



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:22 am BST

PDB ID : 6HUF  
Title : Coping with strong translational non-crystallographic symmetry and extreme anisotropy in molecular replacement with Phaser: human Rab27a  
Authors : Jamshidiha, M.; Perez-Dorado, I.; Murray, J.W.; Tate, E.W.; Cota, E.; Read, R.J.  
Deposited on : 2018-10-08  
Resolution : 2.82 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

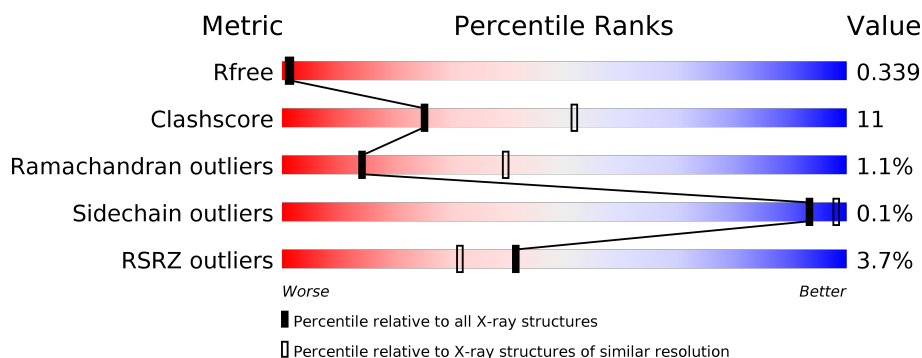
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	182	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 77%, yellow 16%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>16%</span> <span>6%</span> </div> </div>
1	B	182	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 80%, yellow 14%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>14%</span> <span>6%</span> </div> </div>
1	C	182	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 80%, yellow 13%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>13%</span> <span>6%</span> </div> </div>
1	D	182	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 79%, yellow 15%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>79%</span> <span>15%</span> <span>6%</span> </div> </div>
1	E	182	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 81%, yellow 13%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>81%</span> <span>13%</span> <span>6%</span> </div> </div>
1	F	182	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 80%, yellow 14%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>80%</span> <span>14%</span> <span>6%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	182	
1	H	182	
1	I	182	
1	J	182	
1	K	182	
1	L	182	
1	M	182	
1	N	182	
1	O	182	
1	P	182	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18977 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 Ras-related protein Rab-27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1159	728	199	229	3			
1	O	171	Total	C	N	O	S	0	0	0
			1152	723	198	228	3			
1	N	171	Total	C	N	O	S	0	0	0
			1149	720	198	228	3			
1	B	171	Total	C	N	O	S	0	0	0
			1152	723	198	228	3			
1	E	171	Total	C	N	O	S	0	0	0
			1149	720	198	228	3			
1	C	171	Total	C	N	O	S	0	0	0
			1153	722	198	230	3			
1	K	171	Total	C	N	O	S	0	0	0
			1161	732	198	228	3			
1	M	171	Total	C	N	O	S	0	0	0
			1149	720	198	228	3			
1	D	171	Total	C	N	O	S	0	0	0
			1155	726	198	228	3			
1	P	171	Total	C	N	O	S	0	0	0
			1155	726	198	228	3			
1	F	171	Total	C	N	O	S	0	0	0
			1155	726	198	228	3			
1	J	171	Total	C	N	O	S	0	0	0
			1155	726	198	228	3			
1	G	171	Total	C	N	O	S	0	0	0
			1152	721	199	229	3			
1	I	171	Total	C	N	O	S	0	0	0
			1149	720	198	228	3			
1	H	171	Total	C	N	O	S	0	0	0
			1149	720	198	228	3			
1	L	171	Total	C	N	O	S	0	0	0
			1149	720	198	228	3			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P51159
A	?	-	ARG	deletion	UNP P51159
A	50	THR	VAL	conflict	UNP P51159
A	51	ILE	VAL	conflict	UNP P51159
A	?	-	ALA	deletion	UNP P51159
A	?	-	SER	deletion	UNP P51159
A	?	-	GLY	deletion	UNP P51159
A	?	-	PRO	deletion	UNP P51159
A	?	-	ASP	deletion	UNP P51159
