Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 01:09 pm BST

PDB ID	:	7PB1
Title	:	Structure of the human heterotetrameric cis-prenyltransferase complex in complex with magnesium, GGPP and IsPP
Authors	:	Giladi, M.; Lisnyansky Bar-El, M.; Haitin, Y.
Deposited on	:	2021-07-30
Resolution	:	2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

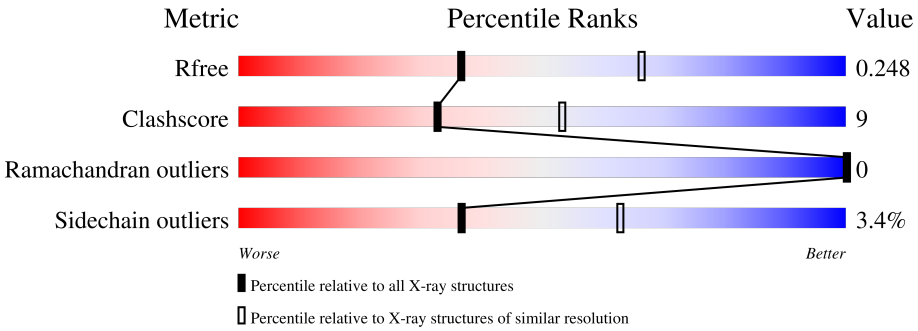
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	340	79% 14% • 6%
2	B	219	70% 13% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3699 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 Dehydrodolichyl diphosphate synthase complex subunit DHDDS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2362	1506	424	417	15			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q86SQ9
A	-5	SER	-	expression tag	UNP Q86SQ9
A	-4	GLY	-	expression tag	UNP Q86SQ9
A	-3	SER	-	expression tag	UNP Q86SQ9
A	-2	GLY	-	expression tag	UNP Q86SQ9
A	-1	SER	-	expression tag	UNP Q86SQ9
A	0	GLY	-	expression tag	UNP Q86SQ9

- Molecule 2 is a protein called Dehydrodolichyl diphosphate synthase complex subunit NUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	1	0
			1291	834	221	230	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	GLY	-	expression tag	UNP Q96E22
B	67	SER	-	expression tag	UNP Q96E22
B	68	GLY	-	expression tag	UNP Q96E22
B	69	SER	-	expression tag	UNP Q96E22
B	70	GLY	-	expression tag	UNP Q96E22
B	71	SER	-	expression tag	UNP Q96E22
B	72	GLY	-	expression tag	UNP Q96E22
B	?	-	TYR	deletion	UNP Q96E22
B	?	-	SER	deletion	UNP Q96E22

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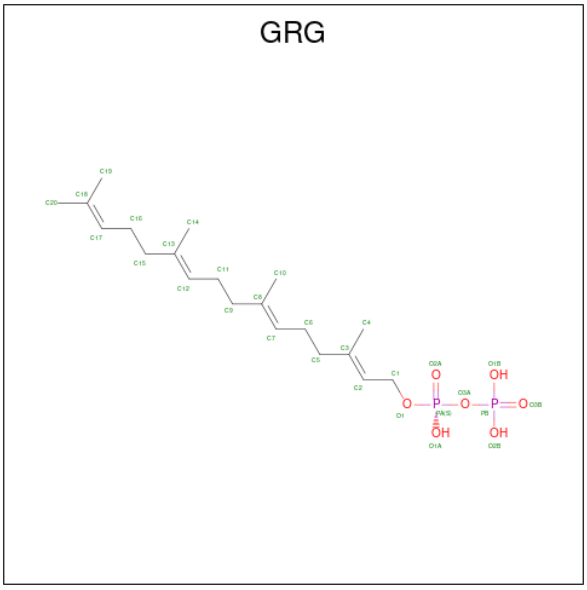
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP Q96E22
B	?	-	GLU	deletion	UNP Q96E22
B	?	-	PHE	deletion	UNP Q96E22
B	?	-	ALA	deletion	UNP Q96E22
B	?	-	ASN	deletion	UNP Q96E22
B	?	-	SER	deletion	UNP Q96E22
B	?	-	ASN	deletion	UNP Q96E22

