wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 09:34 am GMT

PDB ID	:	4D0M
Title	:	Phosphatidylinositol 4-kinase III beta in a complex with Rab11a-GTP-gamma-S and the Rab-binding domain of FIP3
Authors	:	Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.
Deposited on	:	2014-04-29
Resolution	:	6.00 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

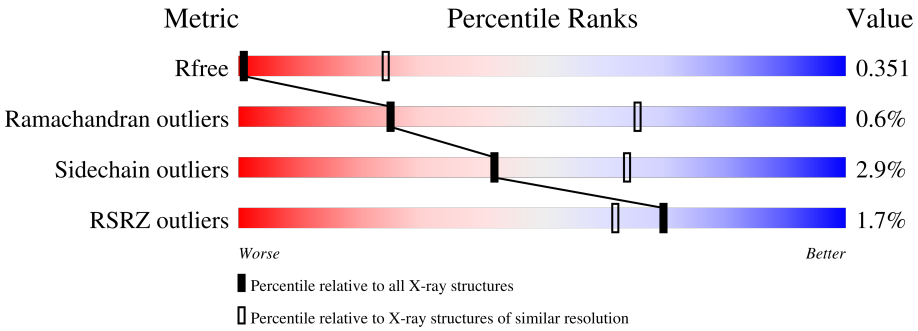
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.00 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	1000 (8.00-3.88)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)
RSRZ outliers	127900	1015 (8.20-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	566	80% · 17%
1	C	566	3% 80% · 17%
1	G	566	79% · 17%
1	I	566	4% 80% · 17%
1	M	566	79% · 17%
1	O	566	79% · 17%

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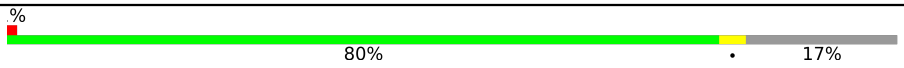
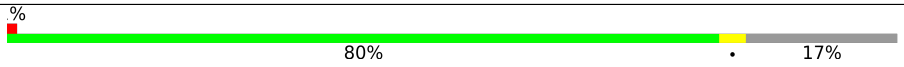
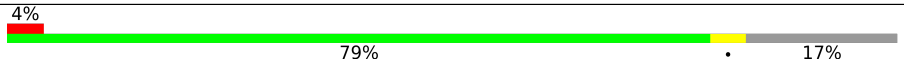
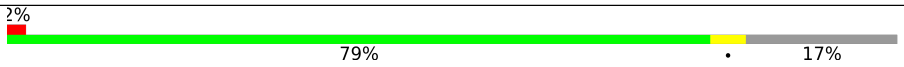
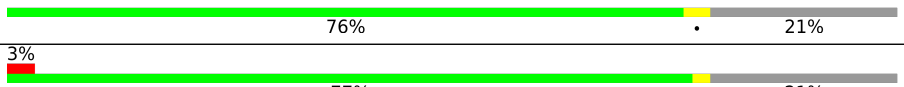
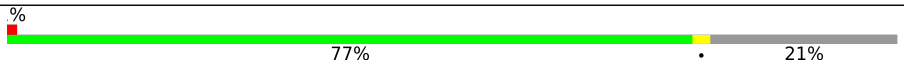
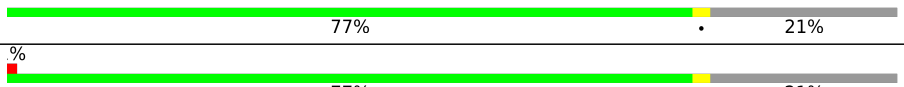
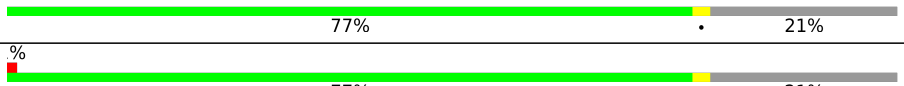
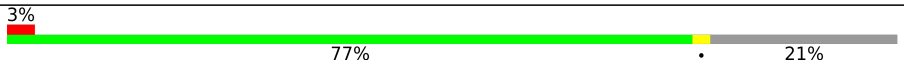
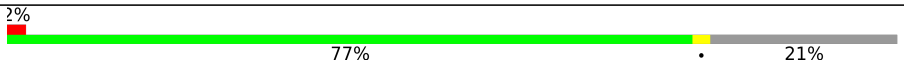
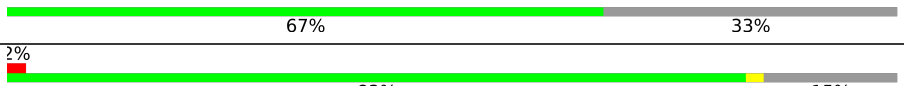
Mol	Chain	Length	Quality of chain
1	Q	566	
1	S	566	
1	W	566	
1	Y	566	
1	c	566	
1	g	566	
2	B	219	
2	D	219	
2	H	219	
2	J	219	
2	N	219	
2	P	219	
2	R	219	
2	T	219	
2	X	219	
2	Z	219	
2	d	219	
2	h	219	
3	E	48	
3	F	48	
3	K	48	
3	L	48	
3	U	48	
3	V	48	
3	a	48	

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Mol	Chain	Length	Quality of chain
3	b	48	67% 33%
3	e	48	2% 83% 15%
3	f	48	67% 33%
3	i	48	83% 15%
3	j	48	67% 33%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 65970 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 PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	C	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	G	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	I	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	M	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	O	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Q	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	S	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	W	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Y	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	c	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	g	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP Q9UBF8
A	120	SER	-	expression tag	UNP Q9UBF8
A	294	ALA	SER	engineered mutation	UNP Q9UBF8
A	507	ARG	LYS	conflict	UNP Q9UBF8
C	119	GLY	-	expression tag	UNP Q9UBF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	120	SER	-	expression tag	UNP Q9UBF8
C	294	ALA	SER	engineered mutation	UNP Q9UBF8
C	507	ARG	LYS	conflict	UNP Q9UBF8
G	119	GLY	-	expression tag	UNP Q9UBF8
G	120	SER	-	expression tag	UNP Q9UBF8
G	294	ALA	SER	engineered mutation	UNP Q9UBF8
G	507	ARG	LYS	conflict	UNP Q9UBF8
I	119	GLY	-	expression tag	UNP Q9UBF8
I	120	SER	-	expression tag	UNP Q9UBF8
I	294	ALA	SER	engineered mutation	UNP Q9UBF8
I	507	ARG	LYS	conflict	UNP Q9UBF8
M	119	GLY	-	expression tag	UNP Q9UBF8
M	120	SER	-	expression tag	UNP Q9UBF8
M	294	ALA	SER	engineered mutation	UNP Q9UBF8
M	507	ARG	LYS	conflict	UNP Q9UBF8
O	119	GLY	-	expression tag	UNP Q9UBF8
O	120	SER	-	expression tag	UNP Q9UBF8
O	294	ALA	SER	engineered mutation	UNP Q9UBF8
O	507	ARG	LYS	conflict	UNP Q9UBF8
Q	119	GLY	-	expression tag	UNP Q9UBF8
Q	120	SER	-	expression tag	UNP Q9UBF8
Q	294	ALA	SER	engineered mutation	UNP Q9UBF8
Q	507	ARG	LYS	conflict	UNP Q9UBF8
S	119	GLY	-	expression tag	UNP Q9UBF8
S	120	SER	-	expression tag	UNP Q9UBF8
S	294	ALA	SER	engineered mutation	UNP Q9UBF8
S	507	ARG	LYS	conflict	UNP Q9UBF8
W	119	GLY	-	expression tag	UNP Q9UBF8
W	120	SER	-	expression tag	UNP Q9UBF8
W	294	ALA	SER	engineered mutation	UNP Q9UBF8
W	507	ARG	LYS	conflict	UNP Q9UBF8
Y	119	GLY	-	expression tag	UNP Q9UBF8
Y	120	SER	-	expression tag	UNP Q9UBF8
Y	294	ALA	SER	engineered mutation	UNP Q9UBF8
Y	507	ARG	LYS	conflict	UNP Q9UBF8
c	119	GLY	-	expression tag	UNP Q9UBF8
c	120	SER	-	expression tag	UNP Q9UBF8
c	294	ALA	SER	engineered mutation	UNP Q9UBF8
c	507	ARG	LYS	conflict	UNP Q9UBF8
g	119	GLY	-	expression tag	UNP Q9UBF8
g	120	SER	-	expression tag	UNP Q9UBF8
g	294	ALA	SER	engineered mutation	UNP Q9UBF8

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Chain	Residue	Modelled	Actual	Comment	Reference
g	507	ARG	LYS	conflict	UNP Q9UBF8

- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	D	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	H	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	J	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	N	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	P	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	R	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	T	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	X	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	Z	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	d	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	h	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62491
B	-1	SER	-	expression tag	UNP P62491
B	0	HIS	-	expression tag	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491
D	-2	GLY	-	expression tag	UNP P62491
D	-1	SER	-	expression tag	UNP P62491
D	0	HIS	-	expression tag	UNP P62491
D	70	LEU	GLN	engineered mutation	UNP P62491
H	-2	GLY	-	expression tag	UNP P62491

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	SER	-	expression tag	UNP P62491
H	0	HIS	-	expression tag	UNP P62491
H	70	LEU	GLN	engineered mutation	UNP P62491
J	-2	GLY	-	expression tag	UNP P62491
J	-1	SER	-	expression tag	UNP P62491
J	0	HIS	-	expression tag	UNP P62491
J	70	LEU	GLN	engineered mutation	UNP P62491
N	-2	GLY	-	expression tag	UNP P62491
N	-1	SER	-	expression tag	UNP P62491
N	0	HIS	-	expression tag	UNP P62491
N	70	LEU	GLN	engineered mutation	UNP P62491
P	-2	GLY	-	expression tag	UNP P62491
P	-1	SER	-	expression tag	UNP P62491
P	0	HIS	-	expression tag	UNP P62491
P	70	LEU	GLN	engineered mutation	UNP P62491
R	-2	GLY	-	expression tag	UNP P62491
R	-1	SER	-	expression tag	UNP P62491
R	0	HIS	-	expression tag	UNP P62491
R	70	LEU	GLN	engineered mutation	UNP P62491
T	-2	GLY	-	expression tag	UNP P62491
T	-1	SER	-	expression tag	UNP P62491
T	0	HIS	-	expression tag	UNP P62491
T	70	LEU	GLN	engineered mutation	UNP P62491
X	-2	GLY	-	expression tag	UNP P62491
X	-1	SER	-	expression tag	UNP P62491
X	0	HIS	-	expression tag	UNP P62491
X	70	LEU	GLN	engineered mutation	UNP P62491
Z	-2	GLY	-	expression tag	UNP P62491
Z	-1	SER	-	expression tag	UNP P62491
Z	0	HIS	-	expression tag	UNP P62491
Z	70	LEU	GLN	engineered mutation	UNP P62491
d	-2	GLY	-	expression tag	UNP P62491
d	-1	SER	-	expression tag	UNP P62491
d	0	HIS	-	expression tag	UNP P62491
d	70	LEU	GLN	engineered mutation	UNP P62491
h	-2	GLY	-	expression tag	UNP P62491
h	-1	SER	-	expression tag	UNP P62491
h	0	HIS	-	expression tag	UNP P62491
h	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 3 is a protein called RAB11 FAMILY-INTERACTING PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	F	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	K	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	L	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	U	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	V	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	a	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	b	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	e	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	f	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	i	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	j	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	709	GLY	-	expression tag	UNP O75154
E	710	SER	-	expression tag	UNP O75154
E	711	HIS	-	expression tag	UNP O75154
E	712	MET	-	expression tag	UNP O75154
F	709	GLY	-	expression tag	UNP O75154
F	710	SER	-	expression tag	UNP O75154
F	711	HIS	-	expression tag	UNP O75154
F	712	MET	-	expression tag	UNP O75154
K	709	GLY	-	expression tag	UNP O75154
K	710	SER	-	expression tag	UNP O75154
K	711	HIS	-	expression tag	UNP O75154
K	712	MET	-	expression tag	UNP O75154
L	709	GLY	-	expression tag	UNP O75154
L	710	SER	-	expression tag	UNP O75154
L	711	HIS	-	expression tag	UNP O75154
L	712	MET	-	expression tag	UNP O75154

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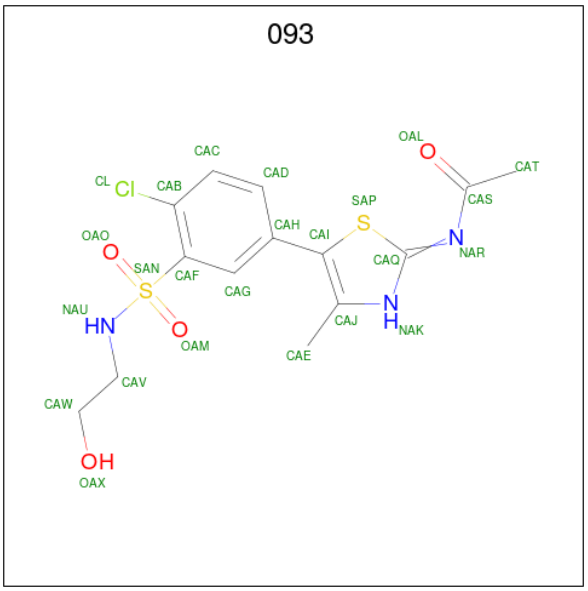
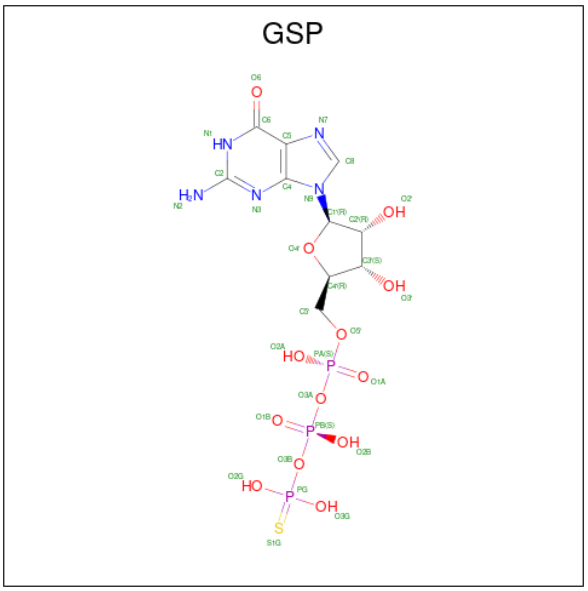
Chain	Residue	Modelled	Actual	Comment	Reference
U	709	GLY	-	expression tag	UNP O75154
U	710	SER	-	expression tag	UNP O75154
U	711	HIS	-	expression tag	UNP O75154
U	712	MET	-	expression tag	UNP O75154
V	709	GLY	-	expression tag	UNP O75154
V	710	SER	-	expression tag	UNP O75154
V	711	HIS	-	expression tag	UNP O75154
V	712	MET	-	expression tag	UNP O75154
a	709	GLY	-	expression tag	UNP O75154
a	710	SER	-	expression tag	UNP O75154
a	711	HIS	-	expression tag	UNP O75154
a	712	MET	-	expression tag	UNP O75154
b	709	GLY	-	expression tag	UNP O75154
b	710	SER	-	expression tag	UNP O75154
b	711	HIS	-	expression tag	UNP O75154
b	712	MET	-	expression tag	UNP O75154
e	709	GLY	-	expression tag	UNP O75154
e	710	SER	-	expression tag	UNP O75154
e	711	HIS	-	expression tag	UNP O75154
e	712	MET	-	expression tag	UNP O75154
f	709	GLY	-	expression tag	UNP O75154
f	710	SER	-	expression tag	UNP O75154
f	711	HIS	-	expression tag	UNP O75154
f	712	MET	-	expression tag	UNP O75154
i	709	GLY	-	expression tag	UNP O75154
i	710	SER	-	expression tag	UNP O75154
i	711	HIS	-	expression tag	UNP O75154
i	712	MET	-	expression tag	UNP O75154
j	709	GLY	-	expression tag	UNP O75154
j	710	SER	-	expression tag	UNP O75154
j	711	HIS	-	expression tag	UNP O75154
j	712	MET	-	expression tag	UNP O75154

- Molecule 4 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: $C_{14}H_{16}ClN_3O_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	C	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	G	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	I	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	M	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	O	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	Q	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	S	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	W	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	Y	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	c	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		
4	g	1	Total	C	Cl	N	O	S	24	0
			24	14	1	3	4	2		

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	H	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	J	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	N	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	P	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	R	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	T	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	X	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	Z	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	d	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	h	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

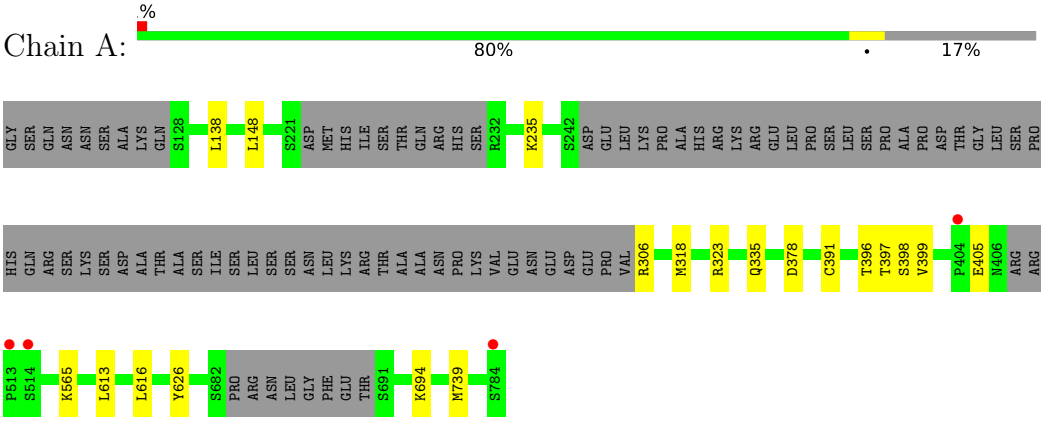
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	H	1	Total Mg 1 1	0	0
6	J	1	Total Mg 1 1	0	0
6	N	1	Total Mg 1 1	0	0
6	P	1	Total Mg 1 1	0	0
6	R	1	Total Mg 1 1	0	0
6	T	1	Total Mg 1 1	0	0
6	X	1	Total Mg 1 1	0	0
6	Z	1	Total Mg 1 1	0	0
6	d	1	Total Mg 1 1	0	0
6	h	1	Total 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.

