN
1	B	96	HIS
1	B	106	ASN
1	B	109	ASN
1	B	121	GLN
1	B	130	HIS
1	B	137	ASN
1	B	144	HIS
1	B	147	GLN
1	B	195	HIS
1	B	204	ASN
1	B	211	GLN
1	B	223	GLN
1	B	255	GLN
1	B	281	GLN
1	B	288	ASN
1	B	298	ASN

### 5.3.3 RNA ⓘ

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, 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$
4	FPP	B	1102	2	21,23,23	2.07	8 (38%)	27,31,31	1.33	5 (18%)
3	PPV	A	1001	-	6,8,8	1.89	1 (16%)	13,13,13	2.04	1 (7%)
4	FPP	A	1101	2	21,23,23	2.07	8 (38%)	27,31,31	1.35	4 (14%)
3	PPV	B	1002	-	6,8,8	1.98	1 (16%)	13,13,13	2.01	1 (7%)

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
4	FPP	B	1102	2	-	7/25/25/25	-
3	PPV	A	1001	-	-	0/6/6/6	-
4	FPP	A	1101	2	-	6/25/25/25	-
3	PPV	B	1002	-	-	0/6/6/6	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	FPP	PB-O1B	3.42	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	FPP	C6-C7	-3.38	1.39	1.50
4	B	1102	FPP	PB-O1B	3.38	1.61	1.50
3	A	1001	PPV	P2-O22	3.37	1.61	1.50
4	A	1101	FPP	C11-C12	-3.37	1.39	1.50
4	B	1102	FPP	C6-C7	-3.37	1.39	1.50
4	B	1102	FPP	C11-C12	-3.35	1.39	1.50
3	B	1002	PPV	P2-O22	3.28	1.61	1.50
4	A	1101	FPP	C1-C2	-3.27	1.39	1.49
4	B	1102	FPP	C1-C2	-3.25	1.39	1.49
4	B	1102	FPP	PA-O1A	3.00	1.61	1.50
4	A	1101	FPP	PA-O1A	2.99	1.61	1.50
4	A	1101	FPP	C7-C8	2.74	1.39	1.33
4	B	1102	FPP	C7-C8	2.73	1.39	1.33
4	A	1101	FPP	C2-C3	2.67	1.39	1.33
4	B	1102	FPP	C2-C3	2.66	1.39	1.33
4	B	1102	FPP	C12-C13	2.48	1.39	1.32
4	A	1101	FPP	C12-C13	2.48	1.39	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	PPV	P2-OPP-P1	-6.64	110.04	132.83
3	A	1001	PPV	P2-OPP-P1	-6.61	110.15	132.83
4	B	1102	FPP	PA-O3A-PB	-3.10	122.18	132.83
4	A	1101	FPP	C10-C8-C9	2.98	120.28	115.27
4	A	1101	FPP	PA-O3A-PB	-2.95	122.70	132.83
4	B	1102	FPP	C4-C3-C5	2.82	120.01	115.27
4	A	1101	FPP	C4-C3-C5	2.80	119.98	115.27
4	B	1102	FPP	C10-C8-C9	2.56	119.58	115.27
4	B	1102	FPP	C15-C13-C14	2.50	120.11	114.60
4	A	1101	FPP	C15-C13-C14	2.46	120.03	114.60
4	B	1102	FPP	O3B-PB-O3A	2.28	112.30	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1102	FPP	O1-C1-C2-C3
4	B	1102	FPP	C1-O1-PA-O3A
4	A	1101	FPP	C1-O1-PA-O3A
4	B	1102	FPP	C4-C3-C5-C6
4	B	1102	FPP	C2-C3-C5-C6

