



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 05:29 am BST

PDB ID : 3AQ0  
Title : Ligand-bound form of Arabidopsis medium/long-chain length prenyl pyrophosphate synthase (surface polar residue mutant)  
Authors : Hsieh, F.-L.; Chang, T.-H.; Ko, T.-P.; Wang, A.H.-J.  
Deposited on : 2010-10-24  
Resolution : 2.65 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

<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

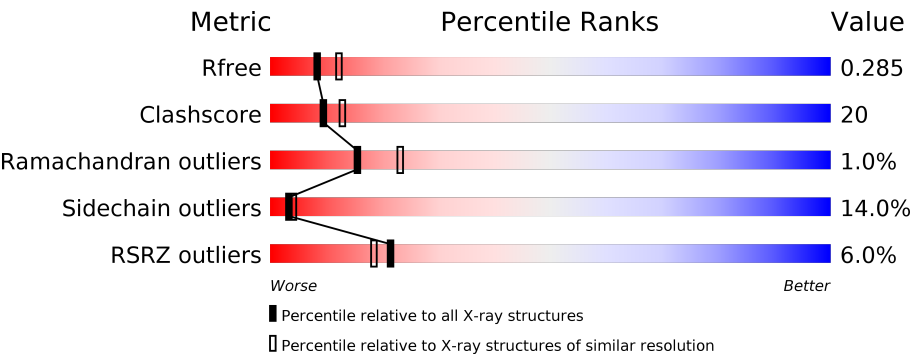
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	348	<div><div>5%</div><div><div></div><div>65%</div><div>25%</div><div>• 6%</div></div></div>
1	B	348	<div><div>5%</div><div><div></div><div>58%</div><div>25%</div><div>7%</div><div>10%</div></div></div>
1	C	348	<div><div>7%</div><div><div></div><div>64%</div><div>24%</div><div>5%</div><div>6%</div></div></div>
1	D	348	<div><div>5%</div><div><div></div><div>62%</div><div>20%</div><div>7%</div><div>• 10%</div></div></div>
1	E	348	<div><div>7%</div><div><div></div><div>66%</div><div>23%</div><div>5%</div><div>7%</div></div></div>
1	F	348	<div><div>5%</div><div><div></div><div>62%</div><div>20%</div><div>6%</div><div>• 11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	348	<div><div></div><div>3%</div><div>60%</div><div>23%</div><div>6%</div><div>10%</div></div>
1	H	348	<div><div></div><div>5%</div><div>65%</div><div>23%</div><div>5%</div><div>7%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20426 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 Geranyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2488	1563	434	479	12			
1	B	313	Total	C	N	O	S	0	0	0
			2394	1507	414	461	12			
1	C	327	Total	C	N	O	S	0	0	0
			2496	1567	434	483	12			
1	D	312	Total	C	N	O	S	0	0	0
			2388	1506	410	460	12			
1	E	325	Total	C	N	O	S	0	0	0
			2478	1556	432	478	12			
1	F	310	Total	C	N	O	S	0	0	0
			2368	1492	408	456	12			
1	G	314	Total	C	N	O	S	0	0	0
			2400	1514	415	459	12			
1	H	324	Total	C	N	O	S	0	0	0
			2471	1552	431	476	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
A	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
A	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
A	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
A	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
B	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
B	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
B	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
B	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
B	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
C	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
C	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
C	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89

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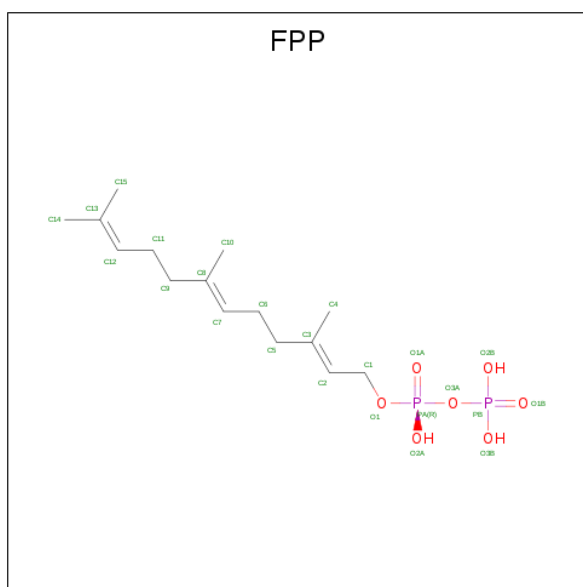
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Chain	Residue	Modelled	Actual	Comment	Reference
C	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
C	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
D	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
D	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
D	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
D	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
D	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
E	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
E	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
E	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
E	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
E	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
F	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
F	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
F	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
F	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
F	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
G	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
G	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
G	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
G	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
G	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89
H	1	GLY	-	EXPRESSION TAG	UNP Q9FT89
H	178	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
H	179	ALA	GLN	ENGINEERED MUTATION	UNP Q9FT89
H	281	ALA	GLU	ENGINEERED MUTATION	UNP Q9FT89
H	282	ALA	LYS	ENGINEERED MUTATION	UNP Q9FT89

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

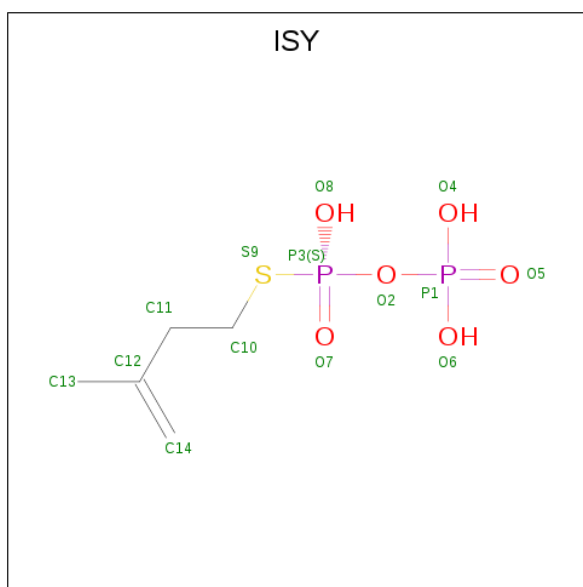
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0

- Molecule 3 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: C<sub>15</sub>H<sub>28</sub>O<sub>7</sub>P<sub>2</sub>).



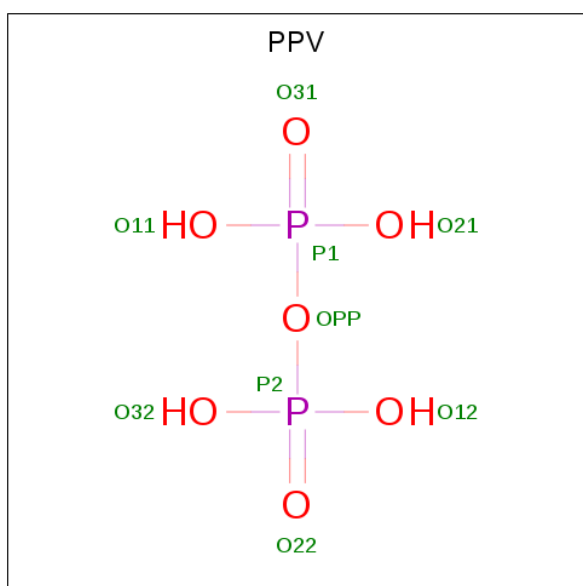
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			24	15	7	2		
3	B	1	Total	C	O	P	0	0
			24	15	7	2		
3	C	1	Total	C	O	P	0	0
			24	15	7	2		
3	E	1	Total	C	O	P	0	0
			24	15	7	2		
3	G	1	Total	C	O	P	0	0
			24	15	7	2		
3	H	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 4 is 3-methylbut-3-enylsulfanyl(phosphonoxy)phosphinic acid (three-letter code: ISY) (formula: C<sub>5</sub>H<sub>12</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
			14	5	6	2	1		
4	H	1	Total	C	O	P	S	0	0
			14	5	6	2	1		

- Molecule 5 is PYROPHOSPHATE (three-letter code: PPV) (formula:  $\text{H}_4\text{O}_7\text{P}_2$ ).