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

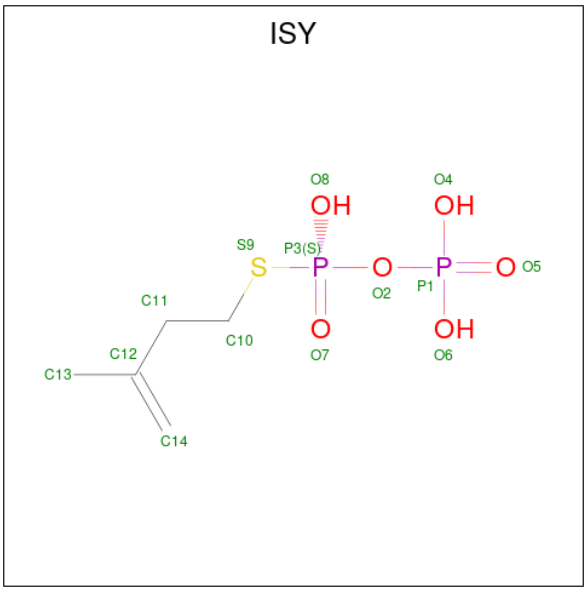
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is GERANYLGERANYL DIPHOSPHATE (three-letter code: GRG) (formula: $C_{20}H_{36}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 29 20 7 2	0	0

- Molecule 5 is 3-methylbut-3-enylsulfanyl(phosphonooxy)phosphinic acid (three-letter code: ISY) (formula: $C_5H_{12}O_6P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O P S 14 5 6 2 1	0	0

- Molecule 6 is water.

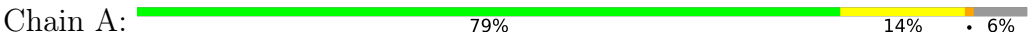
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0

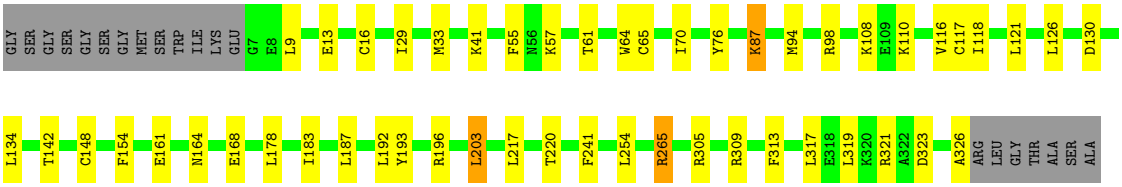
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: Dehydrodolichyl diphosphate synthase complex subunit DHDDS

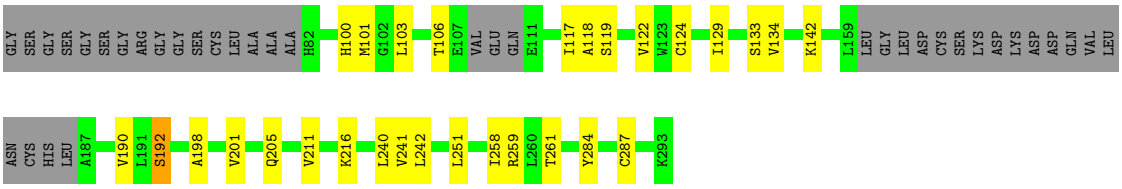
Chain A:





• Molecule 2: Dehydrodolichyl diphosphate synthase complex subunit NUS1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	183.47Å 183.47Å 112.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.86 – 2.59 45.87 – 2.59	Depositor EDS
% Data completeness (in resolution range)	91.2 (45.86-2.59) 91.3 (45.87-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.94 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.205 , 0.249 0.205 , 0.248	Depositor DCC
R_{free} test set	1036 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	76.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.010 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.000 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3699	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GRG, ISY, MG

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	0.30	0/2410	0.44	0/3277
2	B	0.30	0/1322	0.45	0/1809
All	All	0.30	0/3732	0.44	0/5086

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	2362	0	2158	42	0
2	B	1291	0	1153	17	0
3	A	1	0	0	0	0
4	A	29	0	33	7	0
5	A	14	0	9	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	3699	0	3353	61	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 9.