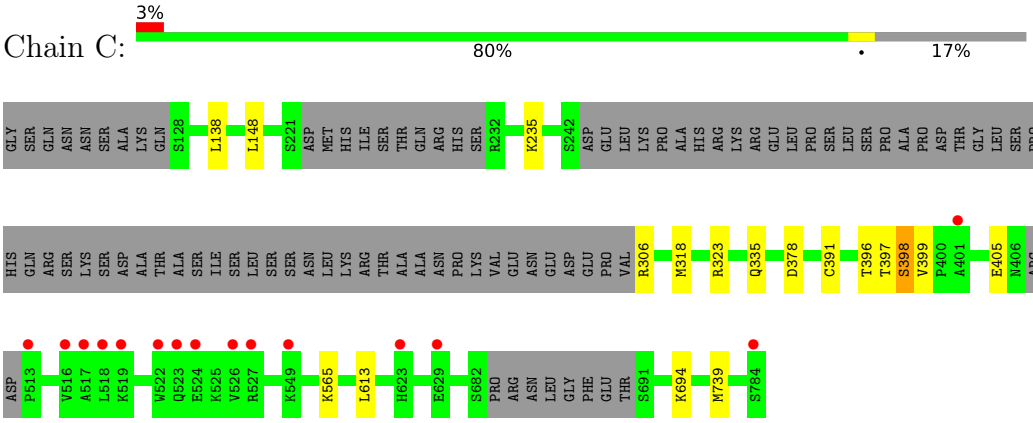
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain A:



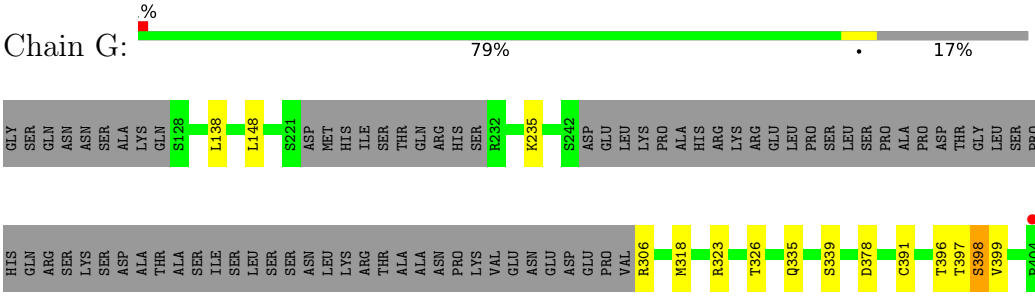
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

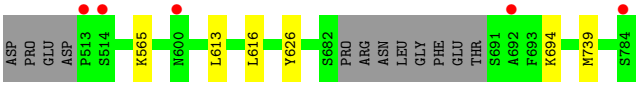
Chain C:



• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

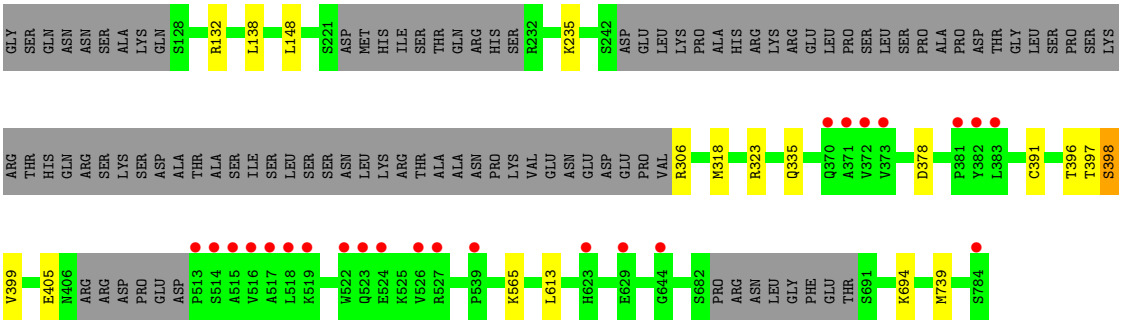
Chain G:





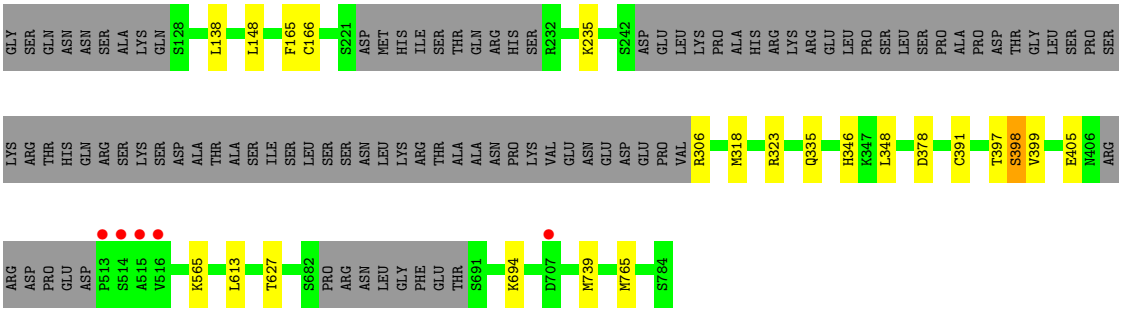
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain I:



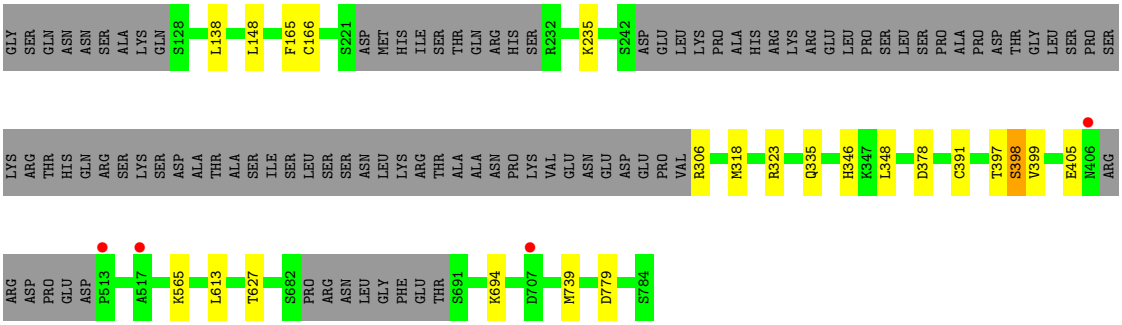
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain M:



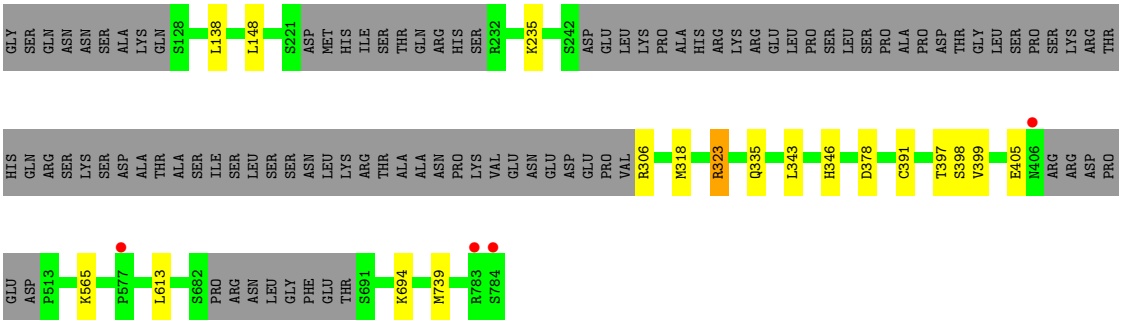
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain O:



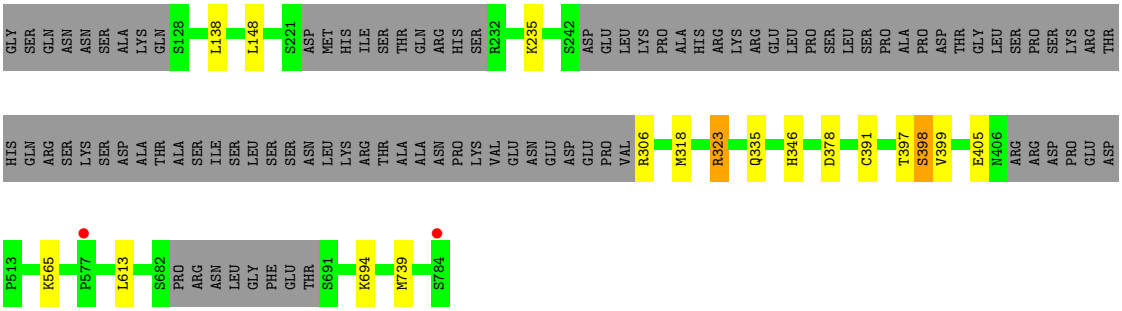
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain Q:



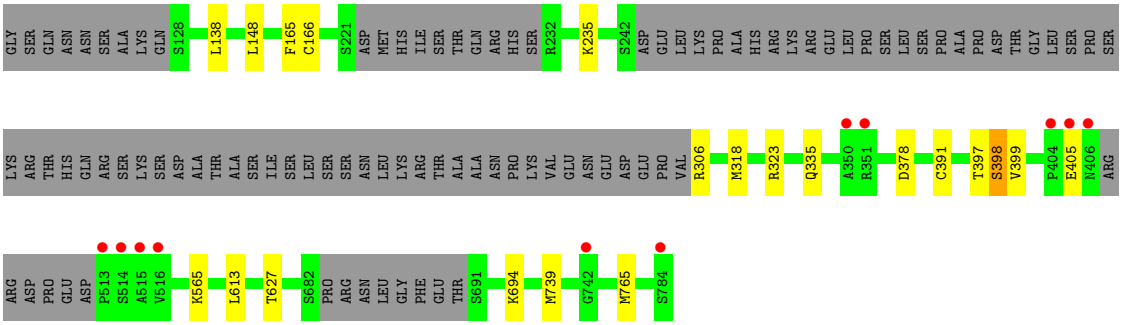
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain S:



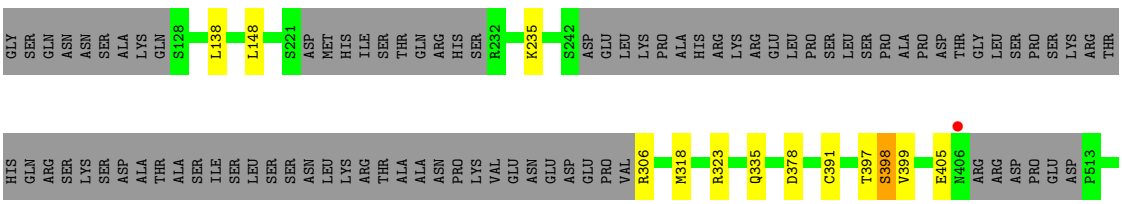
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

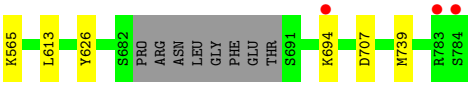
Chain W:



• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

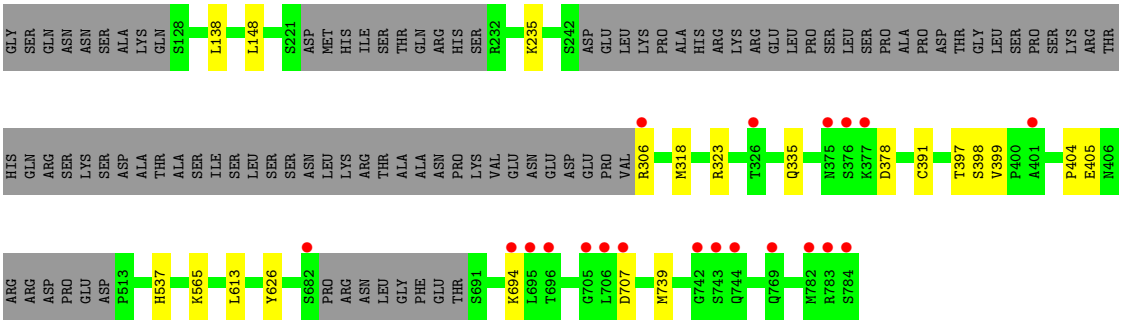
Chain Y:





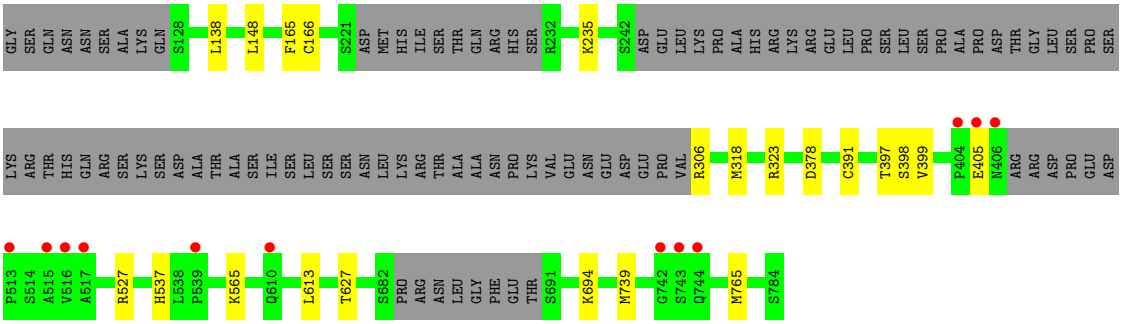
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain c:



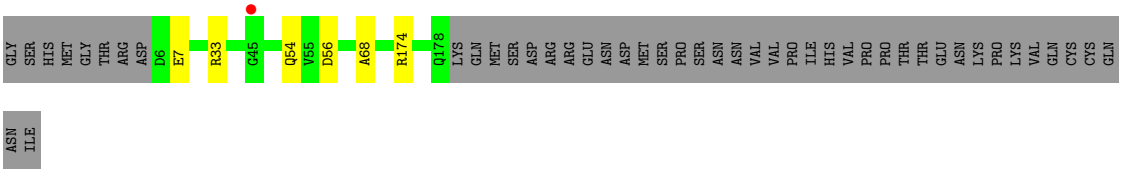
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain g:



• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain B:

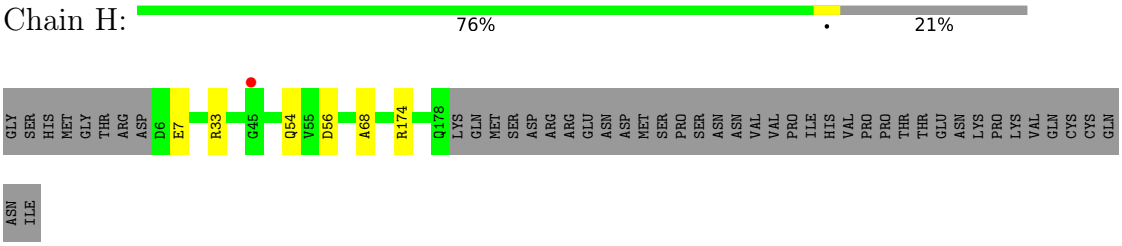


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain D:

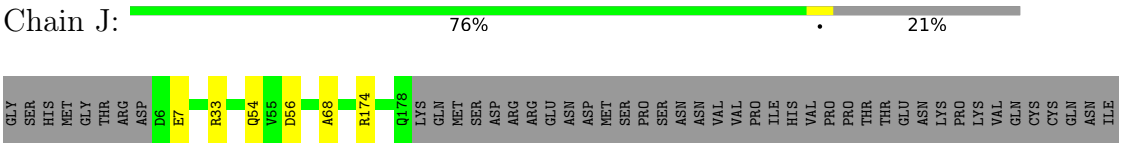
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain H:



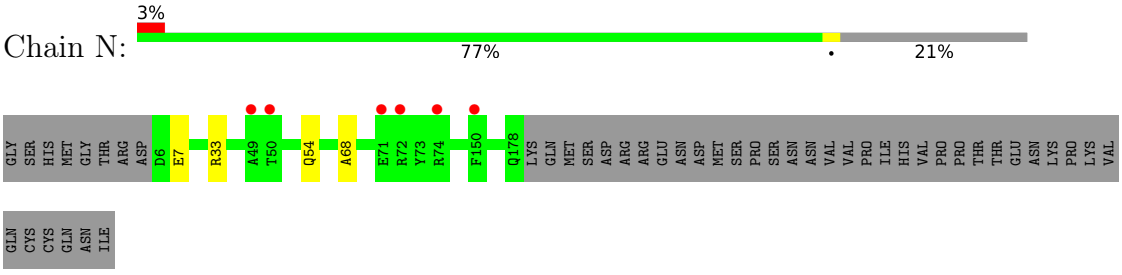
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain J:



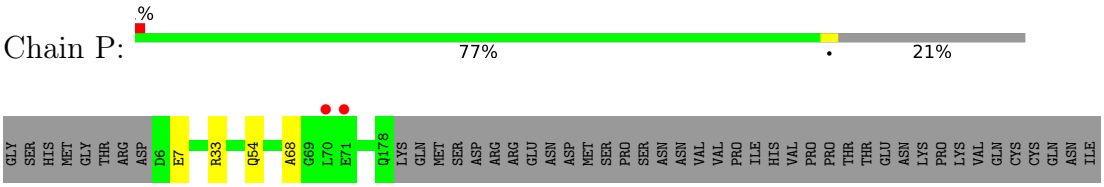
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain N:



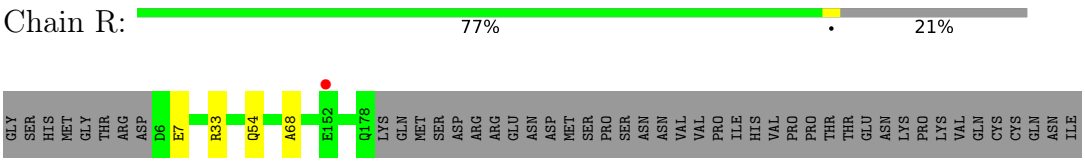
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain P:



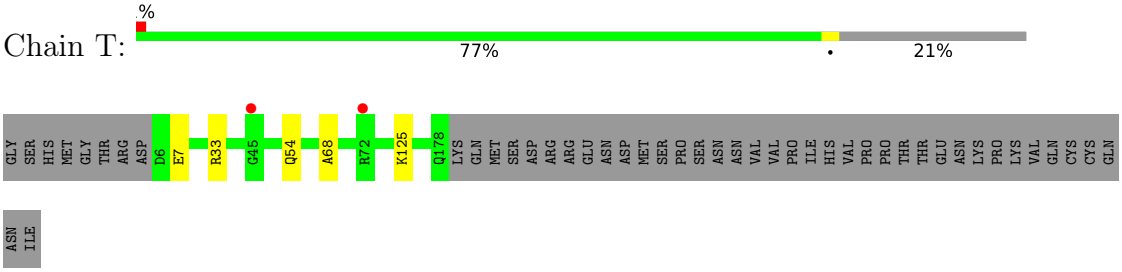
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain R:



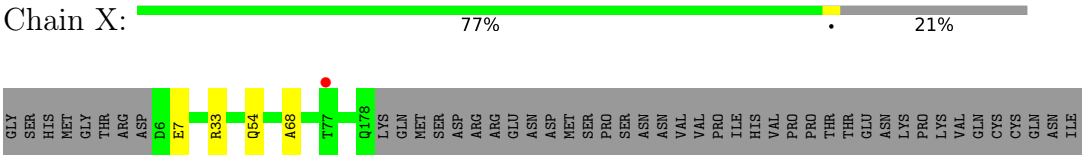
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain T:



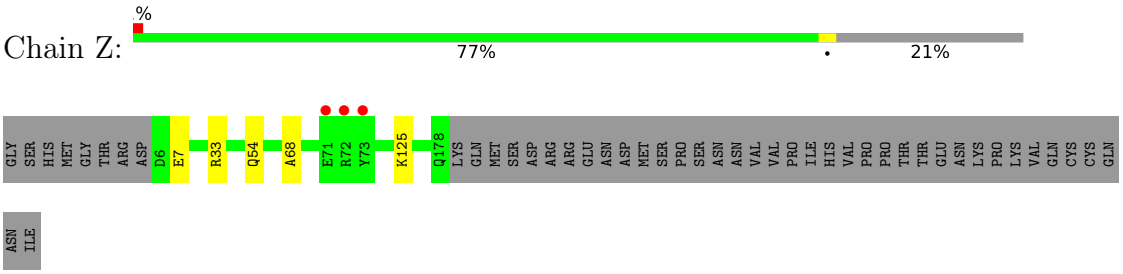
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain X:



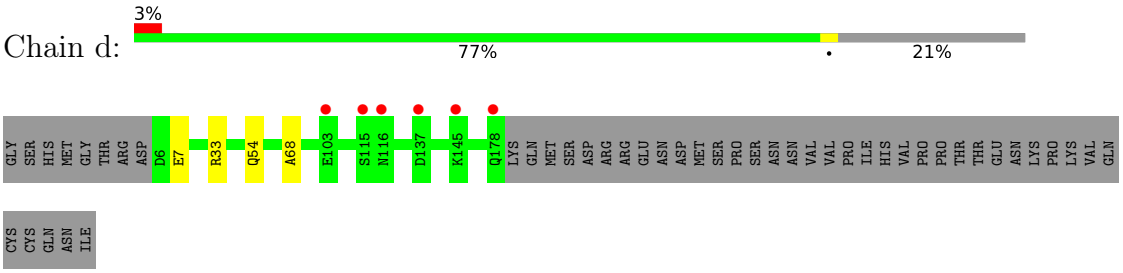
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain Z:



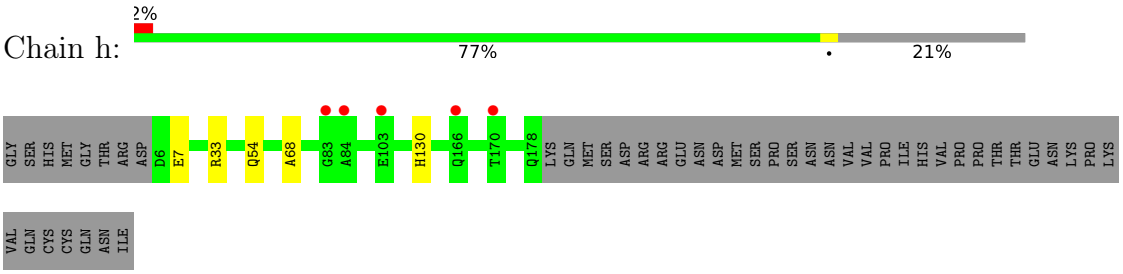
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain d:



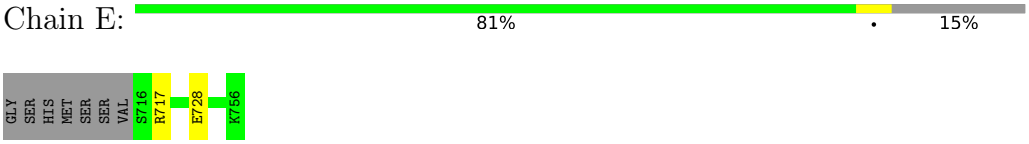
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain h:



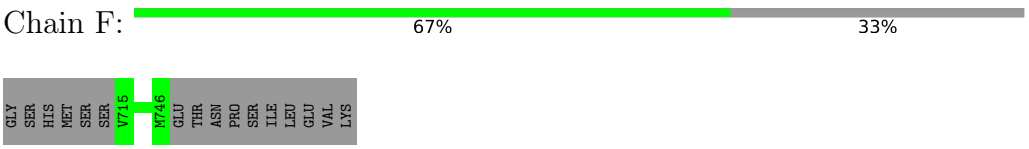
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain E:



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain F:

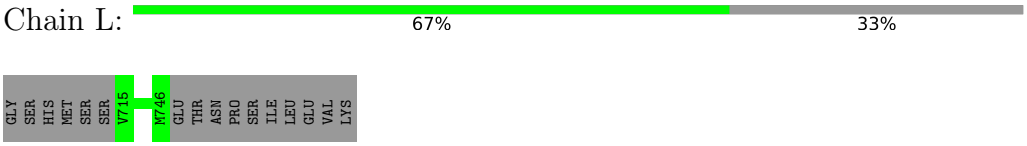


• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain K:

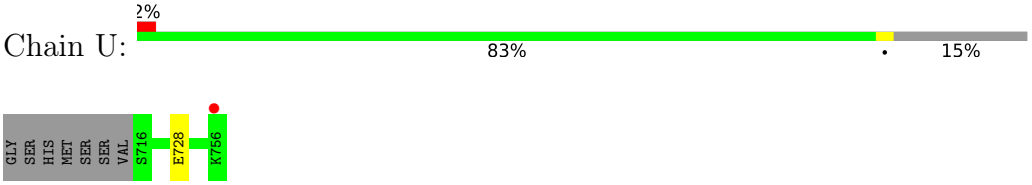
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain L:



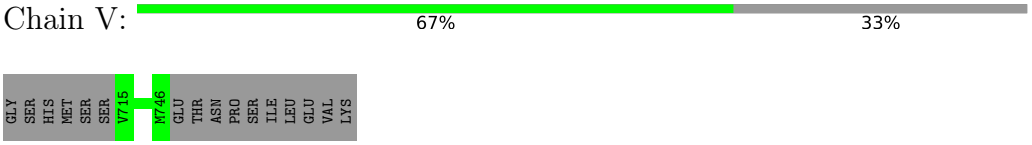
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain U:



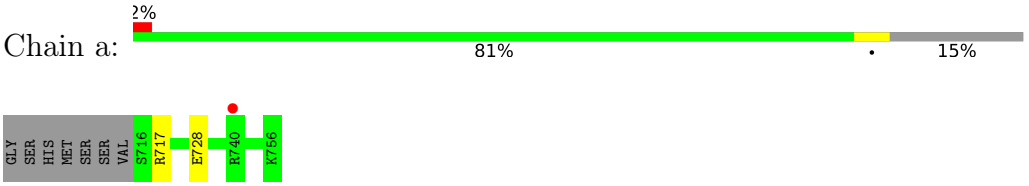
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain V:



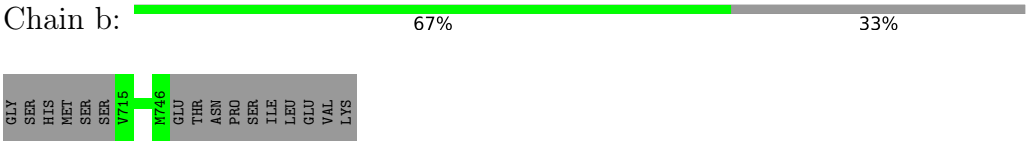
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain a:



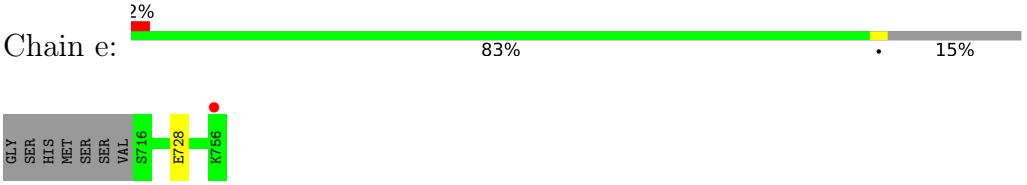
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain b:



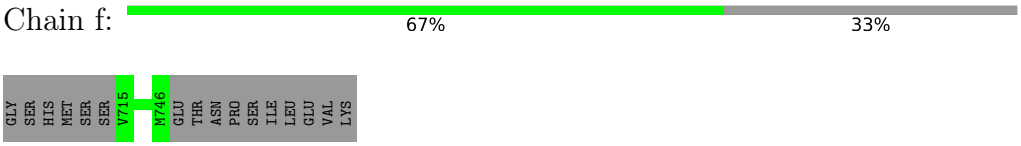
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain e:



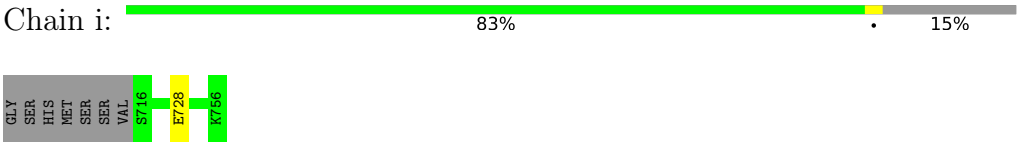
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain f:



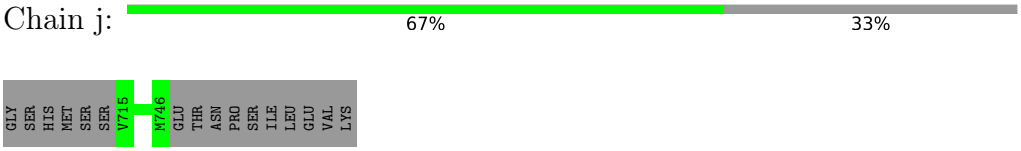
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain i:



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

Chain j:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	199.50Å 134.47Å 294.33Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	294.32 – 6.00 49.88 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (294.32-6.00) 93.0 (49.88-6.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.253 , 0.359 0.252 , 0.351	Depositor DCC
R_{free} test set	1925 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	248.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 117.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	65970	wwPDB-VP
Average B, all atoms (Å^2)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, MG, 093

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	0.59	0/3866	0.72	0/5219
1	C	0.56	0/3866	0.70	0/5219
1	G	0.59	0/3866	0.72	0/5219
1	I	0.56	0/3866	0.69	1/5219 (0.0%)
1	M	0.59	0/3866	0.71	1/5219 (0.0%)
1	O	0.59	0/3866	0.71	0/5219
1	Q	0.57	0/3866	0.70	0/5219
1	S	0.57	0/3866	0.70	0/5219
1	W	0.58	0/3866	0.70	1/5219 (0.0%)
1	Y	0.59	0/3866	0.70	0/5219
1	c	0.60	0/3866	0.71	0/5219
1	g	0.59	0/3866	0.70	2/5219 (0.0%)
2	B	0.64	0/1399	0.76	0/1892
2	D	0.61	0/1399	0.75	0/1892
2	H	0.63	0/1399	0.74	0/1892
2	J	0.63	0/1399	0.75	0/1892
2	N	0.58	0/1399	0.73	0/1892
2	P	0.59	0/1399	0.73	0/1892
2	R	0.59	0/1399	0.72	0/1892
2	T	0.58	0/1399	0.73	0/1892
2	X	0.58	0/1399	0.72	0/1892
2	Z	0.58	0/1399	0.73	0/1892
2	d	0.58	0/1399	0.73	0/1892
2	h	0.59	0/1399	0.72	0/1892
3	E	0.94	1/316 (0.3%)	0.98	1/429 (0.2%)
3	F	0.83	0/238	0.87	0/323
3	K	0.94	1/316 (0.3%)	0.97	1/429 (0.2%)
3	L	0.84	0/238	0.89	0/323
3	U	0.83	0/316	0.82	0/429
3	V	0.90	0/238	0.89	0/323
3	a	0.94	1/316 (0.3%)	0.96	1/429 (0.2%)
3	b	0.86	0/238	0.88	0/323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	e	0.85	0/316	0.86	0/429
3	f	0.88	0/238	0.89	0/323
3	i	0.85	0/316	0.81	0/429
3	j	0.88	0/238	0.87	0/323
All	All	0.60	3/66504 (0.0%)	0.72	8/89844 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	O	0	1
1	Q	0	1
1	S	0	1
1	W	0	1
1	Y	0	1
1	c	0	1
1	g	0	1
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	717	ARG	CD-NE	5.41	1.55	1.46
3	E	717	ARG	CD-NE	5.12	1.55	1.46
3	K	717	ARG	CD-NE	5.07	1.55	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	a	717	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	E	717	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	g	527	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	I	132	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	398	SER	Peptide
1	G	398	SER	Peptide
1	I	398	SER	Peptide
1	M	398	SER	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	460/566 (81%)	442 (96%)	16 (4%)	2 (0%)	34	72
1	C	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	22	62
1	G	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	22	62
1	I	460/566 (81%)	440 (96%)	17 (4%)	3 (1%)	22	62
1	M	460/566 (81%)	441 (96%)	16 (4%)	3 (1%)	22	62
1	O	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	22	62
1	Q	460/566 (81%)	439 (95%)	19 (4%)	2 (0%)	34	72
1	S	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	22	62
1	W	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	22	62
1	Y	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	22	62
1	c	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	34	72
1	g	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	34	72
2	B	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
2	H	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
2	J	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
2	N	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
2	P	171/219 (78%)	162 (95%)	8 (5%)	1 (1%)	25	66
2	R	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
2	T	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	13	50
2	X	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
2	Z	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	13	50
2	d	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
2	h	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	25	66
3	E	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	F	30/48 (62%)	30 (100%)	0	0	100	100
3	K	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	L	30/48 (62%)	30 (100%)	0	0	100	100
3	U	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	V	30/48 (62%)	30 (100%)	0	0	100	100
3	a	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	b	30/48 (62%)	30 (100%)	0	0	100	100
3	e	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	f	30/48 (62%)	30 (100%)	0	0	100	100
3	i	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	j	30/48 (62%)	30 (100%)	0	0	100	100
All	All	7986/9996 (80%)	7645 (96%)	295 (4%)	46 (1%)	25	66