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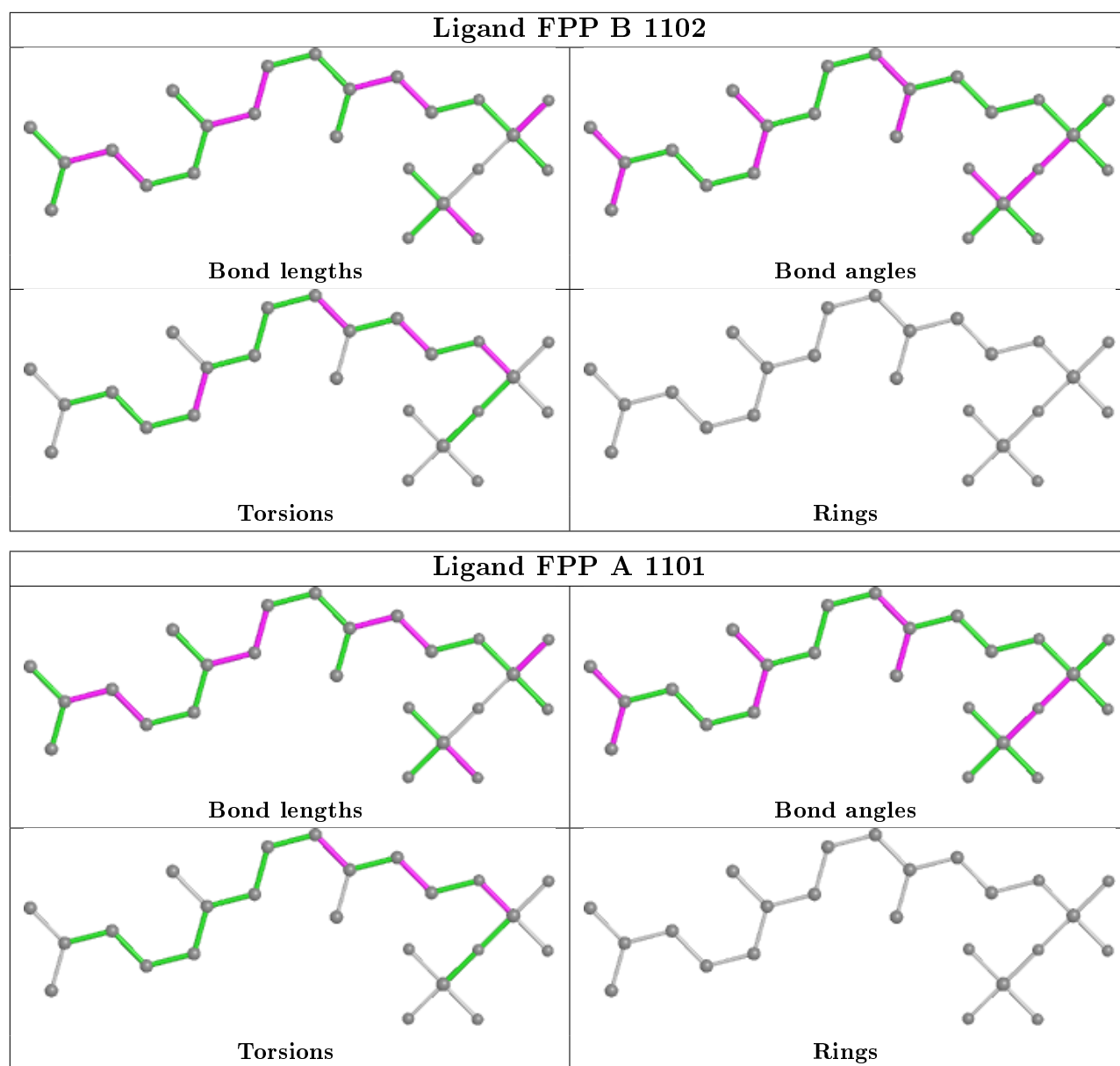
Mol	Chain	Res	Type	Atoms
4	A	1101	FPP	O1-C1-C2-C3
4	B	1102	FPP	C1-O1-PA-O1A
4	B	1102	FPP	C1-O1-PA-O2A
4	A	1101	FPP	C1-O1-PA-O1A
4	A	1101	FPP	C1-O1-PA-O2A
4	A	1101	FPP	C4-C3-C5-C6
4	A	1101	FPP	C2-C3-C5-C6
4	B	1102	FPP	C10-C8-C9-C11

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1102	FPP	14	0
4	A	1101	FPP	4	0
3	B	1002	PPV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 ⓘ