All (61) 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:265:ARG:HH11	1:A:265:ARG:HB3	1.18	1.06
1:A:265:ARG:HH11	1:A:265:ARG:CB	1.89	0.83
1:A:323:ASP:HB3	1:A:326:ALA:HB2	1.68	0.75
1:A:178:LEU:HD21	1:A:187:LEU:HD21	1.73	0.70
1:A:265:ARG:HB3	1:A:265:ARG:NH1	2.03	0.60
1:A:61:THR:HG22	1:A:64:TRP:CZ3	2.37	0.60
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.17	0.58
1:A:55:PHE:HE1	4:A:402:GRG:H162	1.69	0.58
1:A:57:LYS:O	1:A:61:THR:HG23	2.05	0.56
2:B:198:ALA:O	2:B:201:VAL:HG12	2.06	0.55
1:A:118:ILE:H	1:A:142:THR:HG21	1.70	0.55
1:A:118:ILE:H	1:A:142:THR:CG2	2.21	0.54
2:B:119:SER:HA	2:B:122:VAL:HG12	1.91	0.53
1:A:108:LYS:O	1:A:110:LYS:N	2.39	0.53
4:A:402:GRG:H102	4:A:402:GRG:H12	1.91	0.53
1:A:61:THR:HA	1:A:64:TRP:CE3	2.44	0.52
1:A:98:ARG:NH1	1:A:130:ASP:OD1	2.39	0.52
1:A:265:ARG:NH1	1:A:265:ARG:CG	2.72	0.52
2:B:142:LYS:NZ	2:B:192:SER:HB3	2.26	0.51
1:A:65:CYS:HB3	1:A:70:ILE:HB	1.92	0.51
1:A:116:VAL:HG22	1:A:148:CYS:SG	2.52	0.50
1:A:305:ARG:O	1:A:309:ARG:HG3	2.12	0.50
2:B:211:VAL:HA	2:B:216:LYS:O	2.11	0.50
1:A:29:ILE:HG13	1:A:70:ILE:HG21	1.94	0.50
1:A:118:ILE:HB	1:A:142:THR:HG21	1.95	0.49
1:A:98:ARG:HD3	1:A:130:ASP:OD1	2.13	0.49
2:B:134:VAL:HG22	2:B:190:VAL:HG22	1.95	0.48
2:B:100:HIS:NE2	2:B:133:SER:OG	2.44	0.48
2:B:240:LEU:HD13	2:B:284:TYR:HB2	1.96	0.46
1:A:317:LEU:HD23	1:A:321:ARG:HG3	1.96	0.46
2:B:258:ILE:HA	2:B:261:THR:OG1	2.16	0.46
1:A:217:LEU:HD11	2:B:259:ARG:HB3	1.98	0.46
1:A:183:ILE:HB	2:B:205:GLN:HG2	1.98	0.45
1:A:121:LEU:HB3	1:A:193:TYR:HB3	1.98	0.45
1:A:203:LEU:HD13	1:A:220:THR:HG21	1.97	0.45
1:A:57:LYS:HD3	1:A:57:LYS:HA	1.80	0.44
2:B:101:MET:HE3	2:B:242:LEU:HD13	1.97	0.44
1:A:317:LEU:O	1:A:321:ARG:HG3	2.18	0.44
1:A:178:LEU:HD13	1:A:313:PHE:HB2	2.00	0.44
1:A:9:LEU:HB3	1:A:13:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:CYS:HB3	1:A:241:PHE:CZ	2.53	0.44
1:A:265:ARG:HD2	1:A:265:ARG:HA	1.78	0.43
2:B:106:THR:HG22	2:B:251:LEU:HD12	2.01	0.42
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.81	0.42
4:A:402:GRG:H162	4:A:402:GRG:H201	1.74	0.42
2:B:241:VAL:HG23	2:B:261:THR:HG21	2.00	0.42
1:A:161:GLU:OE2	1:A:192:LEU:HB3	2.20	0.42
1:A:134:LEU:HA	1:A:134:LEU:HD23	1.79	0.42
1:A:87:LYS:HE3	1:A:87:LYS:HB3	1.90	0.42
2:B:117:ILE:HG13	2:B:118:ALA:N	2.35	0.42
1:A:116:VAL:O	1:A:142:THR:OG1	2.37	0.42
4:A:402:GRG:H101	4:A:402:GRG:HC61	1.43	0.41
2:B:124:CYS:HB3	2:B:129:ILE:HB	2.01	0.41
1:A:164:ASN:O	1:A:168:GLU:HG2	2.19	0.41
1:A:33:MET:HE3	4:A:402:GRG:HC7	2.02	0.41
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.75	0.41
2:B:103:LEU:HD23	2:B:242:LEU:HB2	2.02	0.41
1:A:117:CYS:HA	1:A:142:THR:OG1	2.21	0.41
2:B:134:VAL:CG2	2:B:190:VAL:HG22	2.50	0.40
1:A:33:MET:O	4:A:402:GRG:HC2	2.21	0.40
4:A:402:GRG:H143	4:A:402:GRG:H161	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/340 (94%)	308 (97%)	10 (3%)	0	100	100
2	B	177/219 (81%)	167 (94%)	10 (6%)	0	100	100
All	All	495/559 (89%)	475 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/295 (72%)	203 (96%)	9 (4%)	30	55
2	B	113/188 (60%)	111 (98%)	2 (2%)	59	80
All	All	325/483 (67%)	314 (97%)	11 (3%)	37	63

