Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:31 PM BST

PDB ID	:	4F86
Title	:	Structure analysis of Geranyl diphosphate methyltransferase in complex with GPP and sinefungin
Authors	:	Ariyawutthiphan, O.; Ose, T.; Minami, A.; Gao, Y.G.; Yao, M.; Oikawa, H.; Tanaka, I.
Deposited on	:	2012-05-17
Resolution	:	3.00 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:

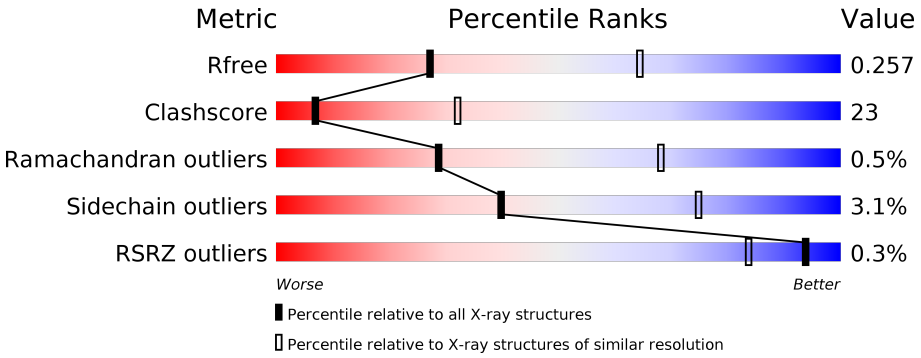
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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% 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	320	52% 32% • 14%
1	B	320	53% 31% • 15%
1	C	320	52% 31% • 14%
1	D	320	53% 30% • 15%
1	E	320	49% 34% • 15%
1	F	320	49% 33% • 16%

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Mol	Chain	Length	Quality of chain
1	G	320	51% 32% • 16%
1	H	320	% 52% 30% • 16%
1	I	320	50% 33% • 15%
1	J	320	53% 31% • 15%
1	K	320	49% 30% • 19%
1	L	320	% 51% 32% • 15%

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	SFG	A	501	-	-	X	-
2	SFG	I	501	-	-	X	-
2	SFG	K	501	-	-	X	-
3	GPP	A	502	-	-	X	-
3	GPP	B	502	-	-	X	-
3	GPP	C	502	-	-	X	-
3	GPP	D	502	-	-	X	-
3	GPP	H	502	-	-	X	-
3	GPP	I	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26078 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 2-C-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2155	1345	392	408	10			
1	B	273	Total	C	N	O	S	0	0	0
			2147	1340	393	404	10			
1	C	274	Total	C	N	O	S	0	0	0
			2142	1338	390	404	10			
1	D	273	Total	C	N	O	S	0	0	0
			2146	1341	392	403	10			
1	E	272	Total	C	N	O	S	0	0	0
			2142	1337	392	403	10			
1	F	269	Total	C	N	O	S	0	0	0
			2113	1321	388	394	10			
1	G	269	Total	C	N	O	S	0	0	0
			2119	1326	386	397	10			
1	H	268	Total	C	N	O	S	0	0	0
			2096	1310	383	393	10			
1	I	273	Total	C	N	O	S	0	0	0
			2143	1338	390	405	10			
1	J	272	Total	C	N	O	S	0	0	0
			2148	1341	392	405	10			
1	K	258	Total	C	N	O	S	0	0	0
			2013	1256	368	379	10			
1	L	273	Total	C	N	O	S	0	0	0
			2150	1343	392	405	10			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
A	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
A	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
A	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
A	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
A	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
A	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
A	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
A	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
A	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
A	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
A	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
A	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
A	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
A	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
A	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
A	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
A	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
A	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
B	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
B	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
B	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
B	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
B	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
B	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
B	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
B	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
B	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
B	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
B	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
B	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
B	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
B	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
B	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
B	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
B	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
B	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
B	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
B	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
C	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
C	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
C	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
C	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
C	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
C	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
C	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
C	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
C	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
C	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
C	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
C	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
C	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
C	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
C	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
C	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
C	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
C	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
C	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
D	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
D	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
D	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
D	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
D	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
D	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
D	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
D	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
D	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
D	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
D	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
D	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
D	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
D	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
D	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
D	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
D	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
D	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
D	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
D	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
E	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
E	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
E	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
E	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
E	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
E	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
E	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
E	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
E	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
E	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
E	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
E	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
E	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
E	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
E	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
E	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
E	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
E	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
E	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
F	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
F	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
F	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
F	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
F	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
F	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
F	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
F	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
F	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
F	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
F	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
F	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
F	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
F	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
F	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
F	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
F	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
F	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
F	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
F	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
G	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
G	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
G	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
G	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
G	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
G	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
G	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
G	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
G	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
G	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
G	-9	SER	-	EXPRESSION TAG	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
G	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
G	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
G	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
G	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
G	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
G	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
G	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
G	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
H	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
H	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
H	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
H	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
H	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
H	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
H	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
H	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
H	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
H	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
H	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
H	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
H	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
H	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
H	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
H	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
H	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
H	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
H	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
H	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
I	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
I	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
I	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
I	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
I	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
I	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
I	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
I	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
I	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
I	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
I	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
I	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
I	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
I	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
I	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
I	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
I	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
I	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
I	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
J	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
J	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
J	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
J	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
J	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
J	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
J	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
J	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
J	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
J	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
J	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
J	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
J	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
J	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
J	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
J	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
J	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
J	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
J	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
J	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
K	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
K	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
K	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
K	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
K	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
K	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
K	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
K	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
K	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
K	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
K	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
K	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
K	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
K	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
K	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3

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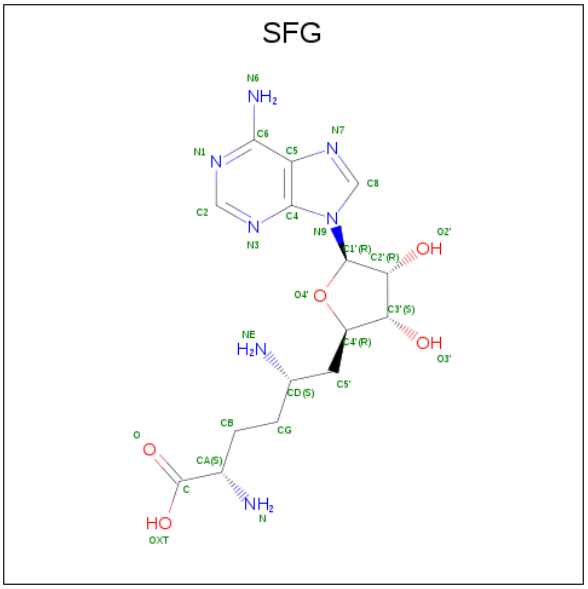
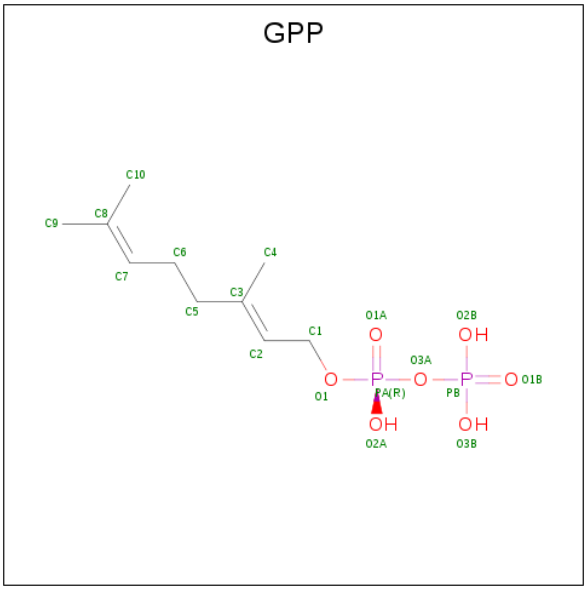
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
K	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
K	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
K	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
K	0	HIS	-	EXPRESSION TAG	UNP D3KYU3
L	-19	MET	-	EXPRESSION TAG	UNP D3KYU3
L	-18	GLY	-	EXPRESSION TAG	UNP D3KYU3
L	-17	SER	-	EXPRESSION TAG	UNP D3KYU3
L	-16	SER	-	EXPRESSION TAG	UNP D3KYU3
L	-15	HIS	-	EXPRESSION TAG	UNP D3KYU3
L	-14	HIS	-	EXPRESSION TAG	UNP D3KYU3
L	-13	HIS	-	EXPRESSION TAG	UNP D3KYU3
L	-12	HIS	-	EXPRESSION TAG	UNP D3KYU3
L	-11	HIS	-	EXPRESSION TAG	UNP D3KYU3
L	-10	HIS	-	EXPRESSION TAG	UNP D3KYU3
L	-9	SER	-	EXPRESSION TAG	UNP D3KYU3
L	-8	SER	-	EXPRESSION TAG	UNP D3KYU3
L	-7	GLY	-	EXPRESSION TAG	UNP D3KYU3
L	-6	LEU	-	EXPRESSION TAG	UNP D3KYU3
L	-5	VAL	-	EXPRESSION TAG	UNP D3KYU3
L	-4	PRO	-	EXPRESSION TAG	UNP D3KYU3
L	-3	ARG	-	EXPRESSION TAG	UNP D3KYU3
L	-2	GLY	-	EXPRESSION TAG	UNP D3KYU3
L	-1	SER	-	EXPRESSION TAG	UNP D3KYU3
L	0	HIS	-	EXPRESSION TAG	UNP D3KYU3

- Molecule 2 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		
2	B	1	Total	C	N	O	0	0
			27	15	7	5		
2	C	1	Total	C	N	O	0	0
			27	15	7	5		
2	D	1	Total	C	N	O	0	0
			27	15	7	5		
2	E	1	Total	C	N	O	0	0
			27	15	7	5		
2	F	1	Total	C	N	O	0	0
			27	15	7	5		
2	G	1	Total	C	N	O	0	0
			27	15	7	5		
2	H	1	Total	C	N	O	0	0
			27	15	7	5		
2	I	1	Total	C	N	O	0	0
			27	15	7	5		
2	J	1	Total	C	N	O	0	0
			27	15	7	5		
2	K	1	Total	C	N	O	0	0
			27	15	7	5		
2	L	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 3 is GERANYL DIPHOSPHATE (three-letter code: GPP) (formula: $C_{10}H_{20}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			19	10	7	2		
3	B	1	Total	C	O	P	0	0
			19	10	7	2		
3	C	1	Total	C	O	P	0	0
			19	10	7	2		
3	D	1	Total	C	O	P	0	0
			19	10	7	2		
3	E	1	Total	C	O	P	0	0
			19	10	7	2		
3	F	1	Total	C	O	P	0	0
			19	10	7	2		
3	G	1	Total	C	O	P	0	0
			19	10	7	2		
3	H	1	Total	C	O	P	0	0
			19	10	7	2		
3	I	1	Total	C	O	P	0	0
			19	10	7	2		
3	J	1	Total	C	O	P	0	0
			19	10	7	2		
3	K	1	Total	C	O	P	0	0
			19	10	7	2		
3	L	1	Total	C	O	P	0	0
			19	10	7	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		

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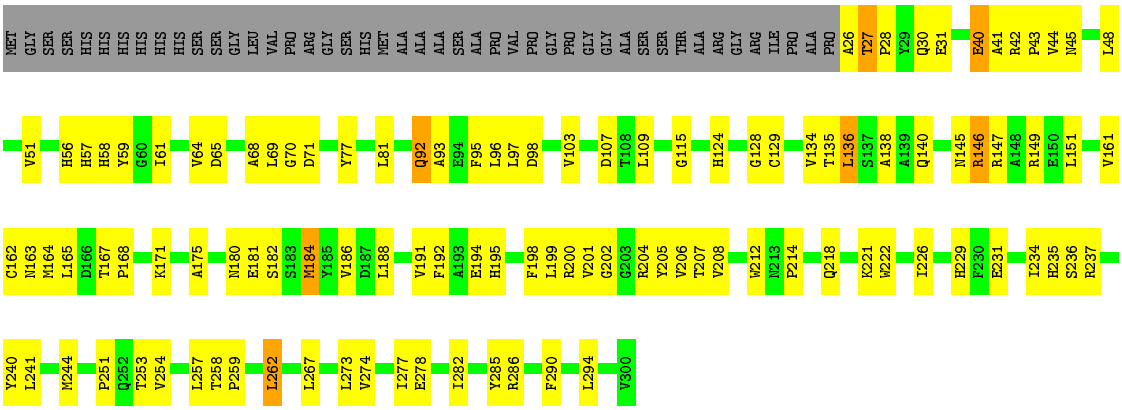
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

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 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.

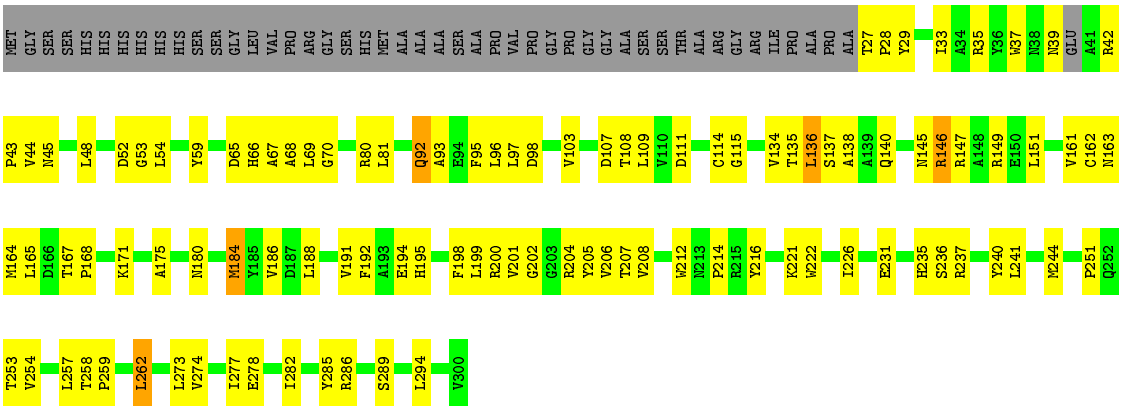
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain A:



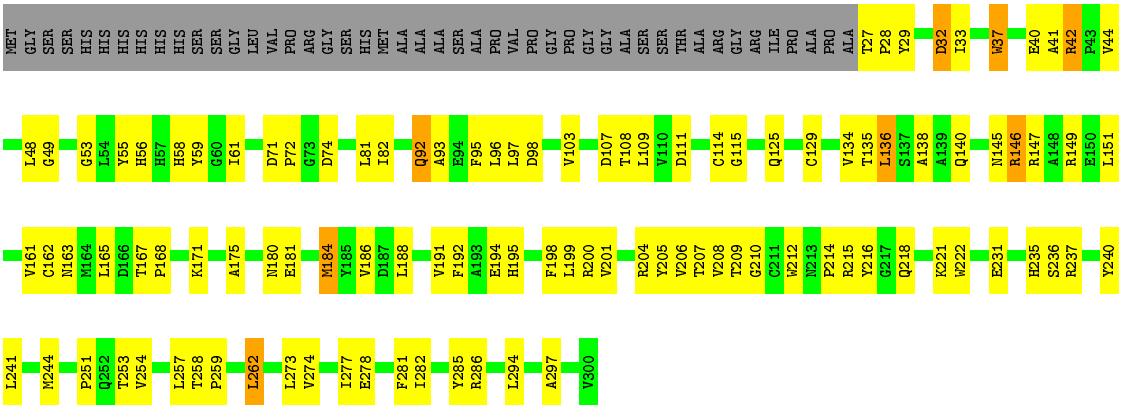
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain B:



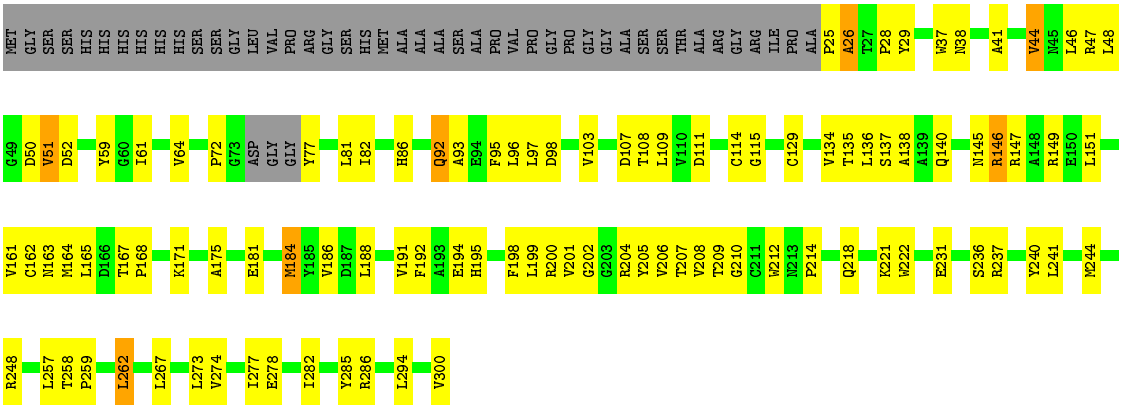
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain C:



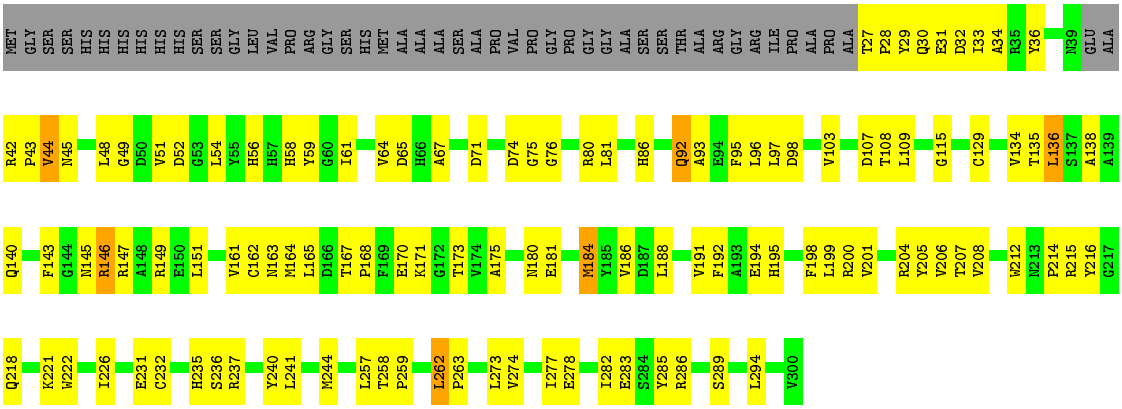
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain D:



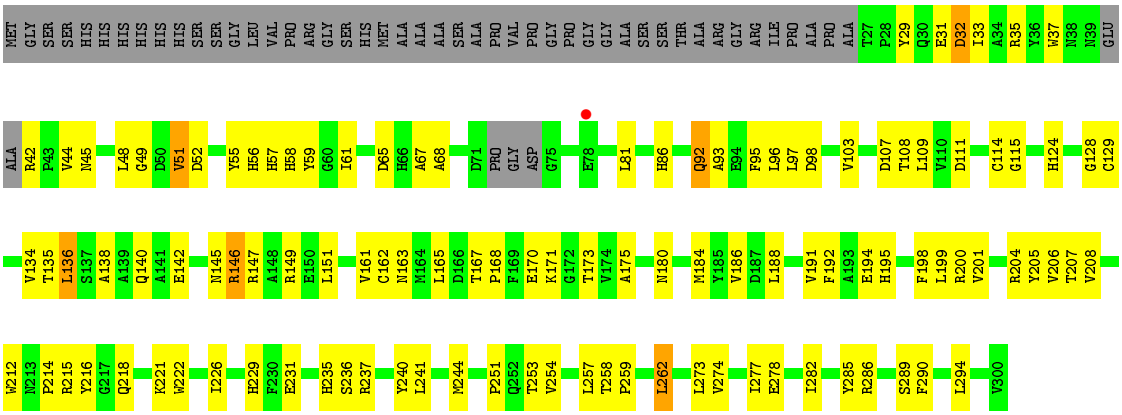
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain E:



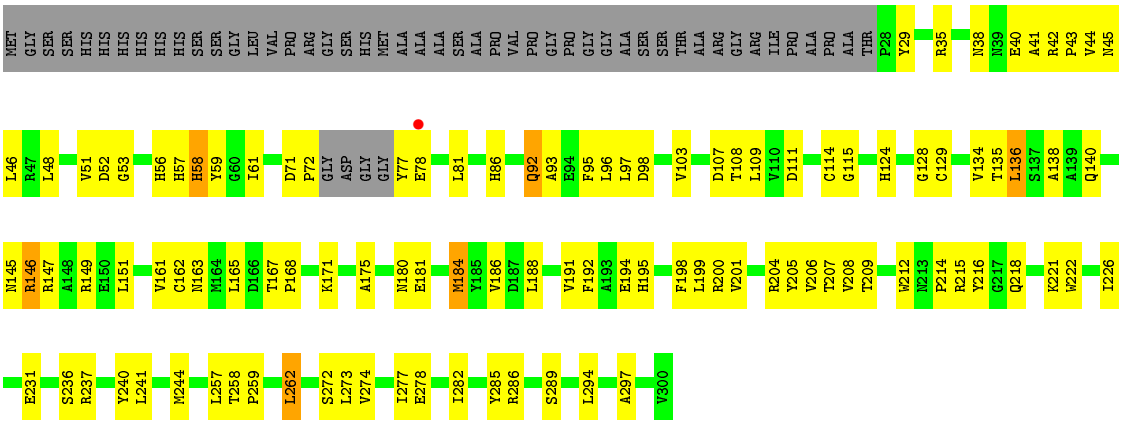
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain F:



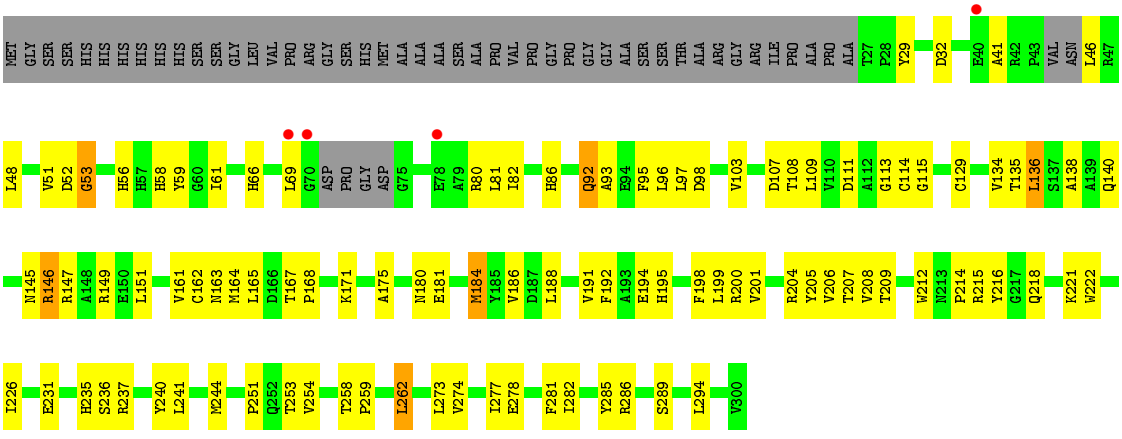
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain G:



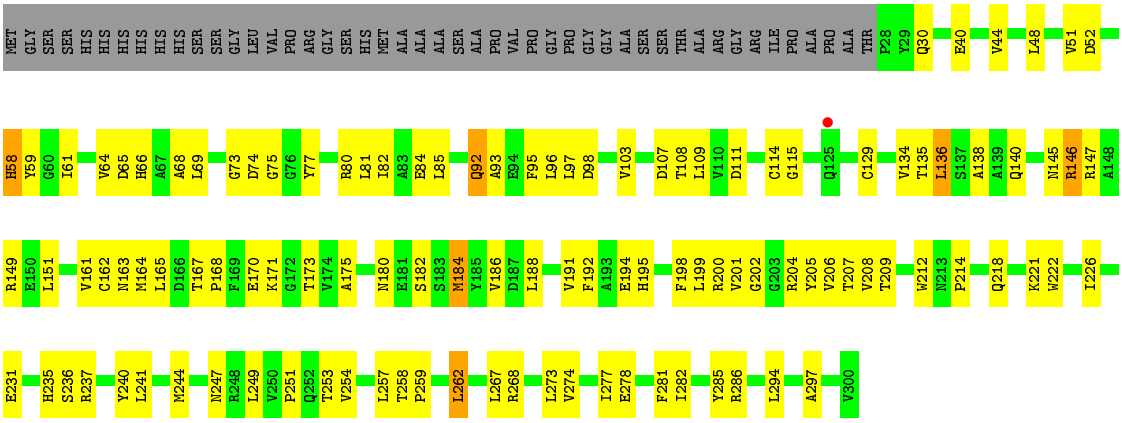
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain H:



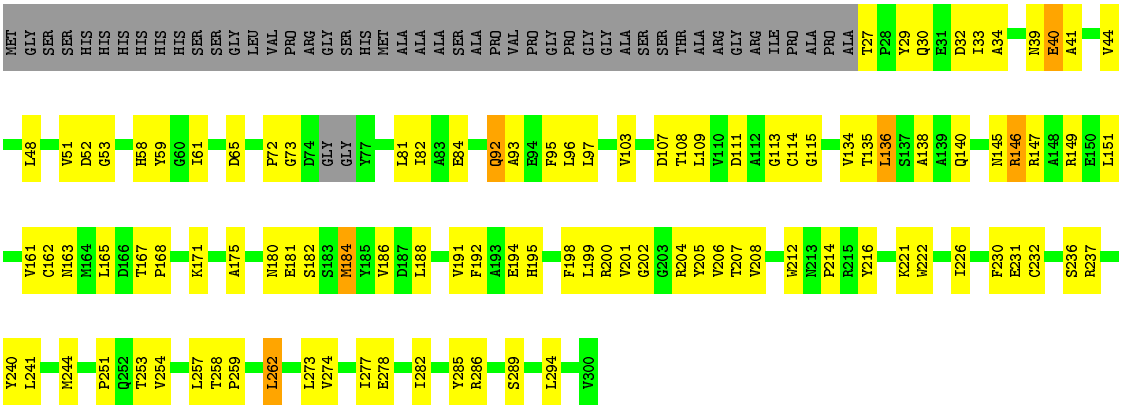
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain I:



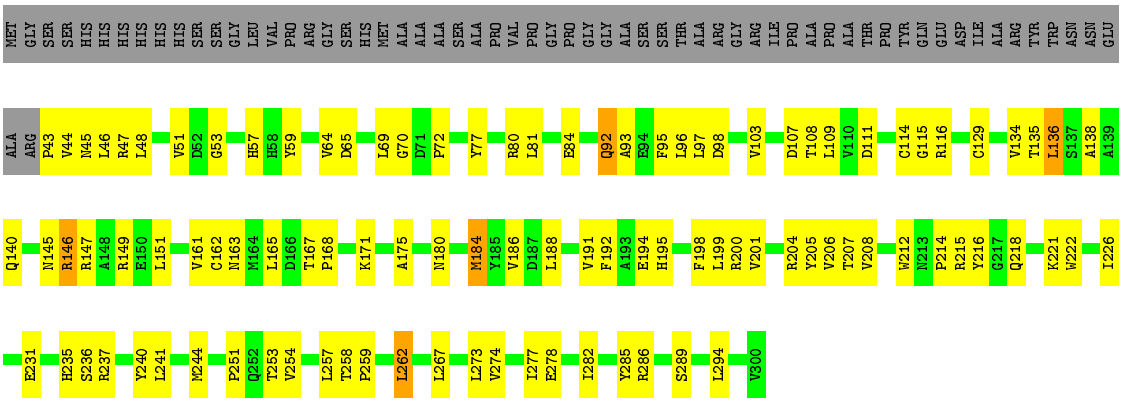
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain J:



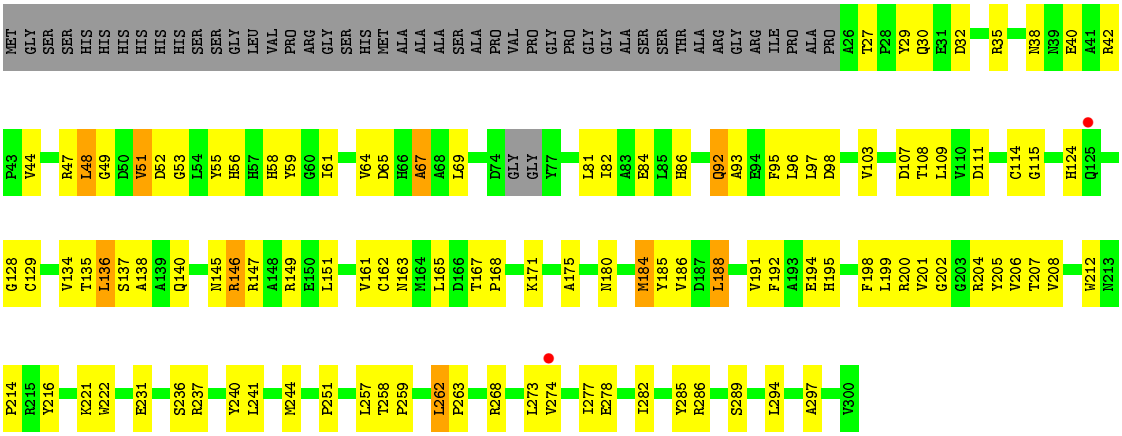
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain K:



• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain L:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA ALA ALA ALA SER ALA PRO VAL PRO GLY PRO GLY GLY ALA SER SER THR ALA ARG GLY ARG ILE PRO ALA PRO A26 T27 P28 Y29 Q30 E31 D32 R35 N38 N39 E40 A41 R42
P43 V44 R47 L48 G49 D50 V51 D52 G53 L54 Y55 H56 H57 H58 Y59 G60 I61 V64 D65 H66 A67 A68 L69 D74 GLY GLY Y77 L81 I82 A83 E84 L85 H86 Q92 A93 E94 F95 L96 L97 D98 V103 D107 T108 L109 V110 D111 C114 G115 H124 Q125
G128 C129 V134 T135 L136 S137 A138 A139 Q140 N145 R146 R147 A148 R149 E150 L151 V161 C162 N163 M164 L165 D166 T167 P168 K171 A175 N180 M184 Y185 V186 D187 L188 V191 F192 A193 E194 H195 F198 L199 R200 V201 G202 G203 R204 Y205 V206 T207 V208 W212 N213
P214 R215 Y216 K221 W222 E231 S236 R237 Y240 L241 M244 P251 L257 T258 P259 L262 P263 R268 L273 V274 I277 E278 I282 Y285 R286 S289 L294 A297 V300

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.94Å 87.73Å 160.22Å 100.01° 96.65° 90.89°	Depositor
Resolution (Å)	46.51 – 3.00 46.51 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.51-3.00) 94.7 (46.51-2.97)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.96Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.279 , 0.298 0.257 , 0.257	Depositor DCC
R_{free} test set	4112 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.891	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 30.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	26078	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% 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: SFG, MG, GPP

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	0.26	0/2208	0.49	0/2999
1	B	0.26	0/2199	0.50	0/2984
1	C	0.27	0/2195	0.49	0/2982
1	D	0.26	0/2199	0.49	0/2985
1	E	0.26	0/2194	0.49	0/2977
1	F	0.27	0/2163	0.48	0/2933
1	G	0.27	0/2171	0.50	0/2947
1	H	0.26	0/2146	0.48	0/2910
1	I	0.26	0/2196	0.49	0/2981
1	J	0.26	0/2200	0.49	0/2986
1	K	0.27	0/2061	0.48	0/2795
1	L	0.27	0/2202	0.48	0/2989
All	All	0.26	0/26134	0.49	0/35468

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	2155	0	2038	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2147	0	2037	100	0
1	C	2142	0	2023	99	3
1	D	2146	0	2033	95	0
1	E	2142	0	2032	105	0
1	F	2113	0	2002	101	3
1	G	2119	0	2009	101	0
1	H	2096	0	1978	97	0
1	I	2143	0	2027	105	0
1	J	2148	0	2037	94	0
1	K	2013	0	1920	97	0
1	L	2150	0	2038	96	0
2	A	27	0	22	10	0
2	B	27	0	22	8	0
2	C	27	0	22	4	0
2	D	27	0	22	1	0
2	E	27	0	22	6	0
2	F	27	0	22	8	0
2	G	27	0	22	5	0
2	H	27	0	22	7	0
2	I	27	0	22	9	0
2	J	27	0	22	7	0
2	K	27	0	22	10	0
2	L	27	0	22	6	0
3	A	19	0	17	8	0
3	B	19	0	17	12	0
3	C	19	0	17	9	0
3	D	19	0	17	8	0
3	E	19	0	17	4	0
3	F	19	0	17	4	0
3	G	19	0	17	5	0
3	H	19	0	17	9	0
3	I	19	0	17	7	0
3	J	19	0	17	6	0
3	K	19	0	17	5	0
3	L	19	0	17	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
All	All	26078	0	24642	1165	3

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 23.