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
2	B	68	ALA
1	C	405	GLU
2	D	68	ALA
1	G	405	GLU

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	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	C	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	G	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	I	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	M	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	O	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	Q	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	S	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	W	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	Y	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	c	422/508 (83%)	408 (97%)	14 (3%)	38	61
1	g	422/508 (83%)	409 (97%)	13 (3%)	40	62
2	B	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	D	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	H	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	J	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	N	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	P	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	R	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	T	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	X	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	Z	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	d	147/191 (77%)	144 (98%)	3 (2%)	55	74
2	h	147/191 (77%)	144 (98%)	3 (2%)	55	74
3	E	31/45 (69%)	30 (97%)	1 (3%)	39	62
3	F	21/45 (47%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	K	31/45 (69%)	30 (97%)	1 (3%)	39 62
3	L	21/45 (47%)	21 (100%)	0	100 100
3	U	31/45 (69%)	30 (97%)	1 (3%)	39 62
3	V	21/45 (47%)	21 (100%)	0	100 100
3	a	31/45 (69%)	30 (97%)	1 (3%)	39 62
3	b	21/45 (47%)	21 (100%)	0	100 100
3	e	31/45 (69%)	30 (97%)	1 (3%)	39 62
3	f	21/45 (47%)	21 (100%)	0	100 100
3	i	31/45 (69%)	30 (97%)	1 (3%)	39 62
3	j	21/45 (47%)	21 (100%)	0	100 100
All	All	7140/8928 (80%)	6931 (97%)	209 (3%)	42 64

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	613	LEU
1	W	318	MET
1	g	391	CYS
2	R	33	ARG
1	S	397	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
3	U	735	GLN
3	b	727	GLN
3	V	727	GLN
1	W	776	GLN
1	c	606	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	GSP	N	2000	6	26,34,34	1.24	4 (15%)	27,54,54	1.50	5 (18%)
4	093	M	2002	-	19,25,25	2.22	8 (42%)	23,36,36	4.91	10 (43%)
5	GSP	P	2000	6	26,34,34	1.28	4 (15%)	27,54,54	1.49	6 (22%)
5	GSP	B	2000	6	26,34,34	1.42	3 (11%)	27,54,54	1.48	4 (14%)
4	093	G	2002	-	19,25,25	2.21	7 (36%)	23,36,36	4.91	10 (43%)
5	GSP	X	2000	6	26,34,34	1.38	5 (19%)	27,54,54	1.52	6 (22%)
4	093	Y	2002	-	19,25,25	2.20	7 (36%)	23,36,36	4.91	10 (43%)
4	093	S	2002	-	19,25,25	2.21	7 (36%)	23,36,36	4.93	10 (43%)
4	093	c	2002	-	19,25,25	2.22	8 (42%)	23,36,36	4.91	10 (43%)
4	093	I	2002	-	19,25,25	2.20	7 (36%)	23,36,36	4.91	10 (43%)
5	GSP	D	2000	6	26,34,34	1.37	5 (19%)	27,54,54	1.47	6 (22%)
5	GSP	J	2000	6	26,34,34	1.43	3 (11%)	27,54,54	1.45	4 (14%)
4	093	g	2002	-	19,25,25	2.20	8 (42%)	23,36,36	4.92	10 (43%)
5	GSP	T	2000	6	26,34,34	1.20	3 (11%)	27,54,54	1.47	6 (22%)
4	093	Q	2002	-	19,25,25	2.21	7 (36%)	23,36,36	4.91	10 (43%)
5	GSP	d	2000	6	26,34,34	1.35	4 (15%)	27,54,54	1.45	5 (18%)
5	GSP	Z	2000	6	26,34,34	1.36	5 (19%)	27,54,54	1.37	5 (18%)
4	093	W	2002	-	19,25,25	2.20	7 (36%)	23,36,36	4.91	10 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	093	A	2002	-	19,25,25	2.19	7 (36%)	23,36,36	4.91	10 (43%)
5	GSP	h	2000	6	26,34,34	1.47	5 (19%)	27,54,54	1.52	5 (18%)
5	GSP	R	2000	6	26,34,34	1.23	2 (7%)	27,54,54	1.40	5 (18%)
4	093	C	2002	-	19,25,25	2.21	8 (42%)	23,36,36	4.91	10 (43%)
4	093	O	2002	-	19,25,25	2.23	8 (42%)	23,36,36	4.91	10 (43%)
5	GSP	H	2000	6	26,34,34	1.29	3 (11%)	27,54,54	1.44	6 (22%)

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
5	GSP	N	2000	6	-	3/17/38/38	0/3/3/3
4	093	M	2002	-	-	6/13/19/19	0/2/2/2
5	GSP	P	2000	6	-	3/17/38/38	0/3/3/3
5	GSP	B	2000	6	-	3/17/38/38	0/3/3/3
4	093	G	2002	-	-	6/13/19/19	0/2/2/2
5	GSP	X	2000	6	-	3/17/38/38	0/3/3/3
4	093	Y	2002	-	-	6/13/19/19	0/2/2/2
4	093	S	2002	-	-	6/13/19/19	0/2/2/2
4	093	c	2002	-	-	6/13/19/19	0/2/2/2
4	093	I	2002	-	-	6/13/19/19	0/2/2/2
5	GSP	D	2000	6	-	3/17/38/38	0/3/3/3
5	GSP	J	2000	6	-	3/17/38/38	0/3/3/3
4	093	g	2002	-	-	6/13/19/19	0/2/2/2
5	GSP	T	2000	6	-	3/17/38/38	0/3/3/3
4	093	Q	2002	-	-	6/13/19/19	0/2/2/2
5	GSP	d	2000	6	-	3/17/38/38	0/3/3/3
5	GSP	Z	2000	6	-	3/17/38/38	0/3/3/3
4	093	W	2002	-	-	6/13/19/19	0/2/2/2
4	093	A	2002	-	-	6/13/19/19	0/2/2/2
5	GSP	h	2000	6	-	3/17/38/38	0/3/3/3
5	GSP	R	2000	6	-	3/17/38/38	0/3/3/3
4	093	C	2002	-	-	6/13/19/19	0/2/2/2
4	093	O	2002	-	-	6/13/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GSP	H	2000	6	-	3/17/38/38	0/3/3/3

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	2002	093	CAQ-NAR	4.19	1.45	1.33
4	S	2002	093	CAQ-NAR	4.18	1.45	1.33
4	W	2002	093	CAQ-NAR	4.17	1.45	1.33
4	O	2002	093	CAQ-NAR	4.17	1.45	1.33
4	g	2002	093	CAQ-NAR	4.16	1.45	1.33

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	2002	093	OAO-SAN-OAM	-20.37	94.51	119.55
4	g	2002	093	OAO-SAN-OAM	-20.35	94.53	119.55
4	Q	2002	093	OAO-SAN-OAM	-20.34	94.55	119.55
4	G	2002	093	OAO-SAN-OAM	-20.33	94.56	119.55
4	C	2002	093	OAO-SAN-OAM	-20.33	94.56	119.55

There are no chirality outliers.

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2000	GSP	C5'-O5'-PA-O2A
5	D	2000	GSP	C5'-O5'-PA-O2A
5	H	2000	GSP	C5'-O5'-PA-O2A
5	J	2000	GSP	C5'-O5'-PA-O2A
5	N	2000	GSP	C5'-O5'-PA-O2A

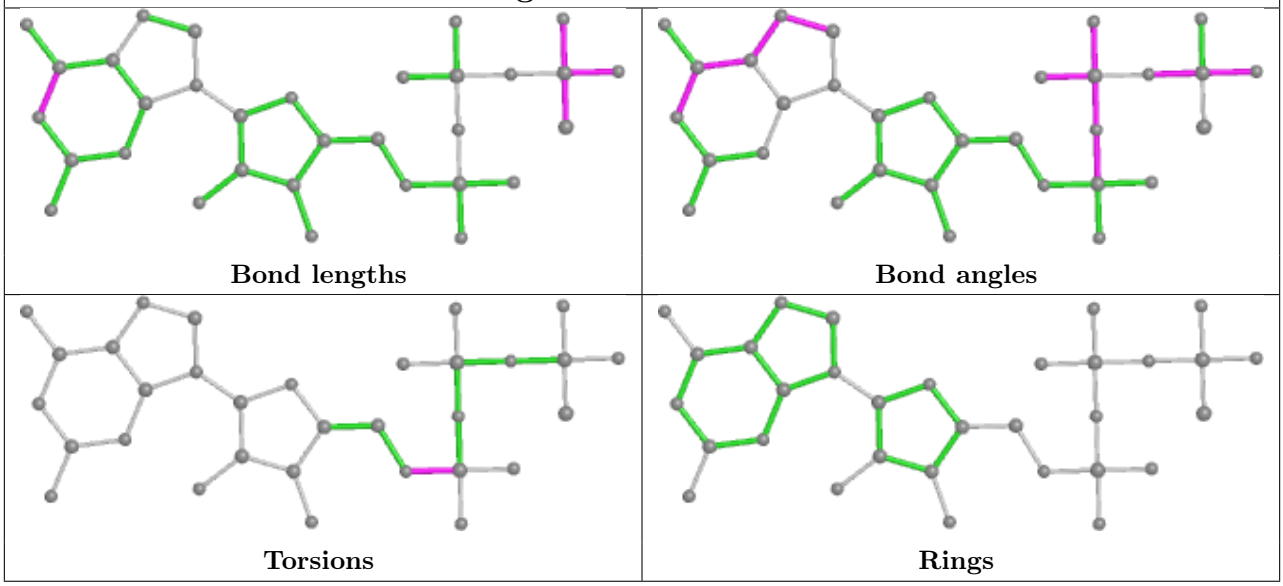
There are no ring outliers.

No monomer is involved in short contacts.

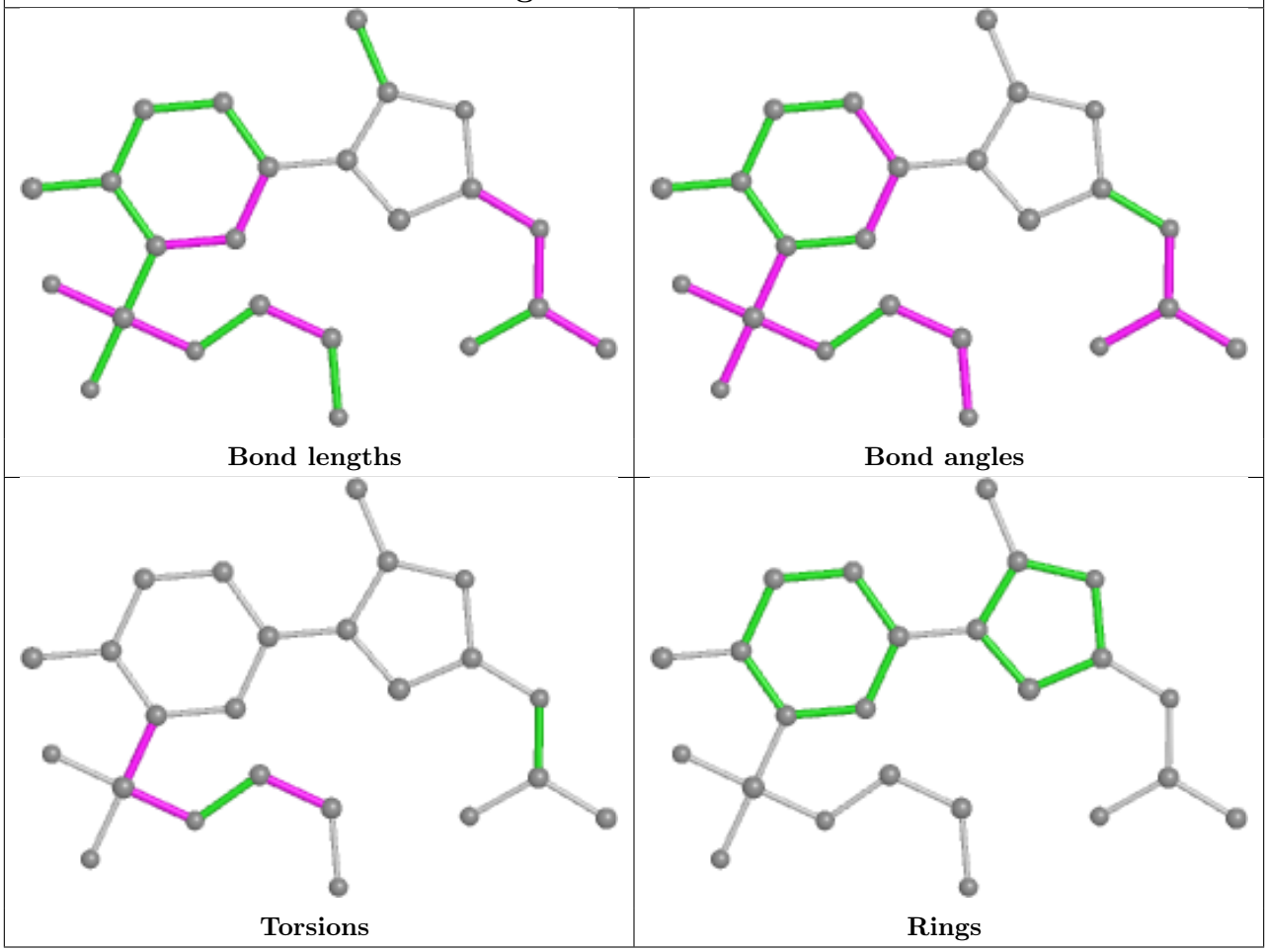
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