A	?	-	GLY	deletion	UNP P51159
A	?	-	ALA	deletion	UNP P51159
A	?	-	THR	deletion	UNP P51159
A	?	-	GLY	deletion	UNP P51159
A	54	ASN	ARG	conflict	UNP P51159
A	55	ASP	GLY	conflict	UNP P51159
A	56	LYS	GLN	conflict	UNP P51159
A	59	LYS	HIS	conflict	UNP P51159
A	68	LEU	GLN	conflict	UNP P51159
A	95	GLU	GLN	conflict	UNP P51159
A	108	LYS	GLN	conflict	UNP P51159
A	109	THR	MET	conflict	UNP P51159
A	113	SER	CYS	conflict	UNP P51159
A	130	GLU	GLN	conflict	UNP P51159
A	134	ALA	LYS	conflict	UNP P51159
A	135	ALA	GLU	conflict	UNP P51159
A	136	ALA	GLU	conflict	UNP P51159
A	139	ARG	ILE	conflict	UNP P51159
A	140	GLN	ALA	conflict	UNP P51159
A	144	HIS	LYS	conflict	UNP P51159
A	178	SER	CYS	conflict	UNP P51159
O	1	GLY	-	expression tag	UNP P51159
O	?	-	ARG	deletion	UNP P51159
O	50	THR	VAL	conflict	UNP P51159
O	51	ILE	VAL	conflict	UNP P51159
O	?	-	ALA	deletion	UNP P51159
O	?	-	SER	deletion	UNP P51159
O	?	-	GLY	deletion	UNP P51159
O	?	-	PRO	deletion	UNP P51159
O	?	-	ASP	deletion	UNP P51159
O	?	-	GLY	deletion	UNP P51159
O	?	-	ALA	deletion	UNP P51159
O	?	-	THR	deletion	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	GLY	deletion	UNP P51159
O	54	ASN	ARG	conflict	UNP P51159
O	55	ASP	GLY	conflict	UNP P51159
O	56	LYS	GLN	conflict	UNP P51159
O	59	LYS	HIS	conflict	UNP P51159
O	68	LEU	GLN	conflict	UNP P51159
O	95	GLU	GLN	conflict	UNP P51159
O	108	LYS	GLN	conflict	UNP P51159
O	109	THR	MET	conflict	UNP P51159
O	113	SER	CYS	conflict	UNP P51159
O	130	GLU	GLN	conflict	UNP P51159
O	134	ALA	LYS	conflict	UNP P51159
O	135	ALA	GLU	conflict	UNP P51159
O	136	ALA	GLU	conflict	UNP P51159
O	139	ARG	ILE	conflict	UNP P51159
O	140	GLN	ALA	conflict	UNP P51159
O	144	HIS	LYS	conflict	UNP P51159
O	178	SER	CYS	conflict	UNP P51159
N	1	GLY	-	expression tag	UNP P51159
N	?	-	ARG	deletion	UNP P51159
N	50	THR	VAL	conflict	UNP P51159
N	51	ILE	VAL	conflict	UNP P51159
N	?	-	ALA	deletion	UNP P51159
N	?	-	SER	deletion	UNP P51159
N	?	-	GLY	deletion	UNP P51159
N	?	-	PRO	deletion	UNP P51159
N	?	-	ASP	deletion	UNP P51159
N	?	-	GLY	deletion	UNP P51159
N	?	-	ALA	deletion	UNP P51159
N	?	-	THR	deletion	UNP P51159
N	?	-	GLY	deletion	UNP P51159
N	54	ASN	ARG	conflict	UNP P51159
N	55	ASP	GLY	conflict	UNP P51159
N	56	LYS	GLN	conflict	UNP P51159
N	59	LYS	HIS	conflict	UNP P51159
N	68	LEU	GLN	conflict	UNP P51159
N	95	GLU	GLN	conflict	UNP P51159
N	108	LYS	GLN	conflict	UNP P51159
N	109	THR	MET	conflict	UNP P51159
N	113	SER	CYS	conflict	UNP P51159
N	130	GLU	GLN	conflict	UNP P51159
N	134	ALA	LYS	conflict	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
N	135	ALA	GLU	conflict	UNP P51159
N	136	ALA	GLU	conflict	UNP P51159
N	139	ARG	ILE	conflict	UNP P51159
N	140	GLN	ALA	conflict	UNP P51159
N	144	HIS	LYS	conflict	UNP P51159
N	178	SER	CYS	conflict	UNP P51159
B	1	GLY	-	expression tag	UNP P51159
B	?	-	ARG	deletion	UNP P51159
B	50	THR	VAL	conflict	UNP P51159
B	51	ILE	VAL	conflict	UNP P51159
B	?	-	ALA	deletion	UNP P51159
B	?	-	SER	deletion	UNP P51159
B	?	-	GLY	deletion	UNP P51159
B	?	-	PRO	deletion	UNP P51159
B	?	-	ASP	deletion	UNP P51159
B	?	-	GLY	deletion	UNP P51159
B	?	-	ALA	deletion	UNP P51159