All (1165) 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:H:180:ASN:HB3	2:H:501:SFG:HN1	1.24	1.02
1:C:171:LYS:HD2	1:C:171:LYS:H	1.28	0.98
1:J:171:LYS:HD2	1:J:171:LYS:H	1.28	0.98
1:K:171:LYS:HD2	1:K:171:LYS:H	1.28	0.98
1:A:171:LYS:HD2	1:A:171:LYS:H	1.28	0.97
1:L:171:LYS:H	1:L:171:LYS:HD2	1.28	0.97
1:G:171:LYS:H	1:G:171:LYS:HD2	1.28	0.97
1:D:171:LYS:H	1:D:171:LYS:HD2	1.30	0.96
1:H:171:LYS:H	1:H:171:LYS:HD2	1.29	0.96
1:I:171:LYS:HD2	1:I:171:LYS:H	1.30	0.96
1:B:171:LYS:H	1:B:171:LYS:HD2	1.30	0.95
1:E:171:LYS:H	1:E:171:LYS:HD2	1.28	0.95
1:F:171:LYS:HD2	1:F:171:LYS:H	1.29	0.94
2:K:501:SFG:HNE2	3:K:502:GPP:H43	1.33	0.93
1:I:231:GLU:HG3	1:J:221:LYS:HB3	1.51	0.92
1:G:221:LYS:HB3	1:H:231:GLU:HG3	1.52	0.90
1:D:44:VAL:HG12	1:D:273:LEU:HB3	1.51	0.89
1:J:48:LEU:HD12	1:J:82:ILE:HG23	1.51	0.88
1:A:231:GLU:HG3	1:B:221:LYS:HB3	1.56	0.88
1:D:208:VAL:HG22	1:D:294:LEU:HD23	1.56	0.88
1:H:208:VAL:HG22	1:H:294:LEU:HD23	1.56	0.88
1:B:146:ARG:HB2	1:B:146:ARG:HH11	1.39	0.88
1:G:231:GLU:HG3	1:H:221:LYS:HB3	1.56	0.87
1:I:208:VAL:HG22	1:I:294:LEU:HD23	1.56	0.87
1:C:208:VAL:HG22	1:C:294:LEU:HD23	1.57	0.86
1:L:208:VAL:HG22	1:L:294:LEU:HD23	1.58	0.85
2:E:501:SFG:HNE2	3:E:502:GPP:H42	1.40	0.85
1:F:208:VAL:HG22	1:F:294:LEU:HD23	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:HG22	1:A:294:LEU:HD23	1.57	0.85
1:K:208:VAL:HG22	1:K:294:LEU:HD23	1.58	0.85
1:J:208:VAL:HG22	1:J:294:LEU:HD23	1.57	0.85
1:E:146:ARG:HH11	1:E:146:ARG:HB2	1.42	0.85
1:E:208:VAL:HG22	1:E:294:LEU:HD23	1.57	0.84
1:G:146:ARG:HH11	1:G:146:ARG:HB2	1.42	0.84
1:D:146:ARG:HH11	1:D:146:ARG:HB2	1.40	0.84
1:E:221:LYS:HB3	1:F:231:GLU:HG3	1.59	0.84
1:L:146:ARG:HB2	1:L:146:ARG:HH11	1.42	0.84
1:K:146:ARG:HH11	1:K:146:ARG:HB2	1.42	0.84
1:I:146:ARG:HH11	1:I:146:ARG:HB2	1.42	0.84
1:J:146:ARG:HH11	1:J:146:ARG:HB2	1.42	0.84
1:H:146:ARG:HB2	1:H:146:ARG:HH11	1.42	0.83
1:C:146:ARG:HH11	1:C:146:ARG:HB2	1.43	0.83
1:K:221:LYS:HB3	1:L:231:GLU:HG3	1.60	0.83
1:G:181:GLU:HB3	3:G:502:GPP:H51	1.59	0.83
1:F:146:ARG:HH11	1:F:146:ARG:HB2	1.44	0.82
1:G:208:VAL:HG22	1:G:294:LEU:HD23	1.60	0.82
1:B:208:VAL:HG22	1:B:294:LEU:HD23	1.61	0.81
1:A:146:ARG:HB2	1:A:146:ARG:HH11	1.44	0.81
1:B:146:ARG:HB2	1:B:146:ARG:NH1	1.95	0.81
1:E:146:ARG:NH1	1:E:146:ARG:HB2	1.97	0.80
1:F:290:PHE:HZ	3:F:502:GPP:H101	1.46	0.80
1:G:59:TYR:O	1:G:92:GLN:HG2	1.82	0.80
1:L:180:ASN:HB3	2:L:501:SFG:HN1	1.46	0.80
1:G:146:ARG:NH1	1:G:146:ARG:HB2	1.97	0.80
1:D:146:ARG:NH1	1:D:146:ARG:HB2	1.96	0.79
1:H:146:ARG:HB2	1:H:146:ARG:NH1	1.97	0.79
1:D:59:TYR:O	1:D:92:GLN:HG2	1.82	0.79
2:E:501:SFG:HNE2	3:E:502:GPP:C4	1.96	0.79
1:H:180:ASN:HB3	2:H:501:SFG:N	1.96	0.79
1:C:146:ARG:HB2	1:C:146:ARG:NH1	1.98	0.78
1:K:146:ARG:HB2	1:K:146:ARG:NH1	1.97	0.78
1:L:48:LEU:HD12	1:L:82:ILE:HG23	1.63	0.78
1:E:231:GLU:HG3	1:F:221:LYS:HB3	1.65	0.78
1:I:146:ARG:NH1	1:I:146:ARG:HB2	1.97	0.78
1:J:146:ARG:NH1	1:J:146:ARG:HB2	1.98	0.78
1:J:59:TYR:O	1:J:92:GLN:HG2	1.84	0.78
1:L:146:ARG:NH1	1:L:146:ARG:HB2	1.98	0.77
1:F:146:ARG:HB2	1:F:146:ARG:NH1	1.99	0.77
1:A:146:ARG:HB2	1:A:146:ARG:NH1	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:HIS:HB2	2:F:501:SFG:HB1	1.67	0.77
1:I:180:ASN:HB3	2:I:501:SFG:HN1	1.49	0.77
1:A:59:TYR:O	1:A:92:GLN:HG2	1.86	0.76
2:I:501:SFG:HNE2	3:I:502:GPP:H42	1.50	0.76
1:E:195:HIS:O	1:E:199:LEU:HB2	1.86	0.75
1:C:195:HIS:O	1:C:199:LEU:HB2	1.86	0.75
1:C:210:GLY:HA3	3:C:502:GPP:H91	1.66	0.75
1:B:171:LYS:N	1:B:171:LYS:HD2	2.02	0.75
1:I:180:ASN:HB3	2:I:501:SFG:N	2.01	0.75
1:C:231:GLU:HG3	1:D:221:LYS:HB3	1.68	0.74
1:C:171:LYS:HD2	1:C:171:LYS:N	2.01	0.74
1:I:66:HIS:HA	1:I:69:LEU:HD23	1.69	0.74
1:J:171:LYS:HD2	1:J:171:LYS:N	2.03	0.74
1:K:171:LYS:HD2	1:K:171:LYS:N	2.01	0.74
1:G:171:LYS:N	1:G:171:LYS:HD2	2.01	0.74
1:H:171:LYS:N	1:H:171:LYS:HD2	2.03	0.74
1:A:26:ALA:O	1:A:27:THR:HG22	1.87	0.74
1:D:41:ALA:HB1	1:D:46:LEU:HD11	1.70	0.74
1:F:51:VAL:HG13	1:F:52:ASP:H	1.50	0.74
1:A:195:HIS:O	1:A:199:LEU:HB2	1.87	0.74
1:D:171:LYS:N	1:D:171:LYS:HD2	2.02	0.74
1:L:163:ASN:HD21	1:L:165:LEU:HB2	1.53	0.74
1:D:184:MET:HE1	3:D:502:GPP:H52	1.68	0.73
1:F:171:LYS:HD2	1:F:171:LYS:N	2.03	0.73
1:I:195:HIS:O	1:I:199:LEU:HB2	1.89	0.73
1:L:47:ARG:HH21	1:L:82:ILE:HD11	1.53	0.73
1:B:195:HIS:O	1:B:199:LEU:HB2	1.88	0.73
1:E:163:ASN:HD21	1:E:165:LEU:HB2	1.53	0.73
3:B:502:GPP:O2A	3:B:502:GPP:H42	1.88	0.73
1:G:195:HIS:O	1:G:199:LEU:HB2	1.89	0.73
1:L:171:LYS:HD2	1:L:171:LYS:N	2.02	0.73
1:B:134:VAL:HG23	1:B:162:CYS:HB3	1.70	0.72
1:B:59:TYR:O	1:B:92:GLN:HG2	1.89	0.72
2:K:501:SFG:HNE2	3:K:502:GPP:C4	2.02	0.72
1:I:163:ASN:HD21	1:I:165:LEU:HB2	1.52	0.72
1:E:59:TYR:O	1:E:92:GLN:HG2	1.88	0.72
1:J:195:HIS:O	1:J:199:LEU:HB2	1.88	0.72
1:C:163:ASN:HD21	1:C:165:LEU:HB2	1.54	0.72
1:H:195:HIS:O	1:H:199:LEU:HB2	1.90	0.72
1:J:134:VAL:HG23	1:J:162:CYS:HB3	1.70	0.72
1:K:195:HIS:O	1:K:199:LEU:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:LYS:N	1:E:171:LYS:HD2	2.03	0.72
1:C:134:VAL:HG23	1:C:162:CYS:HB3	1.71	0.72
1:D:134:VAL:HG23	1:D:162:CYS:HB3	1.70	0.72
1:F:134:VAL:HG23	1:F:162:CYS:HB3	1.72	0.72
1:K:134:VAL:HG23	1:K:162:CYS:HB3	1.72	0.72
1:L:195:HIS:O	1:L:199:LEU:HB2	1.90	0.72
1:I:163:ASN:ND2	1:I:165:LEU:HB2	2.06	0.71
1:D:163:ASN:HD21	1:D:165:LEU:HB2	1.55	0.71
1:L:59:TYR:O	1:L:92:GLN:HG2	1.90	0.71
2:A:501:SFG:HNE2	3:A:502:GPP:H42	1.55	0.71
1:B:163:ASN:HD21	1:B:165:LEU:HB2	1.55	0.71
1:D:195:HIS:O	1:D:199:LEU:HB2	1.91	0.71
1:E:163:ASN:ND2	1:E:165:LEU:HB2	2.06	0.71
1:C:163:ASN:ND2	1:C:165:LEU:HB2	2.06	0.71
1:G:134:VAL:HG23	1:G:162:CYS:HB3	1.72	0.71
1:A:163:ASN:HD21	1:A:165:LEU:HB2	1.55	0.70
1:F:195:HIS:O	1:F:199:LEU:HB2	1.92	0.70
1:G:48:LEU:O	1:G:51:VAL:HG12	1.91	0.70
1:I:134:VAL:HG23	1:I:162:CYS:HB3	1.73	0.70
1:A:171:LYS:HD2	1:A:171:LYS:N	2.02	0.70
1:H:258:THR:HB	1:H:259:PRO:HD3	1.72	0.70
1:H:59:TYR:O	1:H:92:GLN:HG2	1.91	0.70
1:K:163:ASN:HD21	1:K:165:LEU:HB2	1.57	0.70
1:I:69:LEU:HB3	1:I:77:TYR:HE1	1.57	0.70
1:G:258:THR:HB	1:G:259:PRO:HD3	1.74	0.70
1:I:171:LYS:HD2	1:I:171:LYS:N	2.04	0.69
1:A:134:VAL:HG23	1:A:162:CYS:HB3	1.74	0.69
1:A:180:ASN:HB3	2:A:501:SFG:N	2.07	0.69
1:H:163:ASN:HD21	1:H:165:LEU:HB2	1.55	0.69
1:E:134:VAL:HG23	1:E:162:CYS:HB3	1.74	0.69
1:J:163:ASN:HD21	1:J:165:LEU:HB2	1.57	0.69
1:H:134:VAL:HG23	1:H:162:CYS:HB3	1.74	0.69
1:K:171:LYS:CD	1:K:171:LYS:H	2.04	0.69
1:H:171:LYS:H	1:H:171:LYS:CD	2.05	0.69
1:A:163:ASN:ND2	1:A:165:LEU:HB2	2.08	0.69
1:D:171:LYS:CD	1:D:171:LYS:H	2.04	0.69
1:J:29:TYR:OH	1:J:232:CYS:HA	1.93	0.69
1:L:163:ASN:ND2	1:L:165:LEU:HB2	2.07	0.69
1:H:48:LEU:HD12	1:H:82:ILE:HG23	1.73	0.68
1:K:163:ASN:ND2	1:K:165:LEU:HB2	2.08	0.68
1:K:72:PRO:HA	1:K:77:TYR:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:LYS:H	1:L:171:LYS:CD	2.04	0.68
1:I:258:THR:HB	1:I:259:PRO:HD3	1.75	0.68
1:H:59:TYR:HE2	3:H:502:GPP:H103	1.58	0.68
1:C:171:LYS:H	1:C:171:LYS:CD	2.04	0.68
1:H:48:LEU:HG	1:H:86:HIS:HB2	1.75	0.68
1:K:43:PRO:HG2	1:K:46:LEU:HD12	1.76	0.68
1:H:163:ASN:ND2	1:H:165:LEU:HB2	2.09	0.68
1:J:171:LYS:CD	1:J:171:LYS:H	2.04	0.68
1:C:240:TYR:O	1:C:244:MET:HG3	1.94	0.68
1:C:258:THR:HB	1:C:259:PRO:HD3	1.75	0.68
1:J:258:THR:HB	1:J:259:PRO:HD3	1.76	0.68
1:G:163:ASN:HD21	1:G:165:LEU:HB2	1.58	0.68
1:A:258:THR:HB	1:A:259:PRO:HD3	1.76	0.68
1:D:163:ASN:ND2	1:D:165:LEU:HB2	2.08	0.68
1:L:258:THR:HB	1:L:259:PRO:HD3	1.75	0.68
1:B:171:LYS:CD	1:B:171:LYS:H	2.05	0.67
1:B:163:ASN:ND2	1:B:165:LEU:HB2	2.09	0.67
1:K:136:LEU:HD13	2:K:501:SFG:N1	2.09	0.67
1:K:258:THR:HB	1:K:259:PRO:HD3	1.76	0.67
1:K:231:GLU:HG3	1:L:221:LYS:HB3	1.76	0.67
1:L:134:VAL:HG23	1:L:162:CYS:HB3	1.74	0.67
1:G:171:LYS:CD	1:G:171:LYS:H	2.04	0.67
1:F:258:THR:HB	1:F:259:PRO:HD3	1.74	0.67
1:J:30:GLN:HG3	1:J:136:LEU:HD21	1.75	0.67
1:F:171:LYS:CD	1:F:171:LYS:H	2.05	0.67
1:G:163:ASN:ND2	1:G:165:LEU:HB2	2.10	0.67
1:A:180:ASN:HB3	2:A:501:SFG:HN1	1.59	0.66
1:B:258:THR:HB	1:B:259:PRO:HD3	1.77	0.66
1:I:48:LEU:HD12	1:I:82:ILE:HG23	1.78	0.66
1:L:61:ILE:HG12	1:L:92:GLN:HB3	1.77	0.66
1:B:180:ASN:HB3	2:B:501:SFG:HN1	1.60	0.66
1:E:74:ASP:HB3	1:E:80:ARG:HH22	1.60	0.66
1:D:258:THR:HB	1:D:259:PRO:HD3	1.77	0.66
1:J:180:ASN:HB3	2:J:501:SFG:HN1	1.60	0.66
1:J:163:ASN:ND2	1:J:165:LEU:HB2	2.10	0.66
1:B:37:TRP:HH2	3:B:502:GPP:H11	1.61	0.66
1:B:37:TRP:CH2	3:B:502:GPP:H11	2.30	0.66
1:L:240:TYR:O	1:L:244:MET:HG3	1.95	0.66
1:G:240:TYR:O	1:G:244:MET:HG3	1.96	0.66
1:J:53:GLY:HA3	1:J:147:ARG:NH2	2.11	0.66
1:H:147:ARG:O	1:H:151:LEU:HD23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:ASN:HB3	2:L:501:SFG:N	2.10	0.66
2:B:501:SFG:NE	3:B:502:GPP:H43	2.11	0.66
1:E:171:LYS:H	1:E:171:LYS:CD	2.05	0.66
2:A:501:SFG:HNE2	3:A:502:GPP:C4	2.09	0.66
1:F:147:ARG:O	1:F:151:LEU:HD23	1.96	0.66
1:F:163:ASN:ND2	1:F:165:LEU:HB2	2.11	0.66
1:E:258:THR:HB	1:E:259:PRO:HD3	1.78	0.65
1:G:184:MET:HE1	3:G:502:GPP:H52	1.77	0.65
1:C:221:LYS:HB3	1:D:231:GLU:HG3	1.78	0.65
1:F:163:ASN:HD21	1:F:165:LEU:HB2	1.59	0.65
1:H:274:VAL:HG13	1:H:278:GLU:OE1	1.97	0.65
1:G:274:VAL:HG13	1:G:278:GLU:OE1	1.97	0.65
1:F:240:TYR:O	1:F:244:MET:HG3	1.96	0.65
1:C:136:LEU:HD13	2:C:501:SFG:N1	2.11	0.64
1:E:274:VAL:HG13	1:E:278:GLU:OE1	1.97	0.64
1:H:240:TYR:O	1:H:244:MET:HG3	1.96	0.64
1:E:240:TYR:O	1:E:244:MET:HG3	1.98	0.64
1:K:147:ARG:O	1:K:151:LEU:HD23	1.97	0.64
1:G:212:TRP:CE2	1:G:236:SER:HB3	2.32	0.64
1:I:147:ARG:O	1:I:151:LEU:HD23	1.98	0.64
1:D:72:PRO:HA	1:D:77:TYR:CD2	2.33	0.64
1:L:212:TRP:CE2	1:L:236:SER:HB3	2.33	0.64
1:A:171:LYS:H	1:A:171:LYS:CD	2.05	0.64
1:G:136:LEU:HD13	2:G:501:SFG:C2	2.28	0.64
1:I:171:LYS:CD	1:I:171:LYS:H	2.06	0.64
1:J:147:ARG:O	1:J:151:LEU:HD23	1.98	0.64
1:D:240:TYR:O	1:D:244:MET:HG3	1.98	0.63
1:I:212:TRP:CE2	1:I:236:SER:HB3	2.33	0.63
1:I:274:VAL:HG13	1:I:278:GLU:OE1	1.98	0.63
1:A:147:ARG:O	1:A:151:LEU:HD23	1.98	0.63
1:B:147:ARG:O	1:B:151:LEU:HD23	1.98	0.63
1:L:147:ARG:O	1:L:151:LEU:HD23	1.98	0.63
1:G:58:HIS:HE1	1:G:93:ALA:HB2	1.63	0.63
1:J:212:TRP:CE2	1:J:236:SER:HB3	2.33	0.63
1:K:212:TRP:CE2	1:K:236:SER:HB3	2.33	0.63
1:D:212:TRP:CE2	1:D:236:SER:HB3	2.33	0.63
1:J:136:LEU:HD13	2:J:501:SFG:N1	2.14	0.63
1:K:53:GLY:HA3	1:K:147:ARG:NH2	2.13	0.63
2:I:501:SFG:HNE2	3:I:502:GPP:C4	2.11	0.63
1:C:147:ARG:O	1:C:151:LEU:HD23	1.99	0.63
1:F:59:TYR:O	1:F:92:GLN:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ARG:O	1:G:151:LEU:HD23	1.97	0.63
1:B:212:TRP:CE2	1:B:236:SER:HB3	2.34	0.63
1:E:48:LEU:O	1:E:51:VAL:HG22	1.98	0.63
1:F:212:TRP:CE2	1:F:236:SER:HB3	2.34	0.62
1:K:240:TYR:O	1:K:244:MET:HG3	1.99	0.62
1:A:184:MET:CE	3:A:502:GPP:H61	2.30	0.62
1:C:212:TRP:CE2	1:C:236:SER:HB3	2.35	0.62
1:G:184:MET:CE	3:G:502:GPP:H52	2.29	0.62
1:I:240:TYR:O	1:I:244:MET:HG3	1.99	0.62
1:J:32:ASP:HB3	1:J:231:GLU:OE2	1.99	0.62
1:D:237:ARG:O	1:D:241:LEU:HD23	2.00	0.62
1:E:212:TRP:CE2	1:E:236:SER:HB3	2.34	0.62
1:I:281:PHE:HE1	3:I:502:GPP:H92	1.64	0.62
1:A:240:TYR:O	1:A:244:MET:HG3	1.99	0.62
1:D:274:VAL:HG13	1:D:278:GLU:OE1	2.00	0.62
1:I:58:HIS:HE1	1:I:93:ALA:HB2	1.65	0.62
1:K:48:LEU:O	1:K:51:VAL:HG12	2.00	0.62
1:D:147:ARG:O	1:D:151:LEU:HD23	2.00	0.62
1:B:240:TYR:O	1:B:244:MET:HG3	1.99	0.61
1:C:274:VAL:HG13	1:C:278:GLU:OE1	2.00	0.61
1:B:42:ARG:HB2	1:B:45:ASN:HD22	1.64	0.61
1:E:27:THR:HA	1:E:30:GLN:CG	2.31	0.61
1:K:274:VAL:HG13	1:K:278:GLU:OE1	2.01	0.61
1:E:147:ARG:O	1:E:151:LEU:HD23	1.99	0.61
1:K:180:ASN:HB3	2:K:501:SFG:HN1	1.64	0.61
1:A:212:TRP:CE2	1:A:236:SER:HB3	2.35	0.61
1:I:44:VAL:O	1:I:48:LEU:HD13	2.01	0.61
1:I:281:PHE:CE1	3:I:502:GPP:H92	2.36	0.61
1:I:59:TYR:O	1:I:92:GLN:HG2	2.00	0.61
1:C:29:TYR:CE2	1:C:33:ILE:HD11	2.36	0.61
1:F:57:HIS:O	3:F:502:GPP:H12	2.00	0.60
1:K:70:GLY:HA3	1:K:80:ARG:HH21	1.66	0.60
1:H:212:TRP:CE2	1:H:236:SER:HB3	2.36	0.60
1:H:66:HIS:HA	1:H:69:LEU:HB3	1.84	0.60
1:C:181:GLU:HB3	3:C:502:GPP:H51	1.82	0.60
1:H:136:LEU:HD13	2:H:501:SFG:C2	2.32	0.60
1:A:103:VAL:HG21	1:A:109:LEU:HD11	1.84	0.60
2:B:501:SFG:HNE2	3:B:502:GPP:H43	1.65	0.60
1:I:48:LEU:O	1:I:51:VAL:HG12	2.01	0.60
1:D:37:TRP:HH2	3:D:502:GPP:H11	1.66	0.60
1:F:61:ILE:HG12	1:F:92:GLN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:HB3	1:B:231:GLU:HG3	1.84	0.59
1:C:237:ARG:O	1:C:241:LEU:HD23	2.02	0.59
1:K:146:ARG:HA	1:K:149:ARG:NH1	2.17	0.59
1:A:251:PRO:HD2	1:F:241:LEU:HG	1.84	0.59
1:I:48:LEU:HD21	1:I:85:LEU:HB3	1.83	0.59
1:F:274:VAL:HG13	1:F:278:GLU:OE1	2.02	0.59
1:J:240:TYR:O	1:J:244:MET:HG3	2.02	0.59
1:F:52:ASP:HB2	1:F:86:HIS:NE2	2.17	0.59
1:H:93:ALA:O	1:H:97:LEU:HD13	2.02	0.59
1:A:237:ARG:O	1:A:241:LEU:HD23	2.03	0.59
1:B:52:ASP:HB3	1:B:54:LEU:HG	1.83	0.59
1:L:146:ARG:HA	1:L:149:ARG:NH1	2.18	0.59
1:I:103:VAL:HG21	1:I:109:LEU:HD11	1.85	0.59
1:B:146:ARG:HA	1:B:149:ARG:NH1	2.18	0.59
1:I:218:GLN:HB2	1:J:29:TYR:CG	2.38	0.59
2:K:501:SFG:NE	3:K:502:GPP:H43	2.13	0.59
1:B:274:VAL:HG13	1:B:278:GLU:OE1	2.02	0.59
1:E:103:VAL:HG21	1:E:109:LEU:HD11	1.84	0.59
1:J:146:ARG:HA	1:J:149:ARG:NH1	2.18	0.59
1:C:93:ALA:O	1:C:97:LEU:HD13	2.03	0.58
1:G:41:ALA:HA	1:G:46:LEU:HD11	1.84	0.58
1:H:237:ARG:O	1:H:241:LEU:HD23	2.03	0.58
1:D:212:TRP:CZ2	1:D:236:SER:HB3	2.38	0.58
1:D:93:ALA:O	1:D:97:LEU:HD13	2.04	0.58
1:H:53:GLY:HA3	1:H:147:ARG:NH2	2.18	0.58
1:J:180:ASN:HB3	2:J:501:SFG:N	2.18	0.58
1:L:136:LEU:HD13	2:L:501:SFG:N1	2.18	0.58
1:F:237:ARG:O	1:F:241:LEU:HD23	2.03	0.58
1:A:274:VAL:HG13	1:A:278:GLU:OE1	2.03	0.58
1:B:53:GLY:HA3	1:B:147:ARG:NH2	2.18	0.58
1:B:35:ARG:HD2	1:I:73:GLY:O	2.04	0.58
1:G:237:ARG:O	1:G:241:LEU:HD23	2.03	0.58
1:I:146:ARG:HA	1:I:149:ARG:NH1	2.19	0.58
1:K:237:ARG:O	1:K:241:LEU:HD23	2.04	0.58
1:D:146:ARG:HA	1:D:149:ARG:NH1	2.19	0.58
1:G:146:ARG:HA	1:G:149:ARG:NH1	2.18	0.58
1:K:212:TRP:CZ2	1:K:236:SER:HB3	2.39	0.58
1:K:72:PRO:HA	1:K:77:TYR:CG	2.37	0.58
1:A:64:VAL:HG11	1:A:267:LEU:HD22	1.85	0.58
1:B:212:TRP:CZ2	1:B:236:SER:HB3	2.39	0.58
1:B:93:ALA:O	1:B:97:LEU:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLY:HA3	1:C:147:ARG:NH2	2.19	0.58
1:H:103:VAL:HG21	1:H:109:LEU:HD11	1.86	0.58
1:H:146:ARG:HA	1:H:149:ARG:NH1	2.19	0.58
1:J:274:VAL:HG13	1:J:278:GLU:OE1	2.03	0.58
1:A:69:LEU:HB3	1:A:77:TYR:HE1	1.68	0.58
1:E:52:ASP:HB2	1:E:86:HIS:NE2	2.19	0.58
1:L:237:ARG:O	1:L:241:LEU:HD23	2.04	0.58
1:F:212:TRP:CZ2	1:F:236:SER:HB3	2.39	0.57
1:A:146:ARG:HA	1:A:149:ARG:NH1	2.19	0.57
1:E:212:TRP:CZ2	1:E:236:SER:HB3	2.39	0.57
1:I:64:VAL:HG13	1:I:84:GLU:HG2	1.86	0.57
1:J:212:TRP:CZ2	1:J:236:SER:HB3	2.39	0.57
1:L:274:VAL:HG13	1:L:278:GLU:OE1	2.05	0.57
1:C:146:ARG:HA	1:C:149:ARG:NH1	2.20	0.57
1:I:212:TRP:CZ2	1:I:236:SER:HB3	2.39	0.57
1:J:237:ARG:O	1:J:241:LEU:HD23	2.04	0.57
1:C:212:TRP:CZ2	1:C:236:SER:HB3	2.40	0.57
1:J:93:ALA:O	1:J:97:LEU:HD13	2.03	0.57
1:K:93:ALA:O	1:K:97:LEU:HD13	2.05	0.57
1:A:212:TRP:CZ2	1:A:236:SER:HB3	2.39	0.57
1:K:43:PRO:CG	1:K:46:LEU:HD12	2.35	0.57
1:L:212:TRP:CZ2	1:L:236:SER:HB3	2.40	0.57
1:L:93:ALA:O	1:L:97:LEU:HD13	2.04	0.57
1:I:237:ARG:O	1:I:241:LEU:HD23	2.04	0.57
1:K:103:VAL:HG21	1:K:109:LEU:HD11	1.87	0.57
1:B:103:VAL:HG21	1:B:109:LEU:HD11	1.86	0.57
1:B:237:ARG:O	1:B:241:LEU:HD23	2.04	0.57
1:C:103:VAL:HG21	1:C:109:LEU:HD11	1.87	0.57
1:J:136:LEU:HD13	2:J:501:SFG:C2	2.34	0.57
1:F:103:VAL:HG21	1:F:109:LEU:HD11	1.87	0.56
1:F:167:THR:HG22	1:F:194:GLU:OE2	2.05	0.56
1:F:93:ALA:O	1:F:97:LEU:HD13	2.05	0.56
1:G:58:HIS:CE1	1:G:93:ALA:HB2	2.40	0.56
1:G:212:TRP:CZ2	1:G:236:SER:HB3	2.39	0.56
1:D:103:VAL:HG21	1:D:109:LEU:HD11	1.86	0.56
2:H:501:SFG:HNE2	3:H:502:GPP:H42	1.68	0.56
1:G:35:ARG:HA	1:G:38:ASN:HD22	1.70	0.56
1:C:29:TYR:O	1:C:32:ASP:HB2	2.06	0.56
1:E:146:ARG:HA	1:E:149:ARG:NH1	2.21	0.56
1:G:103:VAL:HG21	1:G:109:LEU:HD11	1.86	0.56
1:G:136:LEU:HD13	2:G:501:SFG:N1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:VAL:HG11	1:I:267:LEU:HD22	1.86	0.56
1:I:93:ALA:O	1:I:97:LEU:HD13	2.06	0.56
1:K:44:VAL:HG21	1:K:273:LEU:HB3	1.88	0.56
1:L:103:VAL:HG21	1:L:109:LEU:HD11	1.86	0.56
1:C:180:ASN:HB3	2:C:501:SFG:HN1	1.70	0.56
1:E:167:THR:HG22	1:E:194:GLU:OE2	2.06	0.56
1:F:146:ARG:HA	1:F:149:ARG:NH1	2.21	0.56
1:H:212:TRP:CZ2	1:H:236:SER:HB3	2.41	0.56
1:J:103:VAL:HG21	1:J:109:LEU:HD11	1.86	0.56
1:H:184:MET:SD	3:H:502:GPP:H7	2.46	0.56
1:E:93:ALA:O	1:E:97:LEU:HD13	2.05	0.55
1:E:237:ARG:O	1:E:241:LEU:HD23	2.05	0.55
1:F:48:LEU:O	1:F:51:VAL:HG12	2.05	0.55
1:B:44:VAL:HB	1:B:273:LEU:HB3	1.87	0.55
1:D:184:MET:CE	3:D:502:GPP:H52	2.37	0.55
1:I:167:THR:HG22	1:I:194:GLU:OE2	2.06	0.55
1:K:136:LEU:HD13	2:K:501:SFG:C2	2.36	0.55
1:B:202:GLY:O	1:C:215:ARG:NH1	2.39	0.55
1:G:93:ALA:O	1:G:97:LEU:HD13	2.05	0.55
1:I:136:LEU:HD13	2:I:501:SFG:N1	2.22	0.55
1:K:47:ARG:HG3	1:K:47:ARG:HH11	1.70	0.55
1:L:167:THR:HG22	1:L:194:GLU:OE2	2.07	0.55
1:B:164:MET:HG2	2:B:501:SFG:N1	2.21	0.55
1:C:167:THR:HG22	1:C:194:GLU:OE2	2.06	0.55
1:F:44:VAL:O	1:F:48:LEU:HD13	2.07	0.55
1:G:180:ASN:HB3	2:G:501:SFG:HN1	1.72	0.55
1:H:59:TYR:HE2	3:H:502:GPP:C10	2.18	0.55
1:J:167:THR:HG22	1:J:194:GLU:OE2	2.07	0.55
1:I:58:HIS:CE1	1:I:93:ALA:HB2	2.41	0.55
3:L:502:GPP:H41	3:L:502:GPP:H7	1.87	0.55
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.72	0.55
1:B:282:ILE:O	1:B:286:ARG:HG2	2.07	0.55
1:C:218:GLN:HB2	1:D:29:TYR:CD2	2.42	0.55
1:I:69:LEU:HB3	1:I:77:TYR:CE1	2.39	0.55
1:A:59:TYR:HE2	3:A:502:GPP:H92	1.72	0.55
1:B:167:THR:HG22	1:B:194:GLU:OE2	2.07	0.55
1:D:44:VAL:CG1	1:D:273:LEU:HB3	2.32	0.55
1:E:180:ASN:HB3	2:E:501:SFG:N	2.22	0.55
1:A:167:THR:HG22	1:A:194:GLU:OE2	2.07	0.54
1:A:93:ALA:O	1:A:97:LEU:HD13	2.07	0.54
1:A:241:LEU:HG	1:F:251:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ARG:NH1	1:I:202:GLY:O	2.40	0.54
1:H:167:THR:HG22	1:H:194:GLU:OE2	2.06	0.54
1:F:42:ARG:HB2	1:F:45:ASN:HD22	1.71	0.54
1:C:184:MET:HE1	3:C:502:GPP:H52	1.89	0.54
1:C:61:ILE:HG12	1:C:92:GLN:HB3	1.90	0.54
1:F:136:LEU:HD13	2:F:501:SFG:C6	2.37	0.54
1:I:69:LEU:O	1:I:80:ARG:NH2	2.36	0.54
1:J:48:LEU:O	1:J:51:VAL:HG12	2.07	0.54
1:G:167:THR:HG22	1:G:194:GLU:OE2	2.08	0.54
1:A:26:ALA:O	1:A:27:THR:CG2	2.56	0.54
1:G:218:GLN:HB2	1:H:29:TYR:CD2	2.43	0.54
1:K:167:THR:HG22	1:K:194:GLU:OE2	2.08	0.54
1:E:273:LEU:HD22	1:E:273:LEU:N	2.23	0.53
1:E:180:ASN:HB3	2:E:501:SFG:HN1	1.72	0.53
1:C:56:HIS:HB3	1:C:58:HIS:CE1	2.44	0.53
1:D:44:VAL:HG11	1:D:273:LEU:O	2.09	0.53
1:G:181:GLU:HB3	3:G:502:GPP:C5	2.34	0.53
1:C:184:MET:CE	3:C:502:GPP:H52	2.39	0.53
1:C:29:TYR:CD2	1:D:218:GLN:HB2	2.43	0.53
1:G:61:ILE:HD11	1:G:92:GLN:HA	1.90	0.53
1:J:146:ARG:HA	1:J:149:ARG:HH11	1.74	0.53
1:A:30:GLN:NE2	2:A:501:SFG:HN62	2.07	0.53
1:C:210:GLY:N	3:C:502:GPP:H93	2.24	0.53
1:C:282:ILE:O	1:C:286:ARG:HG2	2.09	0.53
1:C:218:GLN:HB2	1:D:29:TYR:CG	2.44	0.53
1:D:164:MET:HG2	2:D:501:SFG:N1	2.24	0.53
1:H:41:ALA:HB1	1:H:46:LEU:HD11	1.91	0.53
1:K:65:ASP:HB3	1:K:84:GLU:OE1	2.09	0.53
1:A:282:ILE:O	1:A:286:ARG:HG2	2.09	0.53
1:B:42:ARG:HB3	1:B:44:VAL:HG12	1.91	0.53
1:B:180:ASN:HB3	2:B:501:SFG:N	2.22	0.53
1:E:96:LEU:HD23	1:E:96:LEU:C	2.30	0.52
1:I:146:ARG:HA	1:I:149:ARG:HH11	1.75	0.52
1:B:146:ARG:HA	1:B:149:ARG:HH11	1.74	0.52
1:J:251:PRO:HD2	1:K:241:LEU:HG	1.91	0.52
1:D:59:TYR:HE2	3:D:502:GPP:H92	1.74	0.52
1:F:282:ILE:O	1:F:286:ARG:HG2	2.10	0.52
1:B:66:HIS:O	1:B:69:LEU:HB3	2.10	0.52
1:C:273:LEU:HD22	1:C:273:LEU:N	2.25	0.52
1:C:29:TYR:CE2	1:D:218:GLN:HB2	2.44	0.52
1:D:59:TYR:CE2	3:D:502:GPP:H92	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ASN:ND2	1:D:137:SER:HA	2.25	0.52
1:B:251:PRO:HD2	1:C:241:LEU:HG	1.91	0.52
3:B:502:GPP:PA	3:B:502:GPP:H42	2.50	0.52
1:C:27:THR:HB	1:C:28:PRO:HD3	1.91	0.52
1:D:200:ARG:HG2	1:D:201:VAL:N	2.25	0.52
1:L:53:GLY:HA3	1:L:147:ARG:NH2	2.24	0.52
1:E:32:ASP:HB3	1:E:231:GLU:OE2	2.09	0.52
1:G:180:ASN:HB3	2:G:501:SFG:N	2.24	0.52
1:H:273:LEU:HD22	1:H:273:LEU:N	2.25	0.52
1:H:282:ILE:O	1:H:286:ARG:HG2	2.10	0.52
1:B:253:THR:HA	1:C:254:VAL:O	2.10	0.52
1:C:136:LEU:HD13	2:C:501:SFG:C2	2.40	0.52
1:D:273:LEU:N	1:D:273:LEU:HD22	2.25	0.52
1:L:48:LEU:CD1	1:L:82:ILE:HG23	2.38	0.52
1:B:262:LEU:HD21	1:B:285:TYR:HB3	1.92	0.52
1:C:180:ASN:HB3	2:C:501:SFG:N	2.25	0.51
1:L:146:ARG:HA	1:L:149:ARG:HH11	1.75	0.51
1:A:146:ARG:HA	1:A:149:ARG:HH11	1.76	0.51
1:A:273:LEU:HD22	1:A:273:LEU:N	2.25	0.51
1:B:59:TYR:HE2	3:B:502:GPP:H92	1.75	0.51
1:E:200:ARG:HG2	1:E:201:VAL:N	2.25	0.51
1:G:61:ILE:HG12	1:G:92:GLN:HB3	1.92	0.51
1:H:146:ARG:HA	1:H:149:ARG:HH11	1.75	0.51
1:H:200:ARG:HG2	1:H:201:VAL:N	2.24	0.51
1:I:282:ILE:O	1:I:286:ARG:HG2	2.10	0.51
1:G:282:ILE:O	1:G:286:ARG:HG2	2.11	0.51
1:G:29:TYR:CD2	1:H:218:GLN:HB2	2.46	0.51
1:J:61:ILE:CD1	1:J:92:GLN:HA	2.40	0.51
1:K:46:LEU:HD21	1:K:116:ARG:NE	2.25	0.51
1:K:180:ASN:HB3	2:K:501:SFG:N	2.26	0.51
1:B:184:MET:HG2	3:B:502:GPP:H102	1.93	0.51
1:C:200:ARG:HG2	1:C:201:VAL:N	2.25	0.51
1:G:200:ARG:HG2	1:G:201:VAL:N	2.25	0.51
1:C:210:GLY:HA3	3:C:502:GPP:C9	2.37	0.51
1:F:65:ASP:OD1	1:F:68:ALA:HB3	2.10	0.51
1:K:273:LEU:HD22	1:K:273:LEU:N	2.26	0.51
1:A:68:ALA:C	1:A:69:LEU:HD12	2.31	0.51
1:D:72:PRO:HA	1:D:77:TYR:CE2	2.46	0.51
1:F:61:ILE:HD11	1:F:92:GLN:HA	1.93	0.51
1:J:59:TYR:CE2	3:J:502:GPP:H92	2.46	0.51
1:K:146:ARG:HA	1:K:149:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PHE:CZ	3:C:502:GPP:H103	2.46	0.51
1:C:96:LEU:C	1:C:96:LEU:HD23	2.32	0.51
1:A:57:HIS:HB2	2:A:501:SFG:O	2.11	0.50
1:D:282:ILE:O	1:D:286:ARG:HG2	2.11	0.50
1:K:96:LEU:C	1:K:96:LEU:HD23	2.31	0.50
1:B:42:ARG:HB2	1:B:45:ASN:ND2	2.26	0.50
1:F:273:LEU:HD22	1:F:273:LEU:N	2.26	0.50
1:J:282:ILE:O	1:J:286:ARG:HG2	2.11	0.50
1:E:27:THR:O	1:E:31:GLU:HG3	2.11	0.50
1:G:42:ARG:HG2	1:G:43:PRO:HD2	1.94	0.50
1:I:145:ASN:O	1:I:149:ARG:HG3	2.12	0.50
1:I:59:TYR:CZ	3:I:502:GPP:H11	2.47	0.50
1:K:184:MET:CE	3:K:502:GPP:H61	2.41	0.50
1:L:282:ILE:O	1:L:286:ARG:HG2	2.11	0.50
1:D:96:LEU:HD23	1:D:96:LEU:C	2.31	0.50
1:G:146:ARG:HA	1:G:149:ARG:HH11	1.74	0.50
1:G:273:LEU:N	1:G:273:LEU:HD22	2.26	0.50
1:J:202:GLY:O	1:K:215:ARG:NH1	2.44	0.50
1:A:65:ASP:O	1:A:69:LEU:HD13	2.11	0.50
1:E:262:LEU:HD21	1:E:285:TYR:HB3	1.94	0.50
1:K:282:ILE:O	1:K:286:ARG:HG2	2.12	0.50
1:E:29:TYR:O	1:E:32:ASP:HB2	2.11	0.50
1:E:51:VAL:HG23	1:E:52:ASP:N	2.26	0.50
1:F:146:ARG:HA	1:F:149:ARG:HH11	1.77	0.50
1:F:290:PHE:CZ	3:F:502:GPP:H101	2.37	0.50
1:B:70:GLY:HA3	1:B:80:ARG:HE	1.77	0.50
1:E:29:TYR:CZ	1:E:33:ILE:HD11	2.47	0.50
1:F:29:TYR:CZ	1:F:33:ILE:HD11	2.47	0.50
1:G:262:LEU:HD21	1:G:285:TYR:HB3	1.94	0.50
1:H:59:TYR:CE2	3:H:502:GPP:H103	2.45	0.50
1:J:113:GLY:O	2:J:501:SFG:HA	2.12	0.50
1:K:200:ARG:HG2	1:K:201:VAL:N	2.26	0.50
1:L:200:ARG:HG2	1:L:201:VAL:N	2.26	0.50
1:D:262:LEU:HD21	1:D:285:TYR:HB3	1.94	0.50
1:I:273:LEU:N	1:I:273:LEU:HD22	2.27	0.50
1:J:200:ARG:HG2	1:J:201:VAL:N	2.26	0.50
1:J:184:MET:HE3	3:J:502:GPP:H61	1.93	0.50
1:K:44:VAL:O	1:K:48:LEU:HD13	2.12	0.50
1:L:38:ASN:HB3	1:L:137:SER:OG	2.12	0.49
1:L:273:LEU:HD22	1:L:273:LEU:N	2.27	0.49
1:L:44:VAL:HB	1:L:273:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:HIS:HD2	1:F:59:TYR:O	1.95	0.49
1:J:262:LEU:HD21	1:J:285:TYR:HB3	1.94	0.49
1:J:59:TYR:HE2	3:J:502:GPP:H92	1.76	0.49
1:B:200:ARG:HG2	1:B:201:VAL:N	2.27	0.49
1:B:44:VAL:O	1:B:44:VAL:HG22	2.12	0.49
1:B:44:VAL:O	1:B:48:LEU:HD13	2.12	0.49
1:F:96:LEU:C	1:F:96:LEU:HD23	2.33	0.49
1:G:145:ASN:O	1:G:149:ARG:HG3	2.12	0.49
1:H:145:ASN:O	1:H:149:ARG:HG3	2.12	0.49
1:I:218:GLN:HB2	1:J:29:TYR:CD1	2.47	0.49
1:A:200:ARG:HG2	1:A:201:VAL:N	2.26	0.49
1:B:273:LEU:N	1:B:273:LEU:HD22	2.27	0.49
1:G:96:LEU:HD23	1:G:96:LEU:C	2.33	0.49
1:H:96:LEU:HD23	1:H:96:LEU:C	2.33	0.49
1:I:96:LEU:C	1:I:96:LEU:HD23	2.33	0.49
1:I:221:LYS:HB3	1:J:231:GLU:HG3	1.95	0.49
1:J:61:ILE:HD11	1:J:92:GLN:HA	1.95	0.49
1:F:294:LEU:C	1:F:294:LEU:HD13	2.33	0.49
1:E:146:ARG:HA	1:E:149:ARG:HH11	1.76	0.49
1:E:44:VAL:HG22	1:E:44:VAL:O	2.12	0.49
1:J:241:LEU:HG	1:K:251:PRO:HD2	1.94	0.49
1:C:146:ARG:HA	1:C:149:ARG:HH11	1.76	0.49
1:D:146:ARG:HA	1:D:149:ARG:HH11	1.76	0.49
1:I:200:ARG:HG2	1:I:201:VAL:N	2.27	0.49
1:L:96:LEU:C	1:L:96:LEU:HD23	2.32	0.49
1:A:262:LEU:HD21	1:A:285:TYR:HB3	1.93	0.49
1:F:167:THR:OG1	1:F:168:PRO:HD2	2.12	0.49
1:F:56:HIS:HB3	1:F:58:HIS:CE1	2.48	0.49
1:I:167:THR:HG21	1:I:198:PHE:CD2	2.48	0.49
1:A:145:ASN:O	1:A:149:ARG:HG3	2.13	0.49
1:F:262:LEU:HD21	1:F:285:TYR:HB3	1.95	0.49
1:H:136:LEU:HD13	2:H:501:SFG:N1	2.28	0.49
1:B:294:LEU:HD13	1:B:294:LEU:C	2.32	0.48
1:F:200:ARG:HG2	1:F:201:VAL:N	2.27	0.48
1:H:262:LEU:HD21	1:H:285:TYR:HB3	1.94	0.48
1:I:64:VAL:HG13	1:I:84:GLU:CG	2.43	0.48
1:F:145:ASN:O	1:F:149:ARG:HG3	2.13	0.48
1:F:49:GLY:HA3	1:F:55:TYR:CD1	2.48	0.48
1:I:65:ASP:O	1:I:68:ALA:HB3	2.14	0.48
1:J:29:TYR:HH	1:J:232:CYS:HA	1.76	0.48
1:L:145:ASN:O	1:L:149:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:HIS:HA	1:A:181:GLU:OE2	2.14	0.48
1:B:145:ASN:O	1:B:149:ARG:HG3	2.12	0.48
1:C:277:ILE:HG13	1:C:277:ILE:O	2.13	0.48
1:C:294:LEU:HD13	1:C:294:LEU:C	2.33	0.48
1:C:44:VAL:HB	1:C:273:LEU:HB3	1.95	0.48
1:J:96:LEU:C	1:J:96:LEU:HD23	2.33	0.48
1:L:262:LEU:HD21	1:L:285:TYR:HB3	1.95	0.48
1:G:42:ARG:CG	1:G:43:PRO:HD2	2.43	0.48
1:A:96:LEU:C	1:A:96:LEU:HD23	2.34	0.48
1:D:145:ASN:O	1:D:149:ARG:HG3	2.14	0.48
1:E:164:MET:HG2	2:E:501:SFG:N1	2.28	0.48
1:G:56:HIS:HB3	1:G:58:HIS:CD2	2.48	0.48
1:G:61:ILE:CD1	1:G:92:GLN:HA	2.44	0.48
1:I:136:LEU:HD13	2:I:501:SFG:C2	2.43	0.48
1:J:191:VAL:HG13	1:J:192:PHE:N	2.29	0.48
1:L:268:ARG:NH1	3:L:502:GPP:O2B	2.45	0.48
1:A:30:GLN:HB3	1:A:136:LEU:HD21	1.95	0.48
1:D:167:THR:HG22	1:D:194:GLU:OE2	2.13	0.48