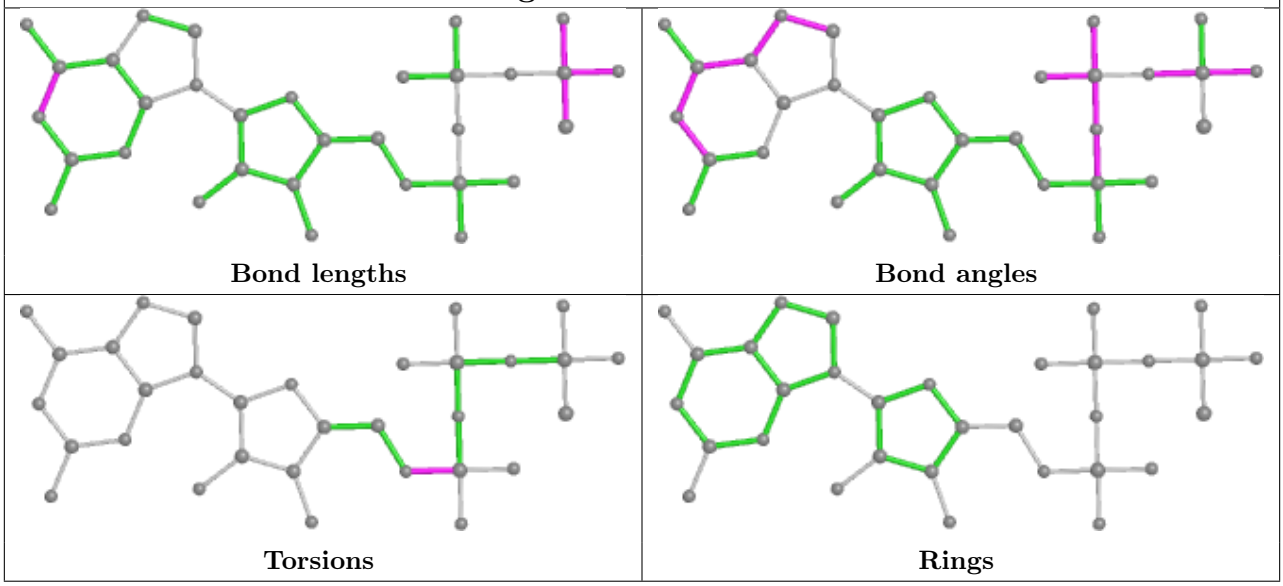
Ligand GSP N 2000



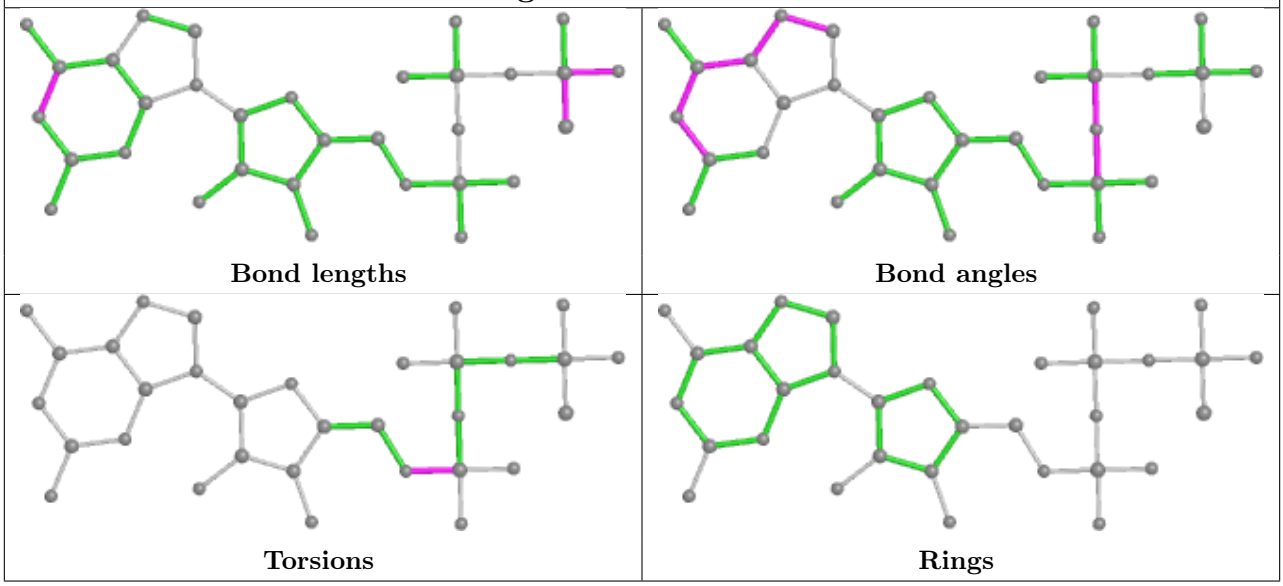
Ligand 093 M 2002



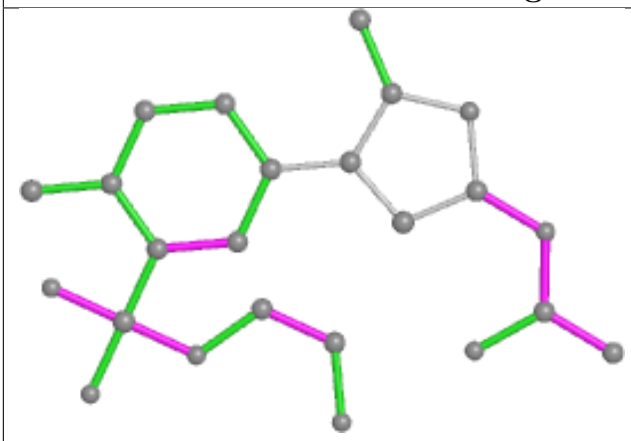
Ligand GSP P 2000



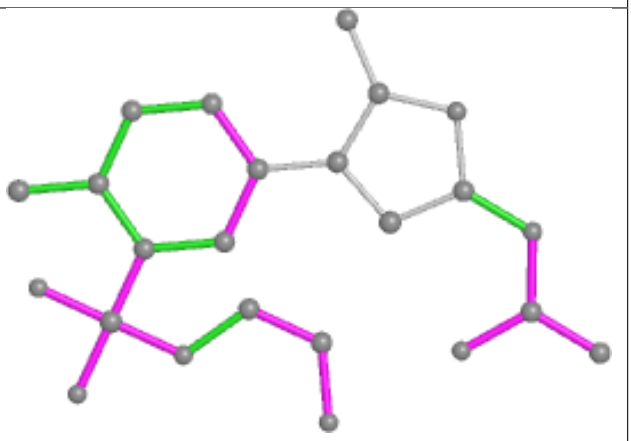
Ligand GSP B 2000



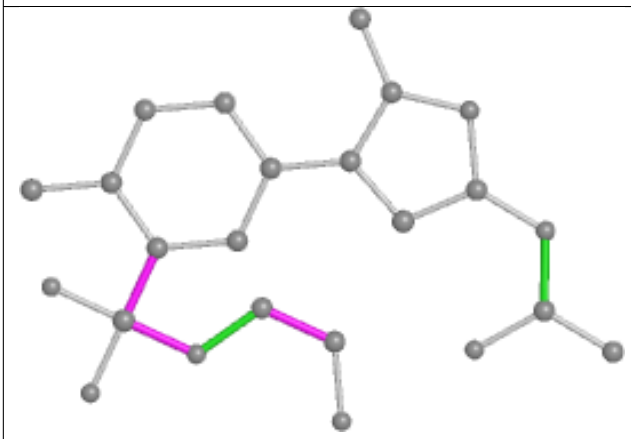
Ligand 093 G 2002



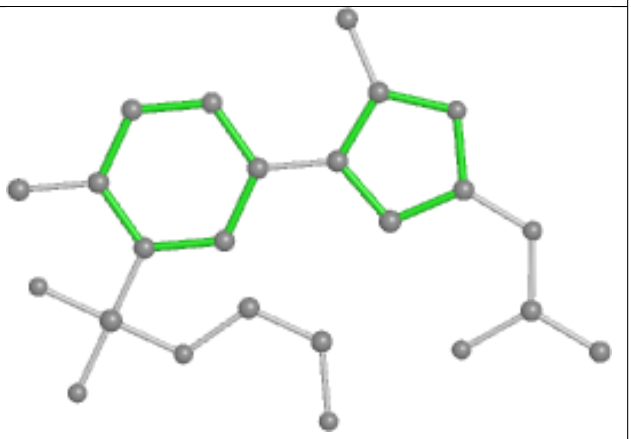
Bond lengths



Bond angles

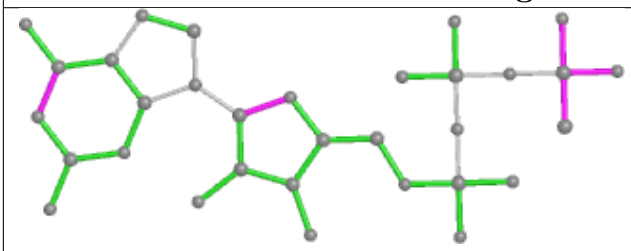


Torsions

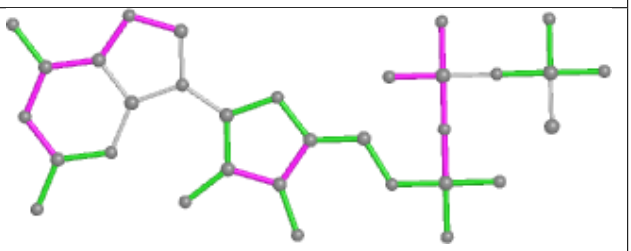


Rings

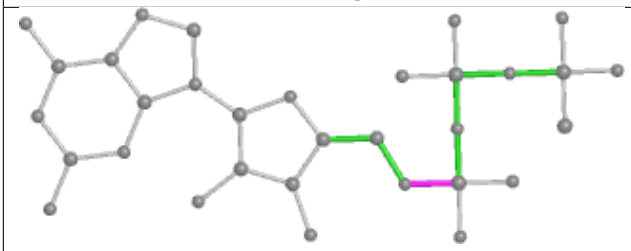
Ligand GSP X 2000



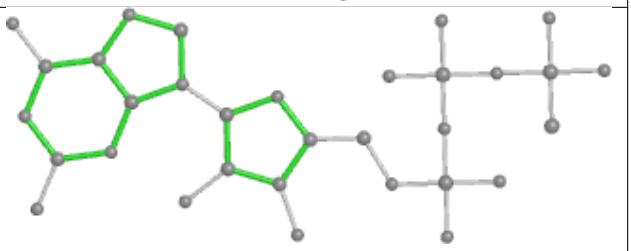
Bond lengths



Bond angles



Torsions



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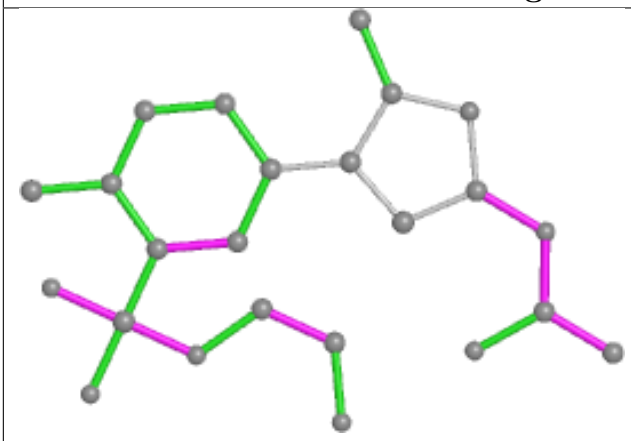

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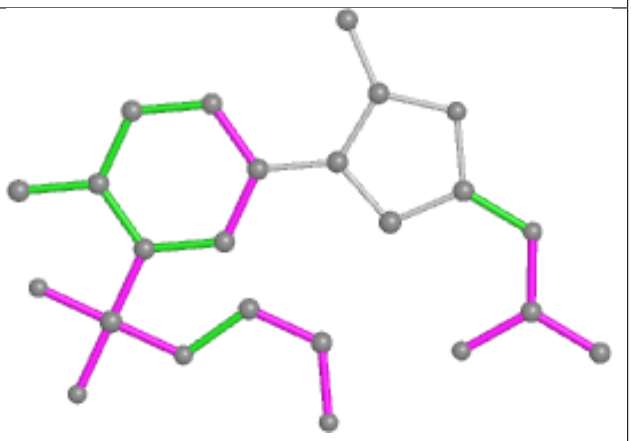

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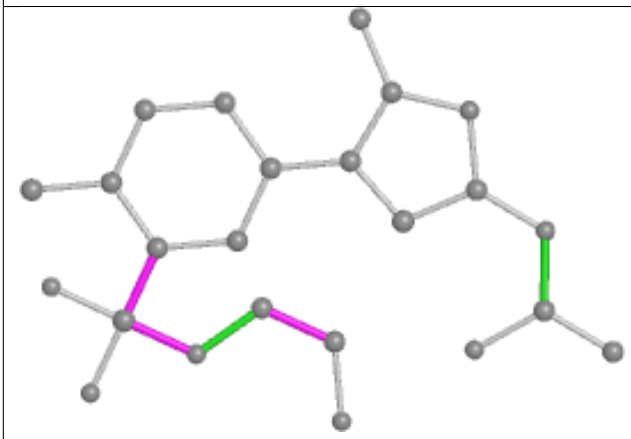

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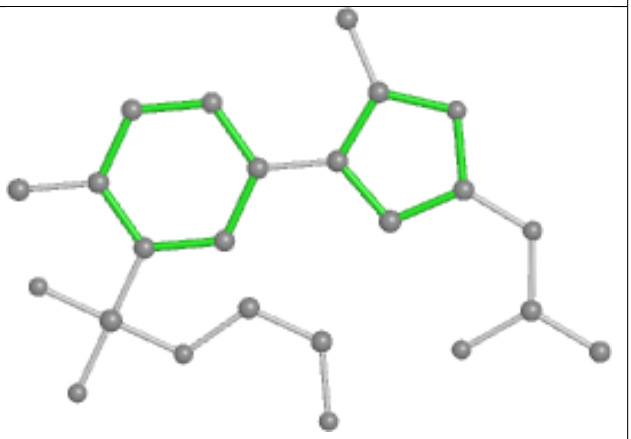

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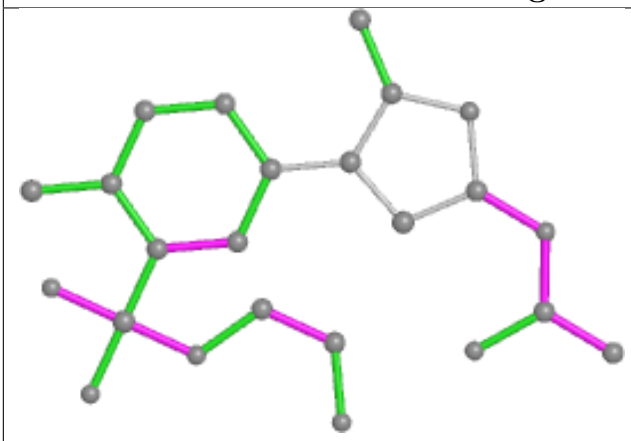

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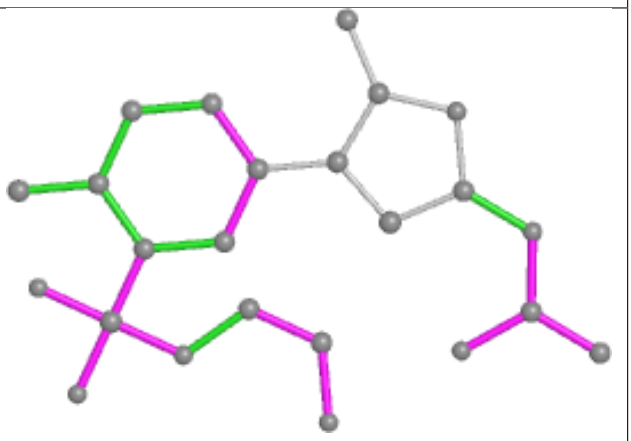

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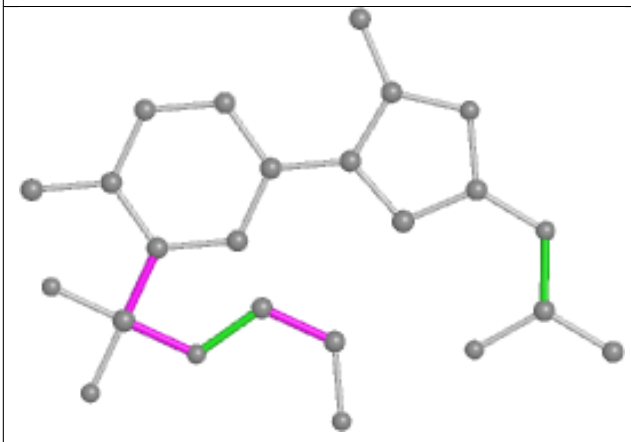

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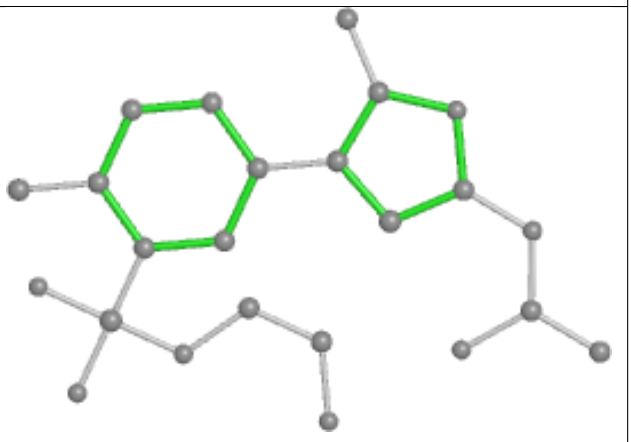