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	76	TYR
1	A	87	LYS
1	A	94	MET
1	A	126	LEU
1	A	154	PHE
1	A	196	ARG
1	A	203	LEU
1	A	265	ARG
2	B	192	SER
2	B	287	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GRG	A	402	3	26,28,28	1.20	1 (3%)	33,37,37	1.73	5 (15%)
5	ISY	A	403	3	9,13,13	0.98	1 (11%)	11,19,19	1.00	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
4	GRG	A	402	3	-	6/31/31/31	-
5	ISY	A	403	3	-	3/9/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	GRG	C9-C8	2.41	1.56	1.51
5	A	403	ISY	P3-O8	-2.11	1.51	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	402	GRG	C6-C7-C8	-4.27	117.37	127.66
4	A	402	GRG	C10-C8-C9	3.88	121.80	115.27
4	A	402	GRG	PA-O3A-PB	-3.74	119.98	132.83
4	A	402	GRG	C4-C3-C5	3.06	120.42	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	402	GRG	C10-C8-C7	-2.49	117.30	123.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

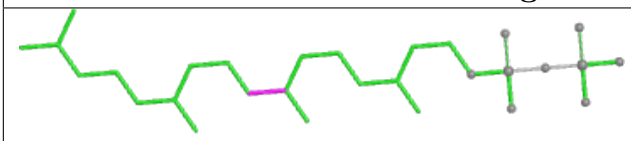
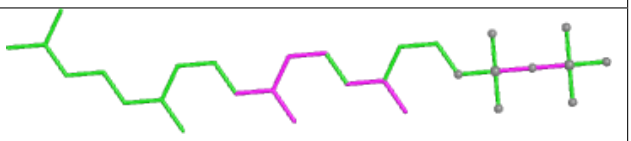
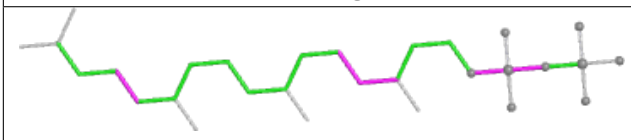
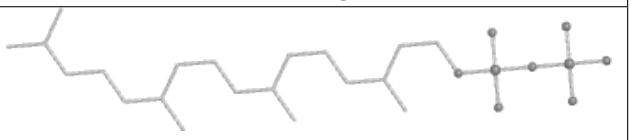
Mol	Chain	Res	Type	Atoms
5	A	403	ISY	P3-O2-P1-O6
4	A	402	GRG	C13-C15-C16-C17
4	A	402	GRG	C3-C5-C6-C7
4	A	402	GRG	PB-O3A-PA-O2A
4	A	402	GRG	C4-C3-C5-C6
4	A	402	GRG	C2-C3-C5-C6
5	A	403	ISY	P3-O2-P1-O4
4	A	402	GRG	C1-O1-PA-O3A
5	A	403	ISY	P3-O2-P1-O5