1:F:138:ALA:HA	1:F:161:VAL:CG2	2.44	0.48
1:A:294:LEU:HD13	1:A:294:LEU:C	2.34	0.48
1:A:44:VAL:HG22	1:A:44:VAL:O	2.13	0.48
1:C:145:ASN:O	1:C:149:ARG:HG3	2.14	0.48
1:D:294:LEU:HD13	1:D:294:LEU:C	2.34	0.48
1:I:61:ILE:HG12	1:I:92:GLN:HB3	1.95	0.48
1:J:273:LEU:N	1:J:273:LEU:HD22	2.28	0.48
1:L:44:VAL:O	1:L:48:LEU:HB2	2.13	0.48
1:F:81:LEU:HD23	1:F:81:LEU:C	2.34	0.48
1:G:167:THR:OG1	1:G:168:PRO:HD2	2.14	0.48
1:H:294:LEU:C	1:H:294:LEU:HD13	2.34	0.48
1:H:56:HIS:HB3	1:H:58:HIS:CE1	2.49	0.48
1:H:241:LEU:HG	1:I:251:PRO:HD2	1.96	0.48
1:K:81:LEU:HD23	1:K:81:LEU:C	2.34	0.48
1:A:138:ALA:HA	1:A:161:VAL:CG2	2.44	0.48
1:I:30:GLN:HB3	1:I:136:LEU:HD21	1.96	0.48
1:L:81:LEU:C	1:L:81:LEU:HD23	2.34	0.48
1:L:61:ILE:HD11	1:L:92:GLN:HA	1.95	0.48
2:F:501:SFG:HNE2	3:F:502:GPP:H42	1.79	0.48
1:G:53:GLY:HA3	1:G:147:ARG:NH2	2.29	0.48
1:K:262:LEU:HD21	1:K:285:TYR:HB3	1.96	0.48
1:L:42:ARG:HG2	1:L:44:VAL:HG12	1.96	0.48
2:B:501:SFG:HNE2	3:B:502:GPP:C4	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:C	1:B:96:LEU:HD23	2.34	0.47
1:H:146:ARG:CB	1:H:146:ARG:HH11	2.22	0.47
1:H:254:VAL:O	1:I:253:THR:HA	2.14	0.47
3:H:502:GPP:H2	3:H:502:GPP:O1A	2.14	0.47
1:I:294:LEU:HD13	1:I:294:LEU:C	2.35	0.47
1:I:81:LEU:C	1:I:81:LEU:HD23	2.35	0.47
1:J:138:ALA:HA	1:J:161:VAL:CG2	2.44	0.47
1:D:138:ALA:HA	1:D:161:VAL:CG2	2.45	0.47
1:F:180:ASN:HB3	2:F:501:SFG:HN1	1.78	0.47
1:K:44:VAL:HG13	1:K:45:ASN:N	2.29	0.47
1:F:136:LEU:HD13	2:F:501:SFG:N1	2.29	0.47
1:H:66:HIS:HA	1:H:69:LEU:CB	2.44	0.47
1:J:135:THR:O	1:J:161:VAL:HA	2.14	0.47
1:J:294:LEU:HD13	1:J:294:LEU:C	2.34	0.47
1:A:184:MET:HE1	3:A:502:GPP:H61	1.95	0.47
1:A:191:VAL:HG13	1:A:192:PHE:N	2.30	0.47
1:D:81:LEU:C	1:D:81:LEU:HD23	2.34	0.47
1:E:115:GLY:O	1:E:140:GLN:HB3	2.14	0.47
1:E:147:ARG:CZ	1:E:151:LEU:HD21	2.45	0.47
1:G:294:LEU:HD13	1:G:294:LEU:C	2.35	0.47
1:H:138:ALA:HA	1:H:161:VAL:CG2	2.44	0.47
1:G:218:GLN:HB2	1:H:29:TYR:CE2	2.50	0.47
1:A:218:GLN:HB2	1:B:29:TYR:CG	2.50	0.47
1:K:107:ASP:HB3	1:K:175:ALA:CB	2.44	0.47
1:K:57:HIS:HB2	2:K:501:SFG:HG2	1.95	0.47
1:B:37:TRP:HH2	3:B:502:GPP:C1	2.25	0.47
1:C:40:GLU:O	1:C:41:ALA:HB3	2.15	0.47
1:G:107:ASP:HB3	1:G:175:ALA:CB	2.45	0.47
1:I:262:LEU:HD21	1:I:285:TYR:HB3	1.95	0.47
1:A:164:MET:HG2	2:A:501:SFG:N1	2.29	0.47
1:L:138:ALA:HA	1:L:161:VAL:CG2	2.45	0.47
1:L:277:ILE:O	1:L:277:ILE:HG13	2.14	0.47
1:C:262:LEU:HD21	1:C:285:TYR:HB3	1.97	0.47
1:D:214:PRO:HD2	1:D:237:ARG:NH1	2.29	0.47
1:I:191:VAL:HG13	1:I:192:PHE:N	2.30	0.47
1:L:294:LEU:C	1:L:294:LEU:HD13	2.36	0.47
1:L:136:LEU:HD13	2:L:501:SFG:C2	2.44	0.47
1:A:253:THR:HA	1:F:254:VAL:O	2.15	0.47
1:A:184:MET:HE3	3:A:502:GPP:H61	1.96	0.47
1:B:191:VAL:HG13	1:B:192:PHE:N	2.30	0.47
1:C:138:ALA:HA	1:C:161:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:LEU:HD13	1:G:129:CYS:SG	2.55	0.47
1:H:109:LEU:HD13	1:H:129:CYS:SG	2.55	0.47
1:J:167:THR:OG1	1:J:168:PRO:HD2	2.15	0.47
1:K:59:TYR:O	1:K:92:GLN:HG2	2.15	0.47
1:L:107:ASP:HB3	1:L:175:ALA:CB	2.45	0.47
1:A:81:LEU:C	1:A:81:LEU:HD23	2.36	0.47
1:B:146:ARG:HH11	1:B:146:ARG:CB	2.19	0.47
1:D:135:THR:O	1:D:161:VAL:HA	2.15	0.47
1:A:109:LEU:HD13	1:A:129:CYS:SG	2.55	0.46
1:A:182:SER:HB3	2:A:501:SFG:H5'2	1.96	0.46
1:H:277:ILE:HG13	1:H:277:ILE:O	2.15	0.46
1:C:107:ASP:HB3	1:C:175:ALA:CB	2.46	0.46
1:D:134:VAL:CG2	1:D:162:CYS:HB3	2.42	0.46
1:E:27:THR:HB	1:E:28:PRO:HD3	1.96	0.46
1:E:294:LEU:C	1:E:294:LEU:HD13	2.35	0.46
1:E:44:VAL:HB	1:E:273:LEU:HB3	1.97	0.46
1:H:147:ARG:CZ	1:H:151:LEU:HD21	2.44	0.46
1:H:58:HIS:HA	1:H:181:GLU:OE2	2.16	0.46
1:I:147:ARG:CZ	1:I:151:LEU:HD21	2.46	0.46
1:K:167:THR:HG21	1:K:198:PHE:CD2	2.50	0.46
1:C:167:THR:HG21	1:C:198:PHE:CD2	2.51	0.46
1:E:29:TYR:CD2	1:F:218:GLN:HB2	2.50	0.46
1:G:147:ARG:CZ	1:G:151:LEU:HD21	2.46	0.46
1:J:145:ASN:O	1:J:149:ARG:HG3	2.14	0.46
1:J:286:ARG:HG3	1:J:286:ARG:HH11	1.80	0.46
2:L:501:SFG:HG2	2:L:501:SFG:O	2.15	0.46
1:A:167:THR:HG21	1:A:198:PHE:CD2	2.51	0.46
1:C:81:LEU:C	1:C:81:LEU:HD23	2.36	0.46
1:D:167:THR:OG1	1:D:168:PRO:HD2	2.16	0.46
1:H:191:VAL:HG13	1:H:192:PHE:N	2.31	0.46
1:K:165:LEU:HD11	1:K:186:VAL:HB	1.98	0.46
1:L:216:TYR:CE2	1:L:289:SER:HB3	2.51	0.46
1:B:138:ALA:HA	1:B:161:VAL:CG2	2.45	0.46
1:E:145:ASN:O	1:E:149:ARG:HG3	2.16	0.46
1:F:31:GLU:O	1:F:35:ARG:HG3	2.16	0.46
1:G:241:LEU:HG	1:L:251:PRO:HD2	1.97	0.46
1:G:81:LEU:HD23	1:G:81:LEU:C	2.35	0.46
1:H:135:THR:O	1:H:161:VAL:HA	2.16	0.46
1:J:81:LEU:HD23	1:J:81:LEU:C	2.35	0.46
1:L:167:THR:HG21	1:L:198:PHE:CD2	2.51	0.46
1:E:138:ALA:HA	1:E:161:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LEU:HD13	1:F:129:CYS:SG	2.55	0.46
2:K:501:SFG:O	2:K:501:SFG:HG2	2.16	0.46
1:K:64:VAL:CG1	1:K:267:LEU:HD22	2.45	0.46
1:A:115:GLY:O	1:A:140:GLN:HB3	2.16	0.46
1:A:277:ILE:O	1:A:277:ILE:HG13	2.15	0.46
1:B:241:LEU:HG	1:C:251:PRO:HD2	1.97	0.46
1:E:135:THR:O	1:E:161:VAL:HA	2.15	0.46
1:E:167:THR:HG21	1:E:198:PHE:CD2	2.51	0.46
1:H:107:ASP:HB3	1:H:175:ALA:CB	2.46	0.46
1:J:134:VAL:CG2	1:J:162:CYS:HB3	2.42	0.46
1:K:277:ILE:HG13	1:K:277:ILE:O	2.16	0.46
1:K:294:LEU:C	1:K:294:LEU:HD13	2.35	0.46
1:B:167:THR:OG1	1:B:168:PRO:HD2	2.16	0.46
1:L:165:LEU:HD11	1:L:186:VAL:HB	1.98	0.46
1:B:167:THR:HG21	1:B:198:PHE:CD2	2.51	0.46
1:B:81:LEU:HD23	1:B:81:LEU:C	2.35	0.46
1:E:167:THR:OG1	1:E:168:PRO:HD2	2.16	0.46
1:E:81:LEU:C	1:E:81:LEU:HD23	2.36	0.46
1:H:81:LEU:HD23	1:H:81:LEU:C	2.36	0.46
1:I:135:THR:O	1:I:161:VAL:HA	2.16	0.46
1:I:146:ARG:HH11	1:I:146:ARG:CB	2.21	0.46
1:I:74:ASP:OD2	1:I:75:GLY:N	2.49	0.46
1:J:107:ASP:HB3	1:J:175:ALA:CB	2.46	0.46
1:J:39:ASN:O	1:J:40:GLU:C	2.53	0.46
1:K:47:ARG:HG3	1:K:47:ARG:NH1	2.31	0.46
1:E:107:ASP:HB3	1:E:175:ALA:CB	2.46	0.46
1:E:34:ALA:C	1:E:36:TYR:H	2.18	0.46
1:F:167:THR:HG21	1:F:198:PHE:CD2	2.51	0.46
1:H:184:MET:CE	3:H:502:GPP:H7	2.45	0.46
1:I:204:ARG:HD3	1:I:205:TYR:N	2.31	0.46
1:A:147:ARG:CZ	1:A:151:LEU:HD21	2.46	0.45
1:B:277:ILE:O	1:B:277:ILE:HG13	2.16	0.45
1:F:147:ARG:CZ	1:F:151:LEU:HD21	2.46	0.45
1:F:134:VAL:CG2	1:F:162:CYS:HB3	2.44	0.45
1:I:115:GLY:O	1:I:140:GLN:HB3	2.17	0.45
1:I:138:ALA:HA	1:I:161:VAL:CG2	2.46	0.45
1:H:251:PRO:HD2	1:I:241:LEU:HG	1.98	0.45
3:J:502:GPP:H7	3:J:502:GPP:C2	2.46	0.45
1:A:135:THR:O	1:A:161:VAL:HA	2.16	0.45
1:G:135:THR:O	1:G:161:VAL:HA	2.16	0.45
1:K:145:ASN:O	1:K:149:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:THR:O	1:L:161:VAL:HA	2.17	0.45
1:G:215:ARG:NH1	1:L:202:GLY:O	2.49	0.45
1:A:42:ARG:HB2	1:A:45:ASN:HD22	1.81	0.45
1:B:59:TYR:CE2	3:B:502:GPP:H92	2.52	0.45
1:F:107:ASP:HB3	1:F:175:ALA:CB	2.46	0.45
1:H:167:THR:OG1	1:H:168:PRO:HD2	2.16	0.45
1:E:218:GLN:HB2	1:F:29:TYR:CE2	2.51	0.45
1:G:134:VAL:CG2	1:G:162:CYS:HB3	2.43	0.45
1:G:167:THR:HG21	1:G:198:PHE:CD2	2.51	0.45
1:J:253:THR:HA	1:K:254:VAL:O	2.16	0.45
1:K:191:VAL:HG13	1:K:192:PHE:N	2.31	0.45
1:L:35:ARG:HG3	1:L:35:ARG:HH11	1.82	0.45
1:B:39:ASN:ND2	1:I:77:TYR:HD2	2.15	0.45
1:B:65:ASP:OD2	1:B:68:ALA:HB3	2.16	0.45
1:D:147:ARG:CZ	1:D:151:LEU:HD21	2.45	0.45
1:H:281:PHE:HZ	3:H:502:GPP:H102	1.81	0.45
1:J:167:THR:HG21	1:J:198:PHE:CD2	2.52	0.45
1:J:58:HIS:HA	1:J:181:GLU:OE2	2.17	0.45
1:K:167:THR:OG1	1:K:168:PRO:HD2	2.16	0.45
1:L:185:TYR:CD2	2:L:501:SFG:H8	2.51	0.45
1:A:43:PRO:C	1:A:45:ASN:H	2.20	0.45
1:C:49:GLY:HA3	1:C:55:TYR:CD1	2.50	0.45
1:G:286:ARG:HH11	1:G:286:ARG:HG3	1.82	0.45
1:J:115:GLY:O	1:J:140:GLN:HB3	2.17	0.45
1:J:182:SER:HB3	2:J:501:SFG:H5'2	1.99	0.45
1:K:138:ALA:HA	1:K:161:VAL:CG2	2.46	0.45
1:K:204:ARG:HD3	1:K:205:TYR:N	2.32	0.45
1:A:30:GLN:NE2	1:A:163:ASN:OD1	2.46	0.45
1:B:134:VAL:CG2	1:B:162:CYS:HB3	2.44	0.45
1:D:48:LEU:CD1	1:D:82:ILE:HG23	2.47	0.45
1:D:48:LEU:HD12	1:D:82:ILE:HG23	1.99	0.45
1:E:146:ARG:HH11	1:E:146:ARG:CB	2.21	0.45
1:F:29:TYR:O	1:F:32:ASP:HB2	2.17	0.45
1:G:138:ALA:HA	1:G:161:VAL:CG2	2.46	0.45
1:H:134:VAL:CG2	1:H:162:CYS:HB3	2.45	0.45
1:H:167:THR:HG21	1:H:198:PHE:CD2	2.51	0.45
1:D:184:MET:CE	3:D:502:GPP:H61	2.47	0.45
1:E:109:LEU:HD13	1:E:129:CYS:SG	2.57	0.45
1:E:61:ILE:HG12	1:E:92:GLN:HB3	1.98	0.45
1:I:167:THR:OG1	1:I:168:PRO:HD2	2.17	0.45
1:K:147:ARG:CZ	1:K:151:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TRP:O	1:A:226:ILE:HG13	2.17	0.45
1:A:286:ARG:HH11	1:A:286:ARG:HG3	1.81	0.45
1:B:286:ARG:HG3	1:B:286:ARG:HH11	1.82	0.45
1:D:277:ILE:O	1:D:277:ILE:HG13	2.16	0.45
1:G:191:VAL:HG13	1:G:192:PHE:N	2.32	0.45
1:I:109:LEU:HD13	1:I:129:CYS:SG	2.57	0.45
1:I:184:MET:CE	3:I:502:GPP:H61	2.47	0.45
1:A:134:VAL:HG22	1:A:162:CYS:O	2.16	0.45
1:A:167:THR:OG1	1:A:168:PRO:HD2	2.17	0.45
1:C:167:THR:OG1	1:C:168:PRO:HD2	2.16	0.45
1:E:165:LEU:HD11	1:E:186:VAL:HB	1.99	0.45
1:G:277:ILE:O	1:G:277:ILE:HG13	2.16	0.45
1:I:69:LEU:H	1:I:69:LEU:HD22	1.82	0.45
1:J:65:ASP:HB3	1:J:84:GLU:OE1	2.17	0.45
1:L:167:THR:OG1	1:L:168:PRO:HD2	2.17	0.45
1:B:42:ARG:NH1	1:B:42:ARG:HG2	2.32	0.44
1:D:165:LEU:HD11	1:D:186:VAL:HB	1.99	0.44
1:E:191:VAL:HG13	1:E:192:PHE:N	2.32	0.44
1:J:277:ILE:HG13	1:J:277:ILE:O	2.16	0.44
1:K:206:VAL:HG12	1:K:207:THR:N	2.32	0.44
1:K:286:ARG:HG3	1:K:286:ARG:HH11	1.81	0.44
1:A:26:ALA:O	1:A:27:THR:CB	2.64	0.44
1:D:95:PHE:CE2	1:D:257:LEU:HD21	2.52	0.44
1:F:57:HIS:HB2	2:F:501:SFG:CB	2.44	0.44
1:H:204:ARG:HD3	1:H:205:TYR:N	2.31	0.44
1:H:61:ILE:HG12	1:H:92:GLN:HB3	2.00	0.44
1:I:107:ASP:HB3	1:I:175:ALA:CB	2.47	0.44
1:I:214:PRO:HD2	1:I:237:ARG:NH1	2.33	0.44
1:K:111:ASP:OD1	1:K:114:CYS:HA	2.18	0.44
1:A:214:PRO:HD2	1:A:237:ARG:NH1	2.33	0.44
1:B:135:THR:O	1:B:161:VAL:HA	2.17	0.44
1:B:35:ARG:HG3	1:B:35:ARG:HH11	1.81	0.44
1:C:108:THR:C	1:C:109:LEU:HD12	2.38	0.44
1:C:95:PHE:CE2	1:C:257:LEU:HD21	2.53	0.44
1:E:218:GLN:HB2	1:F:29:TYR:CD2	2.51	0.44
1:E:282:ILE:O	1:E:286:ARG:HG2	2.17	0.44
1:E:95:PHE:CE2	1:E:257:LEU:HD21	2.53	0.44
1:E:95:PHE:HA	1:E:98:ASP:OD2	2.16	0.44
1:F:204:ARG:HD3	1:F:205:TYR:N	2.32	0.44
1:J:61:ILE:HG12	1:J:92:GLN:HB3	1.98	0.44
1:B:37:TRP:HB3	1:B:137:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ASP:HB3	1:D:175:ALA:CB	2.48	0.44
1:D:167:THR:HG21	1:D:198:PHE:CD2	2.53	0.44
1:F:277:ILE:O	1:F:277:ILE:HG13	2.17	0.44
1:G:214:PRO:HD2	1:G:237:ARG:NH1	2.33	0.44
1:G:29:TYR:CG	1:H:218:GLN:HB2	2.53	0.44
1:I:165:LEU:HD11	1:I:186:VAL:HB	1.99	0.44
1:A:146:ARG:CB	1:A:146:ARG:HH11	2.22	0.44
1:B:165:LEU:HD11	1:B:186:VAL:HB	2.00	0.44
1:C:206:VAL:HG12	1:C:207:THR:N	2.33	0.44
1:E:136:LEU:HD13	2:E:501:SFG:N1	2.33	0.44
1:E:277:ILE:HG13	1:E:277:ILE:O	2.16	0.44
1:F:191:VAL:HG13	1:F:192:PHE:N	2.32	0.44
2:F:501:SFG:HG2	2:F:501:SFG:H4'	1.84	0.44
1:G:188:LEU:O	1:G:191:VAL:HG12	2.17	0.44
1:G:58:HIS:HA	1:G:181:GLU:OE2	2.18	0.44
1:H:209:THR:HG21	1:H:240:TYR:CZ	2.53	0.44
1:H:51:VAL:HG23	1:H:52:ASP:N	2.32	0.44
1:J:147:ARG:CZ	1:J:151:LEU:HD21	2.47	0.44
1:K:221:LYS:HG3	1:K:222:TRP:N	2.33	0.44
1:K:64:VAL:HG11	1:K:267:LEU:HD22	1.98	0.44
1:B:147:ARG:CZ	1:B:151:LEU:HD21	2.47	0.44
1:B:194:GLU:OE1	1:B:194:GLU:HA	2.18	0.44
1:B:48:LEU:N	1:B:48:LEU:HD12	2.32	0.44
1:C:204:ARG:HD3	1:C:205:TYR:N	2.32	0.44
1:D:115:GLY:O	1:D:140:GLN:HB3	2.17	0.44
1:D:206:VAL:HG12	1:D:207:THR:N	2.33	0.44
1:D:202:GLY:O	1:E:215:ARG:NH1	2.51	0.44
1:G:221:LYS:HG3	1:G:222:TRP:N	2.33	0.44
1:G:95:PHE:CE2	1:G:257:LEU:HD21	2.53	0.44
1:H:206:VAL:HG12	1:H:207:THR:N	2.33	0.44
1:H:69:LEU:O	1:H:80:ARG:NE	2.46	0.44
1:K:57:HIS:HB2	2:K:501:SFG:O	2.17	0.44
1:A:136:LEU:HD13	2:A:501:SFG:C2	2.48	0.44
1:B:27:THR:O	1:B:28:PRO:C	2.55	0.44
1:C:134:VAL:CG2	1:C:162:CYS:HB3	2.45	0.44
1:C:165:LEU:HD11	1:C:186:VAL:HB	2.00	0.44
1:C:59:TYR:O	1:C:92:GLN:HG2	2.17	0.44
1:D:61:ILE:HG12	1:D:92:GLN:HB3	2.00	0.44
1:E:221:LYS:HG3	1:E:222:TRP:N	2.33	0.44
1:A:107:ASP:HB3	1:A:175:ALA:CB	2.48	0.44
1:B:107:ASP:HB3	1:B:175:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HD3	1:B:205:TYR:N	2.33	0.44
3:D:502:GPP:O2B	3:D:502:GPP:O2A	2.35	0.44
1:E:56:HIS:HB3	1:E:58:HIS:CE1	2.53	0.44
1:F:214:PRO:HD2	1:F:237:ARG:NH1	2.33	0.44
1:G:206:VAL:HG12	1:G:207:THR:N	2.33	0.44
1:K:95:PHE:CE2	1:K:257:LEU:HD21	2.53	0.44
1:E:64:VAL:HG23	1:E:263:PRO:HB3	1.99	0.44
1:E:76:GLY:O	1:E:80:ARG:NH1	2.51	0.44
1:G:165:LEU:HD11	1:G:186:VAL:HB	2.00	0.44
1:H:188:LEU:O	1:H:191:VAL:HG12	2.18	0.44
1:J:204:ARG:HD3	1:J:205:TYR:N	2.33	0.44
1:L:204:ARG:HD3	1:L:205:TYR:N	2.31	0.44
1:A:59:TYR:CE2	3:A:502:GPP:H92	2.52	0.43
1:C:111:ASP:OD1	1:C:114:CYS:HA	2.18	0.43
1:C:147:ARG:CZ	1:C:151:LEU:HD21	2.48	0.43
1:D:221:LYS:HG3	1:D:222:TRP:N	2.33	0.43
1:F:194:GLU:OE1	1:F:194:GLU:HA	2.18	0.43
1:A:254:VAL:O	1:F:253:THR:HA	2.18	0.43
1:I:221:LYS:HG3	1:I:222:TRP:N	2.33	0.43
1:B:39:ASN:ND2	1:I:77:TYR:CD2	2.86	0.43
1:L:49:GLY:HA2	1:L:86:HIS:CE1	2.53	0.43
1:A:204:ARG:HD3	1:A:205:TYR:N	2.33	0.43
1:B:221:LYS:HG3	1:B:222:TRP:N	2.33	0.43
1:D:109:LEU:HD13	1:D:129:CYS:SG	2.58	0.43
1:A:202:GLY:O	1:F:215:ARG:NH1	2.51	0.43
1:H:286:ARG:HG3	1:H:286:ARG:HH11	1.83	0.43
3:H:502:GPP:H103	3:H:502:GPP:H51	2.00	0.43
1:K:69:LEU:HG	1:K:77:TYR:CE1	2.53	0.43
3:L:502:GPP:O1A	3:L:502:GPP:O1B	2.35	0.43
1:A:221:LYS:HG3	1:A:222:TRP:N	2.34	0.43
1:B:188:LEU:O	1:B:191:VAL:HG12	2.18	0.43
3:B:502:GPP:C4	3:B:502:GPP:O1	2.65	0.43
1:D:64:VAL:HG11	1:D:267:LEU:HD22	2.00	0.43
1:G:204:ARG:HD3	1:G:205:TYR:N	2.33	0.43
1:H:111:ASP:OD1	1:H:114:CYS:HA	2.17	0.43
1:I:188:LEU:O	1:I:191:VAL:HG12	2.18	0.43
1:I:277:ILE:O	1:I:277:ILE:HG13	2.18	0.43
1:J:108:THR:C	1:J:109:LEU:HD12	2.38	0.43
1:J:165:LEU:HD11	1:J:186:VAL:HB	2.00	0.43
1:K:188:LEU:O	1:K:191:VAL:HG12	2.18	0.43
1:L:147:ARG:CZ	1:L:151:LEU:HD21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:LEU:HD13	1:E:235:HIS:CD2	2.54	0.43
1:H:115:GLY:O	1:H:140:GLN:HB3	2.18	0.43
1:H:221:LYS:HG3	1:H:222:TRP:N	2.33	0.43
1:I:194:GLU:OE1	1:I:194:GLU:HA	2.19	0.43
1:K:214:PRO:HD2	1:K:237:ARG:NH1	2.33	0.43
1:K:53:GLY:HA3	1:K:147:ARG:HH21	1.80	0.43
1:L:64:VAL:HG23	1:L:263:PRO:HB3	2.00	0.43
1:A:69:LEU:HB3	1:A:77:TYR:CE1	2.52	0.43
1:C:37:TRP:CD1	1:C:140:GLN:NE2	2.87	0.43
1:C:135:THR:O	1:C:161:VAL:HA	2.17	0.43
1:C:209:THR:HG21	1:C:240:TYR:CZ	2.53	0.43
1:C:281:PHE:HZ	3:C:502:GPP:H103	1.84	0.43
1:D:146:ARG:CB	1:D:146:ARG:HH11	2.20	0.43
1:D:47:ARG:O	1:D:50:ASP:HB2	2.18	0.43
1:E:58:HIS:HA	1:E:181:GLU:OE2	2.19	0.43
1:F:221:LYS:HG3	1:F:222:TRP:N	2.33	0.43
1:H:113:GLY:O	2:H:501:SFG:HA	2.18	0.43
1:J:221:LYS:HG3	1:J:222:TRP:N	2.33	0.43
1:J:44:VAL:HB	1:J:273:LEU:HB3	2.01	0.43
1:C:210:GLY:H	3:C:502:GPP:H93	1.82	0.43
1:E:45:ASN:OD1	3:E:502:GPP:O2A	2.36	0.43
1:F:222:TRP:O	1:F:226:ILE:HG13	2.18	0.43
1:F:188:LEU:HD13	1:F:235:HIS:CD2	2.54	0.43
1:F:95:PHE:HA	1:F:98:ASP:OD2	2.19	0.43
1:G:52:ASP:HB2	1:G:86:HIS:NE2	2.34	0.43
1:K:134:VAL:CG2	1:K:162:CYS:HB3	2.44	0.43
1:C:221:LYS:HG3	1:C:222:TRP:N	2.33	0.43
1:D:188:LEU:O	1:D:191:VAL:HG12	2.19	0.43
1:D:194:GLU:OE1	1:D:194:GLU:HA	2.18	0.43
1:C:29:TYR:CZ	1:D:218:GLN:HB2	2.54	0.43
1:H:222:TRP:O	1:H:226:ILE:HG13	2.19	0.43
1:J:146:ARG:HH11	1:J:146:ARG:CB	2.22	0.43
1:J:206:VAL:HG12	1:J:207:THR:N	2.32	0.43
1:C:191:VAL:HG13	1:C:192:PHE:N	2.34	0.43
1:C:214:PRO:HD2	1:C:237:ARG:NH1	2.33	0.43
1:E:206:VAL:HG12	1:E:207:THR:N	2.33	0.43
1:F:48:LEU:N	1:F:48:LEU:HD12	2.34	0.43
1:F:51:VAL:HG13	1:F:52:ASP:N	2.24	0.43
1:H:165:LEU:HD11	1:H:186:VAL:HB	1.99	0.43
1:H:194:GLU:HA	1:H:194:GLU:OE1	2.19	0.43
1:J:194:GLU:OE1	1:J:194:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:HIS:HB3	1:L:58:HIS:CE1	2.53	0.43
1:L:95:PHE:HA	1:L:98:ASP:OD2	2.19	0.43
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.19	0.43
1:B:43:PRO:C	1:B:45:ASN:H	2.21	0.43
1:K:109:LEU:HD13	1:K:129:CYS:SG	2.59	0.43
1:L:188:LEU:O	1:L:191:VAL:HG12	2.19	0.43
1:L:204:ARG:HD3	1:L:297:ALA:O	2.18	0.43
1:L:29:TYR:O	1:L:32:ASP:HB2	2.18	0.43
1:A:40:GLU:HB3	1:A:41:ALA:H	1.56	0.43
1:A:59:TYR:OH	3:A:502:GPP:H2	2.19	0.43
1:E:188:LEU:O	1:E:191:VAL:HG12	2.18	0.43
1:G:72:PRO:HA	1:G:77:TYR:CE2	2.53	0.43
1:L:184:MET:HE3	3:L:502:GPP:H61	1.99	0.43
1:A:234:ILE:HD13	1:A:290:PHE:CE1	2.54	0.42
1:A:61:ILE:HG23	1:A:92:GLN:HB3	2.01	0.42
1:A:95:PHE:CE2	1:A:257:LEU:HD21	2.54	0.42
1:E:76:GLY:C	1:E:80:ARG:NH1	2.72	0.42
1:F:37:TRP:CE2	2:F:501:SFG:H3'	2.54	0.42
1:G:124:HIS:O	1:G:128:GLY:N	2.41	0.42
1:G:216:TYR:CE2	1:G:289:SER:HB3	2.54	0.42
1:L:206:VAL:HG12	1:L:207:THR:N	2.33	0.42
1:B:115:GLY:O	1:B:140:GLN:HB3	2.19	0.42
1:C:109:LEU:HD13	1:C:129:CYS:SG	2.59	0.42
1:D:108:THR:C	1:D:109:LEU:HD12	2.39	0.42
1:D:191:VAL:HG13	1:D:192:PHE:N	2.33	0.42
1:D:25:PRO:O	1:D:26:ALA:C	2.58	0.42
1:D:95:PHE:HA	1:D:98:ASP:OD2	2.20	0.42
1:E:214:PRO:HD2	1:E:237:ARG:NH1	2.34	0.42
1:E:49:GLY:HA2	1:E:54:LEU:O	2.19	0.42
1:I:222:TRP:O	1:I:226:ILE:HG13	2.19	0.42
1:J:188:LEU:O	1:J:191:VAL:HG12	2.19	0.42
1:L:109:LEU:HD13	1:L:129:CYS:SG	2.59	0.42
1:A:165:LEU:HD11	1:A:186:VAL:HB	2.02	0.42
1:A:188:LEU:O	1:A:191:VAL:HG12	2.19	0.42
1:B:214:PRO:HD2	1:B:237:ARG:NH1	2.34	0.42
1:E:36:TYR:OH	1:E:42:ARG:NH2	2.52	0.42
1:F:42:ARG:HB2	1:F:45:ASN:ND2	2.33	0.42
1:G:115:GLY:O	1:G:140:GLN:HB3	2.19	0.42
1:I:134:VAL:CG2	1:I:162:CYS:HB3	2.45	0.42
1:J:111:ASP:OD1	1:J:114:CYS:HA	2.18	0.42
1:K:147:ARG:NE	1:K:151:LEU:HD21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:THR:C	1:L:109:LEU:HD12	2.40	0.42
1:L:146:ARG:CB	1:L:146:ARG:HH11	2.22	0.42
1:L:191:VAL:HG13	1:L:192:PHE:N	2.33	0.42
1:A:56:HIS:HB3	1:A:58:HIS:CE1	2.54	0.42
1:B:134:VAL:HG22	1:B:162:CYS:O	2.19	0.42
1:B:222:TRP:O	1:B:226:ILE:HG13	2.20	0.42
1:C:286:ARG:HH11	1:C:286:ARG:HG3	1.84	0.42
1:D:286:ARG:HH11	1:D:286:ARG:HG3	1.84	0.42
1:F:135:THR:O	1:F:161:VAL:HA	2.19	0.42
1:G:111:ASP:OD1	1:G:114:CYS:HA	2.19	0.42
1:G:146:ARG:HH11	1:G:146:ARG:CB	2.22	0.42
1:G:222:TRP:O	1:G:226:ILE:HG13	2.19	0.42
1:L:124:HIS:O	1:L:128:GLY:N	2.40	0.42
1:L:286:ARG:HG3	1:L:286:ARG:HH11	1.83	0.42
1:A:136:LEU:HD13	2:A:501:SFG:N1	2.34	0.42
1:C:115:GLY:O	1:C:140:GLN:HB3	2.19	0.42
1:C:42:ARG:HB3	1:C:44:VAL:HG12	2.02	0.42
1:E:107:ASP:O	1:E:129:CYS:HB2	2.20	0.42
1:E:195:HIS:HA	1:E:198:PHE:CZ	2.54	0.42
1:F:216:TYR:CE2	1:F:289:SER:HB3	2.54	0.42
1:G:194:GLU:OE1	1:G:194:GLU:HA	2.19	0.42
1:H:188:LEU:HD13	1:H:235:HIS:CD2	2.55	0.42
1:I:170:GLU:HB2	1:I:173:THR:HG21	2.02	0.42
1:I:182:SER:HB3	2:I:501:SFG:H5'2	2.02	0.42
1:J:134:VAL:HG22	1:J:162:CYS:O	2.19	0.42
1:L:221:LYS:HG3	1:L:222:TRP:N	2.34	0.42
1:L:67:ALA:C	1:L:69:LEU:H	2.22	0.42
1:D:107:ASP:O	1:D:129:CYS:HB2	2.19	0.42
1:E:27:THR:HA	1:E:30:GLN:HG3	1.99	0.42
1:E:43:PRO:C	1:E:45:ASN:H	2.23	0.42
1:E:76:GLY:O	1:E:80:ARG:HG3	2.20	0.42
1:F:107:ASP:O	1:F:129:CYS:HB2	2.20	0.42
1:F:286:ARG:HH11	1:F:286:ARG:HG3	1.85	0.42
1:G:209:THR:HG21	1:G:240:TYR:CZ	2.55	0.42
1:H:253:THR:HA	1:I:254:VAL:O	2.20	0.42
1:H:216:TYR:CE2	1:H:289:SER:HB3	2.55	0.42
1:H:95:PHE:HA	1:H:98:ASP:OD2	2.20	0.42
1:I:164:MET:HG2	2:I:501:SFG:N1	2.35	0.42
1:L:95:PHE:CE2	1:L:257:LEU:HD21	2.55	0.42
1:A:48:LEU:O	1:A:51:VAL:HG12	2.20	0.42
1:B:95:PHE:HA	1:B:98:ASP:OD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ARG:HH11	1:F:146:ARG:CB	2.23	0.42
1:H:214:PRO:HD2	1:H:237:ARG:NH1	2.34	0.42
1:I:134:VAL:HG22	1:I:162:CYS:O	2.19	0.42
1:A:69:LEU:N	1:A:69:LEU:CD1	2.83	0.42
1:C:134:VAL:HG22	1:C:162:CYS:O	2.20	0.42
1:F:111:ASP:OD1	1:F:114:CYS:HA	2.19	0.42
1:G:78:GLU:OE2	1:G:272:SER:OG	2.36	0.42
1:H:147:ARG:NE	1:H:151:LEU:HD21	2.35	0.42
1:K:188:LEU:HD13	1:K:235:HIS:CD2	2.55	0.42
1:L:214:PRO:HD2	1:L:237:ARG:NH1	2.34	0.42
1:E:134:VAL:CG2	1:E:162:CYS:HB3	2.46	0.42
1:E:204:ARG:HD3	1:E:205:TYR:N	2.35	0.42
1:E:27:THR:HA	1:E:30:GLN:HG2	2.00	0.42
1:H:108:THR:C	1:H:109:LEU:HD12	2.40	0.42
1:J:230:PHE:CE1	3:J:502:GPP:H43	2.55	0.42
1:J:214:PRO:HD2	1:J:237:ARG:NH1	2.35	0.42
1:J:216:TYR:CE2	1:J:289:SER:HB3	2.55	0.42
1:L:208:VAL:CG2	1:L:294:LEU:HD23	2.41	0.42
1:E:108:THR:C	1:E:109:LEU:HD12	2.40	0.42
1:E:147:ARG:NE	1:E:151:LEU:HD21	2.35	0.42
1:F:147:ARG:NE	1:F:151:LEU:HD21	2.35	0.42
1:F:229:HIS:CD2	1:F:277:ILE:HB	2.55	0.42
1:H:164:MET:HG2	2:H:501:SFG:N1	2.35	0.42
1:I:95:PHE:CE2	1:I:257:LEU:HD21	2.55	0.42
1:J:254:VAL:O	1:K:253:THR:HA	2.20	0.42
1:L:115:GLY:O	1:L:140:GLN:HB3	2.19	0.42
1:B:206:VAL:HG12	1:B:207:THR:N	2.34	0.41
1:C:194:GLU:OE1	1:C:194:GLU:HA	2.20	0.41
1:C:95:PHE:HA	1:C:98:ASP:OD2	2.19	0.41
1:C:29:TYR:CG	1:D:218:GLN:HB2	2.55	0.41
1:F:206:VAL:HG12	1:F:207:THR:N	2.36	0.41
2:I:501:SFG:NE	3:I:502:GPP:H42	2.27	0.41
1:J:29:TYR:O	1:J:33:ILE:HG12	2.19	0.41
1:K:44:VAL:HG13	1:K:45:ASN:H	1.85	0.41
1:B:95:PHE:CE2	1:B:257:LEU:HD21	2.54	0.41
2:B:501:SFG:HG2	2:B:501:SFG:O	2.20	0.41
1:E:184:MET:HE3	3:E:502:GPP:H61	2.02	0.41
1:E:198:PHE:CD1	1:E:198:PHE:C	2.94	0.41
1:I:95:PHE:HA	1:I:98:ASP:OD2	2.20	0.41
1:J:95:PHE:CE2	1:J:257:LEU:HD21	2.54	0.41
1:K:108:THR:C	1:K:109:LEU:HD12	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:GLU:HA	1:K:194:GLU:OE1	2.20	0.41
1:A:134:VAL:CG2	1:A:162:CYS:HB3	2.47	0.41
1:A:188:LEU:HD13	1:A:235:HIS:CD2	2.55	0.41
1:E:48:LEU:N	1:E:48:LEU:HD12	2.36	0.41
1:F:108:THR:C	1:F:109:LEU:HD12	2.40	0.41
1:F:134:VAL:HG22	1:F:162:CYS:O	2.19	0.41
1:I:206:VAL:HG12	1:I:207:THR:N	2.35	0.41
1:K:135:THR:O	1:K:161:VAL:HA	2.20	0.41
1:G:204:ARG:HD3	1:G:297:ALA:O	2.20	0.41
1:G:43:PRO:C	1:G:45:ASN:H	2.22	0.41
1:I:188:LEU:HD13	1:I:235:HIS:CD2	2.55	0.41
1:I:64:VAL:CG1	1:I:267:LEU:HD22	2.50	0.41
1:B:147:ARG:NE	1:B:151:LEU:HD21	2.36	0.41
1:B:254:VAL:O	1:C:253:THR:HA	2.21	0.41
1:D:204:ARG:HD3	1:D:205:TYR:N	2.35	0.41
1:D:214:PRO:HD2	1:D:237:ARG:HH12	1.85	0.41
1:E:170:GLU:HB2	1:E:173:THR:HG21	2.03	0.41
1:E:65:ASP:OD1	1:E:67:ALA:HB3	2.21	0.41
1:H:208:VAL:CG2	1:H:294:LEU:HD23	2.40	0.41
1:I:286:ARG:HH11	1:I:286:ARG:HG3	1.84	0.41
1:J:113:GLY:O	2:J:501:SFG:CA	2.69	0.41
1:K:218:GLN:HB2	1:L:29:TYR:CD2	2.55	0.41
1:L:49:GLY:HA3	1:L:55:TYR:CD1	2.56	0.41
1:B:108:THR:C	1:B:109:LEU:HD12	2.40	0.41
1:B:188:LEU:HD13	1:B:235:HIS:CD2	2.56	0.41
1:F:124:HIS:O	1:F:128:GLY:N	2.41	0.41
1:I:218:GLN:HB2	1:J:29:TYR:CD2	2.55	0.41
1:K:69:LEU:HG	1:K:77:TYR:HE1	1.86	0.41
1:L:52:ASP:OD2	1:L:86:HIS:NE2	2.54	0.41
1:A:124:HIS:O	1:A:128:GLY:N	2.41	0.41
1:A:27:THR:O	1:A:27:THR:HG23	2.20	0.41
1:F:95:PHE:CE2	1:F:257:LEU:HD21	2.55	0.41
1:I:204:ARG:HD3	1:I:297:ALA:O	2.20	0.41
1:J:30:GLN:O	1:J:34:ALA:N	2.50	0.41
1:K:57:HIS:NE2	1:K:116:ARG:HG3	2.35	0.41
1:L:194:GLU:HA	1:L:194:GLU:OE1	2.20	0.41
1:A:95:PHE:HA	1:A:98:ASP:OD2	2.21	0.41
1:B:216:TYR:CE2	1:B:289:SER:HB3	2.56	0.41
1:E:194:GLU:HA	1:E:194:GLU:OE1	2.20	0.41
1:E:29:TYR:HH	1:E:232:CYS:HA	1.85	0.41
1:E:51:VAL:CG2	1:E:52:ASP:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:GLU:HB2	1:F:173:THR:HG21	2.03	0.41
1:G:108:THR:C	1:G:109:LEU:HD12	2.41	0.41
1:I:247:ASN:O	1:I:249:LEU:HD13	2.20	0.41
1:A:28:PRO:O	1:A:31:GLU:HB3	2.21	0.41
1:B:136:LEU:HD13	2:B:501:SFG:N1	2.36	0.41
1:C:48:LEU:CD1	1:C:82:ILE:HG23	2.51	0.41
1:D:248:ARG:HB3	1:D:300:VAL:OXT	2.21	0.41
1:F:188:LEU:O	1:F:191:VAL:HG12	2.20	0.41
1:G:107:ASP:O	1:G:129:CYS:HB2	2.21	0.41
1:G:95:PHE:HA	1:G:98:ASP:OD2	2.21	0.41
1:I:108:THR:C	1:I:109:LEU:HD12	2.41	0.41
1:J:222:TRP:O	1:J:226:ILE:HG13	2.21	0.41
1:L:147:ARG:NE	1:L:151:LEU:HD21	2.36	0.41
1:A:147:ARG:NE	1:A:151:LEU:HD21	2.35	0.41
1:A:229:HIS:CD2	1:A:277:ILE:HB	2.56	0.41
1:C:188:LEU:HD13	1:C:235:HIS:CD2	2.56	0.41
1:D:181:GLU:HB3	3:D:502:GPP:H51	2.02	0.41
1:E:283:GLU:O	1:E:286:ARG:HB2	2.21	0.41
1:F:165:LEU:HD11	1:F:186:VAL:HB	2.02	0.41
1:K:95:PHE:HA	1:K:98:ASP:OD2	2.20	0.41
1:A:206:VAL:HG12	1:A:207:THR:N	2.36	0.41
1:D:198:PHE:CD1	1:D:198:PHE:C	2.94	0.41
1:H:51:VAL:HG21	1:H:86:HIS:CD2	2.56	0.41
1:L:195:HIS:HA	1:L:198:PHE:CZ	2.56	0.41
1:B:111:ASP:OD1	1:B:114:CYS:HA	2.20	0.40
1:B:198:PHE:C	1:B:198:PHE:CD1	2.95	0.40
1:C:188:LEU:HA	1:C:191:VAL:HG12	2.03	0.40
1:C:71:ASP:HA	1:C:72:PRO:HD3	1.93	0.40
1:E:134:VAL:HG22	1:E:162:CYS:O	2.21	0.40
1:F:198:PHE:C	1:F:198:PHE:CD1	2.95	0.40
1:G:195:HIS:HA	1:G:198:PHE:CZ	2.56	0.40
1:G:57:HIS:HB2	2:G:501:SFG:O	2.21	0.40
1:H:134:VAL:HG22	1:H:162:CYS:O	2.21	0.40
1:K:216:TYR:CE2	1:K:289:SER:HB3	2.55	0.40
1:L:27:THR:HG23	1:L:30:GLN:H	1.86	0.40
1:A:27:THR:HG21	1:A:30:GLN:HG3	2.03	0.40
1:E:216:TYR:CE2	1:E:289:SER:HB3	2.57	0.40
1:G:43:PRO:C	1:G:45:ASN:N	2.74	0.40
1:K:222:TRP:O	1:K:226:ILE:HG13	2.20	0.40
1:K:184:MET:HE1	3:K:502:GPP:H61	2.03	0.40
1:L:134:VAL:CG2	1:L:162:CYS:HB3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:ASP:HB3	1:L:84:GLU:OE1	2.22	0.40
1:B:33:ILE:HA	1:B:33:ILE:HD13	1.95	0.40
1:C:204:ARG:HD3	1:C:297:ALA:O	2.21	0.40
1:C:216:TYR:O	1:D:28:PRO:HD2	2.21	0.40
1:D:51:VAL:CG2	1:D:52:ASP:N	2.84	0.40
1:E:143:PHE:C	1:E:143:PHE:CD1	2.95	0.40
1:I:111:ASP:OD1	1:I:114:CYS:HA	2.21	0.40
1:K:115:GLY:O	1:K:140:GLN:HB3	2.21	0.40
1:L:188:LEU:HA	1:L:191:VAL:HG12	2.03	0.40
1:L:42:ARG:HE	1:L:42:ARG:HB2	1.72	0.40
1:C:147:ARG:NE	1:C:151:LEU:HD21	2.36	0.40
1:D:111:ASP:OD1	1:D:114:CYS:HA	2.22	0.40
1:D:195:HIS:HA	1:D:198:PHE:CZ	2.56	0.40
1:D:209:THR:OG1	1:D:210:GLY:N	2.55	0.40
1:D:51:VAL:HG22	1:D:86:HIS:CD2	2.56	0.40
1:F:115:GLY:O	1:F:140:GLN:HB3	2.21	0.40
1:G:147:ARG:NE	1:G:151:LEU:HD21	2.36	0.40
1:G:43:PRO:O	1:G:45:ASN:N	2.55	0.40
1:G:45:ASN:OD1	3:G:502:GPP:O2A	2.40	0.40
1:I:209:THR:HG21	1:I:240:TYR:CZ	2.57	0.40
1:J:184:MET:CE	3:J:502:GPP:H61	2.52	0.40
1:K:195:HIS:HA	1:K:198:PHE:CZ	2.56	0.40
1:L:111:ASP:OD1	1:L:114:CYS:HA	2.22	0.40
1:A:69:LEU:N	1:A:69:LEU:HD12	2.37	0.40
1:D:147:ARG:NE	1:D:151:LEU:HD21	2.36	0.40
1:E:222:TRP:O	1:E:226:ILE:HG13	2.21	0.40
1:G:218:GLN:HB2	1:H:29:TYR:CG	2.57	0.40
1:I:59:TYR:HE1	1:I:268:ARG:HH12	1.70	0.40
1:K:198:PHE:CD1	1:K:198:PHE:C	2.95	0.40
1:L:51:VAL:CG2	1:L:86:HIS:CD2	3.04	0.40