### 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%)	0.00	21 (7%) 16 19	16, 30, 80, 105	0
1	B	304/340 (89%)	-0.01	17 (5%) 24 29	15, 34, 78, 106	0
All	All	603/680 (88%)	-0.01	38 (6%) 20 23	15, 32, 78, 106	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	SER	6.8
1	A	226	SER	6.7
1	A	308	ASN	6.3
1	A	227	GLU	6.2
1	A	224	MET	5.4
1	B	3	LYS	5.2
1	B	42	ASN	5.0
1	A	309	GLU	4.7
1	B	196	GLY	4.6
1	A	310	ASN	4.3
1	A	311	LYS	3.9
1	A	312	TYR	3.9
1	B	43	PHE	3.8
1	B	230	PHE	3.5
1	B	229	GLY	3.5
1	B	224	MET	3.3
1	A	229	GLY	3.2
1	A	307	ASP	3.2
1	A	305	LYS	3.2
1	B	46	ASN	3.1
1	A	53	ARG	3.0
1	A	191	PRO	3.0
1	A	192	SER	2.9
1	B	49	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	309	GLU	2.6
1	A	306	ASN	2.5
1	B	308	ASN	2.5
1	A	222	PHE	2.5
1	B	306	ASN	2.5
1	B	222	PHE	2.4
1	B	37	LEU	2.4
1	A	46	ASN	2.3
1	B	4	ASN	2.3
1	A	47	LEU	2.3
1	A	197	HIS	2.2
1	B	44	ARG	2.2
1	A	45	LEU	2.1
1	B	90	ARG	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

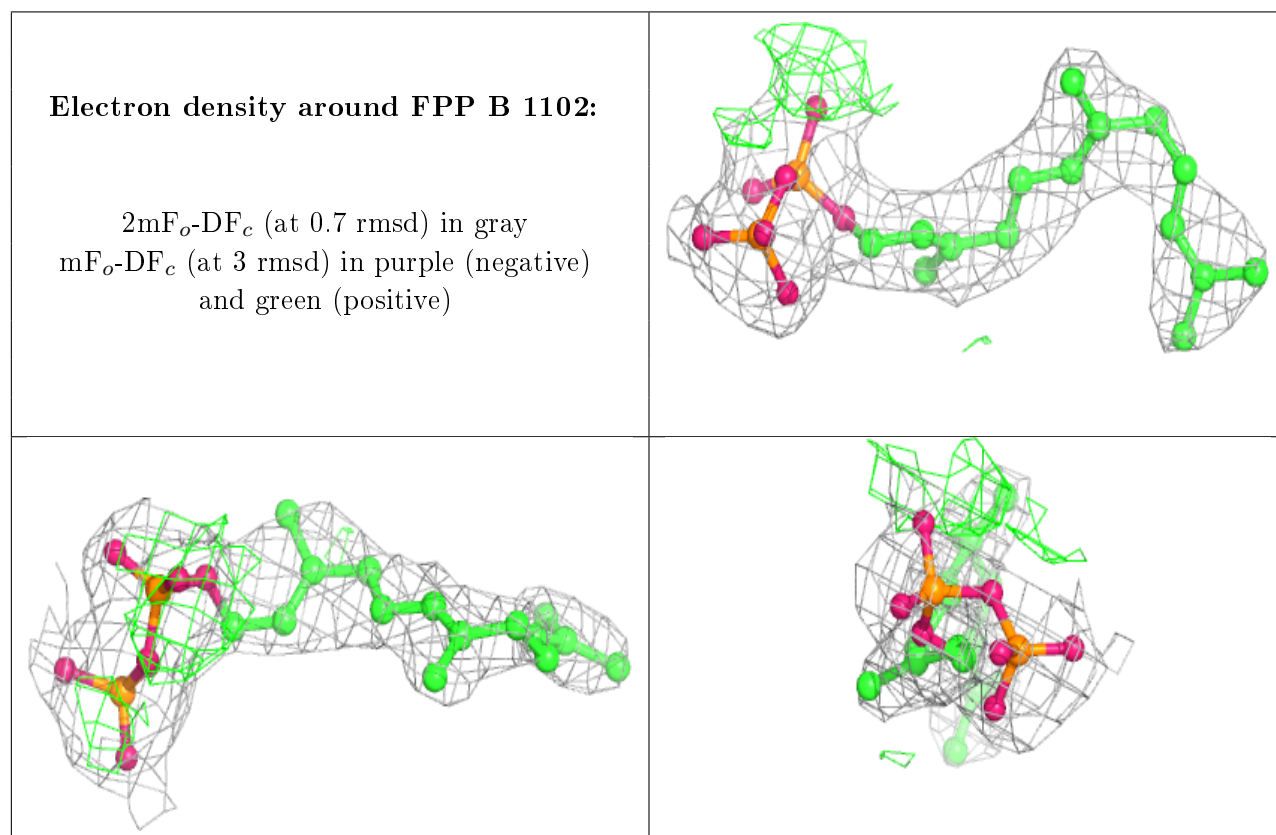
There are no carbohydrates in this entry.