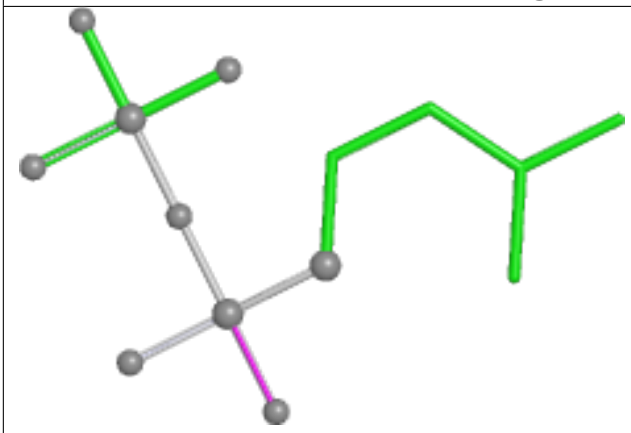
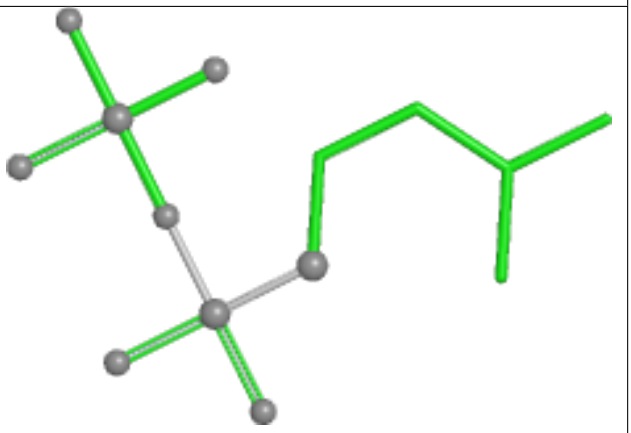
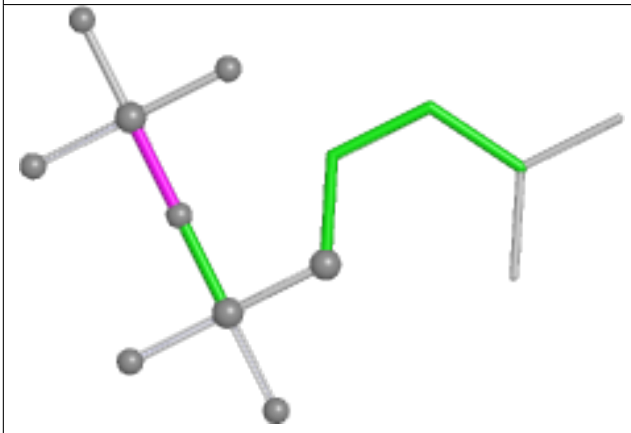
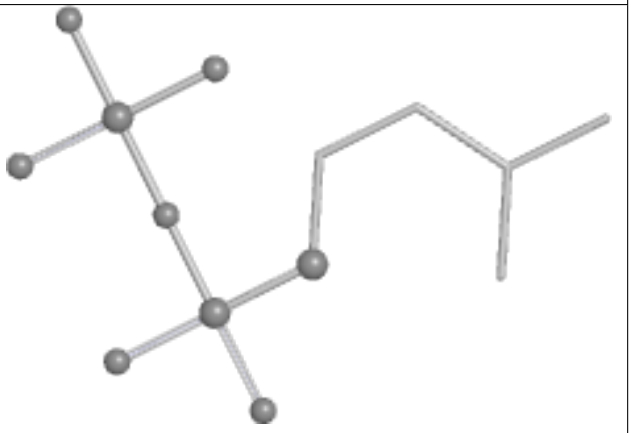
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	GRG	7	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 then 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.