All (3) 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:C:125:GLN:O	1:F:142:GLU:OE1[1_565]	2.05	0.15
1:C:125:GLN:O	1:F:142:GLU:OE2[1_565]	2.07	0.13
1:C:125:GLN:O	1:F:142:GLU:CD[1_565]	2.19	0.01

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	273/320 (85%)	249 (91%)	21 (8%)	3 (1%)	14	50
1	B	269/320 (84%)	251 (93%)	17 (6%)	1 (0%)	34	72
1	C	272/320 (85%)	249 (92%)	23 (8%)	0	100	100
1	D	269/320 (84%)	248 (92%)	20 (7%)	1 (0%)	34	72
1	E	268/320 (84%)	246 (92%)	20 (8%)	2 (1%)	22	60
1	F	263/320 (82%)	240 (91%)	21 (8%)	2 (1%)	19	57
1	G	265/320 (83%)	247 (93%)	17 (6%)	1 (0%)	34	72
1	H	262/320 (82%)	238 (91%)	23 (9%)	1 (0%)	34	72
1	I	271/320 (85%)	254 (94%)	17 (6%)	0	100	100
1	J	268/320 (84%)	245 (91%)	19 (7%)	4 (2%)	10	42
1	K	256/320 (80%)	237 (93%)	19 (7%)	0	100	100
1	L	269/320 (84%)	244 (91%)	23 (9%)	2 (1%)	22	60
All	All	3205/3840 (84%)	2948 (92%)	240 (8%)	17 (0%)	29	68

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	B	67	ALA
1	D	26	ALA
1	F	67	ALA
1	J	41	ALA
1	L	67	ALA
1	F	51	VAL
1	H	53	GLY
1	J	40	GLU
1	L	51	VAL
1	J	72	PRO
1	J	73	GLY