B	?	-	THR	deletion	UNP P51159
B	?	-	GLY	deletion	UNP P51159
B	54	ASN	ARG	conflict	UNP P51159
B	55	ASP	GLY	conflict	UNP P51159
B	56	LYS	GLN	conflict	UNP P51159
B	59	LYS	HIS	conflict	UNP P51159
B	68	LEU	GLN	conflict	UNP P51159
B	95	GLU	GLN	conflict	UNP P51159
B	108	LYS	GLN	conflict	UNP P51159
B	109	THR	MET	conflict	UNP P51159
B	113	SER	CYS	conflict	UNP P51159
B	130	GLU	GLN	conflict	UNP P51159
B	134	ALA	LYS	conflict	UNP P51159
B	135	ALA	GLU	conflict	UNP P51159
B	136	ALA	GLU	conflict	UNP P51159
B	139	ARG	ILE	conflict	UNP P51159
B	140	GLN	ALA	conflict	UNP P51159
B	144	HIS	LYS	conflict	UNP P51159
B	178	SER	CYS	conflict	UNP P51159
E	1	GLY	-	expression tag	UNP P51159
E	?	-	ARG	deletion	UNP P51159
E	50	THR	VAL	conflict	UNP P51159
E	51	ILE	VAL	conflict	UNP P51159
E	?	-	ALA	deletion	UNP P51159
E	?	-	SER	deletion	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP P51159
E	?	-	PRO	deletion	UNP P51159
E	?	-	ASP	deletion	UNP P51159
E	?	-	GLY	deletion	UNP P51159
E	?	-	ALA	deletion	UNP P51159
E	?	-	THR	deletion	UNP P51159
E	?	-	GLY	deletion	UNP P51159
E	54	ASN	ARG	conflict	UNP P51159
E	55	ASP	GLY	conflict	UNP P51159
E	56	LYS	GLN	conflict	UNP P51159
E	59	LYS	HIS	conflict	UNP P51159
E	68	LEU	GLN	conflict	UNP P51159
E	95	GLU	GLN	conflict	UNP P51159
E	108	LYS	GLN	conflict	UNP P51159
E	109	THR	MET	conflict	UNP P51159
E	113	SER	CYS	conflict	UNP P51159
E	130	GLU	GLN	conflict	UNP P51159
E	134	ALA	LYS	conflict	UNP P51159
E	135	ALA	GLU	conflict	UNP P51159
E	136	ALA	GLU	conflict	UNP P51159
E	139	ARG	ILE	conflict	UNP P51159
E	140	GLN	ALA	conflict	UNP P51159
E	144	HIS	LYS	conflict	UNP P51159
E	178	SER	CYS	conflict	UNP P51159
C	1	GLY	-	expression tag	UNP P51159
C	?	-	ARG	deletion	UNP P51159
C	50	THR	VAL	conflict	UNP P51159
C	51	ILE	VAL	conflict	UNP P51159
C	?	-	ALA	deletion	UNP P51159
C	?	-	SER	deletion	UNP P51159
C	?	-	GLY	deletion	UNP P51159
C	?	-	PRO	deletion	UNP P51159
C	?	-	ASP	deletion	UNP P51159
C	?	-	GLY	deletion	UNP P51159
C	?	-	ALA	deletion	UNP P51159
C	?	-	THR	deletion	UNP P51159
C	?	-	GLY	deletion	UNP P51159
C	54	ASN	ARG	conflict	UNP P51159
C	55	ASP	GLY	conflict	UNP P51159
C	56	LYS	GLN	conflict	UNP P51159
C	59	LYS	HIS	conflict	UNP P51159
C	68	LEU	GLN	conflict	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
C	95	GLU	GLN	conflict	UNP P51159
C	108	LYS	GLN	conflict	UNP P51159
C	109	THR	MET	conflict	UNP P51159
C	113	SER	CYS	conflict	UNP P51159
C	130	GLU	GLN	conflict	UNP P51159
C	134	ALA	LYS	conflict	UNP P51159
C	135	ALA	GLU	conflict	UNP P51159
C	136	ALA	GLU	conflict	UNP P51159
C	139	ARG	ILE	conflict	UNP P51159
C	140	GLN	ALA	conflict	UNP P51159
C	144	HIS	LYS	conflict	UNP P51159
C	178	SER	CYS	conflict	UNP P51159
K	1	GLY	-	expression tag	UNP P51159
K	?	-	ARG	deletion	UNP P51159
K	50	THR	VAL	conflict	UNP P51159
K	51	ILE	VAL	conflict	UNP P51159
K	?	-	ALA	deletion	UNP P51159
K	?	-	SER	deletion	UNP P51159
K	?	-	GLY	deletion	UNP P51159
K	?	-	PRO	deletion	UNP P51159
K	?	-	ASP	deletion	UNP P51159
K	?	-	GLY	deletion	UNP P51159
K	?	-	ALA	deletion	UNP P51159
K	?	-	THR	deletion	UNP P51159