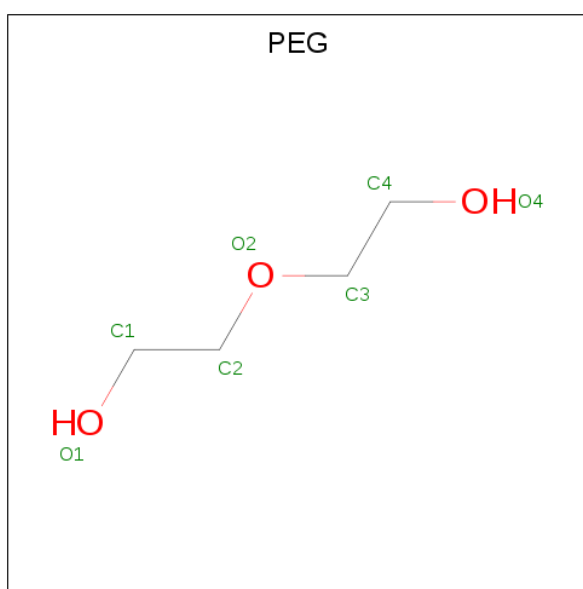
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	C	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			9	7	2		
5	E	1	Total	O	P	0	0
			9	7	2		
5	F	1	Total	O	P	0	0
			9	7	2		
5	G	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	98	Total	O	0	0
			98	98		
7	C	116	Total	O	0	0
			116	116		

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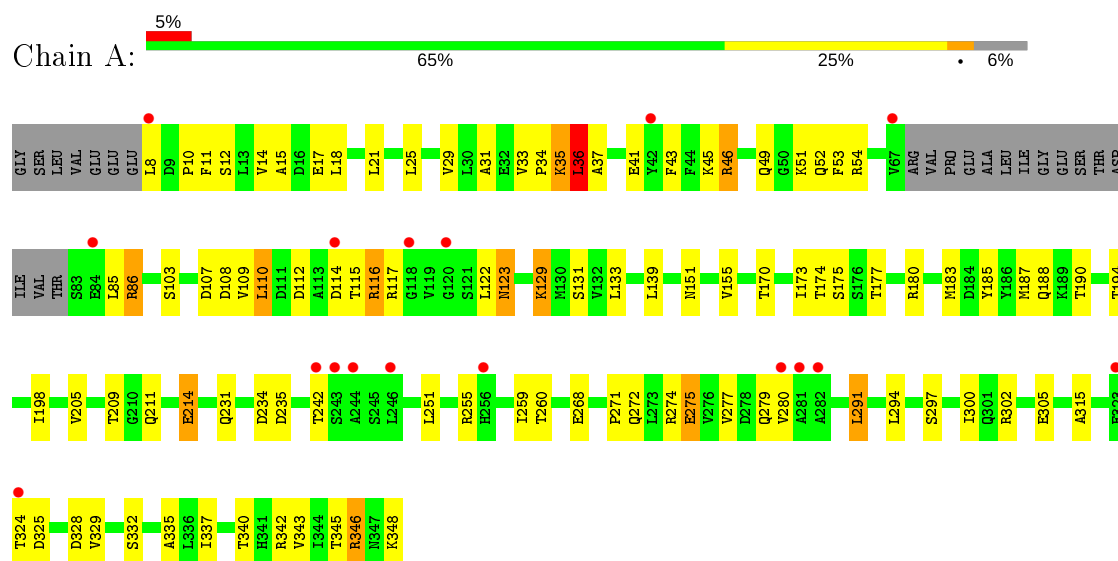
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	100	Total 100	O 100	0	0
7	E	67	Total 67	O 67	0	0
7	F	78	Total 78	O 78	0	0
7	G	77	Total 77	O 77	0	0
7	H	76	Total 76	O 76	0	0

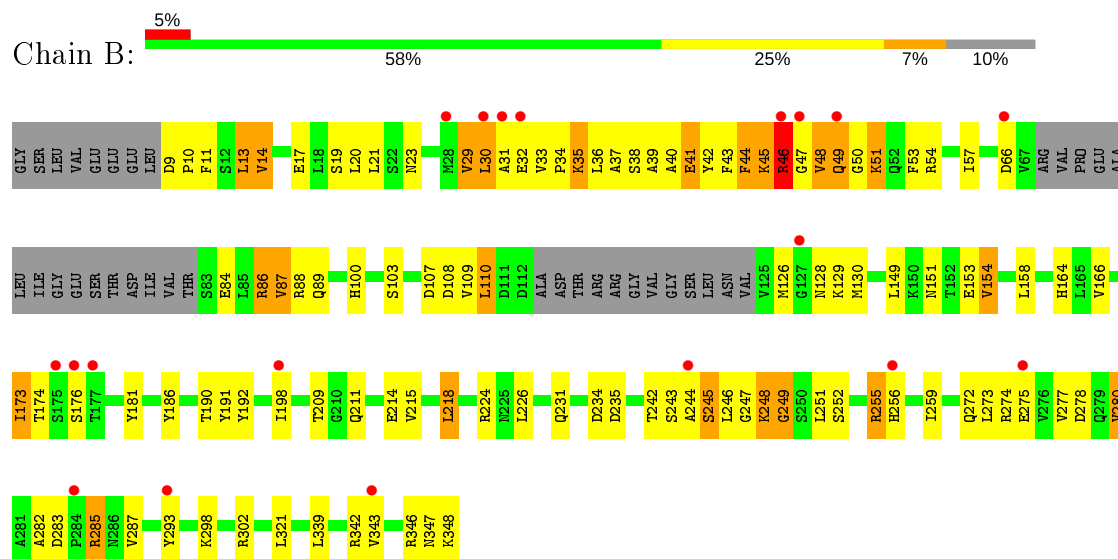
### 3 Residue-property plots [i](#)

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.

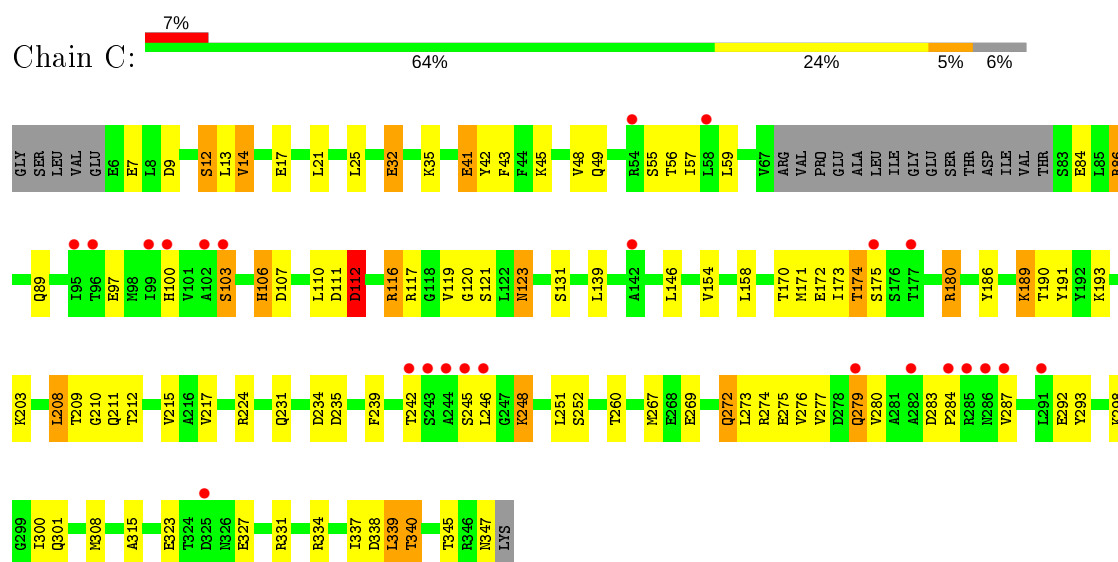
#### • Molecule 1: Geranyl diphosphate synthase



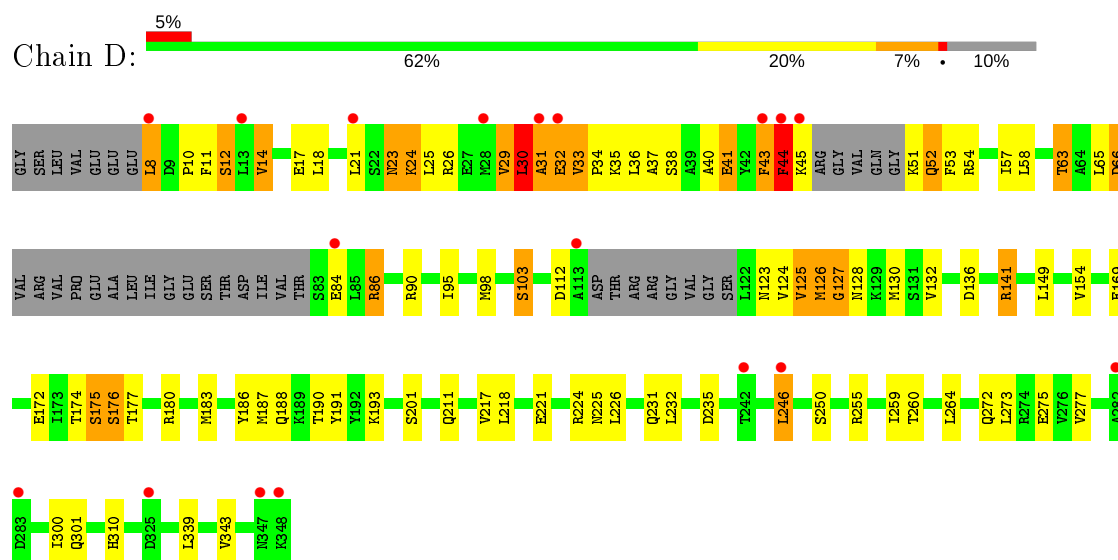
#### • Molecule 1: Geranyl diphosphate synthase