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Mol	Chain	Res	Type
1	A	70	GLY
1	E	44	VAL
1	E	75	GLY
1	G	44	VAL
1	A	71	ASP

5.3.2 Protein sidechains (i)

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	222/254 (87%)	216 (97%)	6 (3%)	44	77
1	B	222/254 (87%)	217 (98%)	5 (2%)	50	80
1	C	220/254 (87%)	211 (96%)	9 (4%)	30	67
1	D	221/254 (87%)	214 (97%)	7 (3%)	39	74
1	E	222/254 (87%)	216 (97%)	6 (3%)	44	77
1	F	217/254 (85%)	211 (97%)	6 (3%)	43	77
1	G	219/254 (86%)	211 (96%)	8 (4%)	34	70
1	H	214/254 (84%)	208 (97%)	6 (3%)	43	77
1	I	221/254 (87%)	213 (96%)	8 (4%)	35	70
1	J	223/254 (88%)	216 (97%)	7 (3%)	40	75
1	K	209/254 (82%)	204 (98%)	5 (2%)	49	79
1	L	222/254 (87%)	214 (96%)	8 (4%)	35	70
All	All	2632/3048 (86%)	2551 (97%)	81 (3%)	40	75

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	92	GLN
1	A	136	LEU
1	A	146	ARG
1	A	184	MET

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Mol	Chain	Res	Type
1	A	262	LEU
1	B	92	GLN
1	B	136	LEU
1	B	146	ARG
1	B	184	MET
1	B	262	LEU
1	C	32	ASP
1	C	37	TRP
1	C	42	ARG
1	C	74	ASP
1	C	92	GLN
1	C	136	LEU
1	C	146	ARG
1	C	184	MET
1	C	262	LEU
1	D	44	VAL
1	D	51	VAL
1	D	92	GLN
1	D	136	LEU
1	D	146	ARG
1	D	184	MET
1	D	262	LEU
1	E	71	ASP
1	E	92	GLN
1	E	136	LEU
1	E	146	ARG
1	E	184	MET
1	E	262	LEU
1	F	32	ASP
1	F	92	GLN
1	F	136	LEU
1	F	146	ARG
1	F	184	MET
1	F	262	LEU
1	G	40	GLU
1	G	58	HIS
1	G	71	ASP
1	G	92	GLN
1	G	136	LEU
1	G	146	ARG
1	G	184	MET
1	G	262	LEU

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Mol	Chain	Res	Type
1	H	32	ASP
1	H	92	GLN
1	H	136	LEU
1	H	146	ARG
1	H	184	MET
1	H	262	LEU
1	I	40	GLU
1	I	52	ASP
1	I	58	HIS
1	I	92	GLN
1	I	136	LEU
1	I	146	ARG
1	I	184	MET
1	I	262	LEU
1	J	27	THR
1	J	52	ASP
1	J	92	GLN
1	J	136	LEU
1	J	146	ARG
1	J	184	MET
1	J	262	LEU
1	K	92	GLN
1	K	136	LEU
1	K	146	ARG
1	K	184	MET
1	K	262	LEU
1	L	40	GLU
1	L	48	LEU
1	L	92	GLN
1	L	136	LEU
1	L	146	ARG
1	L	184	MET
1	L	188	LEU
1	L	262	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	45	ASN
1	A	252	GLN
1	B	45	ASN

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Mol	Chain	Res	Type
1	B	252	GLN
1	C	45	ASN
1	C	140	GLN
1	C	252	GLN
1	D	252	GLN
1	E	45	ASN
1	E	252	GLN
1	F	45	ASN
1	F	252	GLN
1	G	38	ASN
1	G	45	ASN
1	G	163	ASN
1	G	252	GLN
1	H	163	ASN
1	H	252	GLN
1	I	252	GLN
1	J	252	GLN
1	K	252	GLN
1	L	45	ASN
1	L	252	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	GPP	A	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.42	4 (19%)
2	SFG	H	501	-	22,29,29	0.73	1 (4%)	18,42,42	1.65	2 (11%)
3	GPP	D	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.35	4 (19%)
2	SFG	L	501	-	22,29,29	0.73	1 (4%)	18,42,42	1.64	2 (11%)
2	SFG	F	501	-	22,29,29	0.72	0	18,42,42	1.58	3 (16%)
3	GPP	J	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.40	4 (19%)
2	SFG	K	501	-	22,29,29	0.74	1 (4%)	18,42,42	1.73	3 (16%)
2	SFG	I	501	-	22,29,29	0.74	1 (4%)	18,42,42	1.65	2 (11%)
2	SFG	E	501	-	22,29,29	0.75	1 (4%)	18,42,42	1.64	3 (16%)
2	SFG	C	501	-	22,29,29	0.74	1 (4%)	18,42,42	1.67	3 (16%)
3	GPP	F	502	4	16,18,18	1.93	5 (31%)	21,25,25	1.44	4 (19%)
2	SFG	J	501	-	22,29,29	0.73	1 (4%)	18,42,42	1.63	2 (11%)
3	GPP	G	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.43	4 (19%)
2	SFG	D	501	-	22,29,29	0.75	1 (4%)	18,42,42	1.57	3 (16%)
2	SFG	B	501	-	22,29,29	0.73	0	18,42,42	1.60	2 (11%)
3	GPP	H	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.39	4 (19%)
2	SFG	G	501	-	22,29,29	0.74	1 (4%)	18,42,42	1.60	2 (11%)
3	GPP	B	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.51	5 (23%)
2	SFG	A	501	-	22,29,29	0.72	0	18,42,42	1.56	2 (11%)
3	GPP	K	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.43	4 (19%)
3	GPP	I	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.39	4 (19%)
3	GPP	C	502	4	16,18,18	1.93	5 (31%)	21,25,25	1.49	4 (19%)
3	GPP	E	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.41	4 (19%)
3	GPP	L	502	4	16,18,18	1.94	5 (31%)	21,25,25	1.45	4 (19%)

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	GPP	A	502	4	-	0/19/19/19	-
2	SFG	H	501	-	-	0/9/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GPP	D	502	4	-	5/19/19/19	-
2	SFG	L	501	-	-	0/9/33/33	0/3/3/3
2	SFG	F	501	-	-	0/9/33/33	0/3/3/3
3	GPP	J	502	4	-	3/19/19/19	-
2	SFG	K	501	-	-	0/9/33/33	0/3/3/3
2	SFG	I	501	-	-	0/9/33/33	0/3/3/3
2	SFG	E	501	-	-	0/9/33/33	0/3/3/3
2	SFG	C	501	-	-	0/9/33/33	0/3/3/3
3	GPP	F	502	4	-	9/19/19/19	-
2	SFG	J	501	-	-	0/9/33/33	0/3/3/3
3	GPP	G	502	4	-	0/19/19/19	-
2	SFG	D	501	-	-	1/9/33/33	0/3/3/3
2	SFG	B	501	-	-	0/9/33/33	0/3/3/3
3	GPP	H	502	4	-	2/19/19/19	-
2	SFG	G	501	-	-	0/9/33/33	0/3/3/3
3	GPP	B	502	4	-	3/19/19/19	-
2	SFG	A	501	-	-	0/9/33/33	0/3/3/3
3	GPP	K	502	4	-	3/19/19/19	-
3	GPP	I	502	4	-	4/19/19/19	-
3	GPP	C	502	4	-	1/19/19/19	-
3	GPP	E	502	4	-	2/19/19/19	-
3	GPP	L	502	4	-	3/19/19/19	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	502	GPP	PB-O1B	3.41	1.61	1.50
3	I	502	GPP	PB-O1B	3.41	1.61	1.50
3	A	502	GPP	PB-O1B	3.39	1.61	1.50
3	J	502	GPP	PB-O1B	3.39	1.61	1.50
3	F	502	GPP	C6-C7	-3.39	1.39	1.50
3	K	502	GPP	PB-O1B	3.39	1.61	1.50
3	D	502	GPP	C6-C7	-3.38	1.39	1.50
3	L	502	GPP	PB-O1B	3.38	1.61	1.50
3	D	502	GPP	PB-O1B	3.38	1.61	1.50
3	K	502	GPP	C6-C7	-3.38	1.39	1.50
3	C	502	GPP	C6-C7	-3.38	1.39	1.50
3	E	502	GPP	PB-O1B	3.38	1.61	1.50
3	B	502	GPP	PB-O1B	3.37	1.61	1.50
3	B	502	GPP	C6-C7	-3.37	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	GPP	PB-O1B	3.37	1.61	1.50
3	I	502	GPP	C6-C7	-3.37	1.39	1.50
3	F	502	GPP	PB-O1B	3.36	1.61	1.50
3	A	502	GPP	C6-C7	-3.36	1.39	1.50
3	G	502	GPP	PB-O1B	3.36	1.61	1.50
3	J	502	GPP	C6-C7	-3.36	1.39	1.50
3	H	502	GPP	C6-C7	-3.36	1.39	1.50
3	E	502	GPP	C6-C7	-3.36	1.39	1.50
3	G	502	GPP	C6-C7	-3.36	1.39	1.50
3	L	502	GPP	C6-C7	-3.35	1.39	1.50
3	G	502	GPP	C1-C2	-3.27	1.39	1.49
3	A	502	GPP	C1-C2	-3.25	1.39	1.49
3	C	502	GPP	C1-C2	-3.25	1.39	1.49
3	H	502	GPP	C1-C2	-3.25	1.39	1.49
3	L	502	GPP	C1-C2	-3.25	1.39	1.49
3	J	502	GPP	C1-C2	-3.24	1.39	1.49
3	F	502	GPP	C1-C2	-3.24	1.39	1.49
3	K	502	GPP	C1-C2	-3.24	1.39	1.49
3	E	502	GPP	C1-C2	-3.24	1.39	1.49
3	I	502	GPP	C1-C2	-3.24	1.39	1.49
3	D	502	GPP	C1-C2	-3.23	1.39	1.49
3	B	502	GPP	C1-C2	-3.19	1.39	1.49
3	B	502	GPP	C2-C3	2.73	1.39	1.33
3	K	502	GPP	C2-C3	2.73	1.39	1.33
3	A	502	GPP	C2-C3	2.71	1.39	1.33
3	H	502	GPP	C2-C3	2.71	1.39	1.33
3	C	502	GPP	C2-C3	2.71	1.39	1.33
3	L	502	GPP	C2-C3	2.70	1.39	1.33
3	J	502	GPP	C2-C3	2.70	1.39	1.33
3	F	502	GPP	C2-C3	2.70	1.39	1.33
3	E	502	GPP	C2-C3	2.69	1.39	1.33
3	I	502	GPP	C2-C3	2.69	1.39	1.33
3	D	502	GPP	C2-C3	2.69	1.39	1.33
3	G	502	GPP	C2-C3	2.68	1.39	1.33
3	B	502	GPP	C7-C8	2.50	1.39	1.32
3	J	502	GPP	C7-C8	2.50	1.39	1.32
3	A	502	GPP	C7-C8	2.50	1.39	1.32
3	E	502	GPP	C7-C8	2.49	1.39	1.32
3	K	502	GPP	C7-C8	2.48	1.39	1.32
3	H	502	GPP	C7-C8	2.47	1.39	1.32
3	L	502	GPP	C7-C8	2.46	1.39	1.32
3	F	502	GPP	C7-C8	2.46	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	502	GPP	C7-C8	2.45	1.39	1.32
3	D	502	GPP	C7-C8	2.45	1.39	1.32
3	I	502	GPP	C7-C8	2.44	1.39	1.32
3	C	502	GPP	C7-C8	2.43	1.39	1.32
2	D	501	SFG	O4'-C1'	2.14	1.44	1.41
2	E	501	SFG	O4'-C1'	2.13	1.44	1.41
2	C	501	SFG	O4'-C1'	2.10	1.44	1.41
2	G	501	SFG	O4'-C1'	2.05	1.43	1.41
2	I	501	SFG	O4'-C1'	2.04	1.43	1.41
2	K	501	SFG	O4'-C1'	2.03	1.43	1.41
2	J	501	SFG	O4'-C1'	2.02	1.43	1.41
2	H	501	SFG	O4'-C1'	2.01	1.43	1.41
2	L	501	SFG	O4'-C1'	2.00	1.43	1.41

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	501	SFG	N3-C2-N1	-4.51	121.63	128.68
2	J	501	SFG	N3-C2-N1	-4.48	121.68	128.68
2	A	501	SFG	N3-C2-N1	-4.47	121.69	128.68
2	H	501	SFG	N3-C2-N1	-4.47	121.70	128.68
2	F	501	SFG	N3-C2-N1	-4.47	121.70	128.68
2	C	501	SFG	N3-C2-N1	-4.46	121.70	128.68
2	G	501	SFG	N3-C2-N1	-4.44	121.73	128.68
2	D	501	SFG	N3-C2-N1	-4.44	121.74	128.68
2	L	501	SFG	N3-C2-N1	-4.42	121.76	128.68
2	I	501	SFG	N3-C2-N1	-4.42	121.77	128.68
2	E	501	SFG	N3-C2-N1	-4.41	121.79	128.68
2	B	501	SFG	N3-C2-N1	-4.40	121.80	128.68
2	L	501	SFG	O4'-C1'-C2'	-4.40	100.49	106.93
2	I	501	SFG	O4'-C1'-C2'	-4.28	100.67	106.93
2	J	501	SFG	O4'-C1'-C2'	-4.25	100.71	106.93
2	B	501	SFG	O4'-C1'-C2'	-4.25	100.71	106.93
2	H	501	SFG	O4'-C1'-C2'	-4.21	100.77	106.93
2	K	501	SFG	O4'-C1'-C2'	-4.19	100.81	106.93
2	E	501	SFG	O4'-C1'-C2'	-3.96	101.13	106.93
2	C	501	SFG	O4'-C1'-C2'	-3.95	101.15	106.93
2	A	501	SFG	O4'-C1'-C2'	-3.89	101.25	106.93
2	G	501	SFG	O4'-C1'-C2'	-3.88	101.26	106.93
3	B	502	GPP	PA-O3A-PB	-3.87	119.55	132.83
3	A	502	GPP	PA-O3A-PB	-3.79	119.81	132.83
3	J	502	GPP	PA-O3A-PB	-3.73	120.04	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	502	GPP	PA-O3A-PB	-3.64	120.35	132.83
3	H	502	GPP	PA-O3A-PB	-3.60	120.48	132.83
3	C	502	GPP	PA-O3A-PB	-3.59	120.50	132.83
3	I	502	GPP	PA-O3A-PB	-3.54	120.67	132.83
3	K	502	GPP	PA-O3A-PB	-3.52	120.74	132.83
3	E	502	GPP	PA-O3A-PB	-3.46	120.94	132.83
3	L	502	GPP	PA-O3A-PB	-3.46	120.95	132.83
3	G	502	GPP	PA-O3A-PB	-3.33	121.41	132.83
2	F	501	SFG	O4'-C1'-C2'	-3.13	102.36	106.93
3	D	502	GPP	PA-O3A-PB	-3.11	122.16	132.83
3	L	502	GPP	C4-C3-C5	3.08	120.45	115.27
3	C	502	GPP	C4-C3-C5	3.07	120.44	115.27
3	G	502	GPP	C4-C3-C5	2.98	120.29	115.27
3	K	502	GPP	C4-C3-C5	2.83	120.03	115.27
3	E	502	GPP	C4-C3-C5	2.81	120.00	115.27
3	F	502	GPP	C4-C3-C5	2.77	119.93	115.27
2	D	501	SFG	C3'-C2'-C1'	-2.61	97.05	100.98
3	I	502	GPP	C4-C3-C5	2.58	119.61	115.27
3	A	502	GPP	C4-C3-C5	2.54	119.55	115.27
3	D	502	GPP	C4-C3-C5	2.54	119.54	115.27
3	B	502	GPP	C4-C3-C5	2.53	119.52	115.27
3	J	502	GPP	C4-C3-C5	2.52	119.51	115.27
3	C	502	GPP	C10-C8-C9	2.50	120.13	114.60
2	D	501	SFG	O4'-C1'-C2'	-2.47	103.31	106.93
3	F	502	GPP	C10-C8-C9	2.47	120.05	114.60
3	G	502	GPP	C10-C8-C9	2.47	120.05	114.60
3	L	502	GPP	O3B-PB-O3A	2.46	112.90	104.64
3	K	502	GPP	C10-C8-C9	2.46	120.03	114.60
3	L	502	GPP	C10-C8-C9	2.44	120.00	114.60
3	D	502	GPP	C10-C8-C9	2.44	119.98	114.60
2	K	501	SFG	C3'-C2'-C1'	-2.44	97.31	100.98
3	B	502	GPP	O3B-PB-O3A	2.42	112.76	104.64
3	K	502	GPP	O3B-PB-O3A	2.40	112.68	104.64
3	E	502	GPP	C10-C8-C9	2.40	119.90	114.60
3	A	502	GPP	C10-C8-C9	2.40	119.90	114.60
3	E	502	GPP	O3B-PB-O3A	2.39	112.66	104.64
3	I	502	GPP	C10-C8-C9	2.38	119.85	114.60
3	C	502	GPP	O3B-PB-O3A	2.37	112.59	104.64
3	I	502	GPP	O3B-PB-O3A	2.37	112.58	104.64
3	H	502	GPP	C4-C3-C5	2.35	119.23	115.27
3	H	502	GPP	C10-C8-C9	2.35	119.79	114.60
2	C	501	SFG	C3'-C2'-C1'	-2.35	97.45	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	502	GPP	O3B-PB-O3A	2.34	112.49	104.64
3	A	502	GPP	O3B-PB-O3A	2.34	112.48	104.64
3	J	502	GPP	C10-C8-C9	2.33	119.75	114.60
3	G	502	GPP	O3B-PB-O3A	2.33	112.43	104.64
3	B	502	GPP	C10-C8-C9	2.32	119.73	114.60
3	F	502	GPP	O3B-PB-O3A	2.31	112.38	104.64
2	F	501	SFG	O4'-C4'-C5'	2.29	113.30	109.35
3	D	502	GPP	O3B-PB-O3A	2.29	112.32	104.64
3	J	502	GPP	O3B-PB-O3A	2.29	112.31	104.64
3	B	502	GPP	C1-C2-C3	2.11	129.69	126.04
2	E	501	SFG	C3'-C2'-C1'	-2.09	97.83	100.98

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	GPP	PA-O3A-PB-O2B
3	J	502	GPP	O1-C1-C2-C3
3	F	502	GPP	C1-O1-PA-O1A
3	F	502	GPP	C1-O1-PA-O2A
3	F	502	GPP	PA-O3A-PB-O2B
3	H	502	GPP	C2-C1-O1-PA
3	B	502	GPP	O1-C1-C2-C3
3	K	502	GPP	C1-O1-PA-O1A
3	K	502	GPP	C1-O1-PA-O2A
3	I	502	GPP	C1-O1-PA-O1A
3	I	502	GPP	C1-O1-PA-O2A
3	L	502	GPP	O1-C1-C2-C3
3	F	502	GPP	O1-C1-C2-C3
3	E	502	GPP	C2-C1-O1-PA
3	K	502	GPP	C1-O1-PA-O3A
3	E	502	GPP	PA-O3A-PB-O1B
3	J	502	GPP	PB-O3A-PA-O1A
3	I	502	GPP	O1-C1-C2-C3
3	F	502	GPP	C4-C3-C5-C6
3	F	502	GPP	C2-C3-C5-C6
3	D	502	GPP	PB-O3A-PA-O1A
3	H	502	GPP	C5-C6-C7-C8
3	D	502	GPP	PA-O3A-PB-O1B
3	F	502	GPP	PA-O3A-PB-O1B
3	C	502	GPP	C3-C5-C6-C7
3	D	502	GPP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	F	502	GPP	PA-O3A-PB-O3B
3	L	502	GPP	PA-O3A-PB-O2B
3	F	502	GPP	C1-O1-PA-O3A
3	I	502	GPP	C1-O1-PA-O3A
3	D	502	GPP	PB-O3A-PA-O2A
3	J	502	GPP	PB-O3A-PA-O2A
3	B	502	GPP	PB-O3A-PA-O1A
3	B	502	GPP	PB-O3A-PA-O2A
3	L	502	GPP	PB-O3A-PA-O2A
2	D	501	SFG	C4'-C5'-CD-CG

There are no ring outliers.

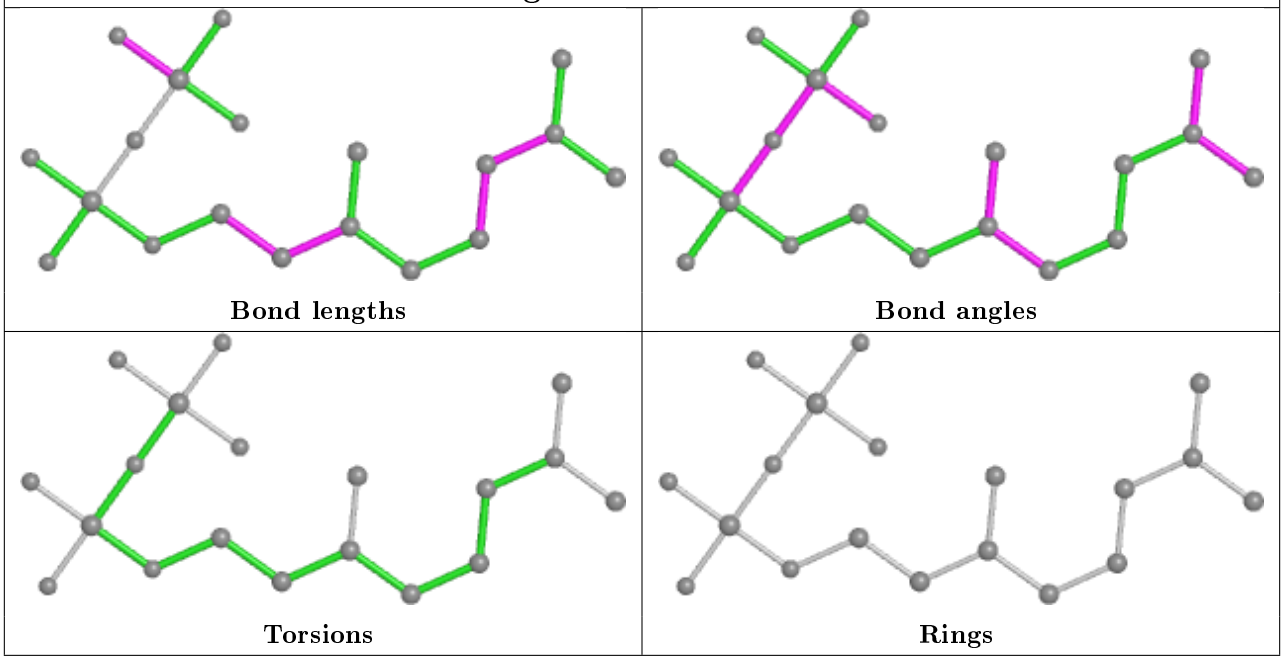
24 monomers are involved in 147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GPP	8	0
2	H	501	SFG	7	0
3	D	502	GPP	8	0
2	L	501	SFG	6	0
2	F	501	SFG	8	0
3	J	502	GPP	6	0
2	K	501	SFG	10	0
2	I	501	SFG	9	0
2	E	501	SFG	6	0
2	C	501	SFG	4	0
3	F	502	GPP	4	0
2	J	501	SFG	7	0
3	G	502	GPP	5	0
2	D	501	SFG	1	0
2	B	501	SFG	8	0
3	H	502	GPP	9	0
2	G	501	SFG	5	0
3	B	502	GPP	12	0
2	A	501	SFG	10	0
3	K	502	GPP	5	0
3	I	502	GPP	7	0
3	C	502	GPP	9	0
3	E	502	GPP	4	0
3	L	502	GPP	4	0

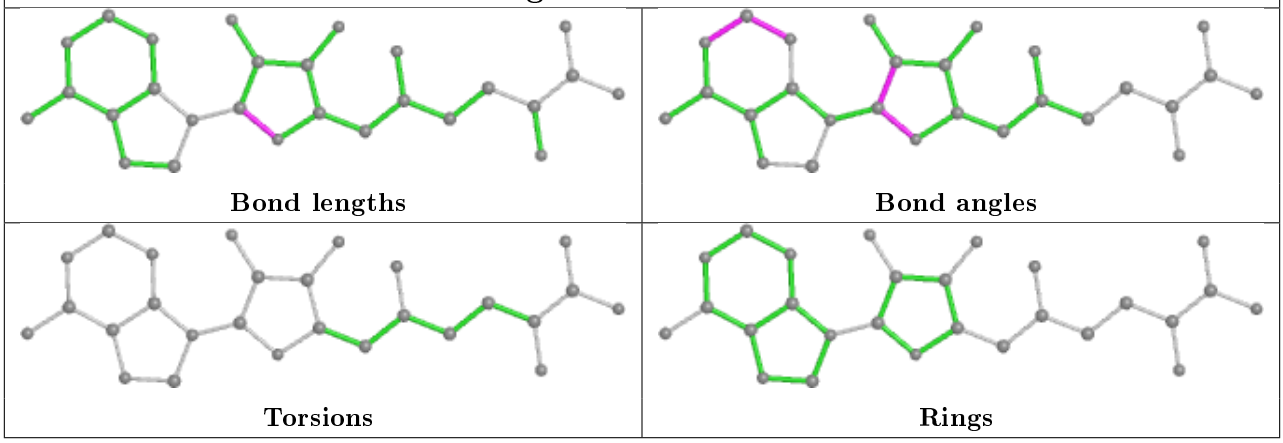
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

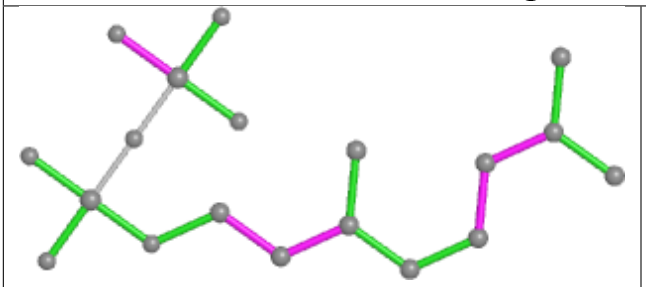
Ligand GPP A 502



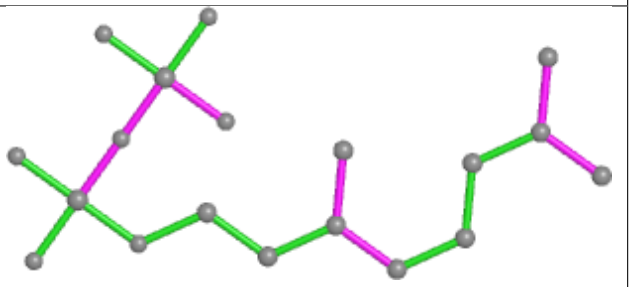
Ligand SFG H 501



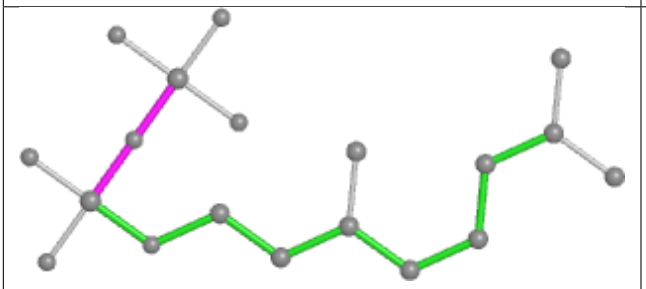
Ligand GPP D 502



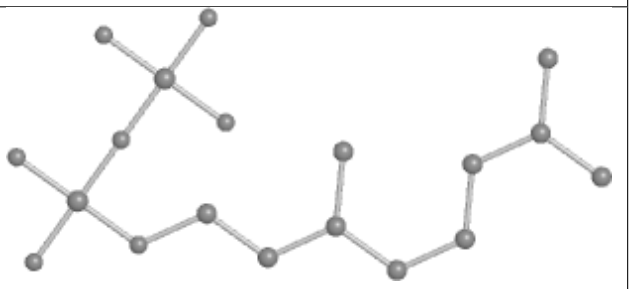
Bond lengths



Bond angles

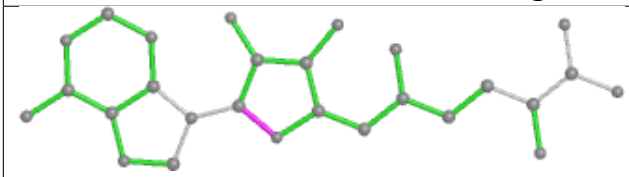


Torsions

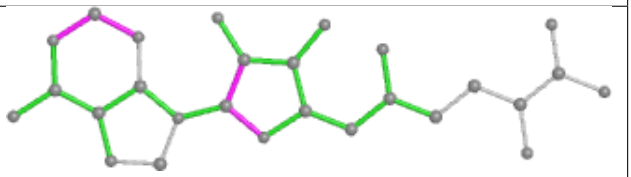


Rings

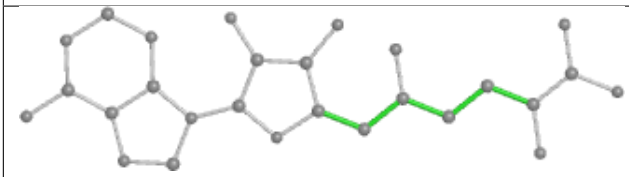
Ligand SFG L 501



Bond lengths



Bond angles



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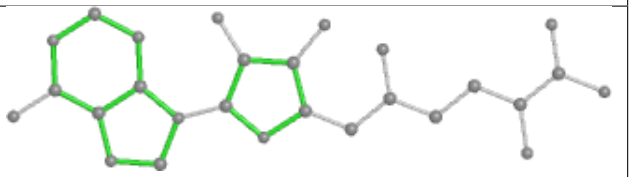
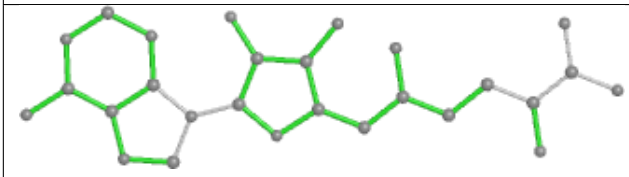
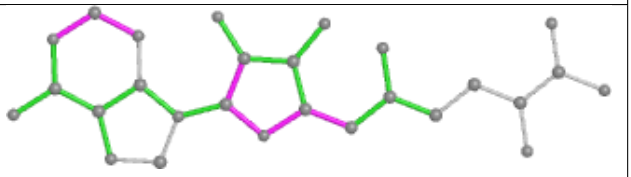


Rings

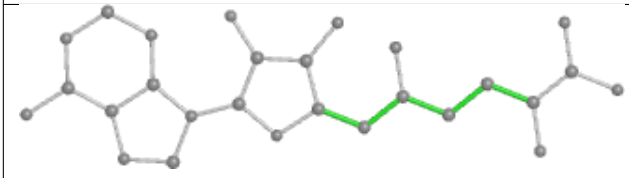
Ligand SFG F 501



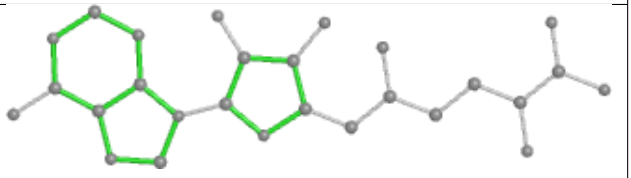
Bond lengths



Bond angles

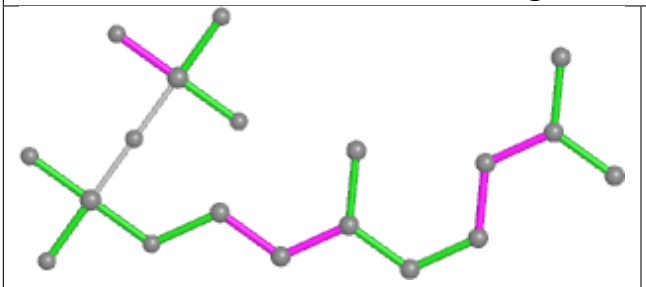


Torsions

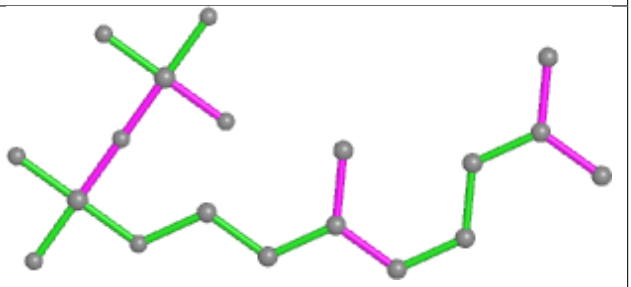


Rings

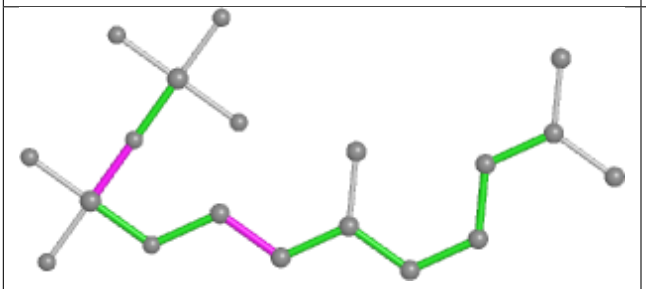
Ligand GPP J 502



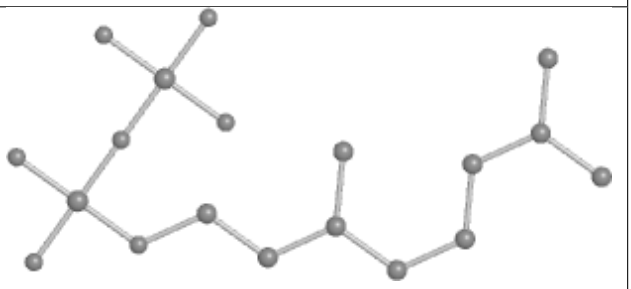
Bond lengths



Bond angles

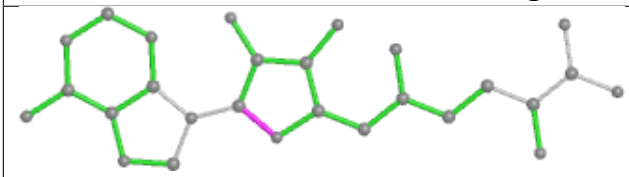


Torsions



Rings

Ligand SFG K 501



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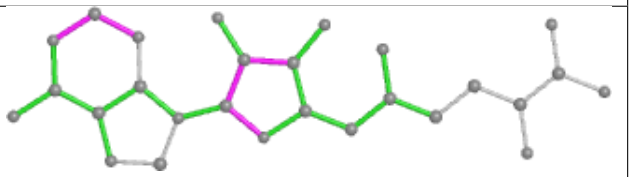