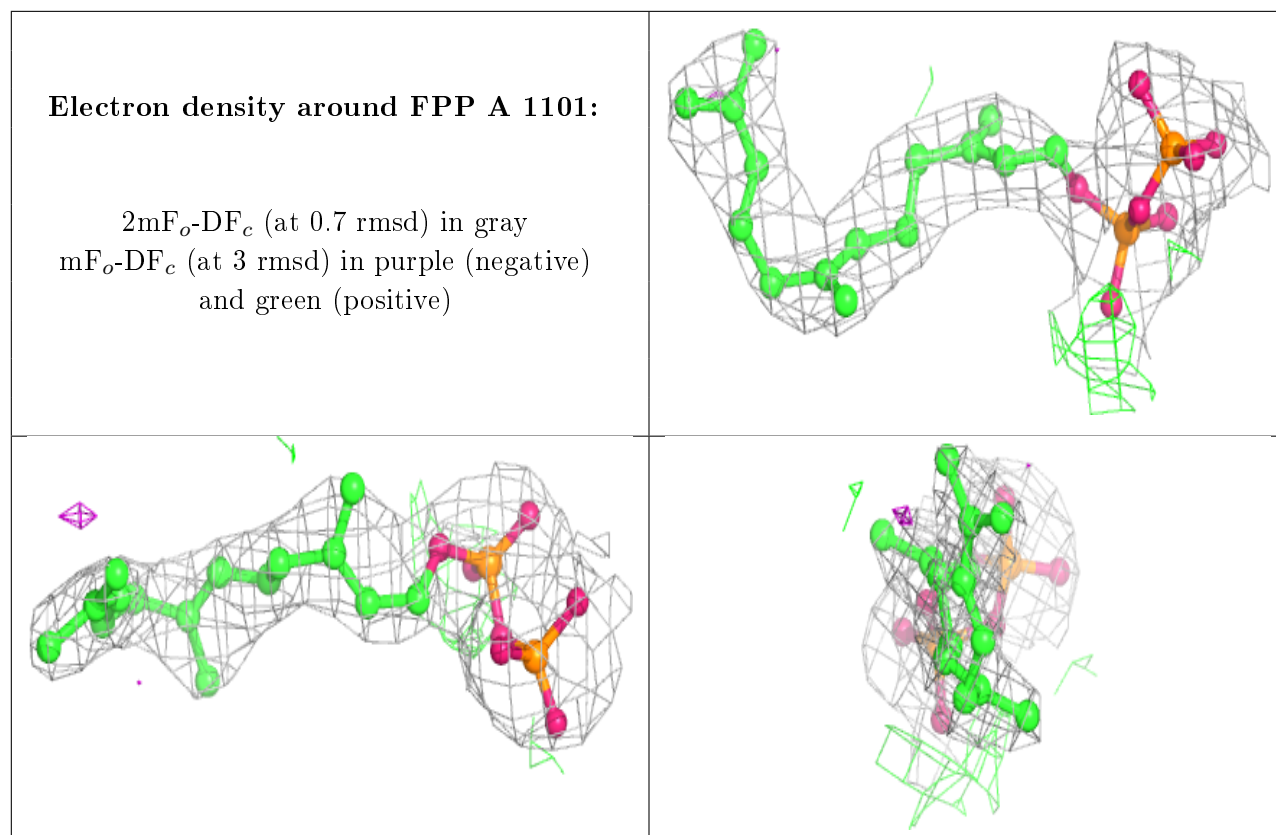
## 6.4 Ligands ⓘ

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1202	1/1	0.81	0.15	22,22,22,22	0
2	MG	B	1203	1/1	0.86	0.24	19,19,19,19	0
3	PPV	B	1002	9/9	0.89	0.20	101,102,105,105	0
3	PPV	A	1001	9/9	0.90	0.20	86,87,93,93	0
2	MG	A	1201	1/1	0.91	0.24	7,7,7,7	0
2	MG	B	1204	1/1	0.94	0.31	9,9,9,9	0
4	FPP	B	1102	24/24	0.96	0.24	41,44,47,47	0
4	FPP	A	1101	24/24	0.96	0.17	36,40,44,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.