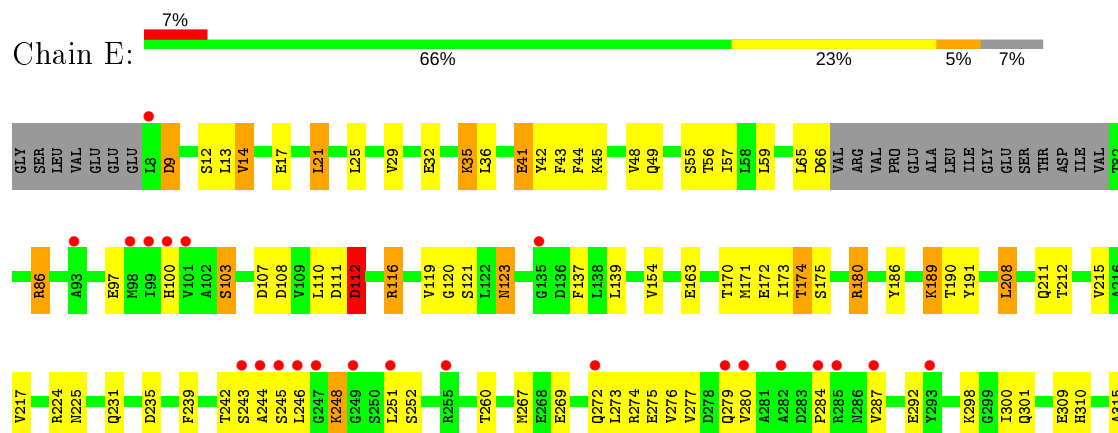
#### • Molecule 1: Geranyl diphosphate synthase



• Molecule 1: Geranyl diphosphate synthase

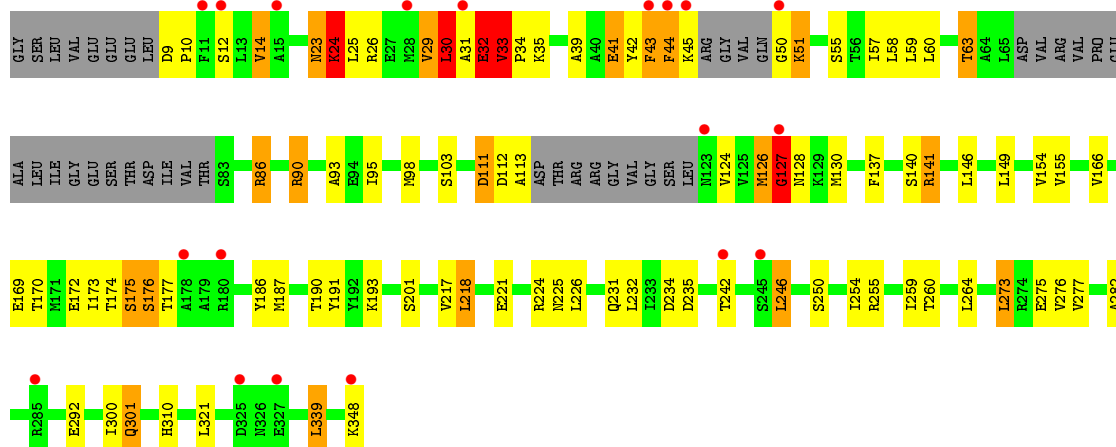


• Molecule 1: Geranyl diphosphate synthase

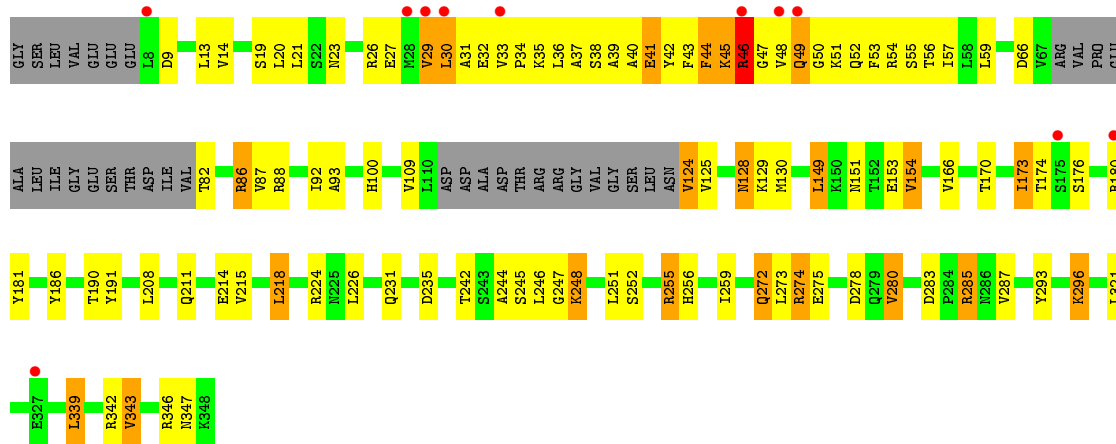




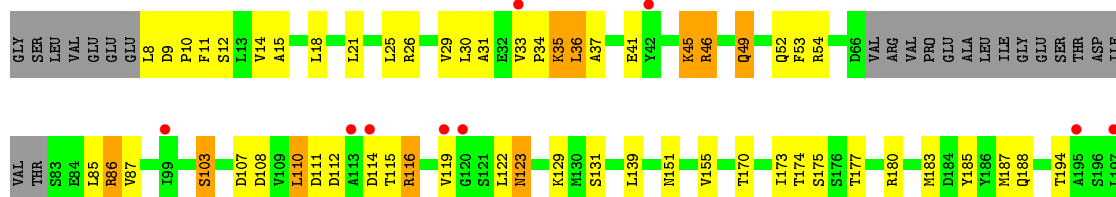
• Molecule 1: Geranyl diphosphate synthase

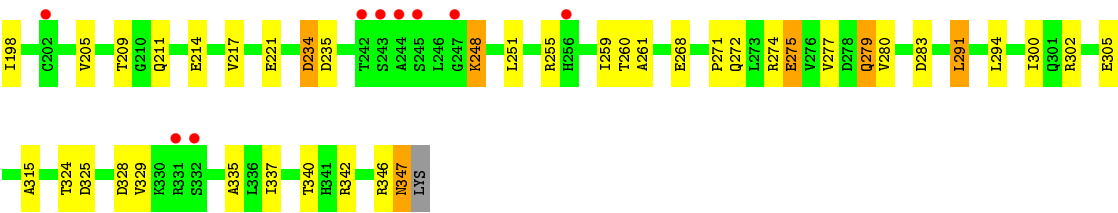


• Molecule 1: Geranyl diphosphate synthase



• Molecule 1: Geranyl diphosphate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.96Å 115.96Å 385.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.65 29.83 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.65) 98.7 (29.83-2.65)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.64Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.222 , 0.274 0.250 , 0.285	Depositor DCC
$R_{free}$ test set	4167 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 61.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.944 for H, K, L 0.056 for -H-K, K, -L	Depositor
Outliers	0 of 83457 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PPV, MG, PEG, ISY, FPP

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	0.45	0/2516	0.64	2/3399 (0.1%)
1	B	0.61	0/2421	0.70	1/3269 (0.0%)
1	C	0.56	1/2524 (0.0%)	0.68	2/3412 (0.1%)
1	D	0.53	0/2414	0.67	0/3260
1	E	0.47	1/2506 (0.0%)	0.66	1/3388 (0.0%)
1	F	0.49	0/2394	0.67	3/3232 (0.1%)
1	G	0.61	0/2427	0.71	1/3278 (0.0%)
1	H	0.42	0/2499	0.62	0/3378
All	All	0.52	2/19701 (0.0%)	0.67	10/26616 (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	B	0	1
1	D	0	2
1	F	0	1
1	G	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	VAL	CB-CG1	-6.83	1.38	1.52
1	E	217	VAL	CB-CG2	-6.45	1.39	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LEU	CA-CB-CG	6.40	130.03	115.30
1	G	149	LEU	CA-CB-CG	6.23	129.63	115.30
1	E	217	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	F	32	GLU	CB-CA-C	-6.09	98.22	110.40
1	F	127	GLY	N-CA-C	5.83	127.67	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	35	LYS	Peptide
1	D	31	ALA	Peptide
1	D	32	GLU	Peptide
1	F	32	GLU	Peptide
1	G	35	LYS	Peptide

## 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	2488	0	2546	67	2
1	B	2394	0	2446	161	0
1	C	2496	0	2545	91	0
1	D	2388	0	2442	131	0
1	E	2478	0	2531	81	0
1	F	2368	0	2419	115	0
1	G	2400	0	2465	169	0
1	H	2471	0	2524	74	2
2	A	2	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	0	0
2	H	2	0	0	0	0
3	A	24	0	25	1	0
3	B	24	0	25	6	0
3	C	24	0	25	7	0
3	E	24	0	25	2	0
3	G	24	0	25	4	0
3	H	24	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	9	3	0
4	H	14	0	9	2	0
5	B	9	0	0	3	0
5	C	9	0	0	0	0
5	D	9	0	0	0	0
5	E	9	0	0	0	0
5	F	9	0	0	0	0
5	G	9	0	0	0	0
6	B	7	0	10	1	0
6	D	7	0	10	0	0
7	A	83	0	0	5	0
7	B	98	0	0	8	0
7	C	116	0	0	5	0
7	D	100	0	0	6	0
7	E	67	0	0	0	0
7	F	78	0	0	3	0
7	G	77	0	0	5	0
7	H	76	0	0	3	0
All	All	20426	0	20106	781	2

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.