Ligand GRG A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ISY A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

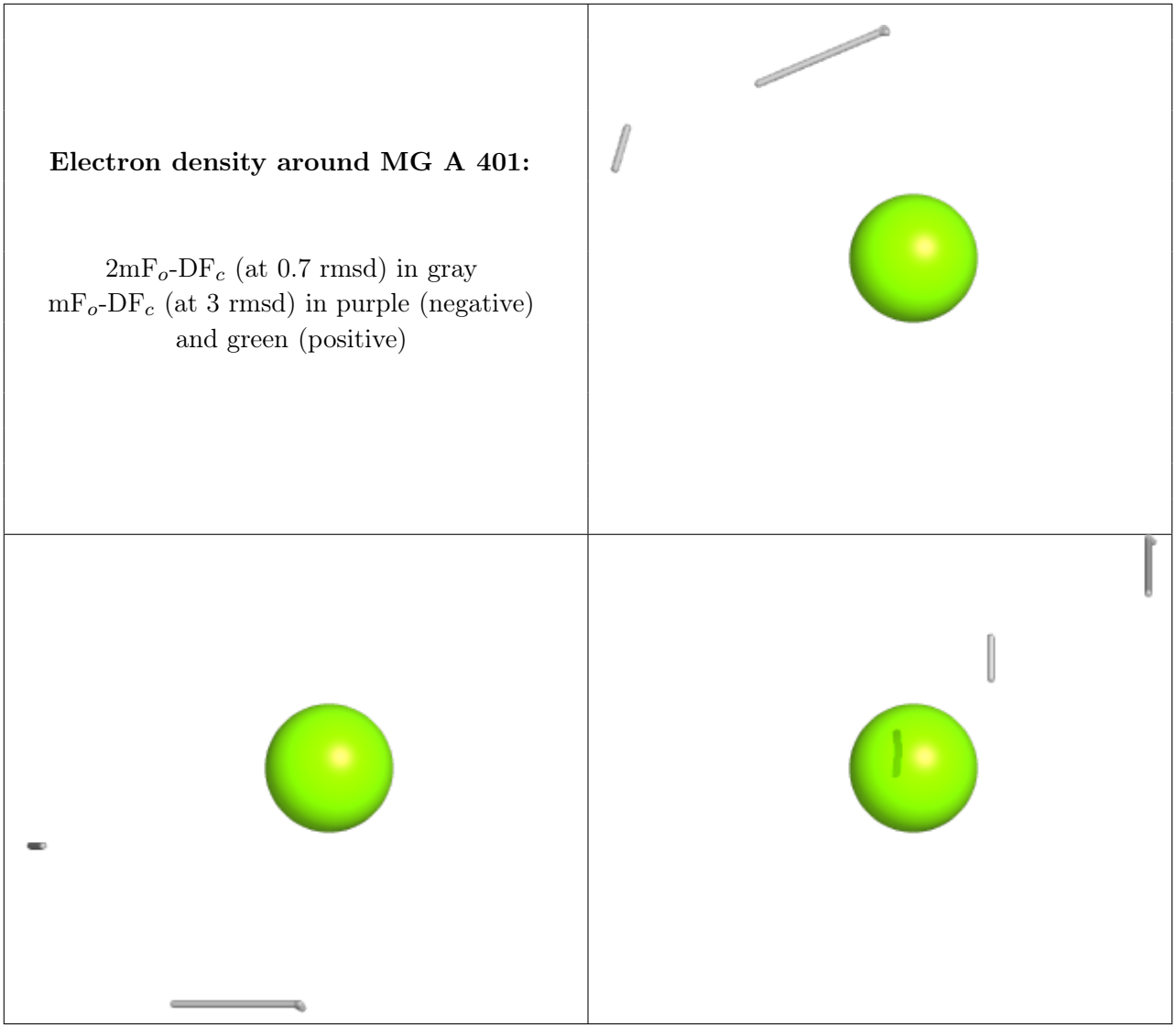
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