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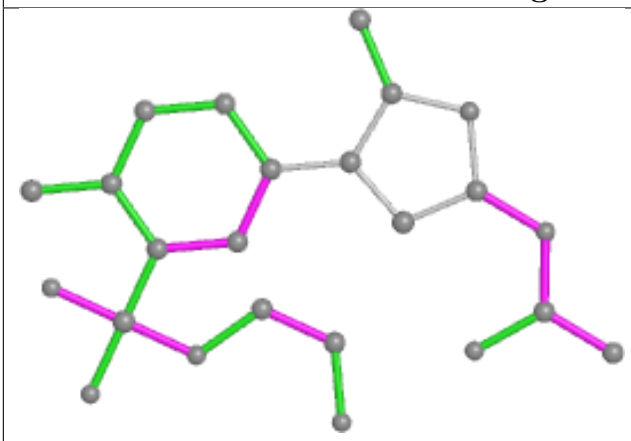

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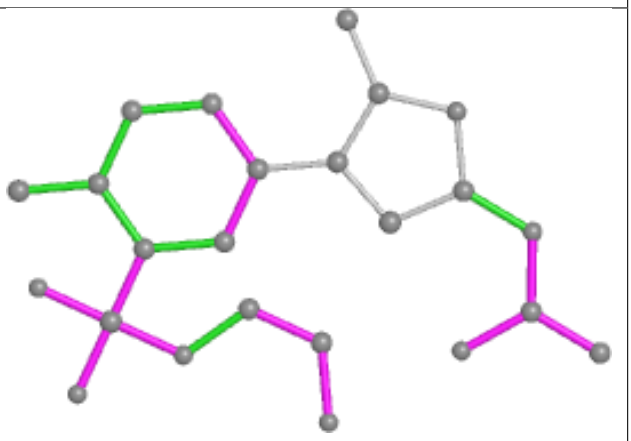

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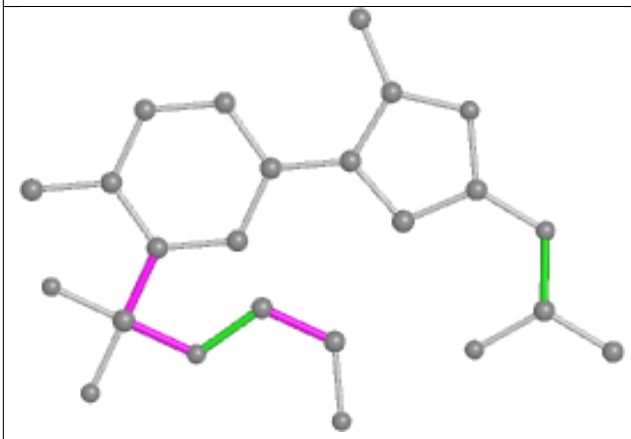

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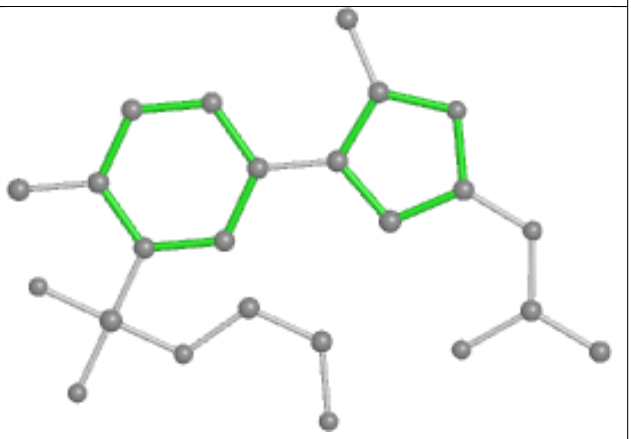

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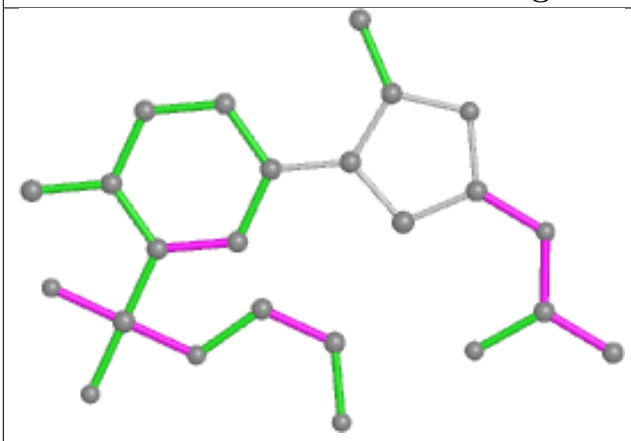

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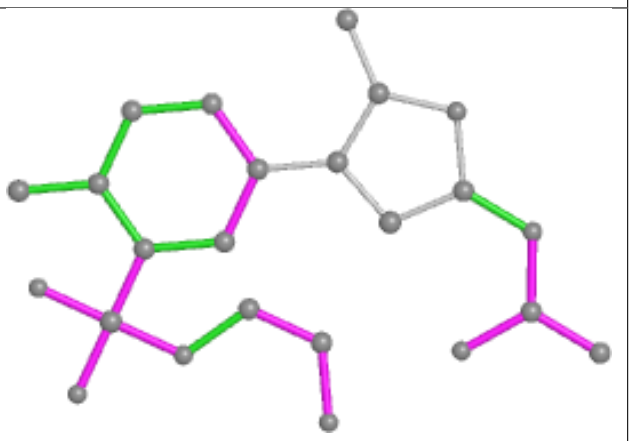

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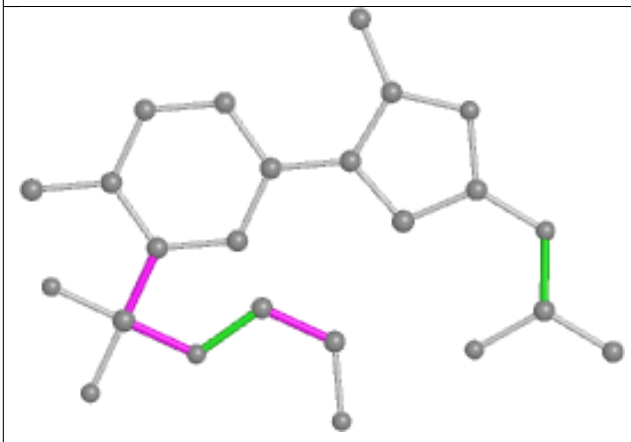

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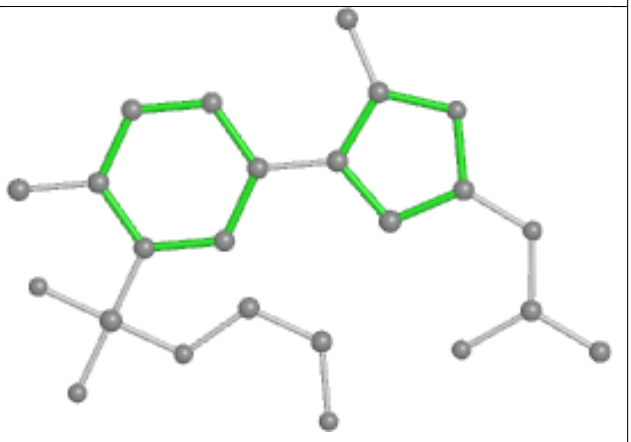

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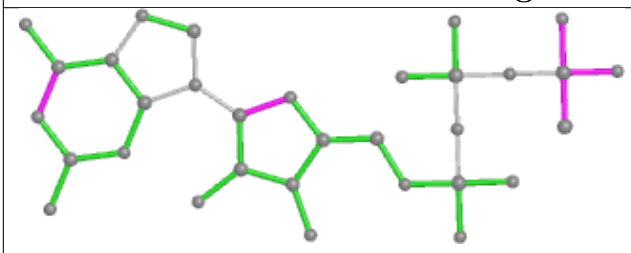

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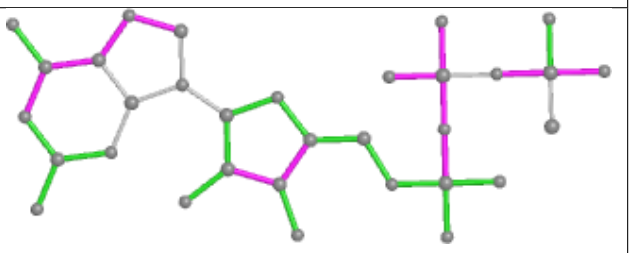

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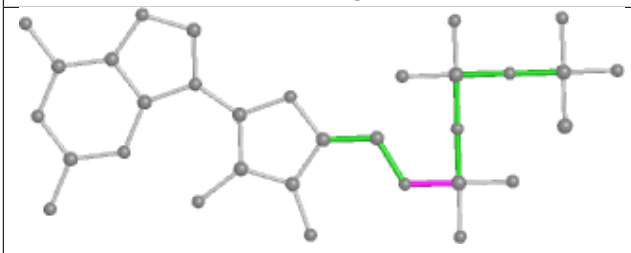

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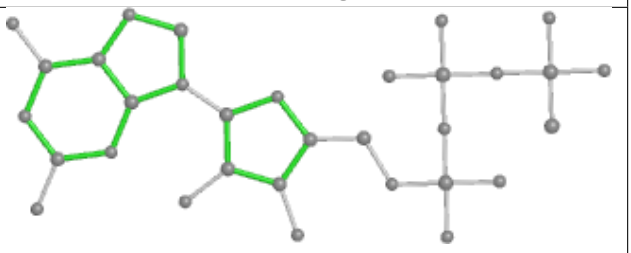

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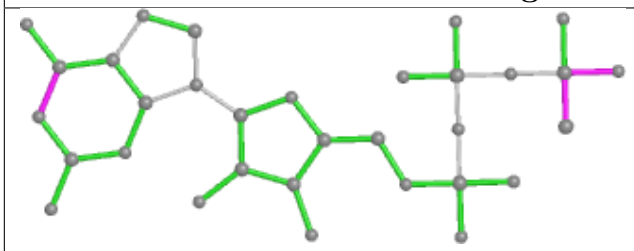

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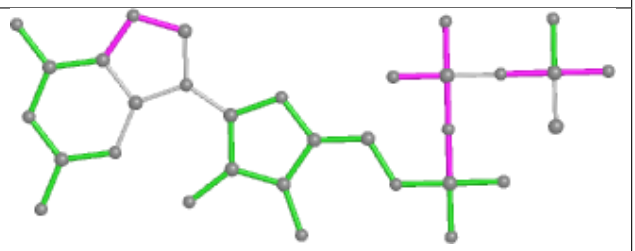

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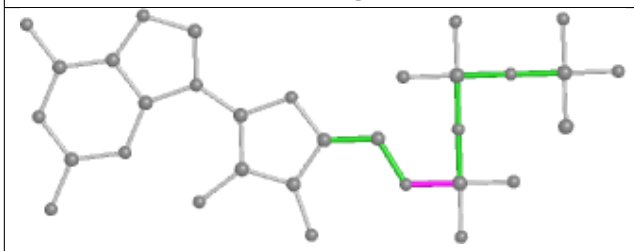

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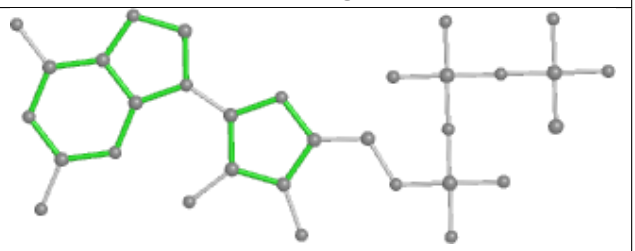

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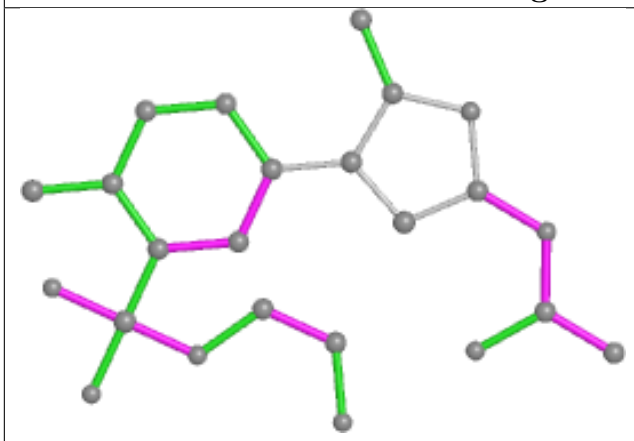

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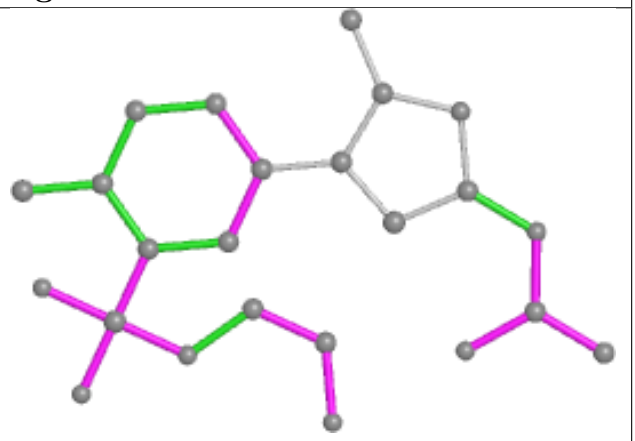

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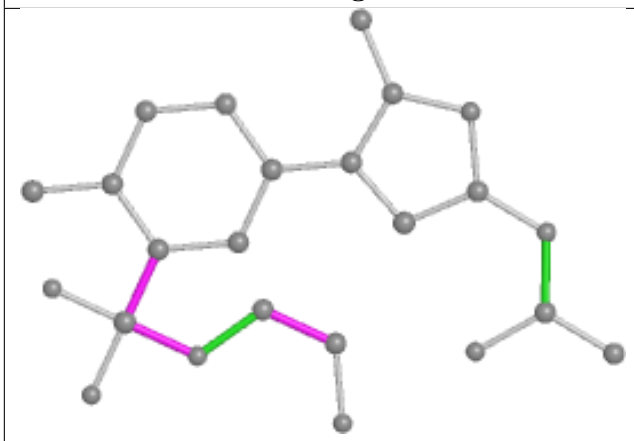

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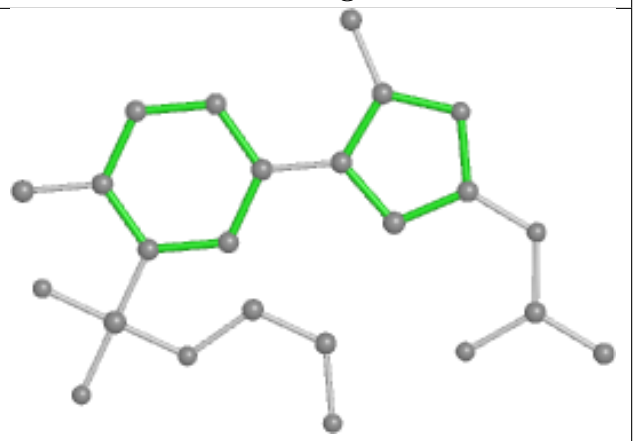

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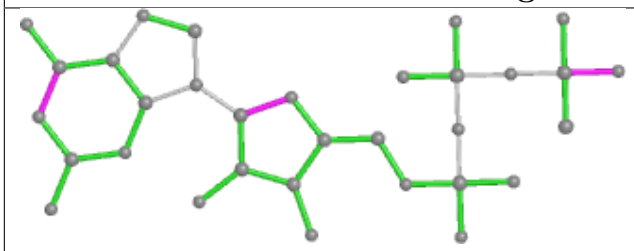

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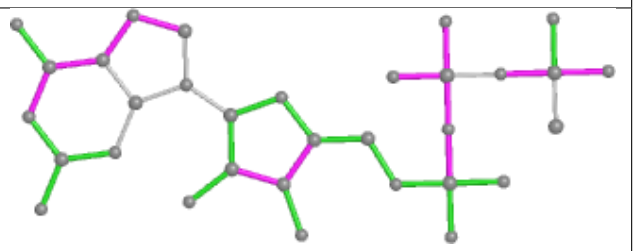

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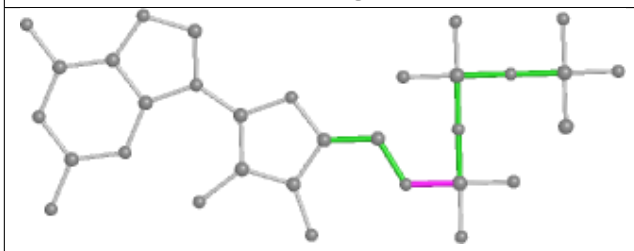