The worst 5 of 781 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:B:48:VAL:HG13	1:B:49:GLN:CA	1.34	1.55
1:G:46:ARG:HD2	1:G:49:GLN:CA	1.43	1.49
1:C:274:ARG:NH2	1:F:30:LEU:HD11	1.15	1.39
1:B:48:VAL:HG22	1:B:50:GLY:N	1.40	1.34
1:G:46:ARG:CD	1:G:49:GLN:HA	1.60	1.31

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ALA:O	1:H:46:ARG:NH1[1_665]	1.98	0.22
1:A:46:ARG:NH1	1:H:15:ALA:O[1_665]	2.19	0.01

## 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	322/348 (92%)	312 (97%)	9 (3%)	1 (0%)	41	56
1	B	307/348 (88%)	289 (94%)	15 (5%)	3 (1%)	15	23
1	C	323/348 (93%)	311 (96%)	11 (3%)	1 (0%)	41	56
1	D	304/348 (87%)	280 (92%)	14 (5%)	10 (3%)	4	4
1	E	321/348 (92%)	308 (96%)	12 (4%)	1 (0%)	41	56
1	F	302/348 (87%)	282 (93%)	14 (5%)	6 (2%)	7	10
1	G	308/348 (88%)	291 (94%)	16 (5%)	1 (0%)	41	56
1	H	320/348 (92%)	308 (96%)	11 (3%)	1 (0%)	41	56
All	All	2507/2784 (90%)	2381 (95%)	102 (4%)	24 (1%)	15	23

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	ARG
1	B	48	VAL
1	C	112	ASP
1	D	30	LEU
1	D	31	ALA

### 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	266/285 (93%)	231 (87%)	35 (13%)	4 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	256/285 (90%)	218 (85%)	38 (15%)	3	3
1	C	267/285 (94%)	226 (85%)	41 (15%)	2	3
1	D	256/285 (90%)	225 (88%)	31 (12%)	5	6
1	E	265/285 (93%)	230 (87%)	35 (13%)	4	5
1	F	253/285 (89%)	217 (86%)	36 (14%)	3	4
1	G	257/285 (90%)	221 (86%)	36 (14%)	3	4
1	H	264/285 (93%)	225 (85%)	39 (15%)	3	3
All	All	2084/2280 (91%)	1793 (86%)	291 (14%)	3	4

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	126	MET
1	E	174	THR
1	H	103	SER
1	D	175	SER
1	E	14	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	211	GLN
1	E	272	GLN
1	H	211	GLN
1	D	310	HIS
1	E	279	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	FPP	A	1002	2	21,23,23	1.98	7 (33%)	27,31,31	1.22	3 (11%)
3	FPP	G	1001	-	21,23,23	2.03	8 (38%)	27,31,31	1.52	4 (14%)
5	PPV	G	1000	-	6,8,8	2.61	4 (66%)	13,13,13	1.61	3 (23%)
5	PPV	B	1000	-	6,8,8	2.56	4 (66%)	13,13,13	1.69	3 (23%)
5	PPV	D	1000	-	6,8,8	2.67	2 (33%)	13,13,13	1.65	3 (23%)
5	PPV	F	1000	-	6,8,8	2.58	2 (33%)	13,13,13	1.57	3 (23%)
5	PPV	C	1003	-	6,8,8	2.52	2 (33%)	13,13,13	1.31	2 (15%)
6	PEG	B	1002	-	6,6,6	0.41	0	5,5,5	0.80	0
3	FPP	H	1002	2	21,23,23	2.08	8 (38%)	27,31,31	1.27	2 (7%)
5	PPV	E	1003	-	6,8,8	2.46	2 (33%)	13,13,13	1.64	3 (23%)
3	FPP	E	1002	2	21,23,23	2.00	7 (33%)	27,31,31	1.20	4 (14%)
4	ISY	H	1003	-	9,13,13	3.41	4 (44%)	11,19,19	1.87	2 (18%)
3	FPP	C	1002	2	21,23,23	2.04	9 (42%)	27,31,31	1.30	2 (7%)
4	ISY	A	1003	-	9,13,13	3.39	4 (44%)	11,19,19	2.01	2 (18%)
3	FPP	B	1001	-	21,23,23	1.99	8 (38%)	27,31,31	1.16	2 (7%)
6	PEG	D	1002	-	6,6,6	0.86	0	5,5,5	0.74	0

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	FPP	A	1002	2	-	4/25/25/25	-
3	FPP	G	1001	-	-	5/25/25/25	-
5	PPV	G	1000	-	-	0/6/6/6	-
5	PPV	B	1000	-	-	3/6/6/6	-
5	PPV	D	1000	-	-	1/6/6/6	-
5	PPV	F	1000	-	-	1/6/6/6	-
5	PPV	C	1003	-	-	0/6/6/6	-
6	PEG	B	1002	-	-	3/4/4/4	-
3	FPP	H	1002	2	-	5/25/25/25	-
5	PPV	E	1003	-	-	0/6/6/6	-
3	FPP	E	1002	2	-	3/25/25/25	-
4	ISY	H	1003	-	-	3/9/13/13	-
3	FPP	C	1002	2	-	6/25/25/25	-
4	ISY	A	1003	-	-	4/9/13/13	-
3	FPP	B	1001	-	-	3/25/25/25	-
6	PEG	D	1002	-	-	3/4/4/4	-

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1003	ISY	C14-C12	6.62	1.51	1.33
4	A	1003	ISY	C14-C12	6.41	1.51	1.33
4	A	1003	ISY	C11-C12	-6.08	1.40	1.51
4	H	1003	ISY	C11-C12	-6.00	1.40	1.51
3	G	1001	FPP	PA-O1A	4.11	1.65	1.50

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1001	FPP	PA-O3A-PB	-4.41	117.71	132.83
4	A	1003	ISY	O8-P3-O7	4.30	120.23	109.82
3	H	1002	FPP	PA-O3A-PB	-4.16	118.57	132.83
4	H	1003	ISY	O8-P3-O7	4.12	119.80	109.82
3	A	1002	FPP	PA-O3A-PB	-3.97	119.20	132.83