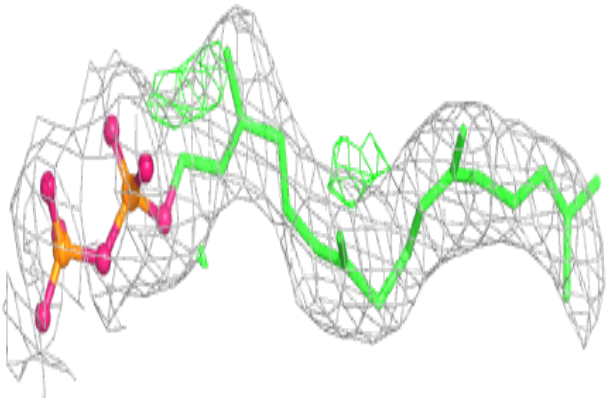
Electron density around MG A 401:

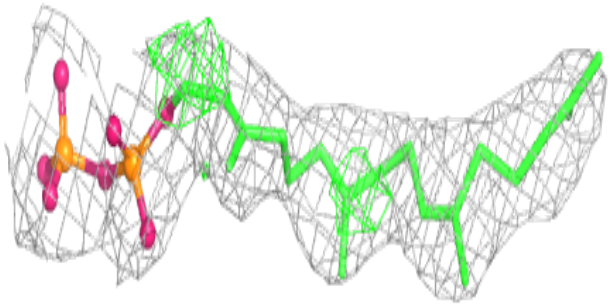
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GRG A 402:

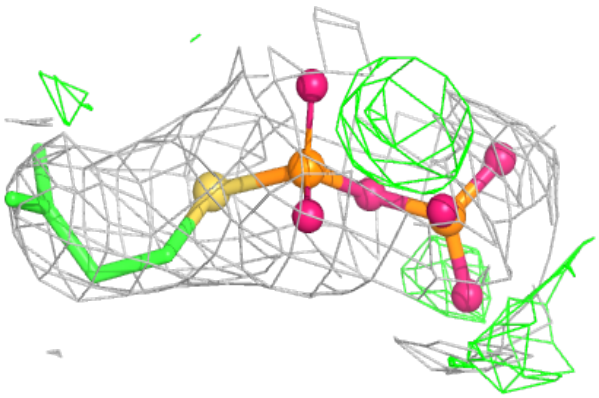
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

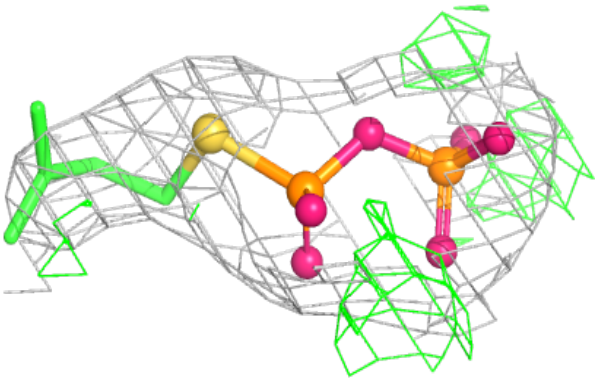


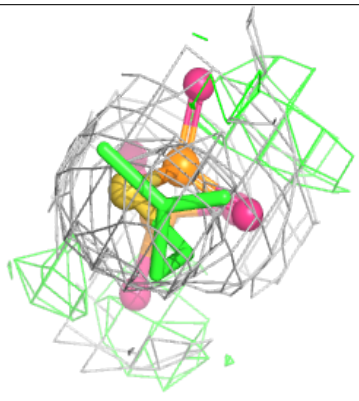


Electron density around ISY A 403:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.