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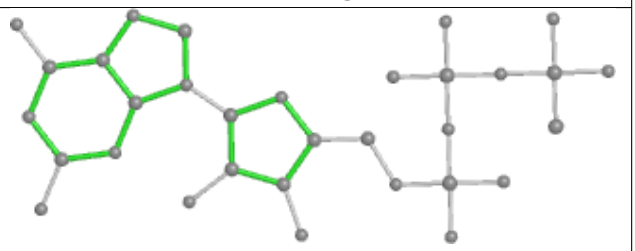

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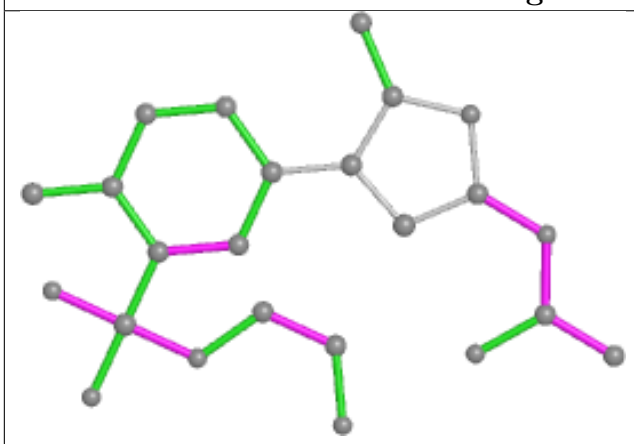

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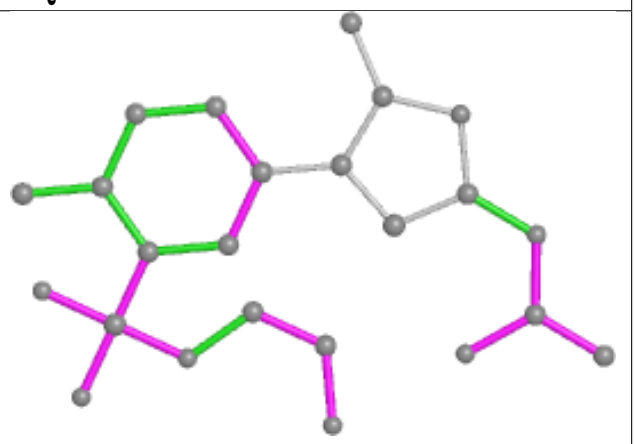

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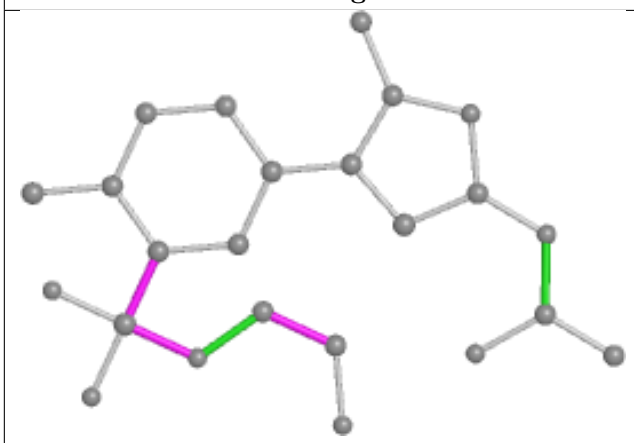

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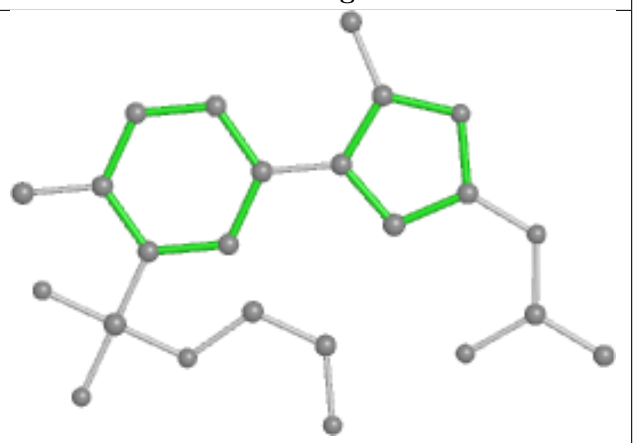

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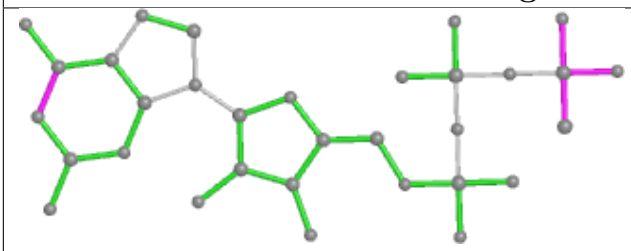

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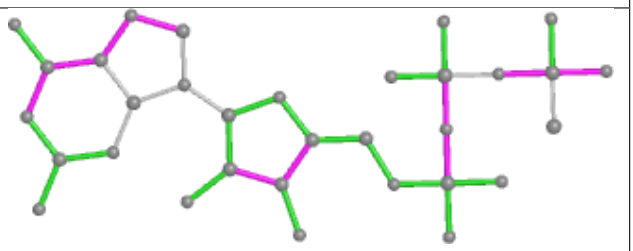

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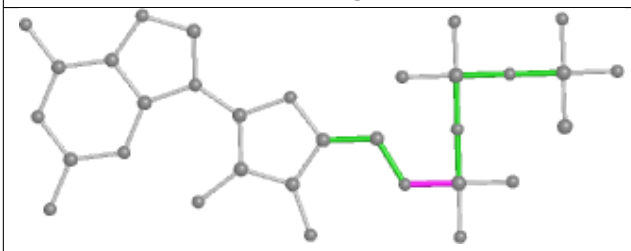

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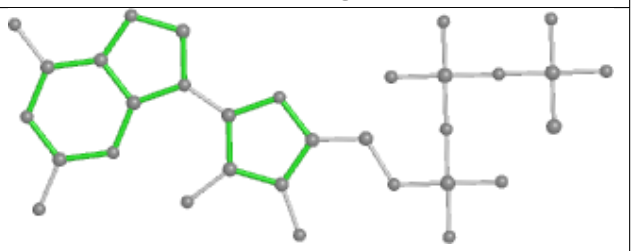

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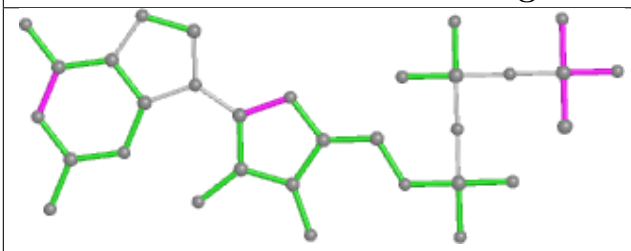

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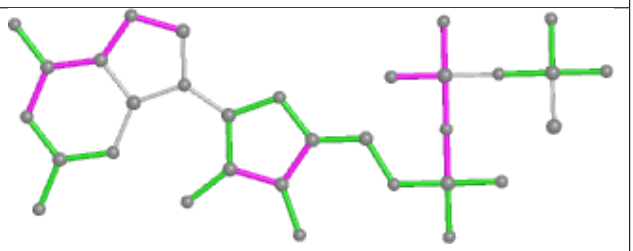

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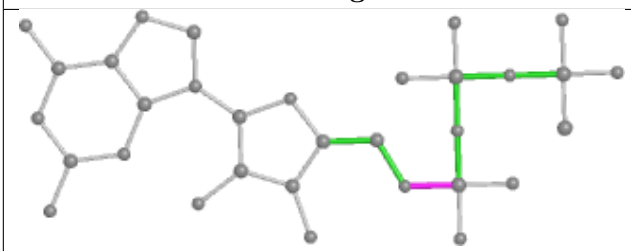

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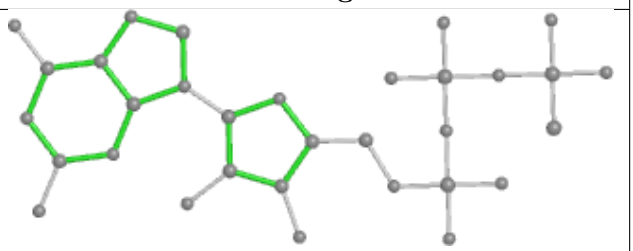

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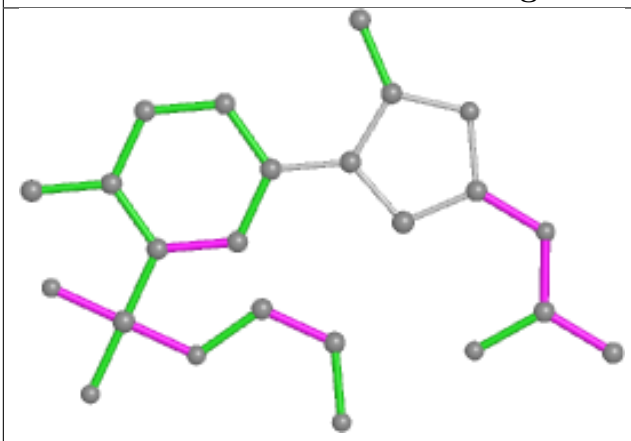

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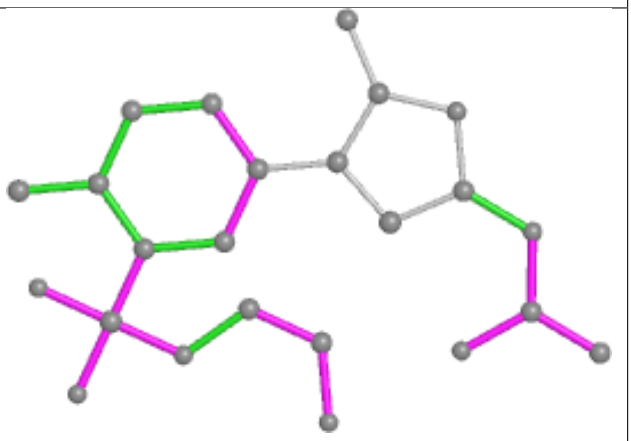

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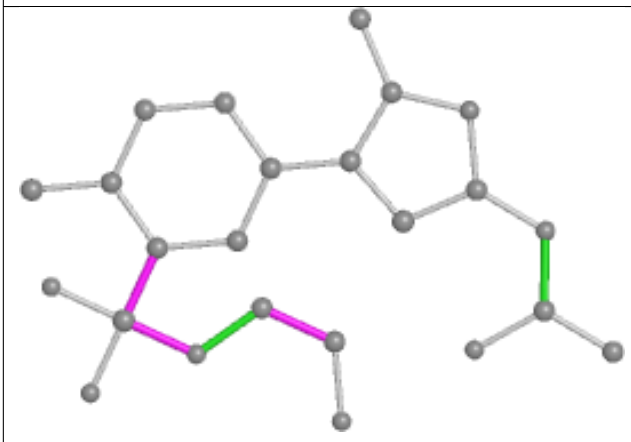

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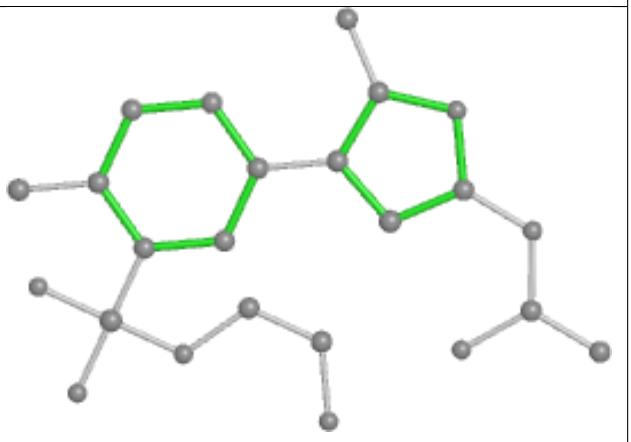

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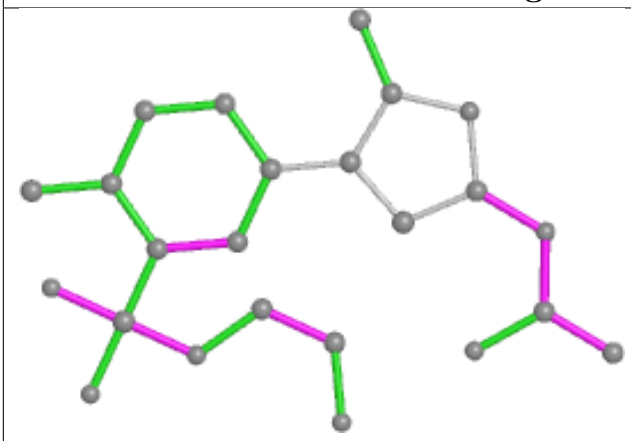

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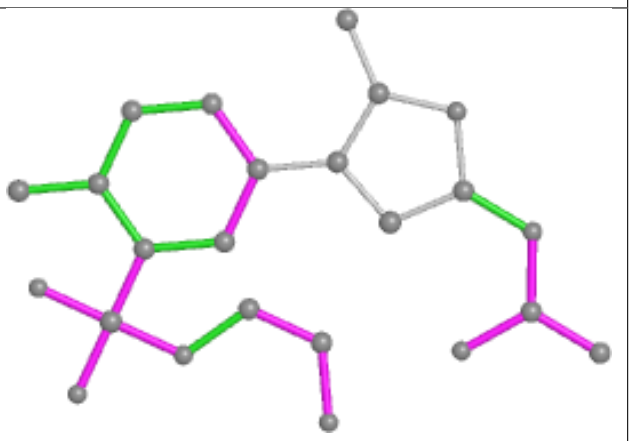

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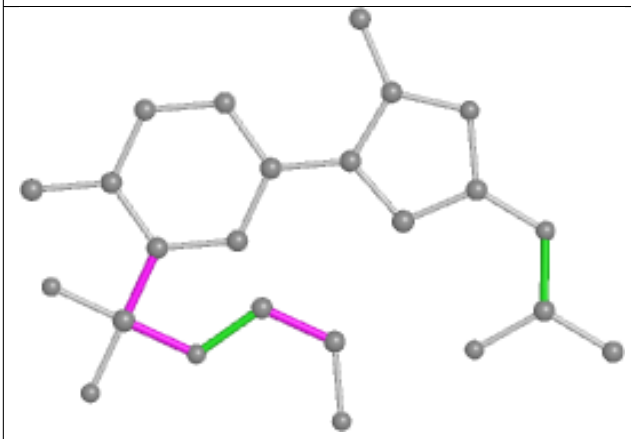

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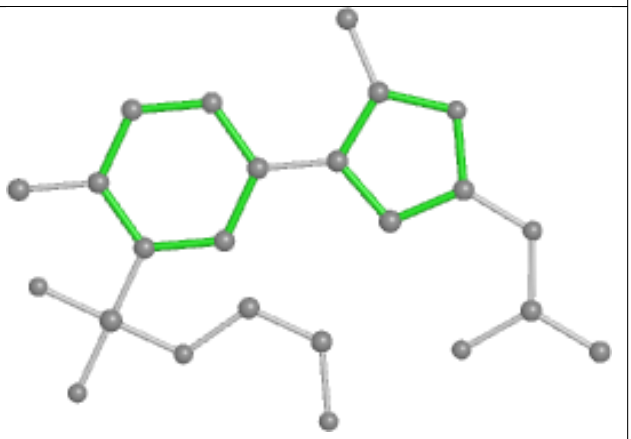

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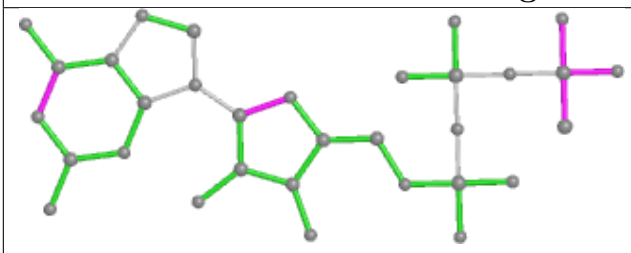

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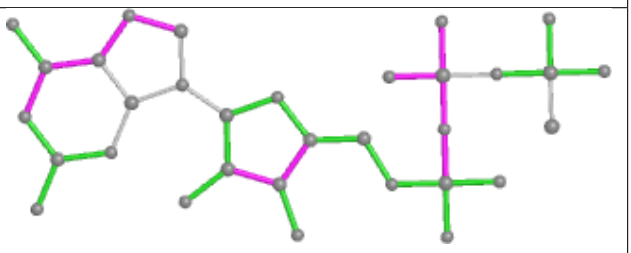