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1001	FPP	C1-O1-PA-O1A

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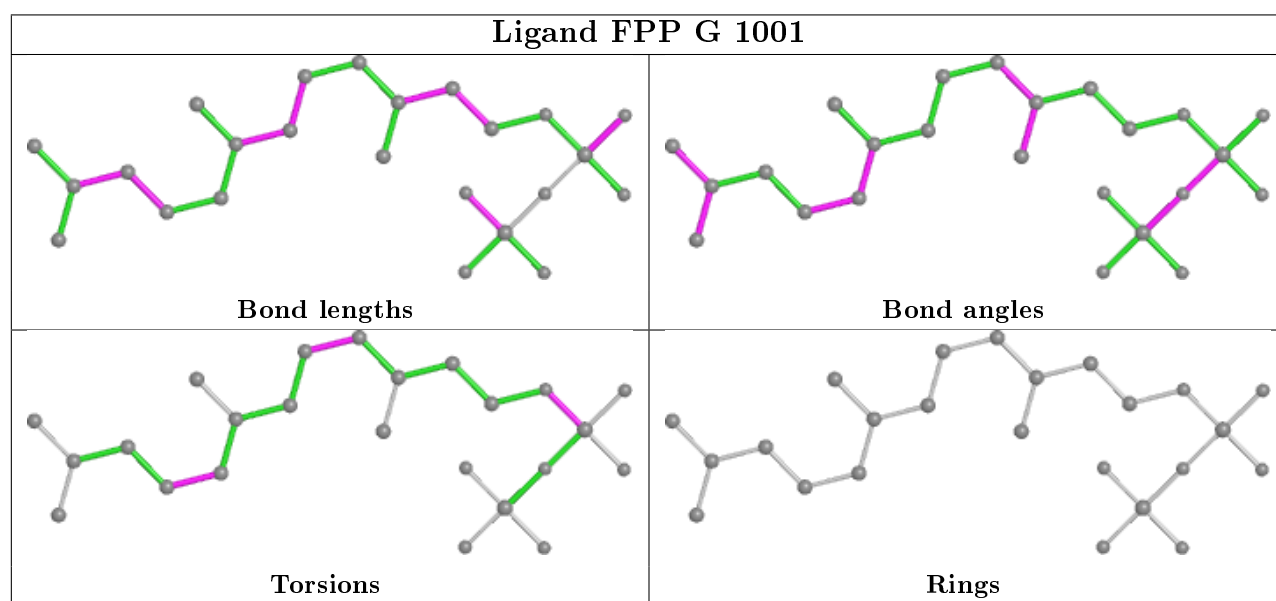
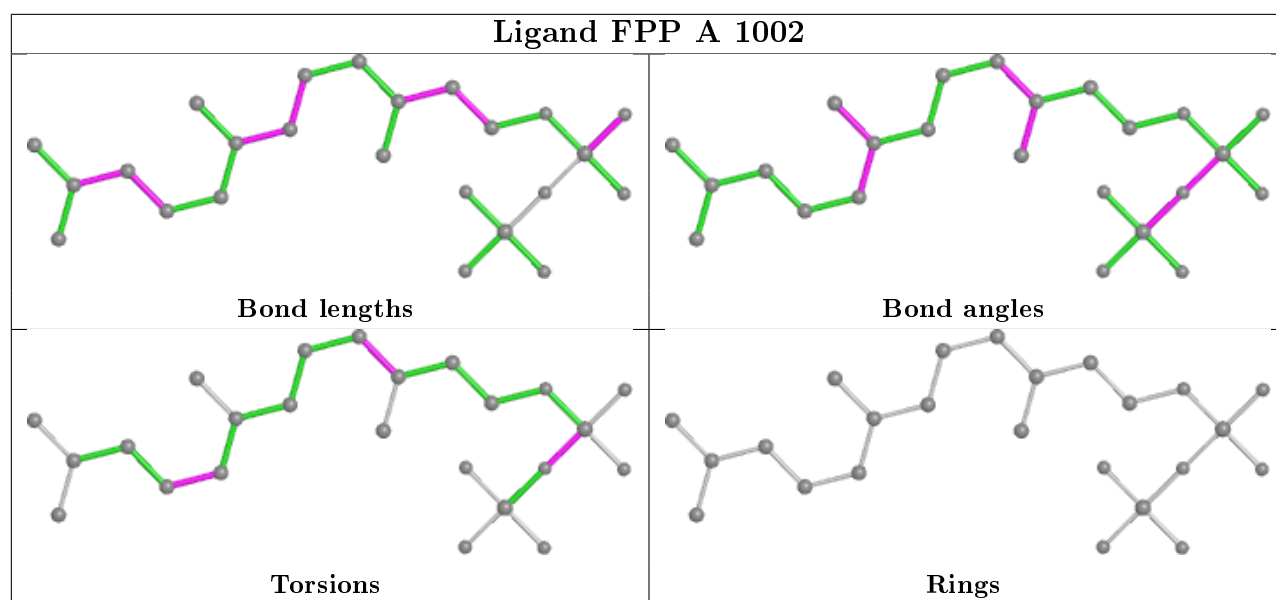
Mol	Chain	Res	Type	Atoms
3	G	1001	FPP	C1-O1-PA-O2A
4	H	1003	ISY	S9-C10-C11-C12
4	H	1003	ISY	C10-C11-C12-C13
4	H	1003	ISY	C10-C11-C12-C14

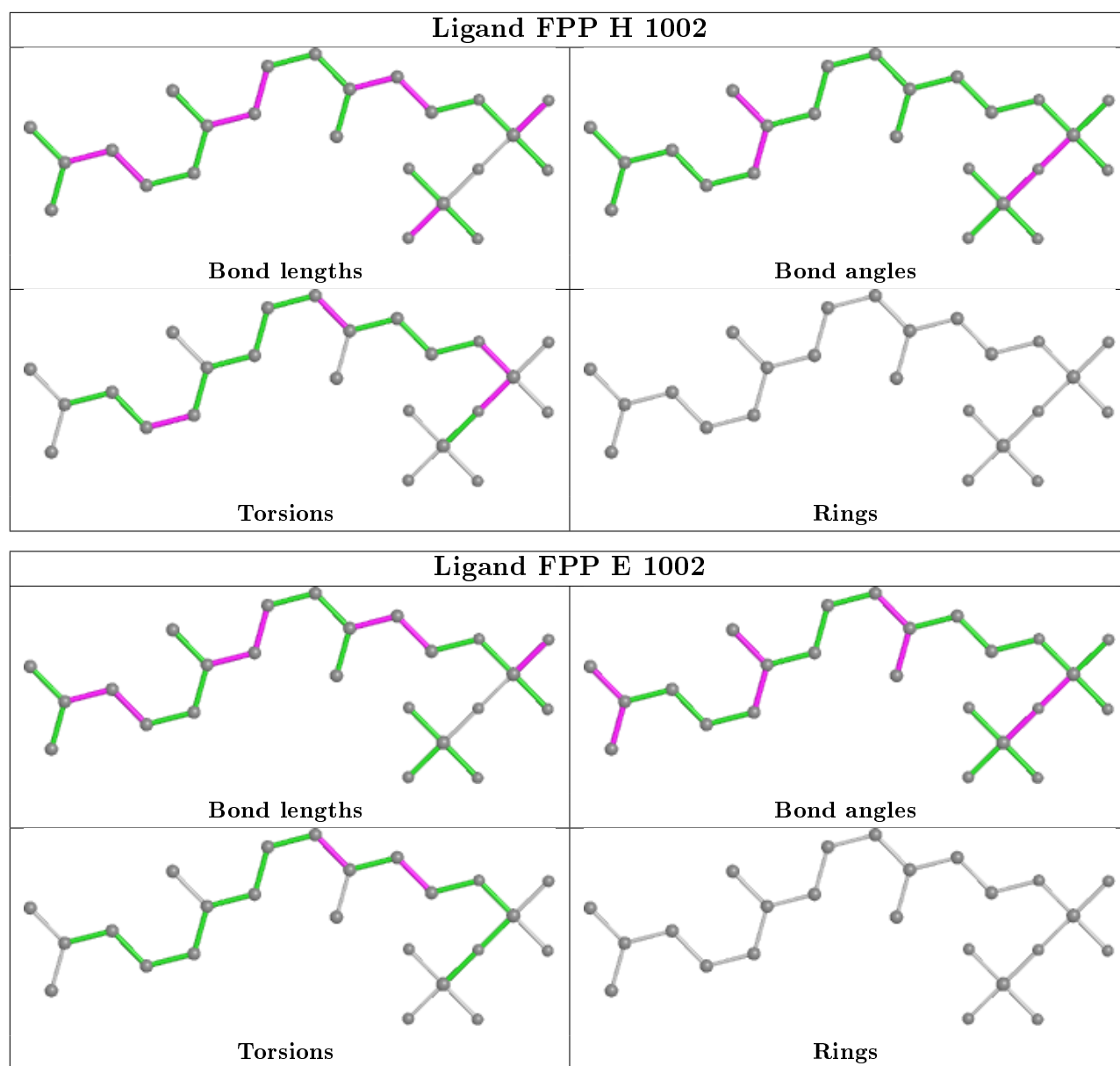
There are no ring outliers.

10 monomers are involved in 31 short contacts:

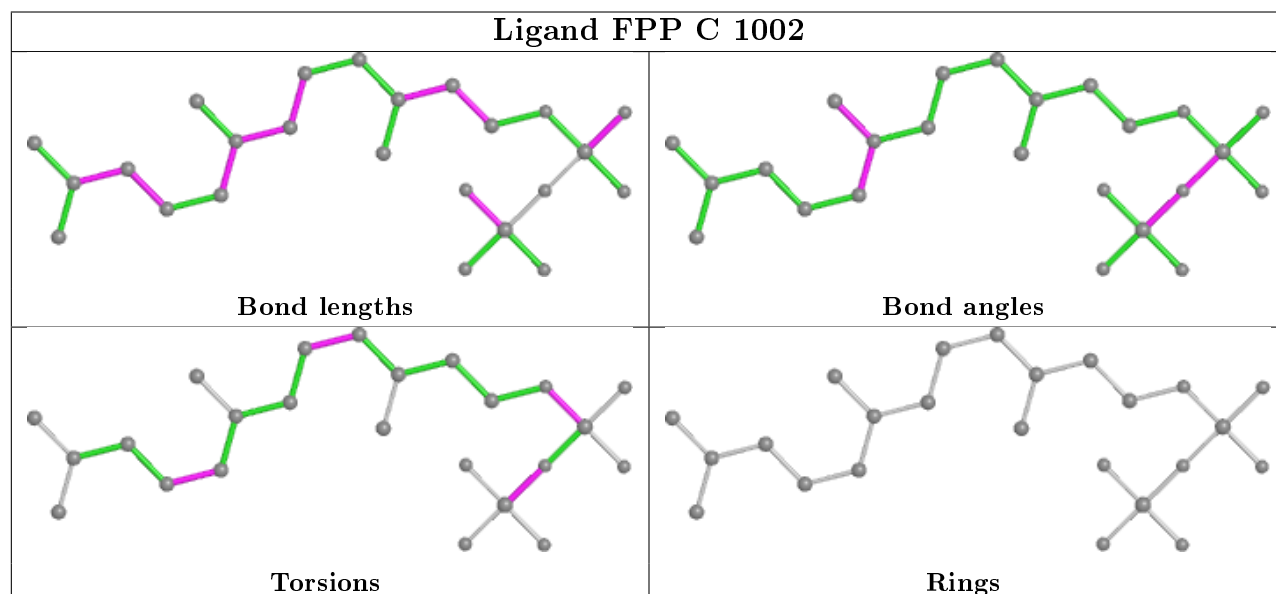
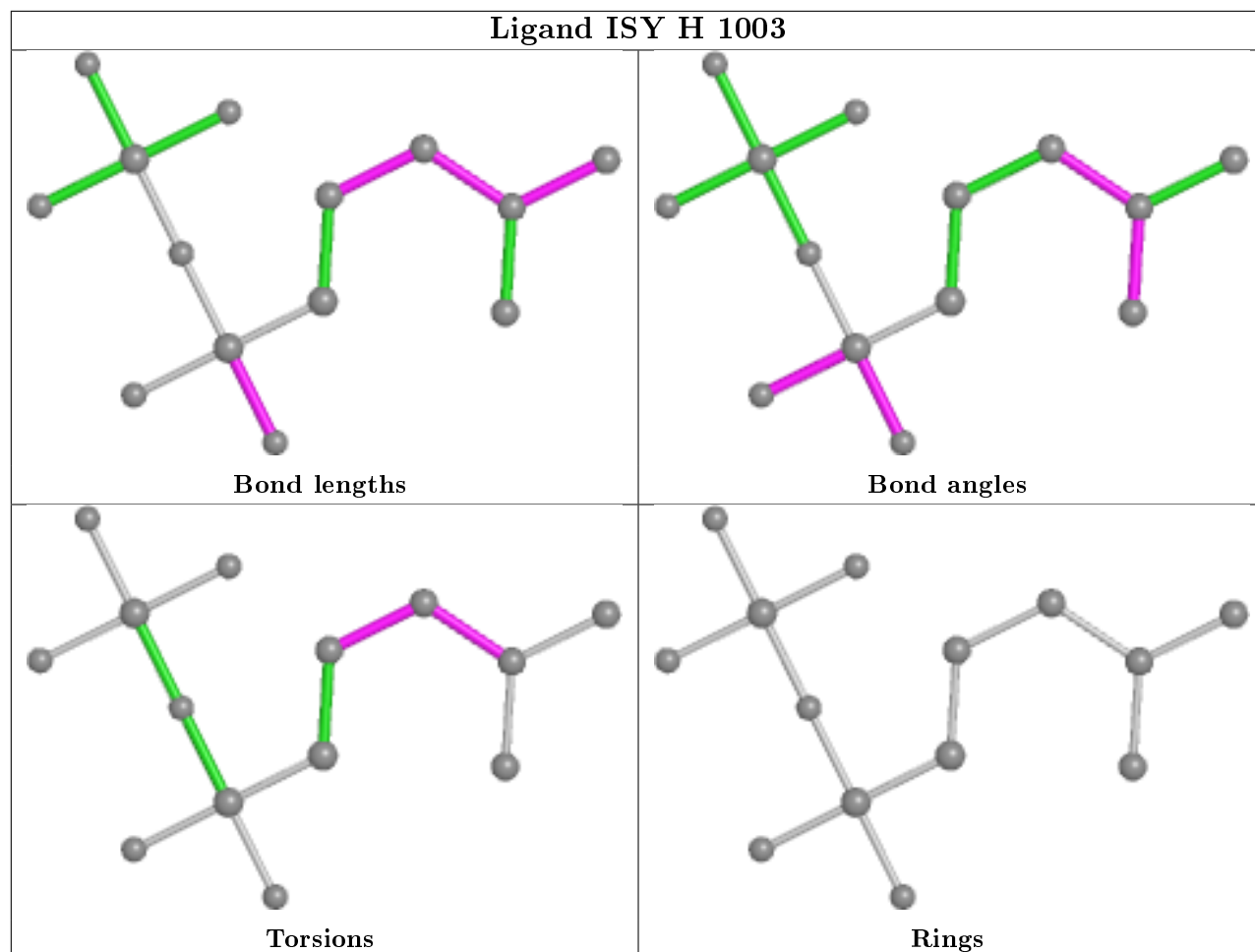
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	FPP	1	0
3	G	1001	FPP	4	0
5	B	1000	PPV	3	0
6	B	1002	PEG	1	0
3	H	1002	FPP	2	0
3	E	1002	FPP	2	0
4	H	1003	ISY	2	0
3	C	1002	FPP	7	0
4	A	1003	ISY	3	0
3	B	1001	FPP	6	0

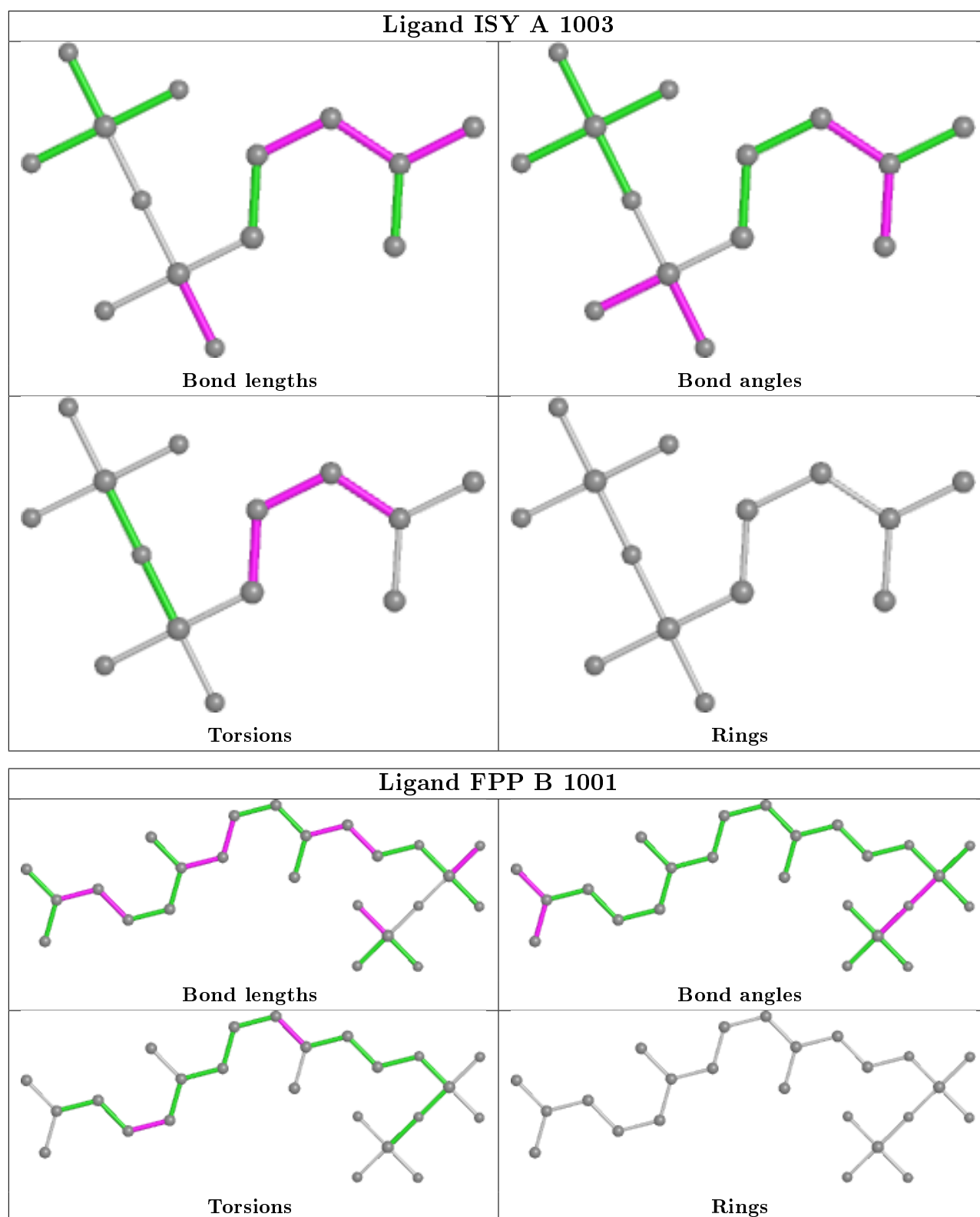
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