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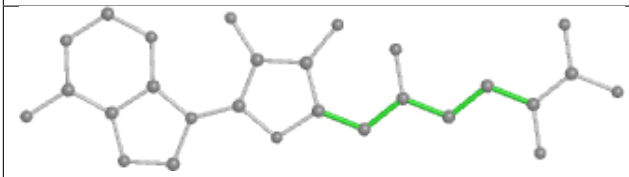

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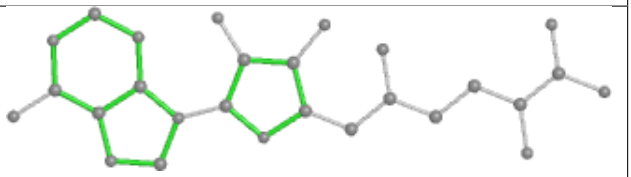

Rings

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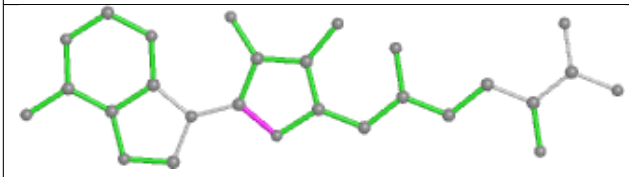

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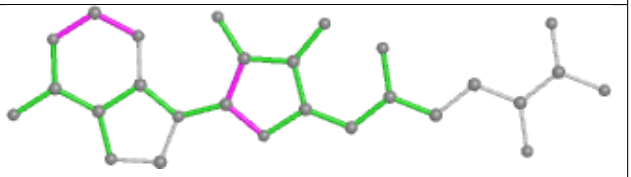

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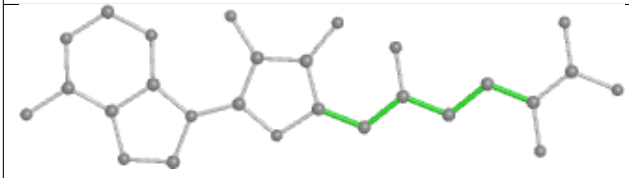

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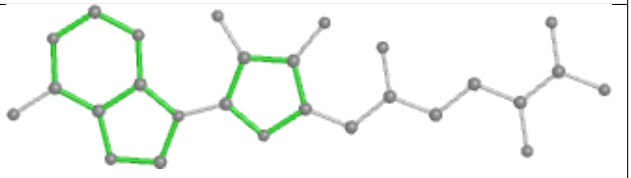

Rings

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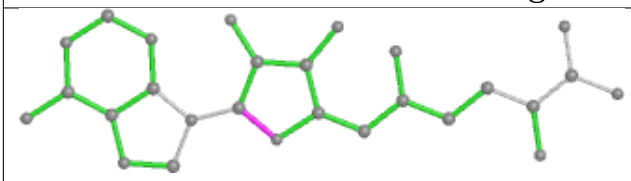

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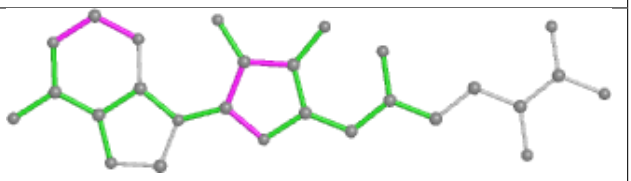

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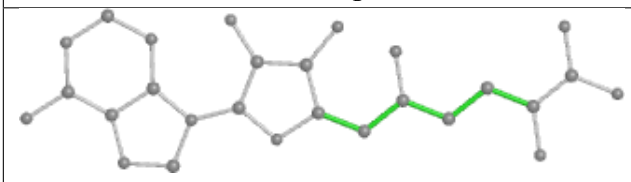

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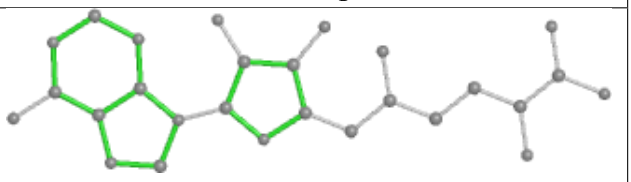
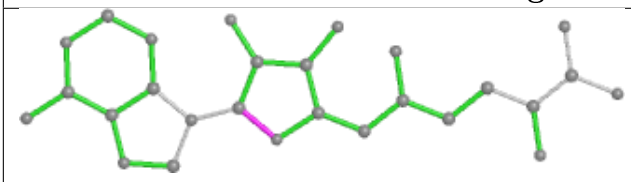


Rings

Ligand SFG C 501



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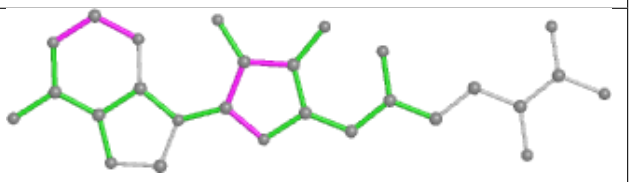

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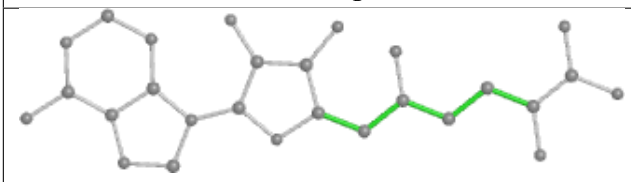

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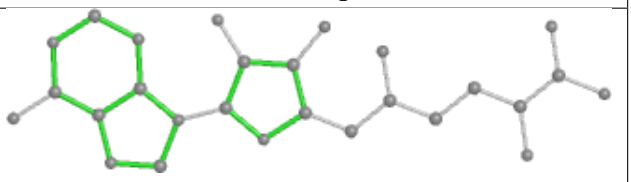
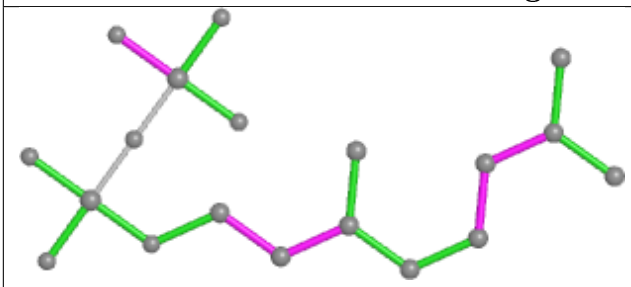


Rings

Ligand GPP F 502



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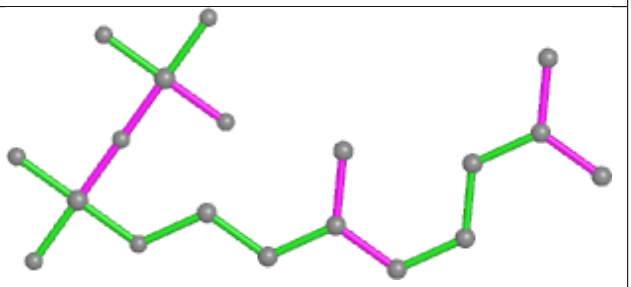
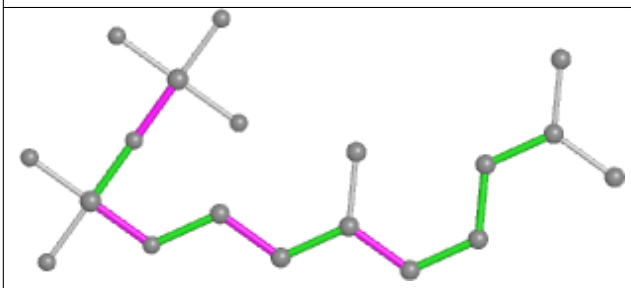


Bond angles



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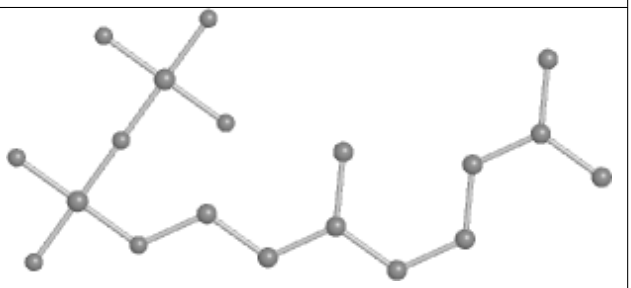
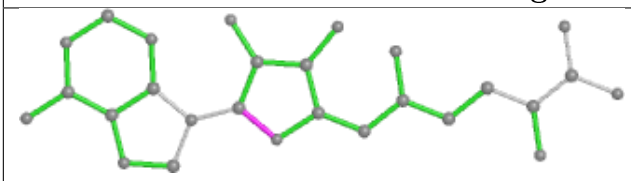


Rings

Ligand SFG J 501



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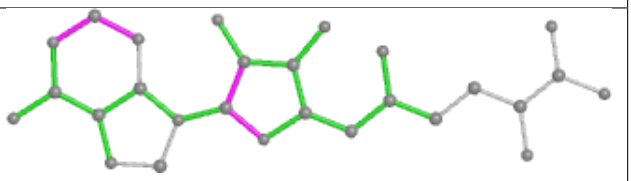

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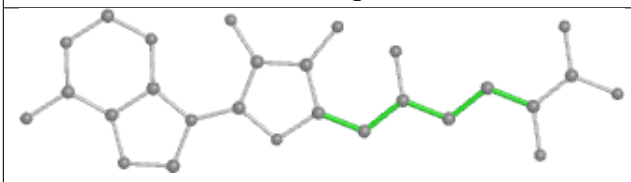

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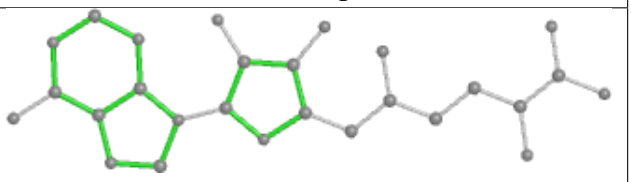
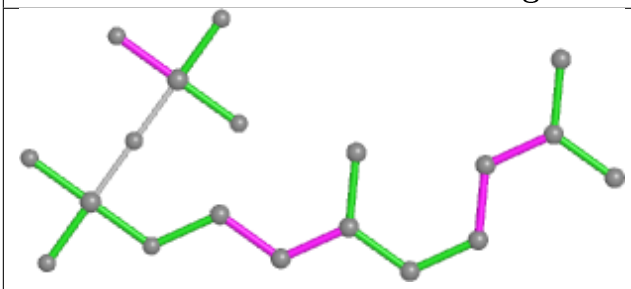


Rings

Ligand GPP G 502



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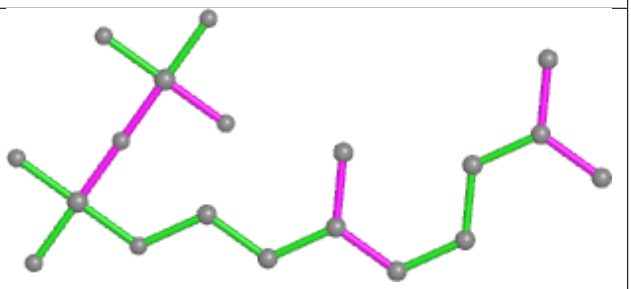

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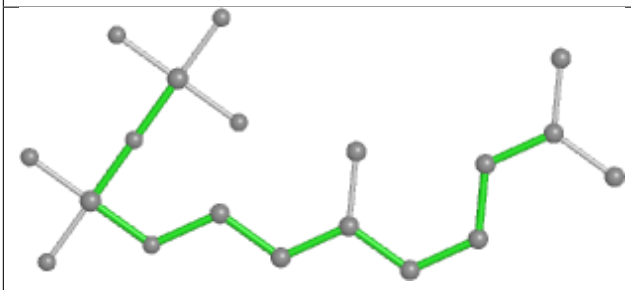

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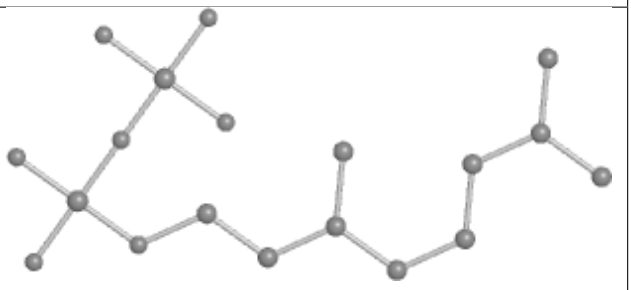
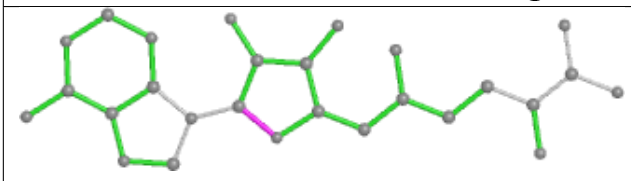


Rings

Ligand SFG D 501



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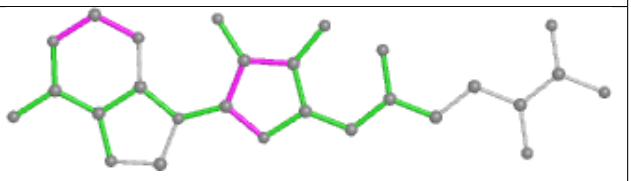

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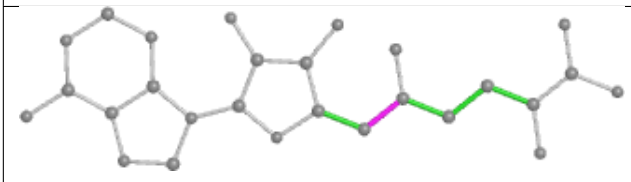

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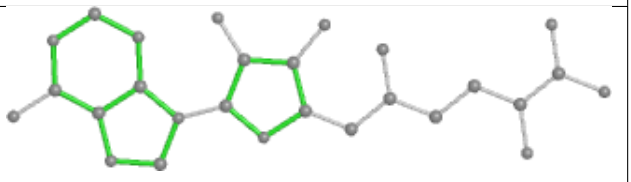

Rings

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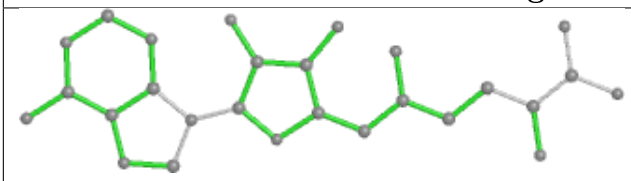

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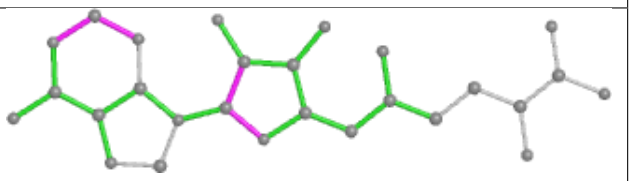

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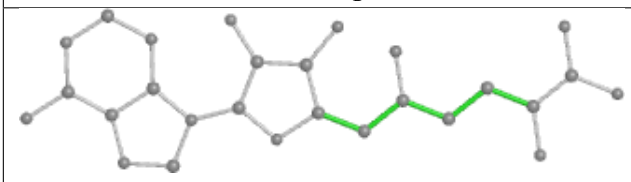

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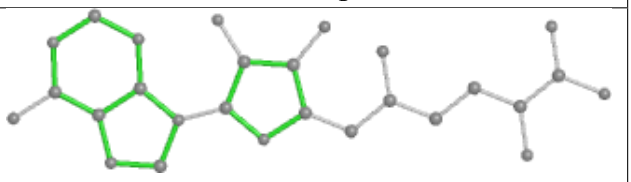
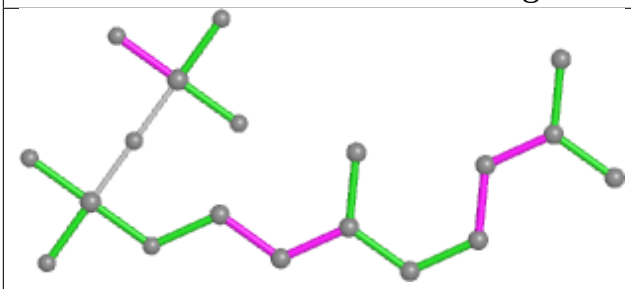


Rings

Ligand GPP H 502



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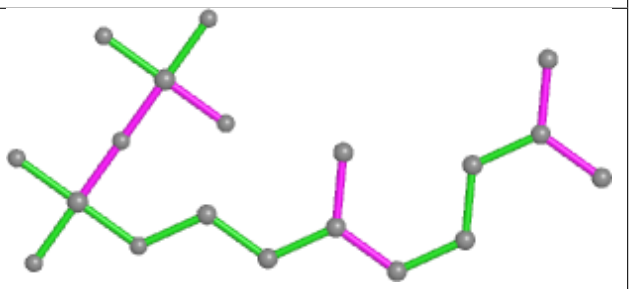

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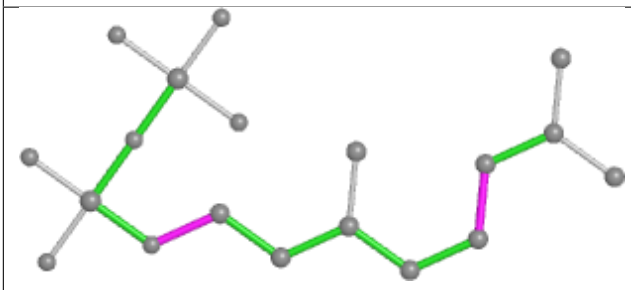

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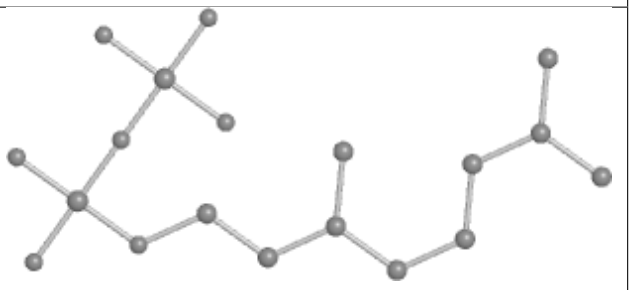
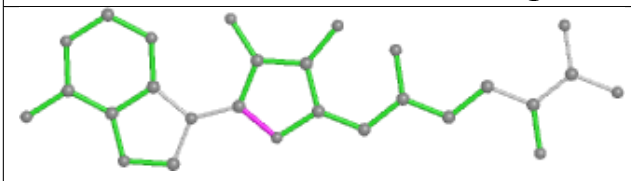


Rings

Ligand SFG G 501



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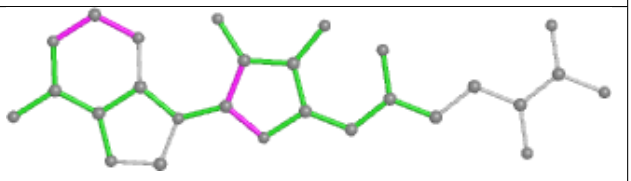

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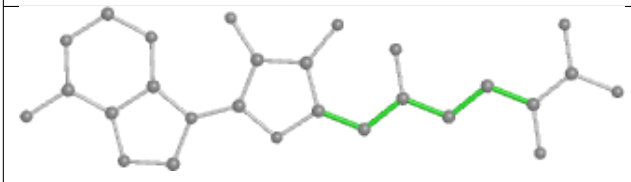

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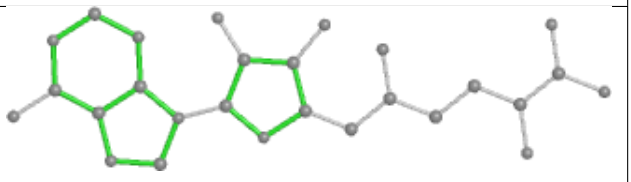
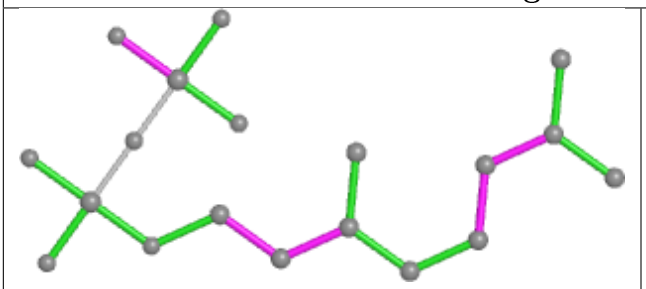


Rings

Ligand GPP B 502



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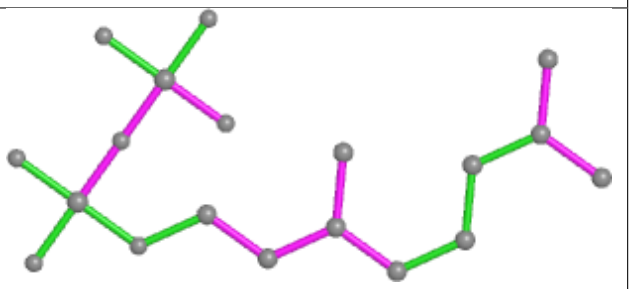

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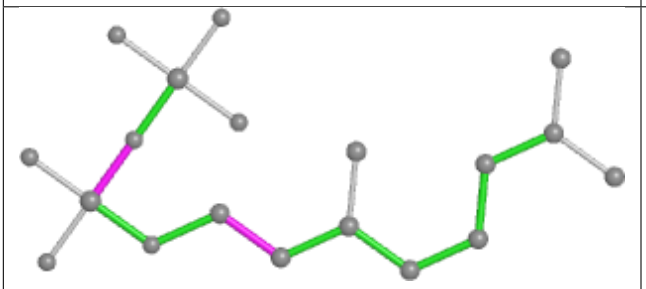

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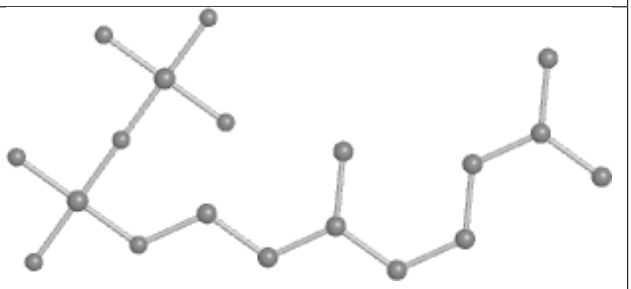
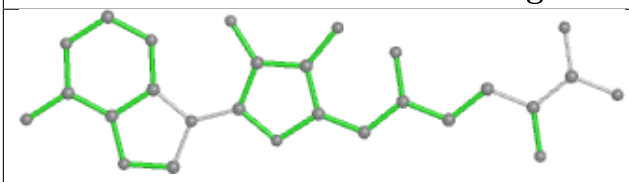


Rings

Ligand SFG A 501



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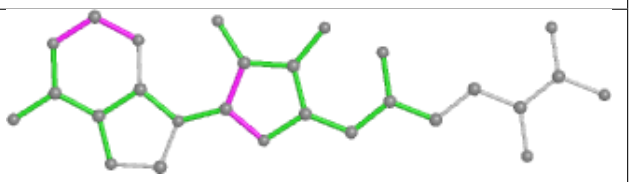
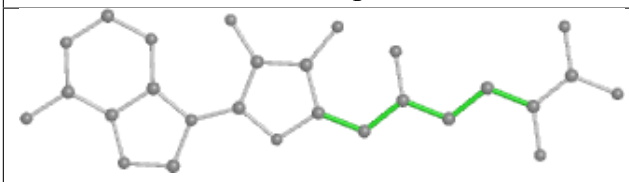


Bond angles



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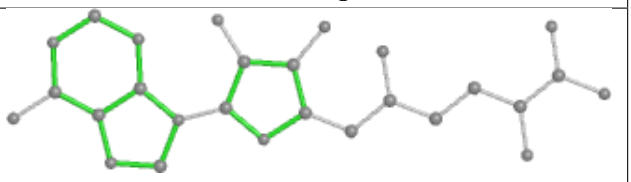
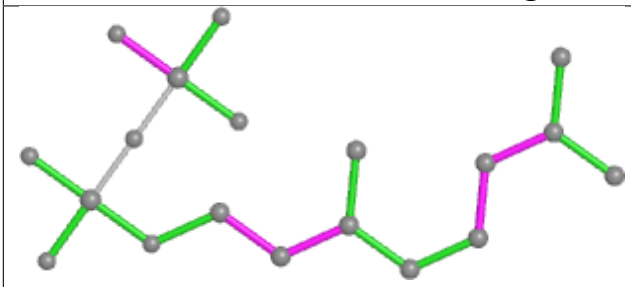


Rings

Ligand GPP K 502



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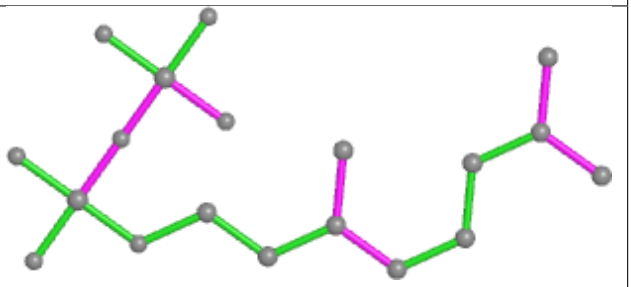
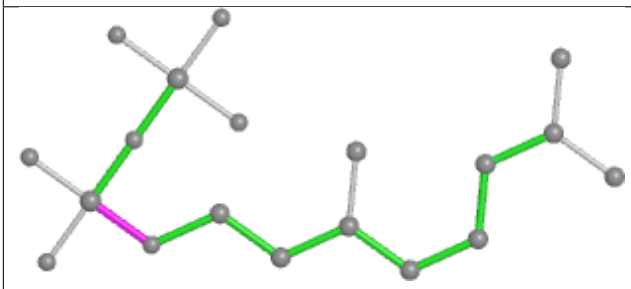


Bond angles



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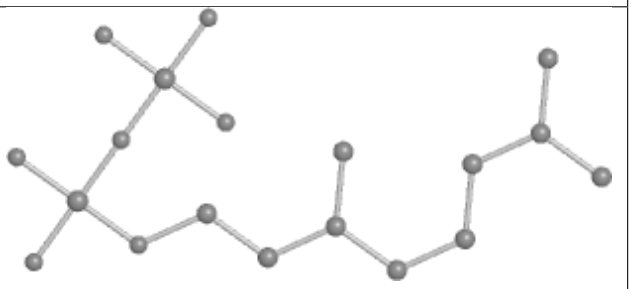
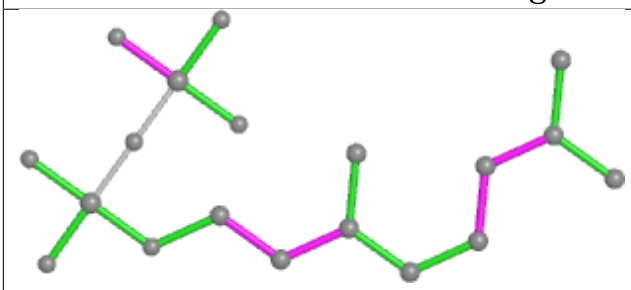