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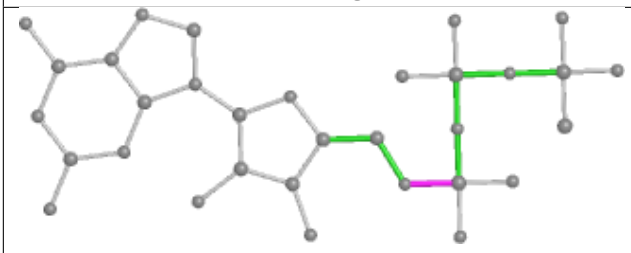

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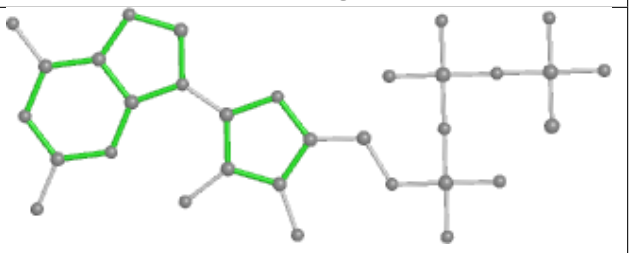

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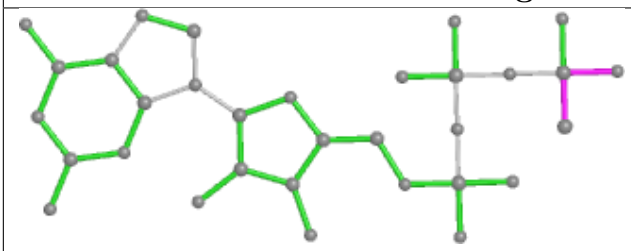
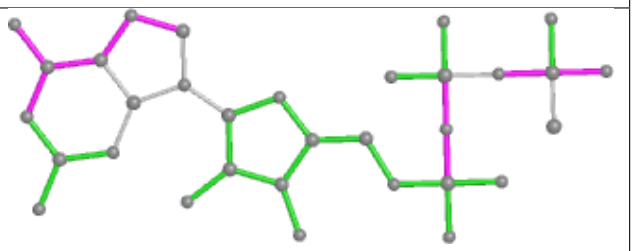
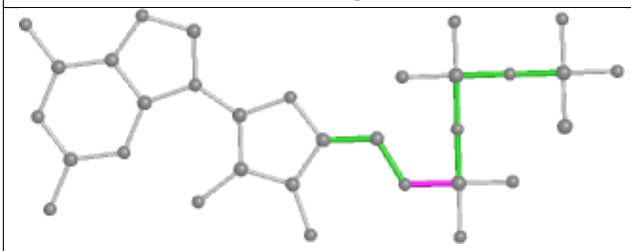


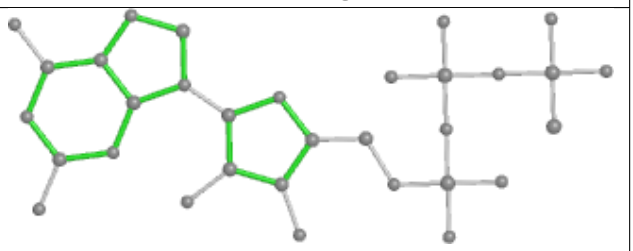
Bond lengths



Bond angles

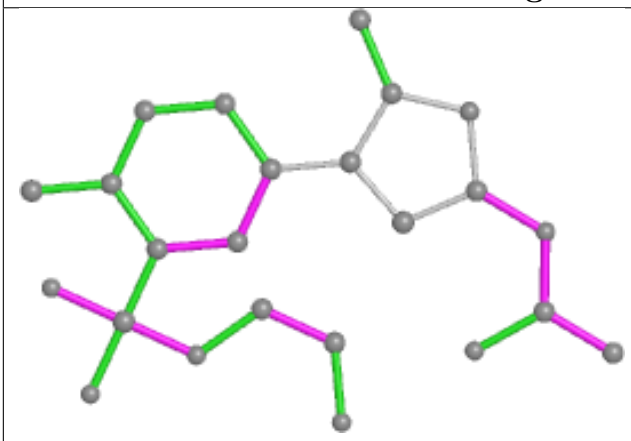


Torsions

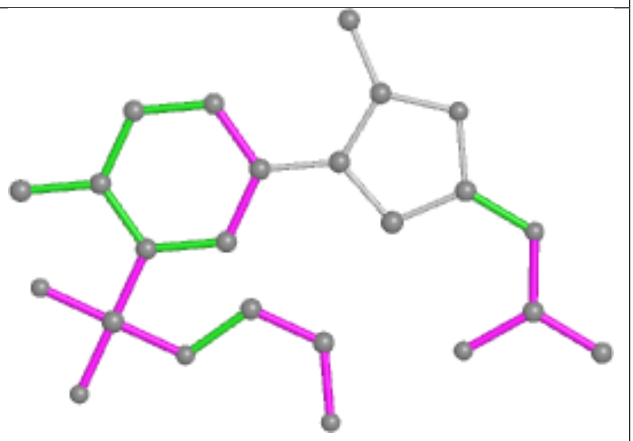


Rings

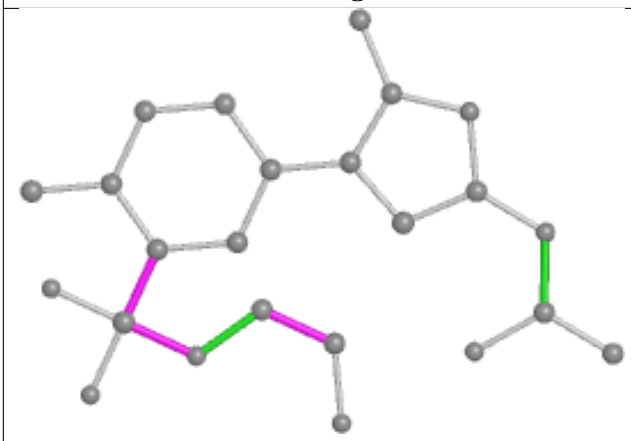
Ligand 093 C 2002



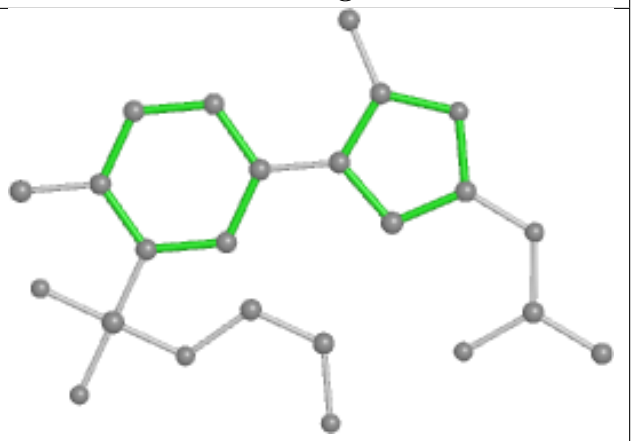
Bond lengths



Bond angles

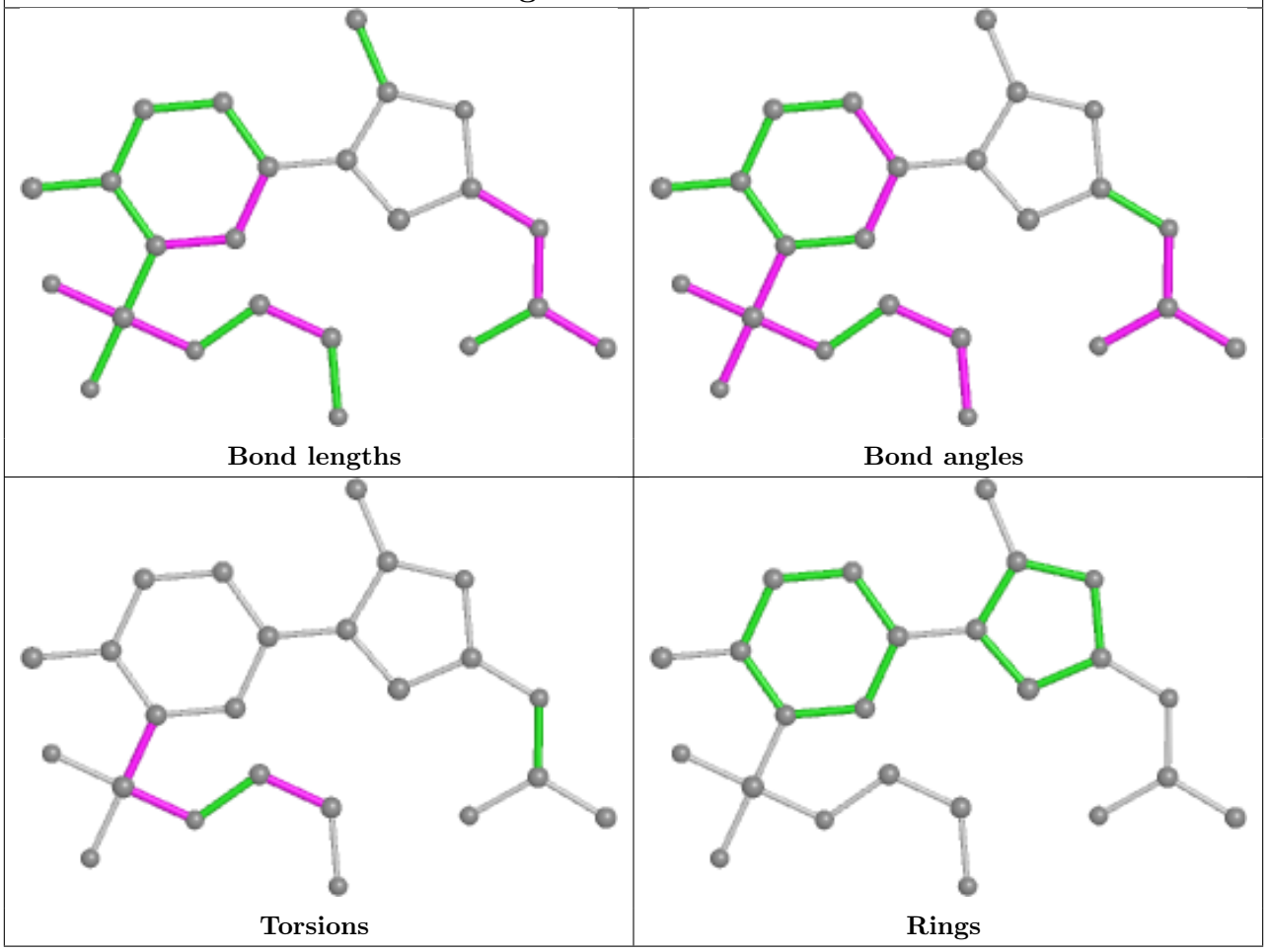


Torsions

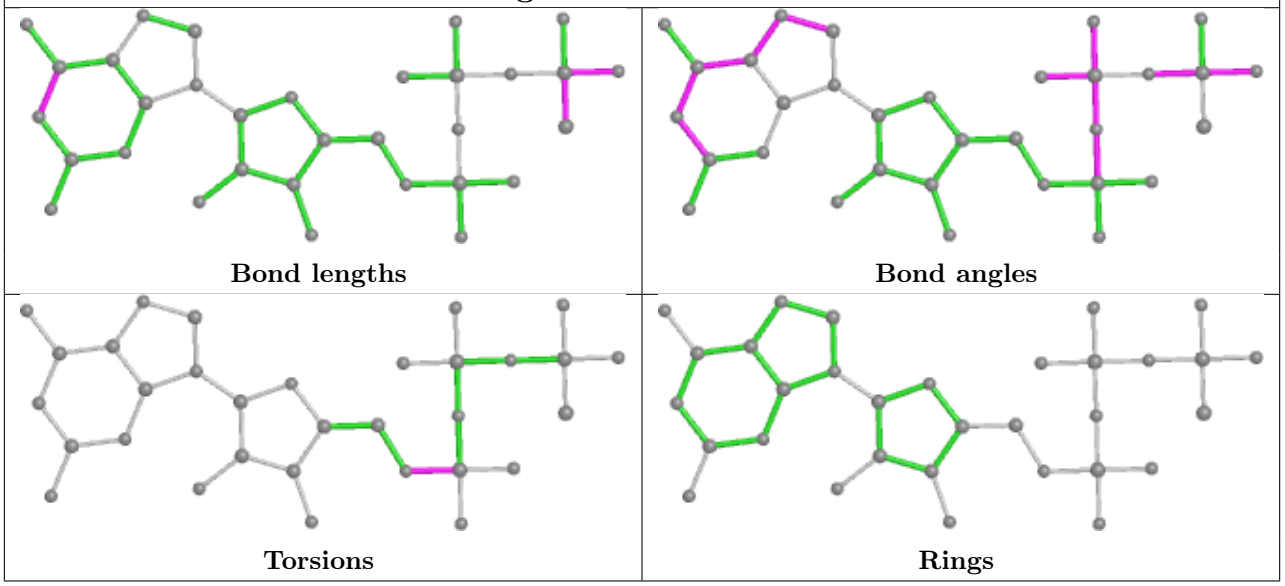


Rings

Ligand 093 O 2002



Ligand GSP H 2000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	470/566 (83%)	-0.59	4 (0%) 84 77	95, 212, 331, 500	0
1	C	470/566 (83%)	-0.19	15 (3%) 47 41	126, 300, 456, 500	0
1	G	470/566 (83%)	-0.52	6 (1%) 77 68	98, 214, 342, 500	0
1	I	470/566 (83%)	-0.06	24 (5%) 28 27	124, 306, 474, 500	0
1	M	470/566 (83%)	-0.57	5 (1%) 80 73	95, 217, 341, 500	0
1	O	470/566 (83%)	-0.59	4 (0%) 84 77	102, 208, 335, 500	0
1	Q	470/566 (83%)	-0.40	4 (0%) 84 77	102, 247, 364, 498	0
1	S	470/566 (83%)	-0.38	2 (0%) 92 87	114, 251, 389, 500	0
1	W	470/566 (83%)	-0.42	11 (2%) 60 53	99, 253, 387, 500	0
1	Y	470/566 (83%)	-0.47	4 (0%) 84 77	115, 250, 364, 474	0
1	c	470/566 (83%)	-0.09	20 (4%) 35 32	119, 305, 478, 500	0
1	g	470/566 (83%)	-0.31	12 (2%) 56 49	126, 268, 416, 500	0
2	B	173/219 (78%)	-0.61	1 (0%) 89 84	94, 201, 375, 493	0
2	D	173/219 (78%)	-0.46	0 100 100	95, 220, 341, 488	0
2	H	173/219 (78%)	-0.49	1 (0%) 89 84	94, 207, 382, 499	0
2	J	173/219 (78%)	-0.49	0 100 100	92, 198, 338, 500	0
2	N	173/219 (78%)	-0.04	6 (3%) 44 39	137, 282, 424, 496	0
2	P	173/219 (78%)	-0.10	2 (1%) 79 71	132, 277, 432, 496	0
2	R	173/219 (78%)	-0.30	1 (0%) 89 84	139, 269, 415, 496	0
2	T	173/219 (78%)	-0.53	2 (1%) 79 71	136, 266, 407, 493	0
2	X	173/219 (78%)	-0.25	1 (0%) 89 84	146, 282, 453, 500	0
2	Z	173/219 (78%)	-0.36	3 (1%) 70 62	165, 262, 362, 494	0
2	d	173/219 (78%)	-0.21	6 (3%) 44 39	146, 308, 447, 500	0
2	h	173/219 (78%)	-0.05	5 (2%) 51 44	158, 294, 440, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	E	41/48 (85%)	-0.44	0 100 100	153, 251, 365, 489	0
3	F	32/48 (66%)	-0.78	0 100 100	169, 285, 399, 466	0
3	K	41/48 (85%)	-0.34	0 100 100	131, 240, 410, 465	0
3	L	32/48 (66%)	-0.73	0 100 100	170, 263, 384, 436	0
3	U	41/48 (85%)	-0.15	1 (2%) 59 52	175, 284, 408, 494	0
3	V	32/48 (66%)	-0.65	0 100 100	170, 260, 403, 435	0
3	a	41/48 (85%)	-0.16	1 (2%) 59 52	195, 318, 423, 476	0
3	b	32/48 (66%)	0.14	0 100 100	213, 309, 428, 479	0
3	e	41/48 (85%)	-0.48	1 (2%) 59 52	175, 255, 384, 478	0
3	f	32/48 (66%)	-0.64	0 100 100	194, 288, 337, 363	0
3	i	41/48 (85%)	-0.05	0 100 100	202, 325, 441, 500	0
3	j	32/48 (66%)	-0.43	0 100 100	194, 282, 404, 462	0
All	All	8154/9996 (81%)	-0.37	142 (1%) 70 62	92, 255, 416, 500	0

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	523	GLN	6.9
1	C	517	ALA	6.0
1	g	406	ASN	5.7
1	g	405	GLU	5.6
1	C	523	GLN	5.6

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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.