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	326/348 (93%)	0.36	17 (5%) 27 24	53, 82, 121, 153	0
1	B	313/348 (89%)	0.45	19 (6%) 21 18	49, 69, 125, 175	0
1	C	327/348 (93%)	0.30	24 (7%) 15 12	46, 69, 110, 141	0
1	D	312/348 (89%)	0.28	18 (5%) 23 19	49, 70, 109, 142	0
1	E	325/348 (93%)	0.36	26 (8%) 12 9	54, 79, 117, 144	0
1	F	310/348 (89%)	0.34	19 (6%) 21 18	52, 76, 108, 141	0
1	G	314/348 (90%)	0.28	11 (3%) 44 40	46, 66, 119, 166	0
1	H	324/348 (93%)	0.34	18 (5%) 24 21	57, 85, 121, 147	0
All	All	2551/2784 (91%)	0.34	152 (5%) 21 18	46, 75, 118, 175	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	244	ALA	9.7
1	A	244	ALA	8.2
1	H	243	SER	7.7
1	G	30	LEU	7.3
1	E	244	ALA	6.5

### 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 ⓘ

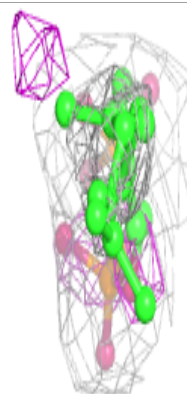
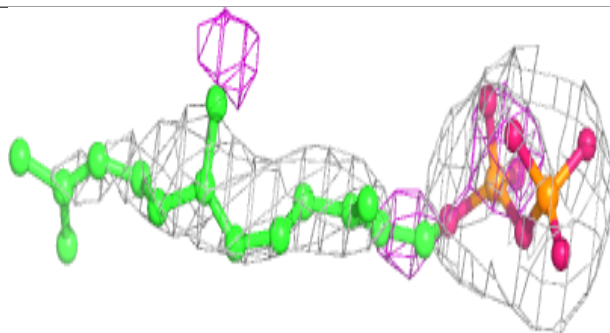
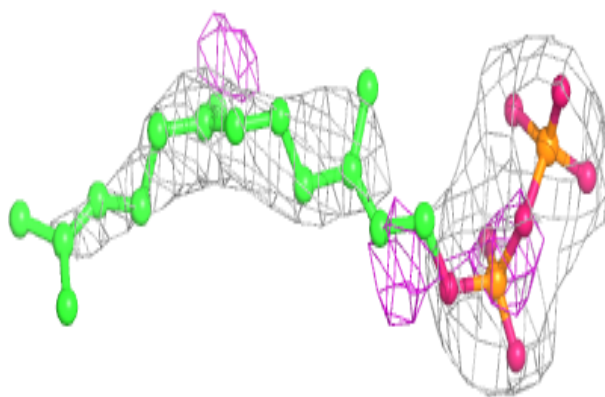
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	E	1001	1/1	0.77	0.10	47,47,47,47	0
2	MG	C	1000	1/1	0.82	0.28	53,53,53,53	0
5	PPV	F	1000	9/9	0.83	0.20	131,131,131,132	0
5	PPV	D	1000	9/9	0.84	0.22	109,109,110,110	0
2	MG	C	1001	1/1	0.87	0.12	36,36,36,36	0
2	MG	E	1000	1/1	0.88	0.17	62,62,62,62	0
5	PPV	B	1000	9/9	0.90	0.14	57,59,62,62	0
6	PEG	B	1002	7/7	0.90	0.42	22,23,24,27	0
2	MG	A	1001	1/1	0.91	0.23	63,63,63,63	0
3	FPP	B	1001	24/24	0.92	0.23	65,67,68,69	0
2	MG	H	1001	1/1	0.92	0.14	61,61,61,61	0
5	PPV	G	1000	9/9	0.93	0.12	69,70,70,71	0
6	PEG	D	1002	7/7	0.93	0.35	3,4,5,8	0
3	FPP	G	1001	24/24	0.94	0.21	51,56,62,63	0
3	FPP	A	1002	24/24	0.94	0.15	25,37,44,45	0
3	FPP	H	1002	24/24	0.94	0.17	20,40,42,43	0
5	PPV	C	1003	9/9	0.94	0.13	25,29,32,33	0
4	ISY	A	1003	14/14	0.94	0.15	33,40,44,45	0
2	MG	A	1000	1/1	0.96	0.10	46,46,46,46	0
2	MG	H	1000	1/1	0.96	0.14	42,42,42,42	0
4	ISY	H	1003	14/14	0.96	0.14	38,41,44,45	0
3	FPP	E	1002	24/24	0.96	0.13	40,42,45,45	0
3	FPP	C	1002	24/24	0.97	0.13	26,35,40,40	0
5	PPV	E	1003	9/9	0.97	0.11	31,33,35,36	0

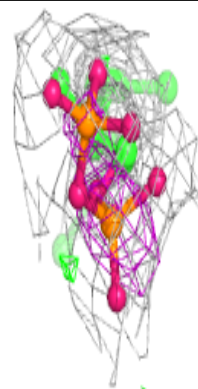
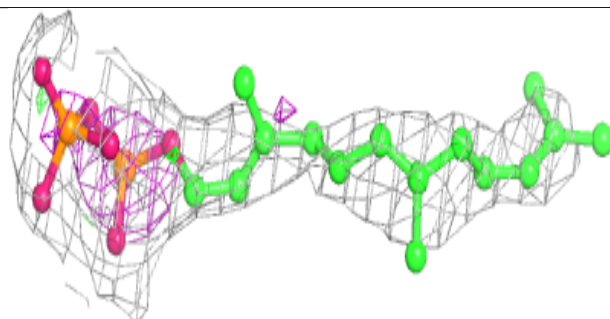
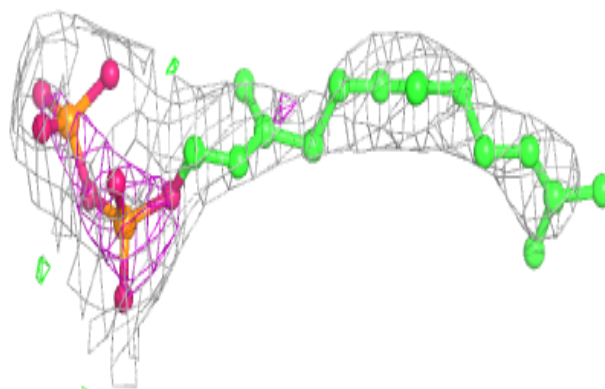
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FPP B 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

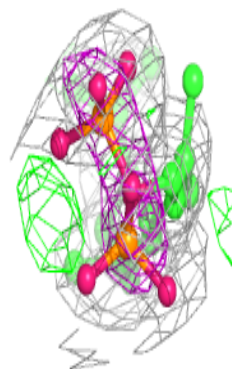
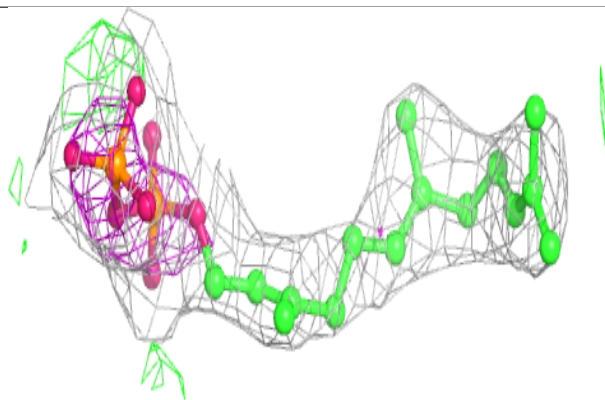
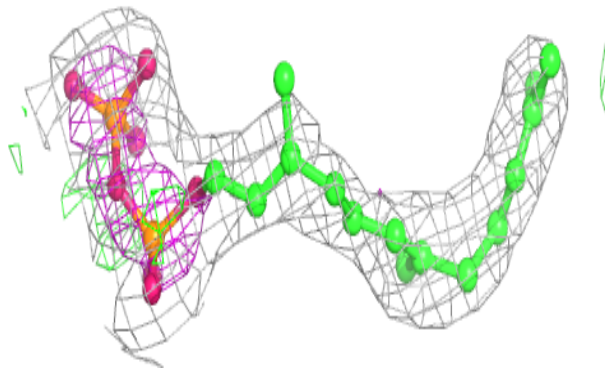
**Electron density around FPP G 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