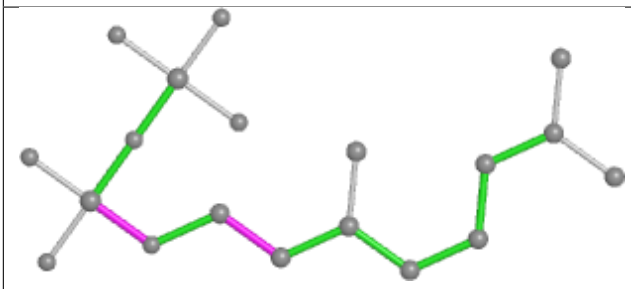
Rings

Ligand GPP I 502

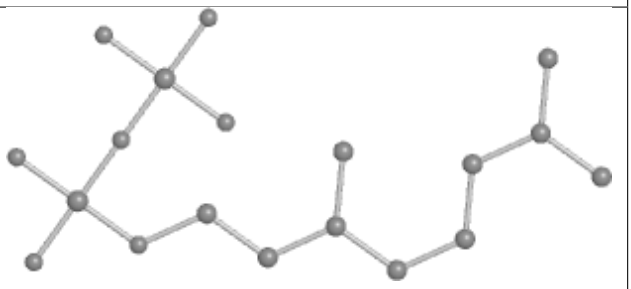


Bond lengths

Bond angles

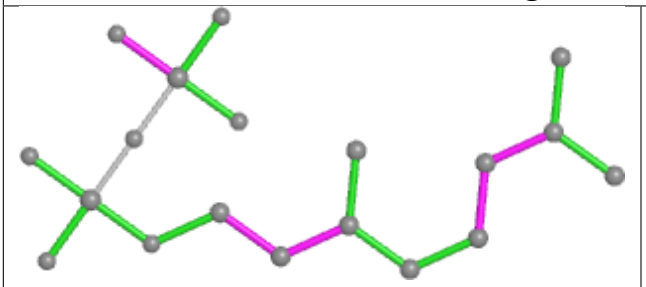


Torsions

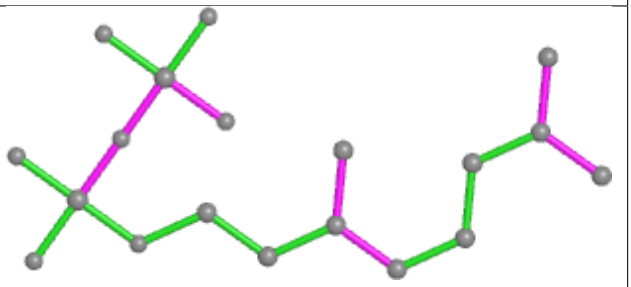


Rings

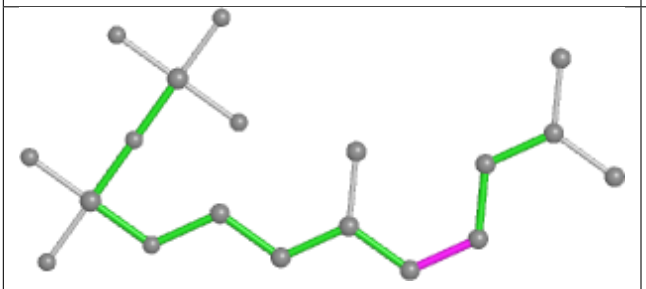
Ligand GPP C 502



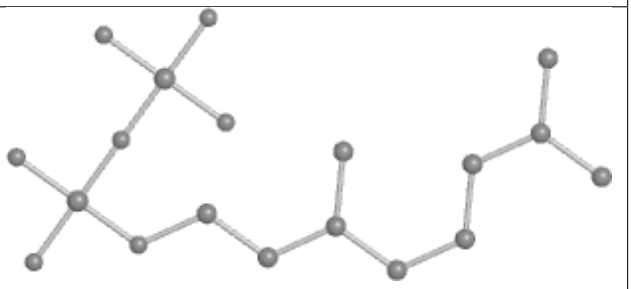
Bond lengths



Bond angles

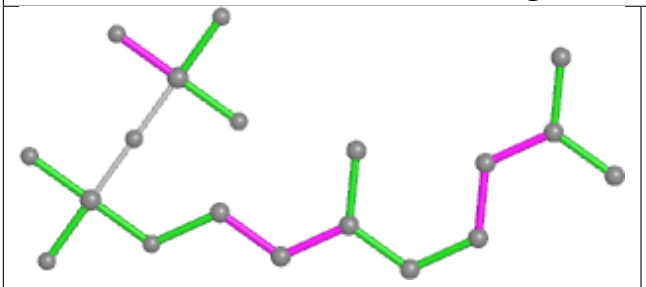


Torsions



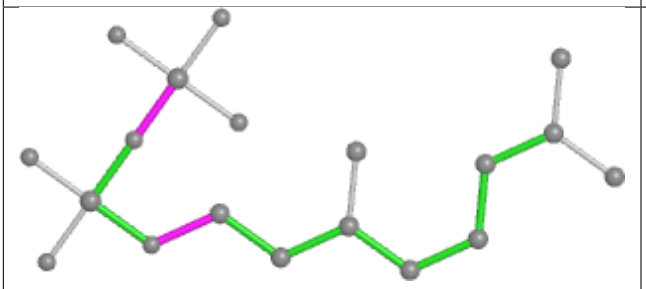
Rings

Ligand GPP E 502

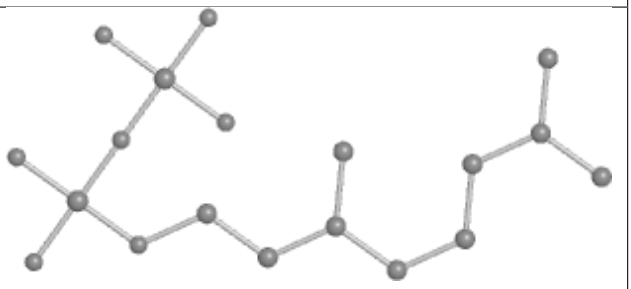


Bond lengths

Bond angles

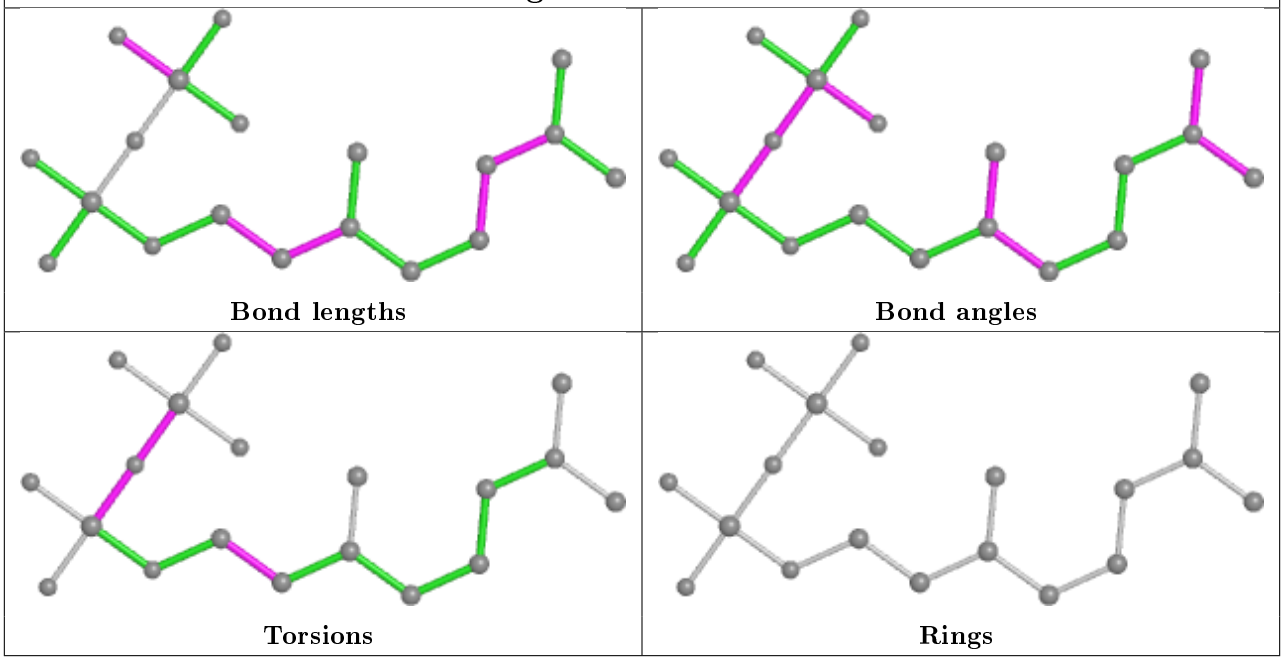


Torsions



Rings

Ligand GPP L 502



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	275/320 (85%)	-0.28	0 100 100	36, 47, 63, 77	0
1	B	273/320 (85%)	-0.28	0 100 100	30, 47, 73, 91	0
1	C	274/320 (85%)	-0.15	0 100 100	37, 50, 80, 93	0
1	D	273/320 (85%)	-0.27	0 100 100	34, 48, 65, 79	0
1	E	272/320 (85%)	-0.18	0 100 100	34, 49, 71, 87	0
1	F	269/320 (84%)	-0.13	1 (0%) 92 79	37, 50, 74, 81	0
1	G	269/320 (84%)	-0.29	1 (0%) 92 79	37, 47, 63, 81	0
1	H	268/320 (83%)	-0.10	4 (1%) 73 46	38, 50, 76, 90	0
1	I	273/320 (85%)	-0.28	1 (0%) 92 79	36, 48, 64, 77	0
1	J	272/320 (85%)	-0.26	0 100 100	31, 47, 67, 92	0
1	K	258/320 (80%)	-0.19	0 100 100	37, 49, 72, 90	0
1	L	273/320 (85%)	-0.10	2 (0%) 87 69	38, 50, 80, 96	0
All	All	3249/3840 (84%)	-0.21	9 (0%) 94 84	30, 48, 71, 96	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	69	LEU	3.2
1	H	78	GLU	3.2
1	H	70	GLY	2.6
1	H	40	GLU	2.4
1	L	274	VAL	2.3
1	G	78	GLU	2.3
1	I	125	GLN	2.1
1	L	125	GLN	2.1
1	F	78	GLU	2.1

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
4	MG	F	503	1/1	0.77	0.23	36,36,36,36	0
4	MG	K	503	1/1	0.85	0.22	49,49,49,49	0
2	SFG	L	501	27/27	0.86	0.26	64,66,70,71	0
4	MG	E	503	1/1	0.86	0.16	45,45,45,45	0
2	SFG	K	501	27/27	0.87	0.20	52,54,57,57	0
2	SFG	H	501	27/27	0.88	0.21	64,68,70,71	0
2	SFG	C	501	27/27	0.89	0.21	47,52,53,54	0
2	SFG	F	501	27/27	0.89	0.21	57,59,69,71	0
4	MG	J	503	1/1	0.89	0.16	21,21,21,21	0
2	SFG	D	501	27/27	0.90	0.21	37,45,47,49	0
4	MG	D	503	1/1	0.90	0.20	31,31,31,31	0
2	SFG	A	501	27/27	0.90	0.17	34,40,50,50	0
2	SFG	J	501	27/27	0.90	0.20	37,42,46,49	0
2	SFG	E	501	27/27	0.91	0.20	46,50,53,54	0
2	SFG	I	501	27/27	0.91	0.20	41,46,53,55	0
2	SFG	B	501	27/27	0.91	0.21	42,43,45,46	0
4	MG	I	503	1/1	0.92	0.25	43,43,43,43	0
2	SFG	G	501	27/27	0.93	0.18	40,47,52,54	0
3	GPP	B	502	19/19	0.93	0.24	54,56,62,63	0
4	MG	A	503	1/1	0.93	0.26	17,17,17,17	0
4	MG	L	503	1/1	0.93	0.13	31,31,31,31	0
3	GPP	I	502	19/19	0.94	0.24	44,47,53,53	0
4	MG	H	503	1/1	0.94	0.10	35,35,35,35	0
3	GPP	G	502	19/19	0.95	0.20	34,39,42,42	0
3	GPP	F	502	19/19	0.95	0.15	50,56,61,61	0
4	MG	C	503	1/1	0.95	0.25	58,58,58,58	0
3	GPP	K	502	19/19	0.95	0.15	37,49,54,54	0

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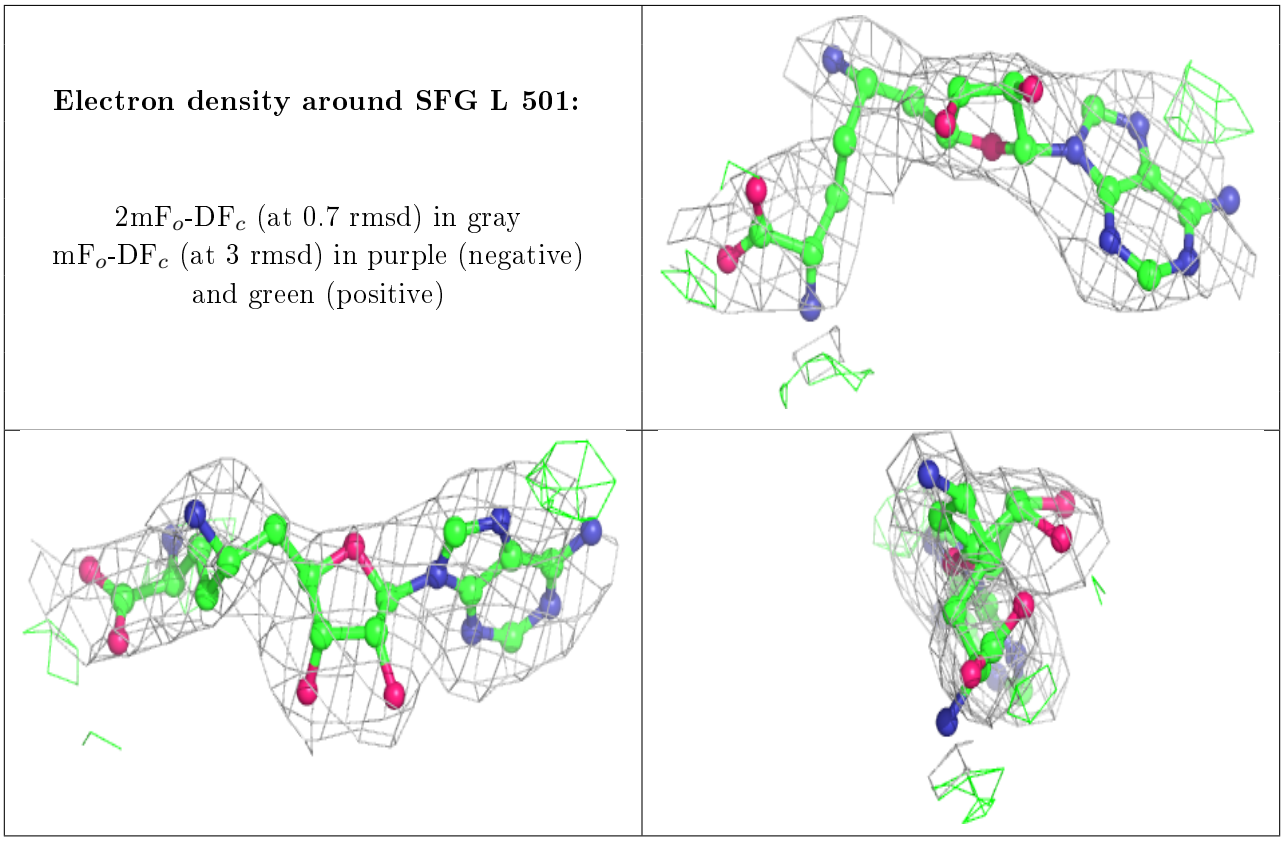
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GPP	H	502	19/19	0.95	0.18	50,54,61,62	0
3	GPP	C	502	19/19	0.95	0.18	56,57,58,58	0
3	GPP	D	502	19/19	0.95	0.19	34,43,48,48	0
3	GPP	E	502	19/19	0.95	0.19	49,57,61,61	0
3	GPP	J	502	19/19	0.96	0.18	28,38,47,48	0
3	GPP	A	502	19/19	0.96	0.16	33,40,44,45	0
4	MG	G	503	1/1	0.96	0.23	38,38,38,38	0
3	GPP	L	502	19/19	0.96	0.23	58,68,71,71	0
4	MG	B	503	1/1	0.97	0.25	9,9,9,9	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.

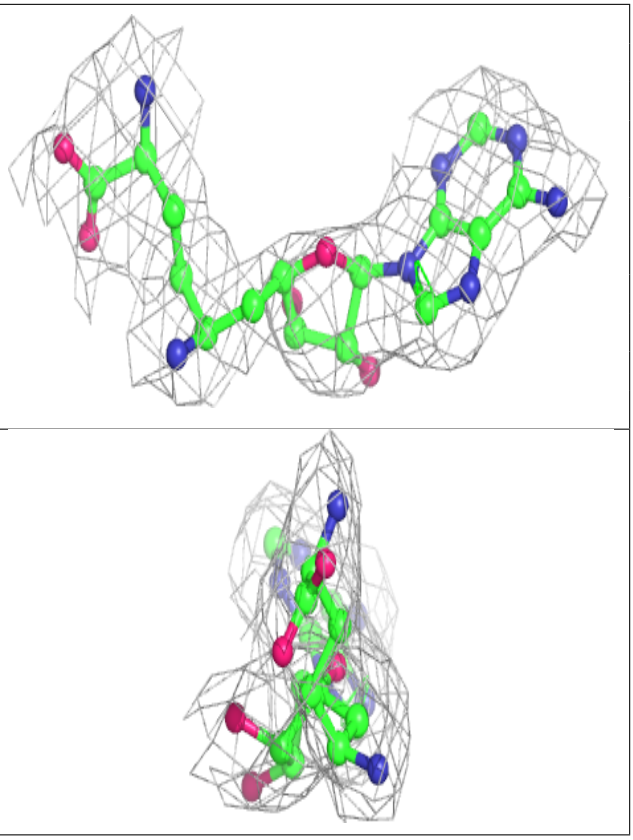
Electron density around SFG L 501:

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



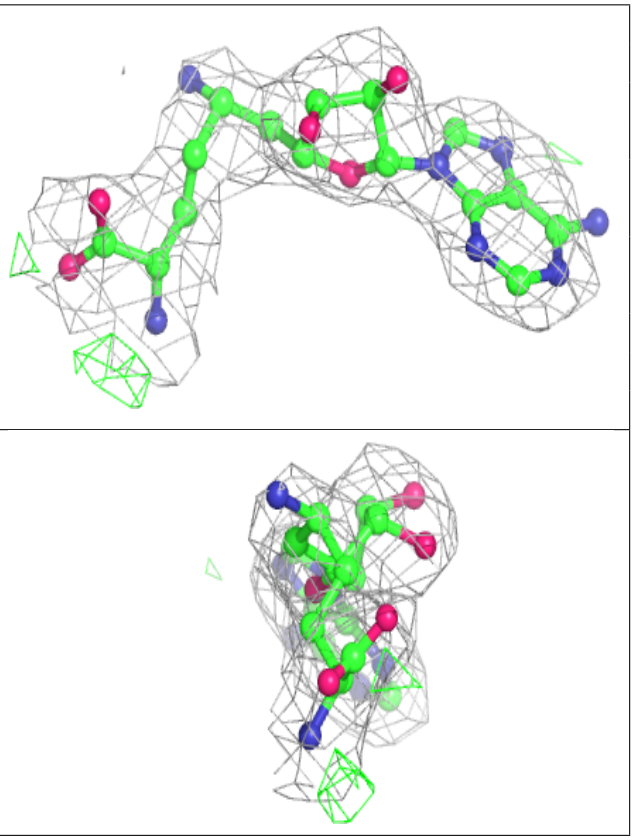
Electron density around SFG K 501:

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



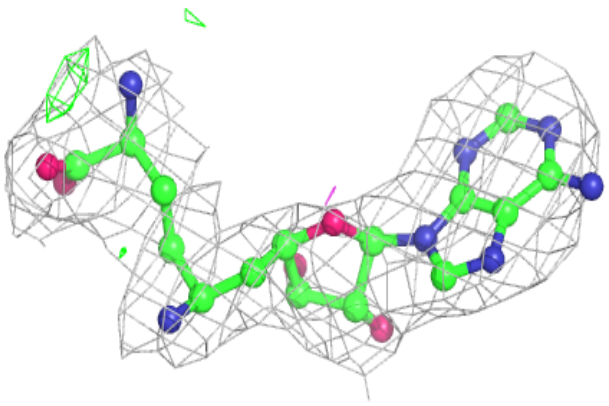
Electron density around SFG H 501:

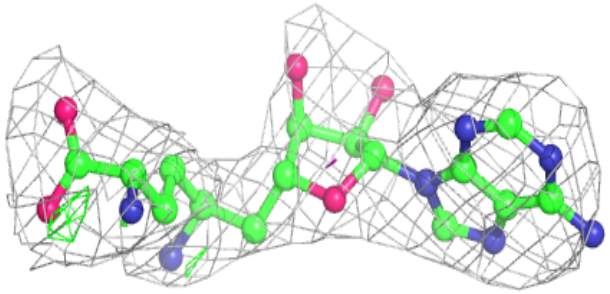
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

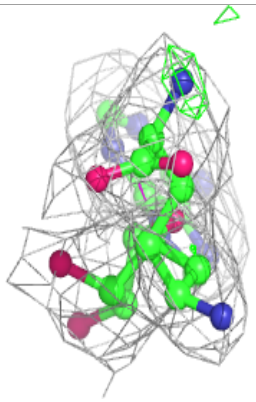


Electron density around SFG C 501:

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

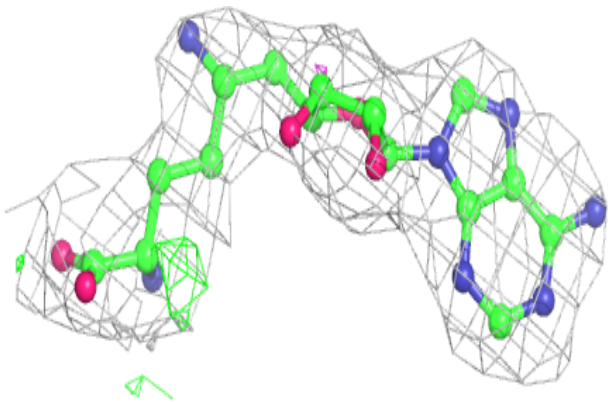


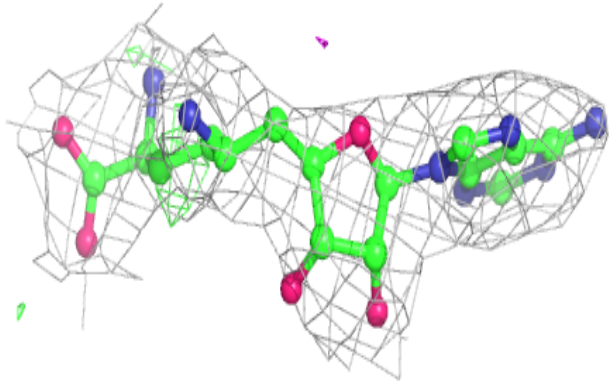


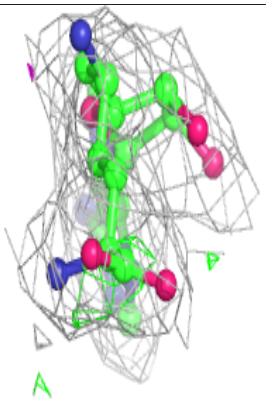


Electron density around SFG F 501:

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

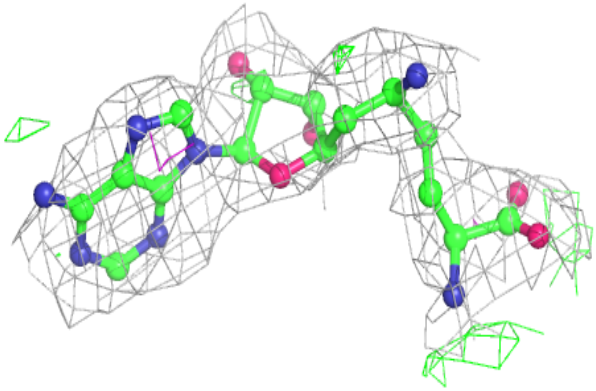


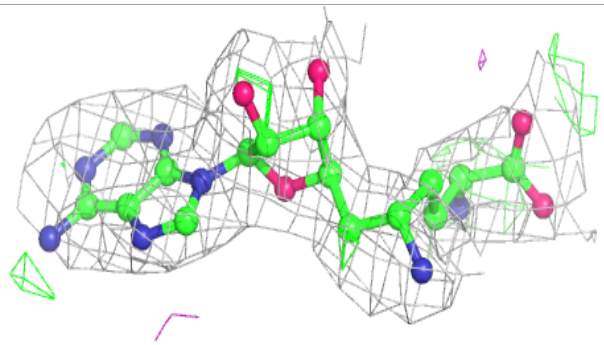


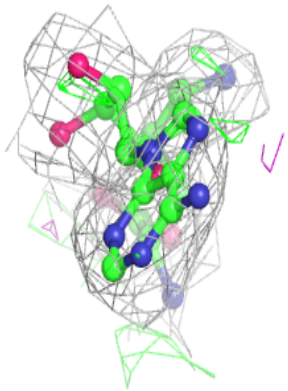


Electron density around SFG D 501:

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

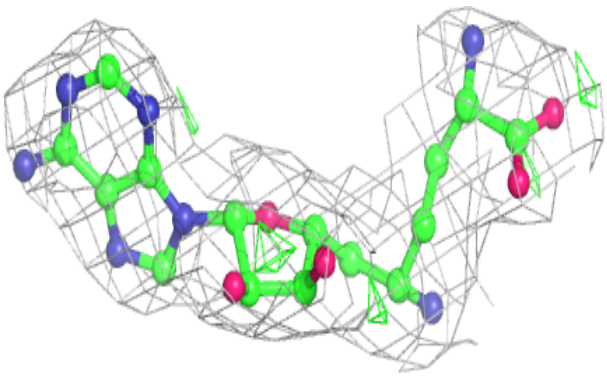


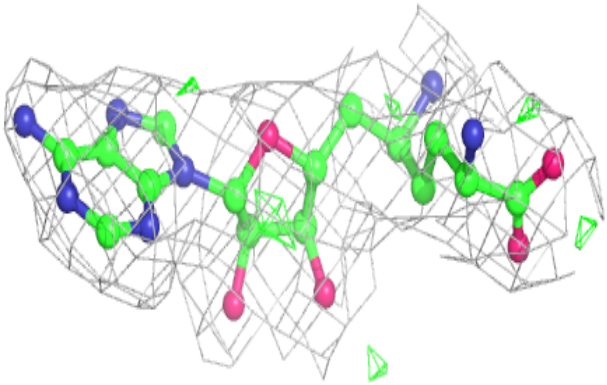


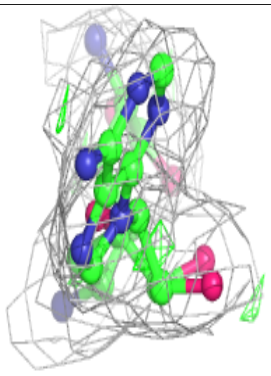


Electron density around SFG A 501:

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

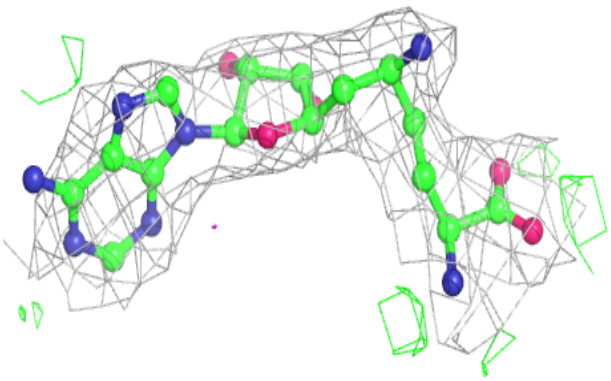


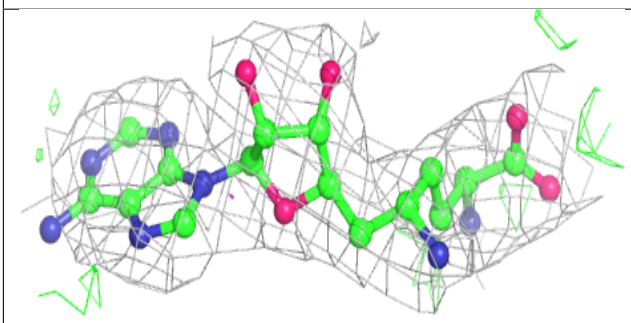


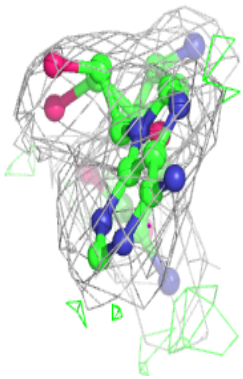


Electron density around SFG J 501:

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

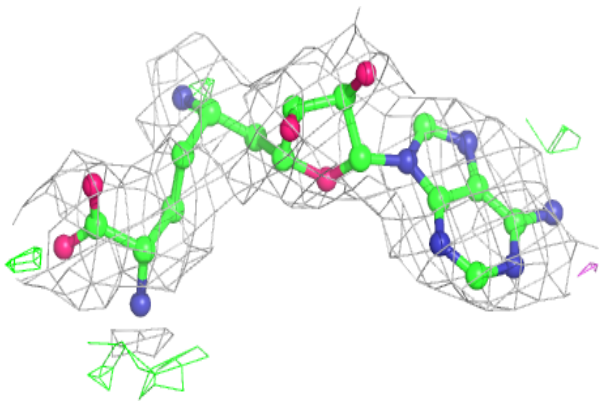


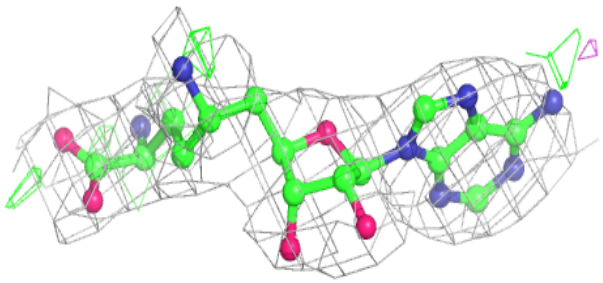


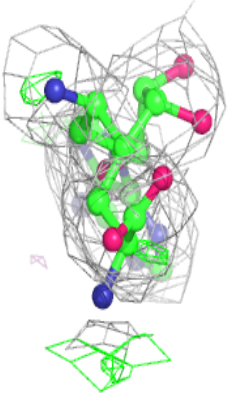


Electron density around SFG E 501:

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

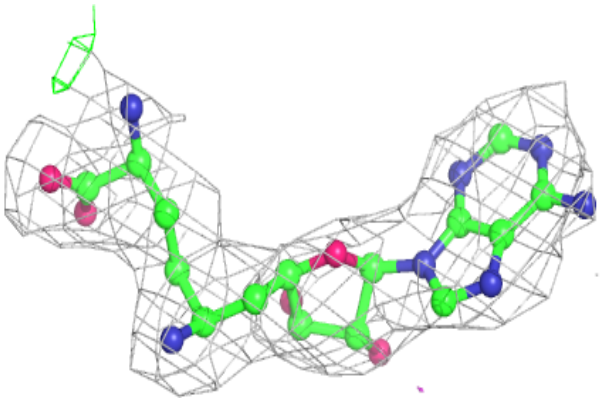


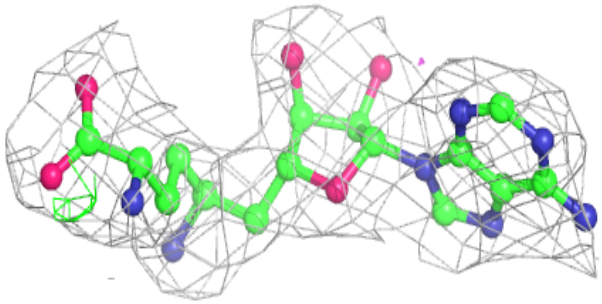


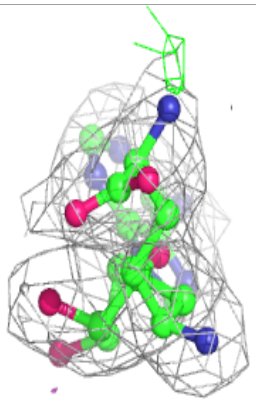


Electron density around SFG I 501:

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

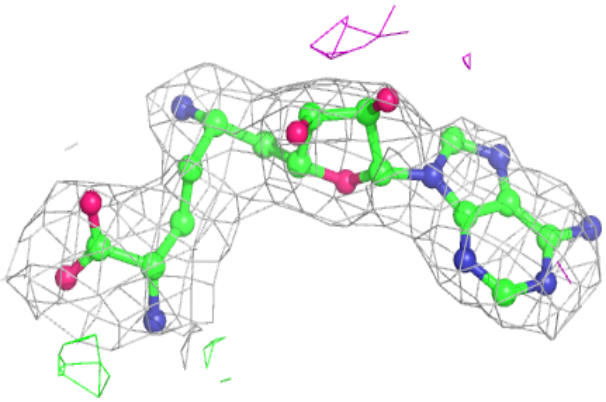


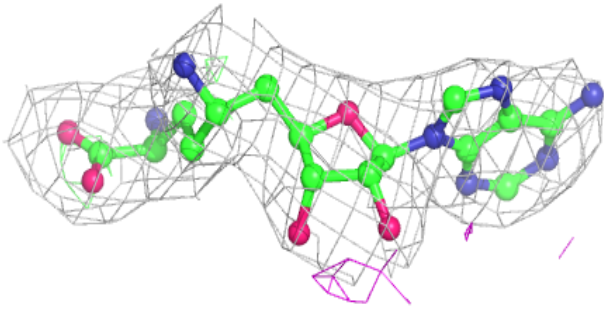


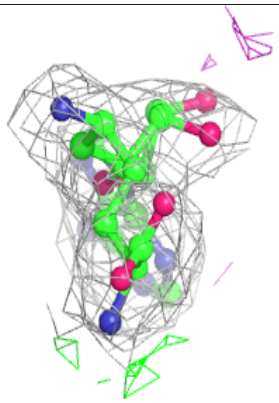


Electron density around SFG B 501:

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

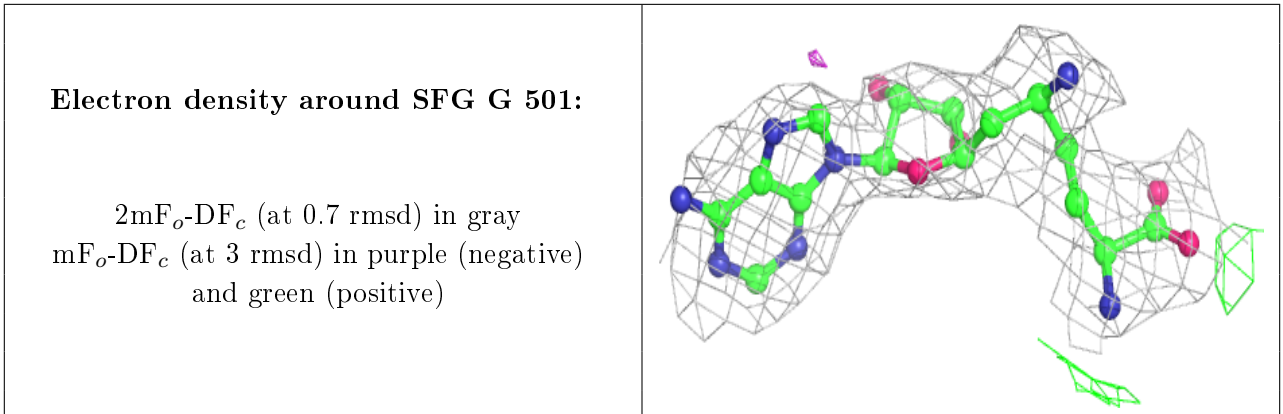


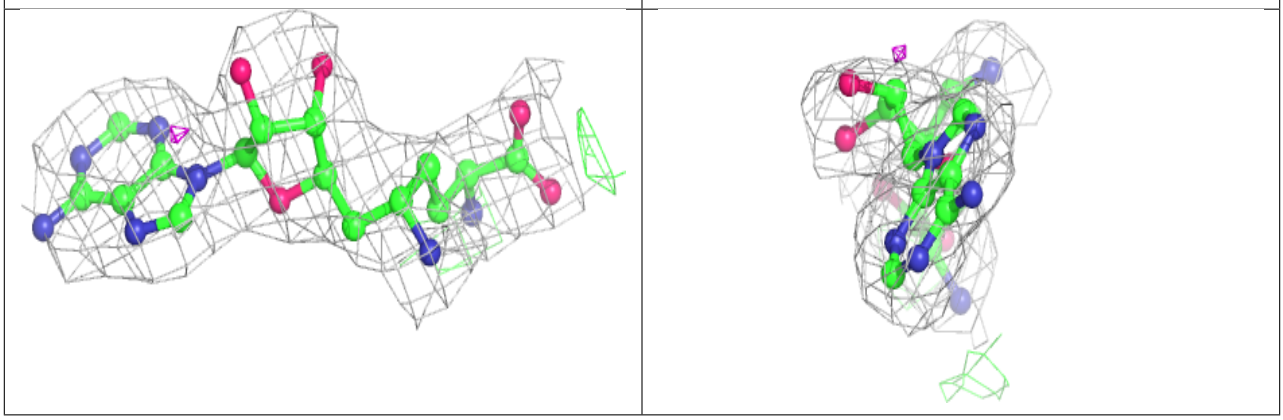




Electron density around SFG G 501:

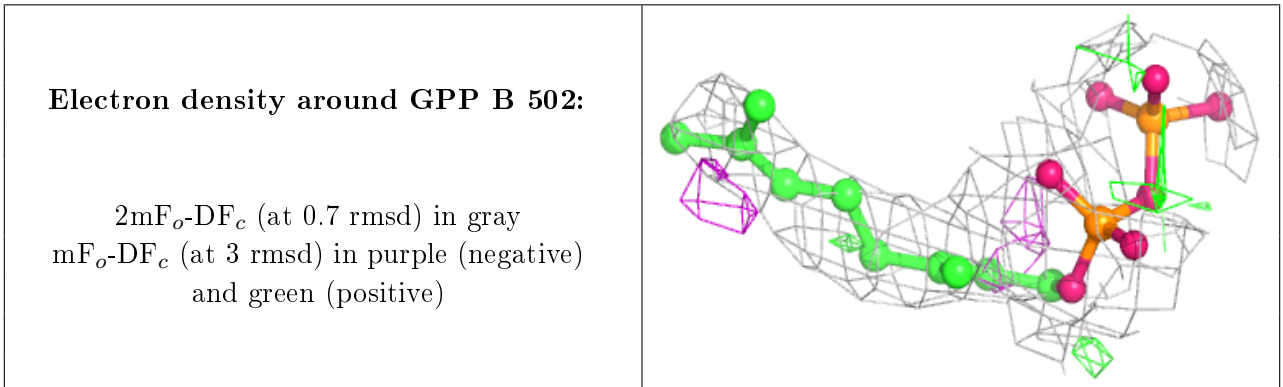
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

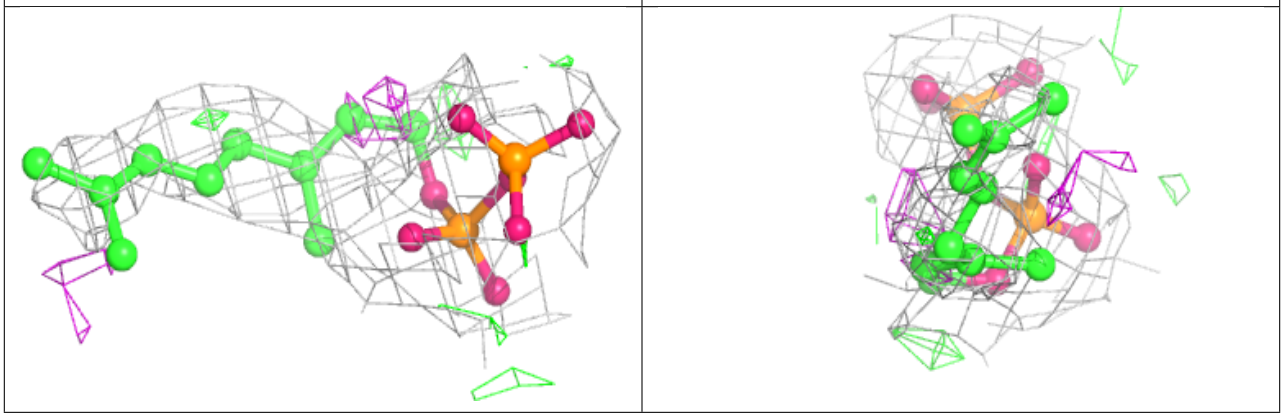




Electron density around GPP B 502:

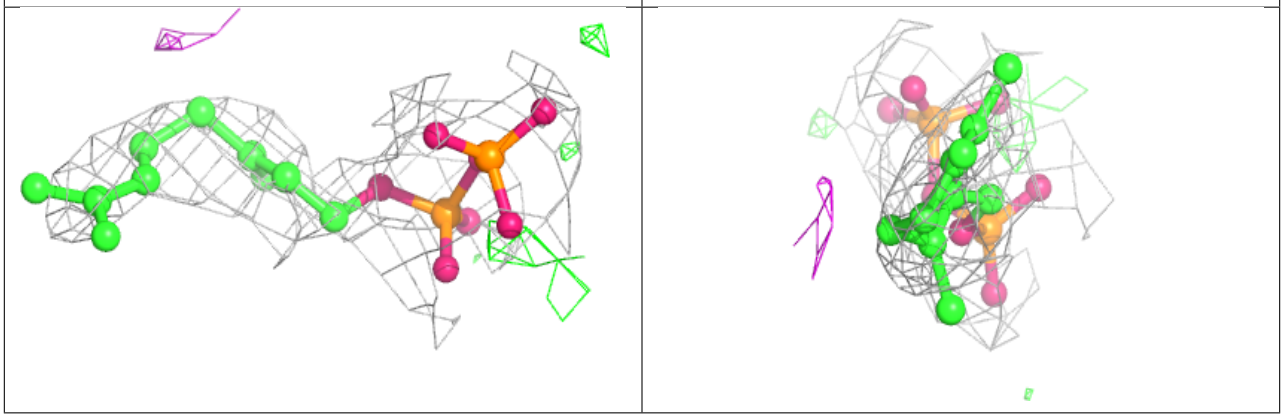
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





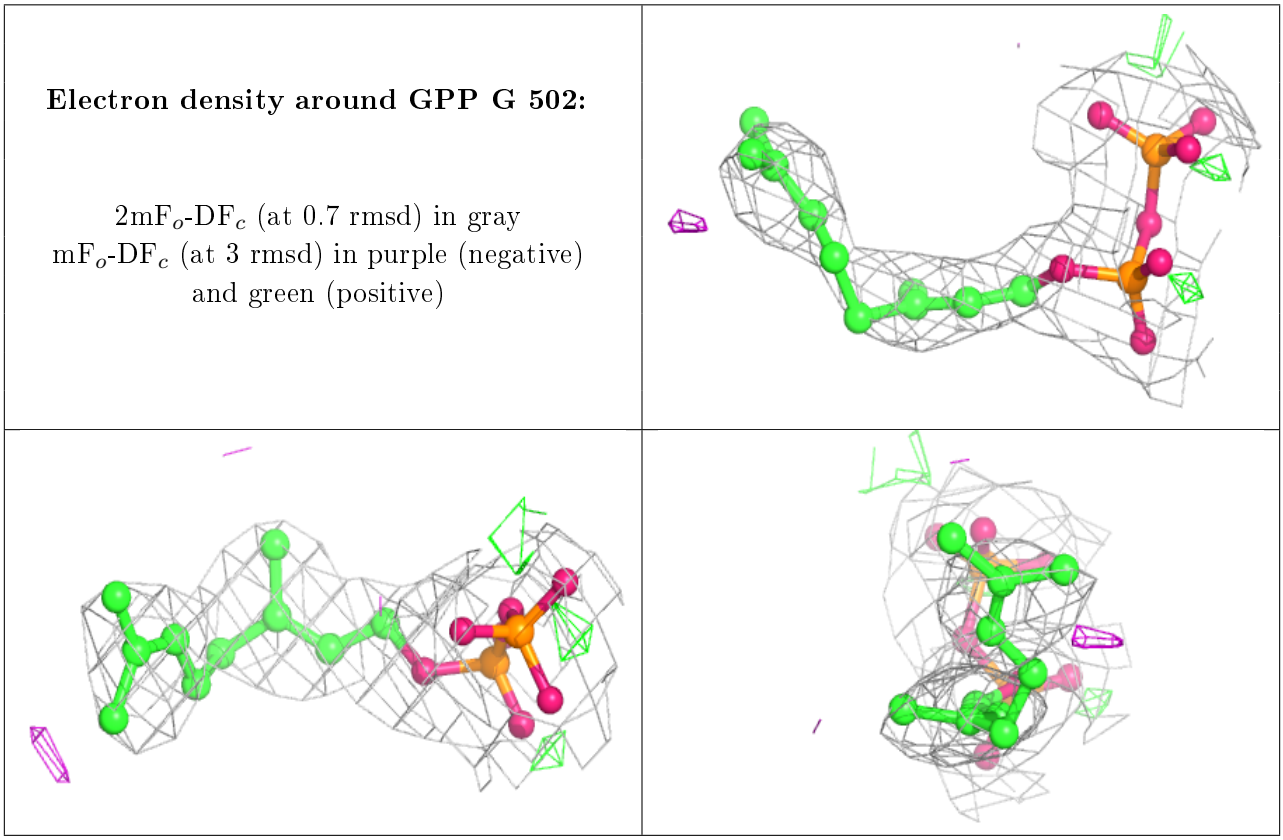
Electron density around GPP I 502:

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



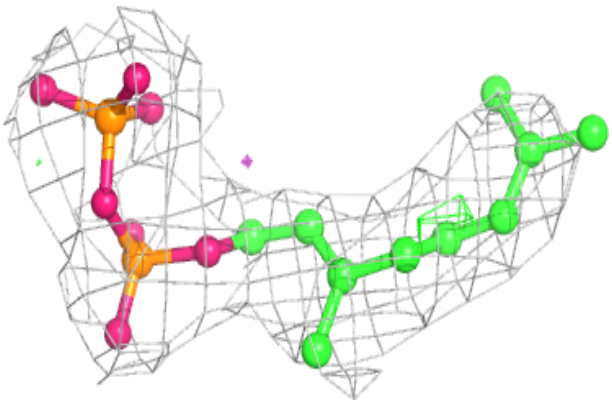
Electron density around GPP G 502:

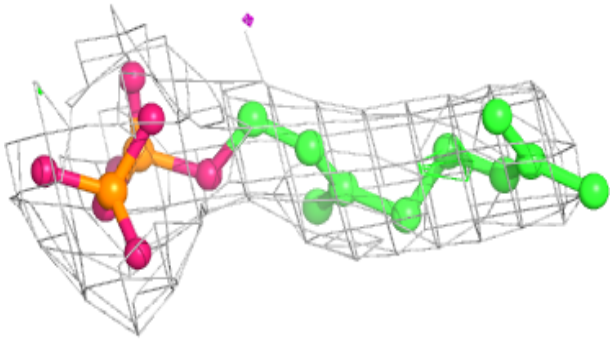
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

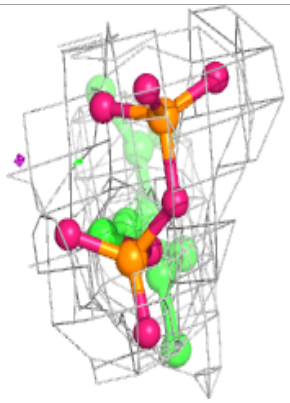


Electron density around GPP F 502:

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

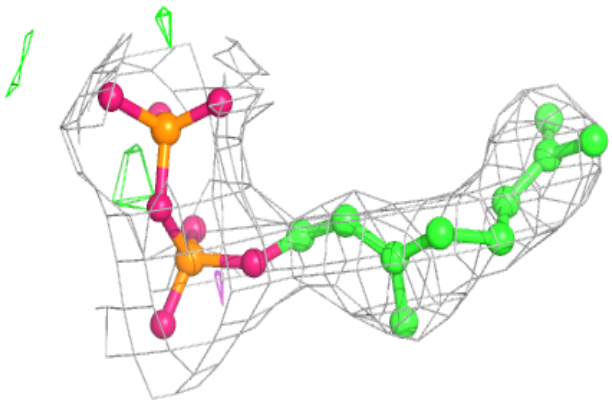


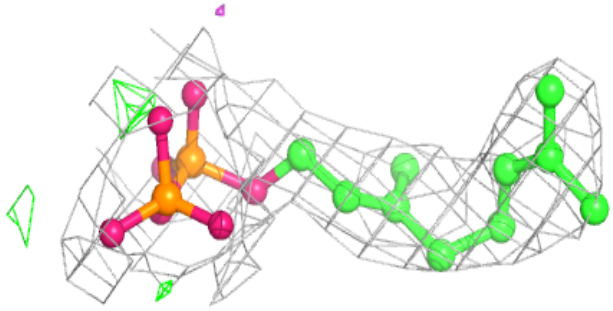


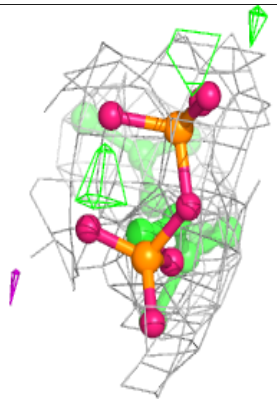


Electron density around GPP K 502:

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

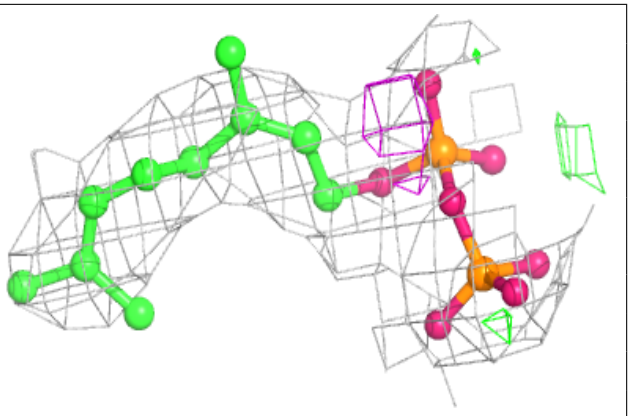


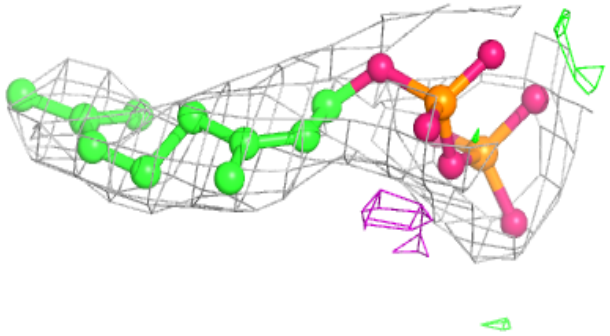


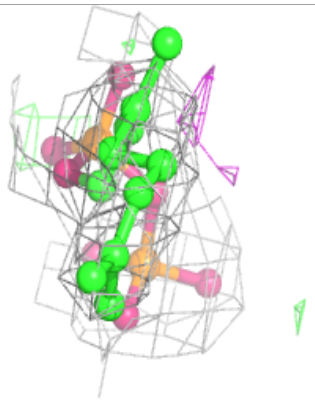


Electron density around GPP H 502:

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

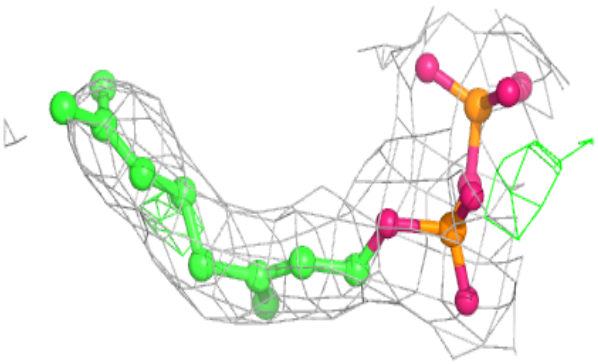


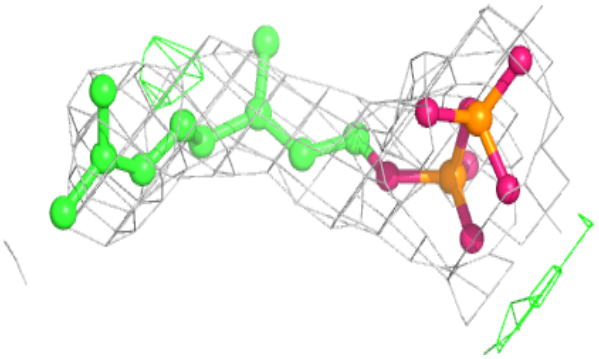




Electron density around GPP C 502:

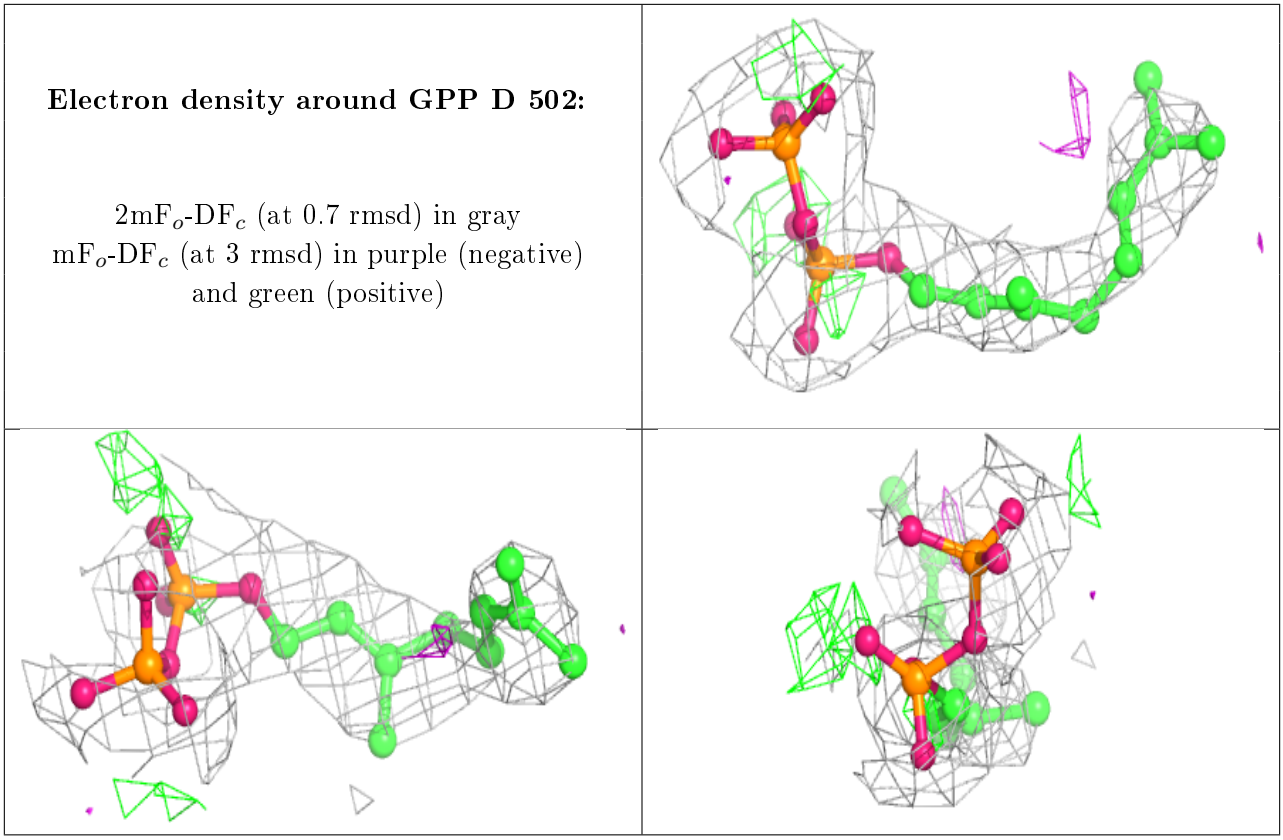
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





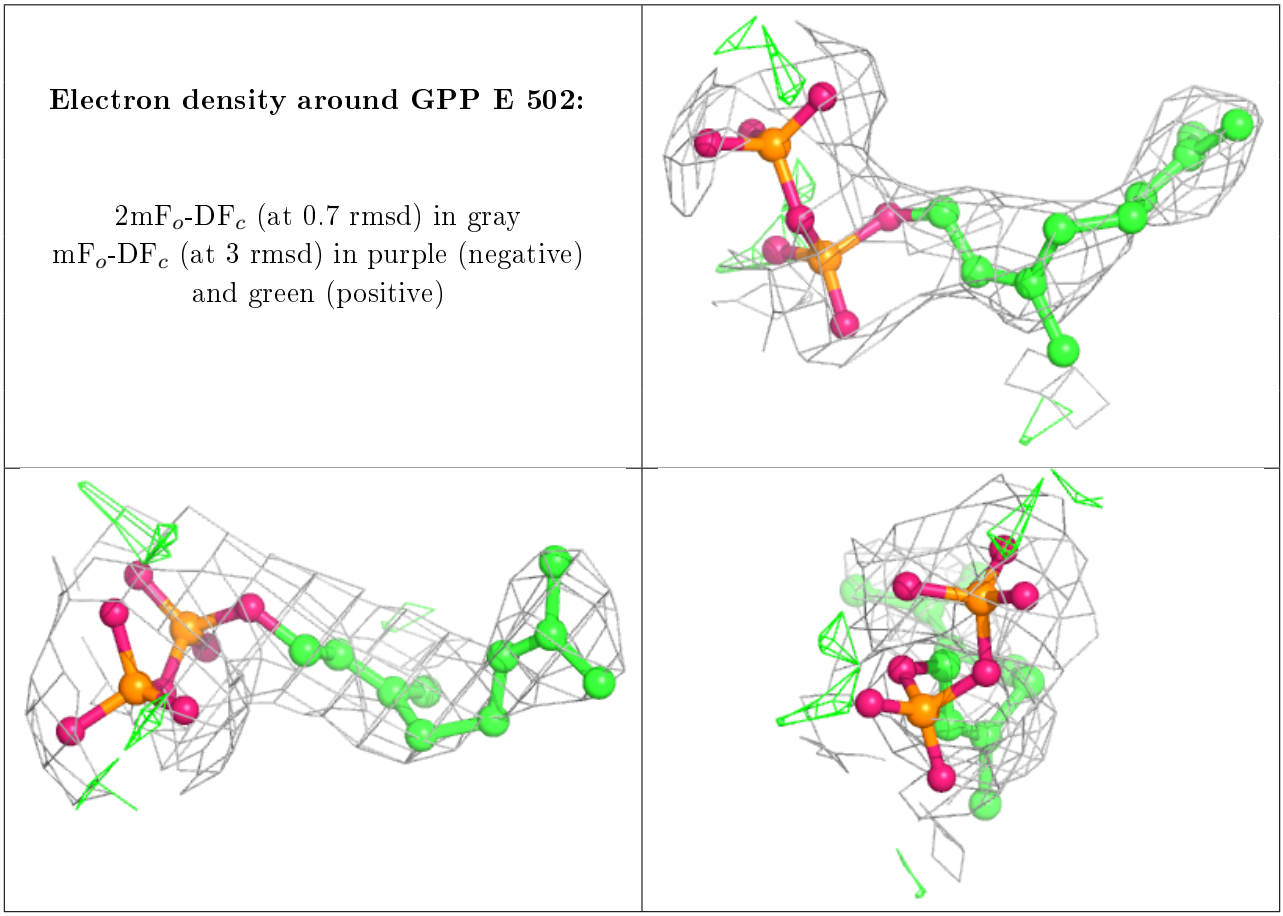
Electron density around GPP D 502:

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



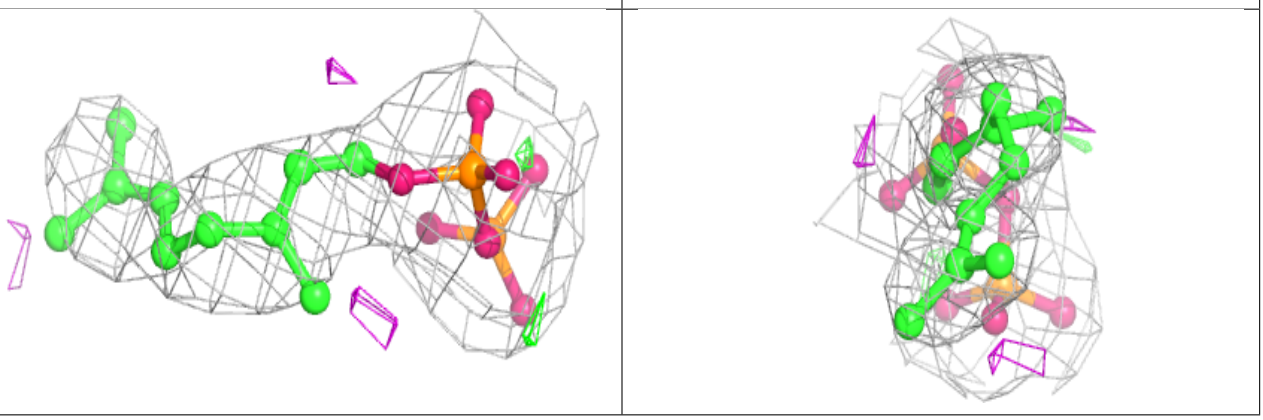
Electron density around GPP E 502:

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



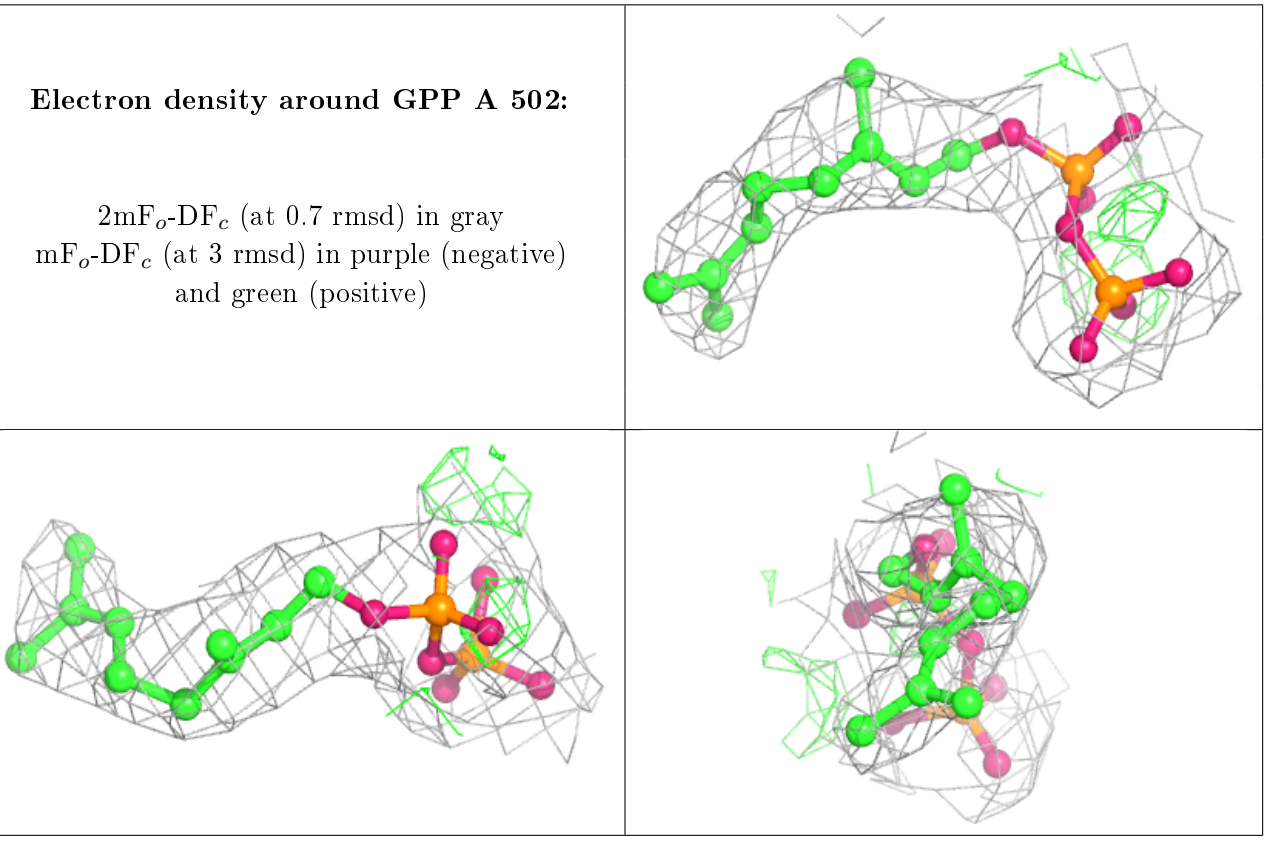
Electron density around GPP J 502:

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



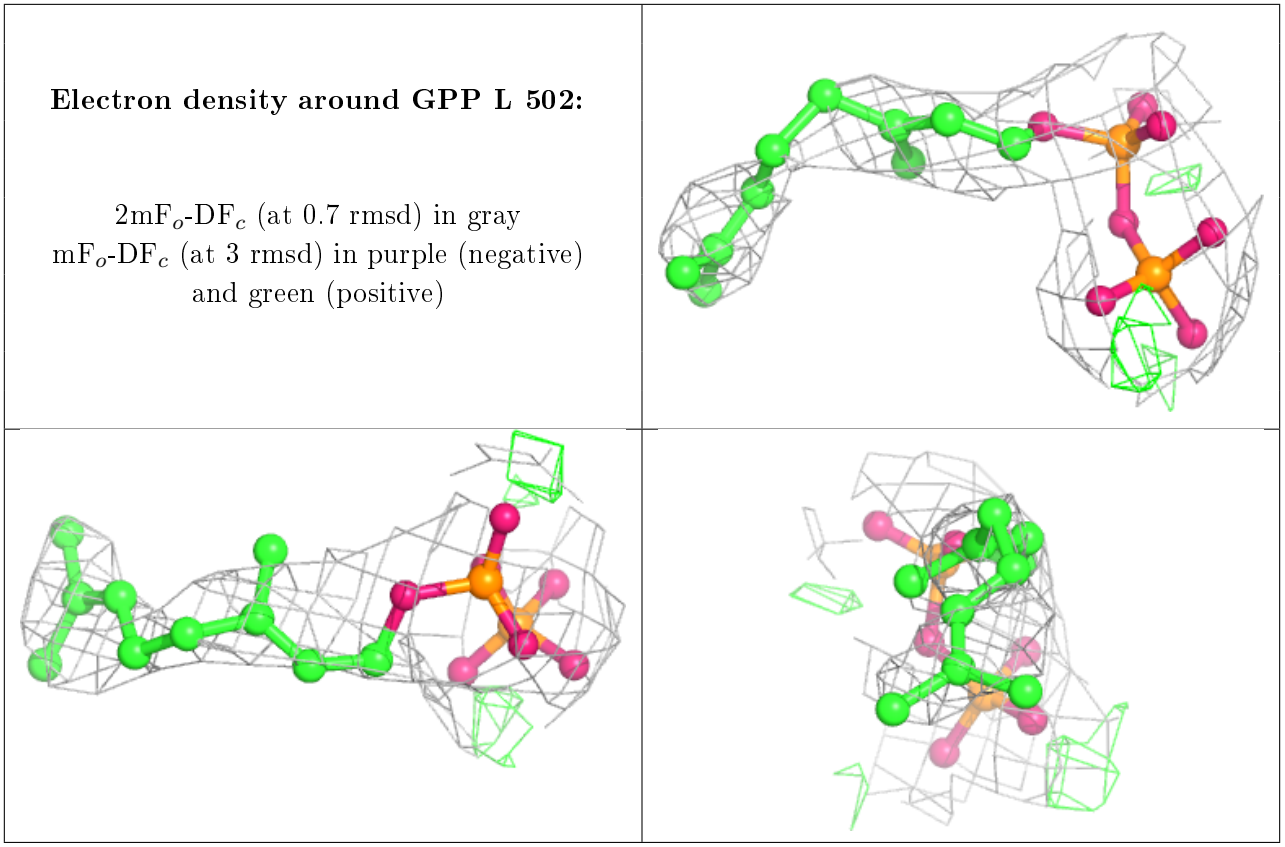
Electron density around GPP A 502:

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



Electron density around GPP L 502:

$2mF_o$-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.