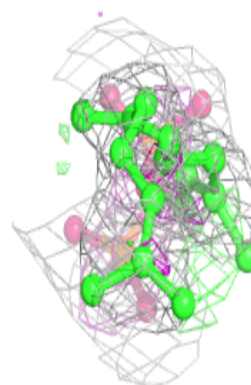
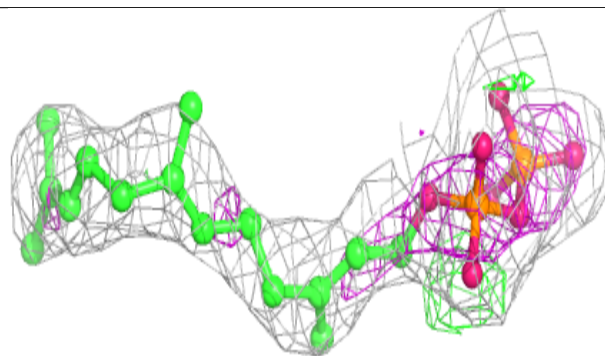
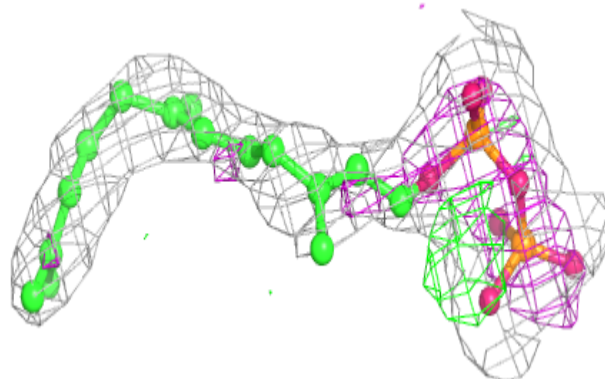


**Electron density around FPP A 1002:**

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and green (positive)

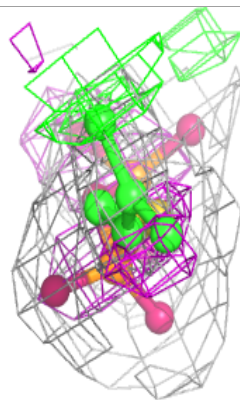
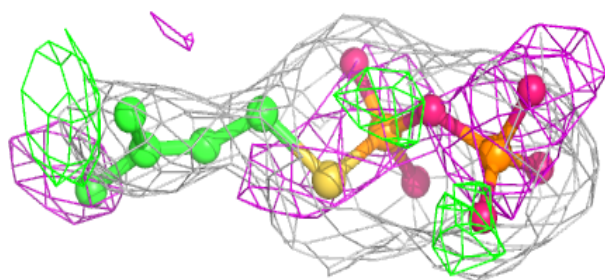
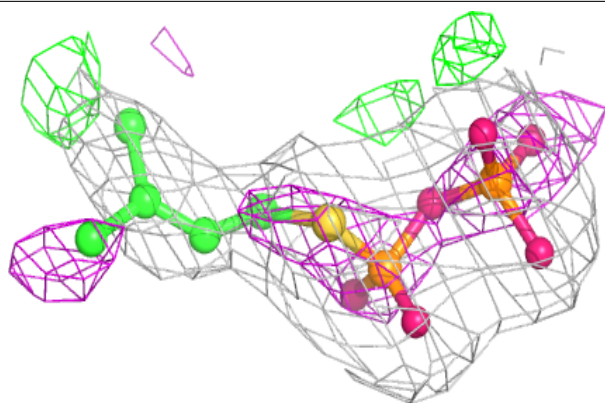
**Electron density around FPP H 1002:**

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and green (positive)

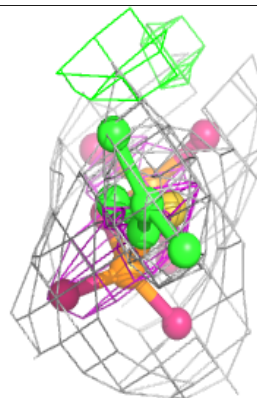
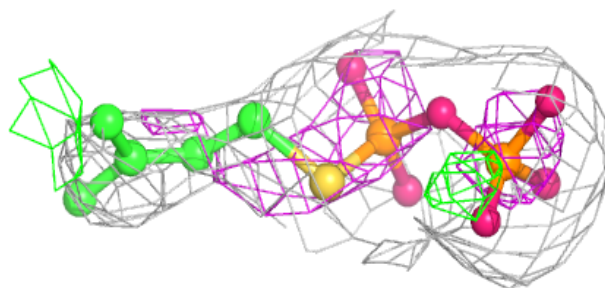
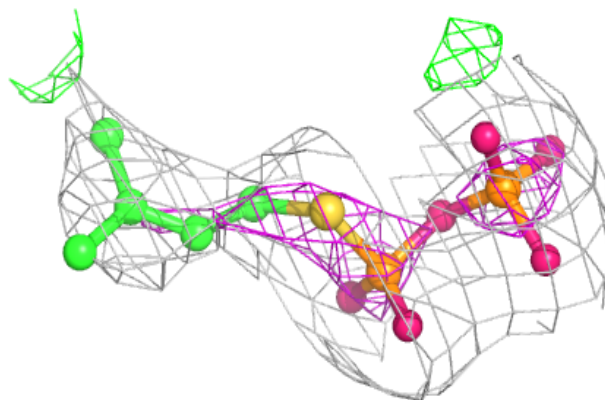


**Electron density around ISY A 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ISY H 1003:**

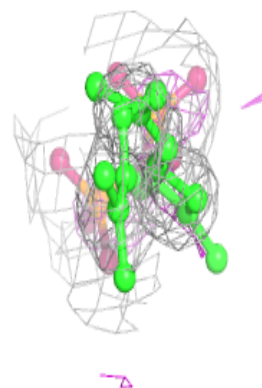
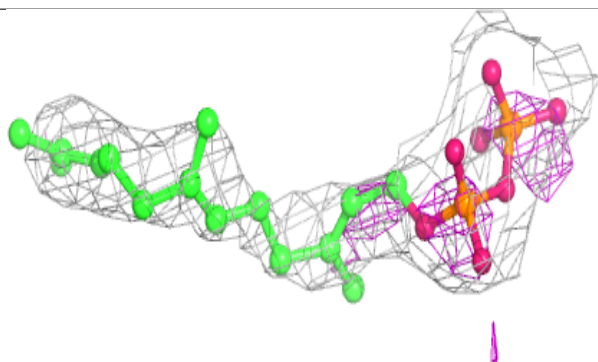
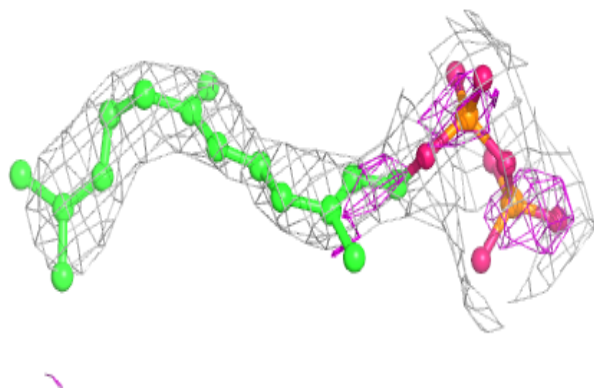
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



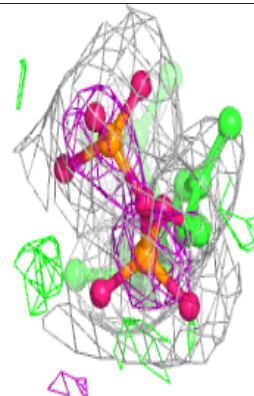
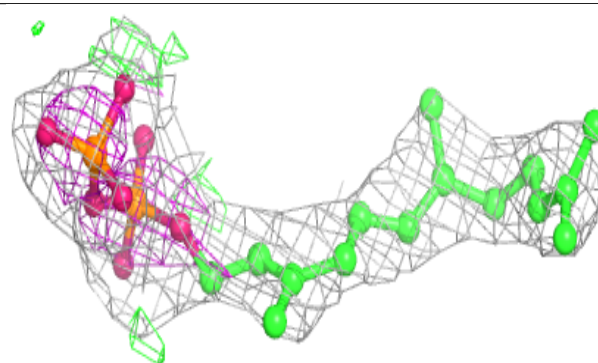
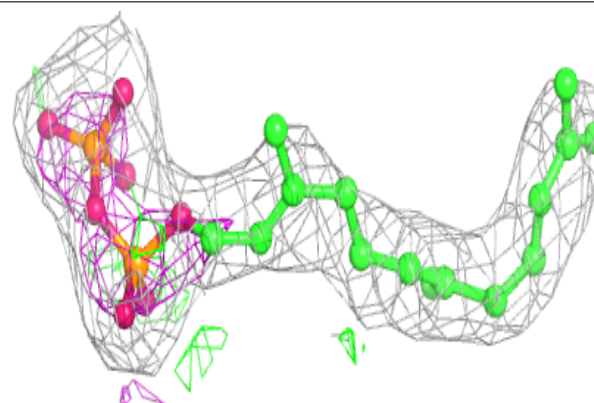


**Electron density around FPP E 1002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FPP C 1002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.