K	?	-	GLY	deletion	UNP P51159
K	54	ASN	ARG	conflict	UNP P51159
K	55	ASP	GLY	conflict	UNP P51159
K	56	LYS	GLN	conflict	UNP P51159
K	59	LYS	HIS	conflict	UNP P51159
K	68	LEU	GLN	conflict	UNP P51159
K	95	GLU	GLN	conflict	UNP P51159
K	108	LYS	GLN	conflict	UNP P51159
K	109	THR	MET	conflict	UNP P51159
K	113	SER	CYS	conflict	UNP P51159
K	130	GLU	GLN	conflict	UNP P51159
K	134	ALA	LYS	conflict	UNP P51159
K	135	ALA	GLU	conflict	UNP P51159
K	136	ALA	GLU	conflict	UNP P51159
K	139	ARG	ILE	conflict	UNP P51159
K	140	GLN	ALA	conflict	UNP P51159
K	144	HIS	LYS	conflict	UNP P51159
K	178	SER	CYS	conflict	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1	GLY	-	expression tag	UNP P51159
M	?	-	ARG	deletion	UNP P51159
M	50	THR	VAL	conflict	UNP P51159
M	51	ILE	VAL	conflict	UNP P51159
M	?	-	ALA	deletion	UNP P51159
M	?	-	SER	deletion	UNP P51159
M	?	-	GLY	deletion	UNP P51159
M	?	-	PRO	deletion	UNP P51159
M	?	-	ASP	deletion	UNP P51159
M	?	-	GLY	deletion	UNP P51159
M	?	-	ALA	deletion	UNP P51159
M	?	-	THR	deletion	UNP P51159
M	?	-	GLY	deletion	UNP P51159
M	54	ASN	ARG	conflict	UNP P51159
M	55	ASP	GLY	conflict	UNP P51159
M	56	LYS	GLN	conflict	UNP P51159
M	59	LYS	HIS	conflict	UNP P51159
M	68	LEU	GLN	conflict	UNP P51159
M	95	GLU	GLN	conflict	UNP P51159
M	108	LYS	GLN	conflict	UNP P51159
M	109	THR	MET	conflict	UNP P51159
M	113	SER	CYS	conflict	UNP P51159
M	130	GLU	GLN	conflict	UNP P51159
M	134	ALA	LYS	conflict	UNP P51159
M	135	ALA	GLU	conflict	UNP P51159
M	136	ALA	GLU	conflict	UNP P51159
M	139	ARG	ILE	conflict	UNP P51159
M	140	GLN	ALA	conflict	UNP P51159
M	144	HIS	LYS	conflict	UNP P51159
M	178	SER	CYS	conflict	UNP P51159
D	1	GLY	-	expression tag	UNP P51159
D	?	-	ARG	deletion	UNP P51159
D	50	THR	VAL	conflict	UNP P51159
D	51	ILE	VAL	conflict	UNP P51159
D	?	-	ALA	deletion	UNP P51159
D	?	-	SER	deletion	UNP P51159
D	?	-	GLY	deletion	UNP P51159
D	?	-	PRO	deletion	UNP P51159
D	?	-	ASP	deletion	UNP P51159
D	?	-	GLY	deletion	UNP P51159
D	?	-	ALA	deletion	UNP P51159
D	?	-	THR	deletion	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP P51159
D	54	ASN	ARG	conflict	UNP P51159
D	55	ASP	GLY	conflict	UNP P51159
D	56	LYS	GLN	conflict	UNP P51159
D	59	LYS	HIS	conflict	UNP P51159
D	68	LEU	GLN	conflict	UNP P51159
D	95	GLU	GLN	conflict	UNP P51159
D	108	LYS	GLN	conflict	UNP P51159
D	109	THR	MET	conflict	UNP P51159
D	113	SER	CYS	conflict	UNP P51159
D	130	GLU	GLN	conflict	UNP P51159
D	134	ALA	LYS	conflict	UNP P51159
D	135	ALA	GLU	conflict	UNP P51159
D	136	ALA	GLU	conflict	UNP P51159
D	139	ARG	ILE	conflict	UNP P51159
D	140	GLN	ALA	conflict	UNP P51159
D	144	HIS	LYS	conflict	UNP P51159
D	178	SER	CYS	conflict	UNP P51159
P	1	GLY	-	expression tag	UNP P51159
P	?	-	ARG	deletion	UNP P51159
P	50	THR	VAL	conflict	UNP P51159
P	51	ILE	VAL	conflict	UNP P51159
P	?	-	ALA	deletion	UNP P51159
P	?	-	SER	deletion	UNP P51159
P	?	-	GLY	deletion	UNP P51159
P	?	-	PRO	deletion	UNP P51159
P	?	-	ASP	deletion	UNP P51159
P	?	-	GLY	deletion	UNP P51159
P	?	-	ALA	deletion	UNP P51159
P	?	-	THR	deletion	UNP P51159
P	?	-	GLY	deletion	UNP P51159
P	54	ASN	ARG	conflict	UNP P51159
P	55	ASP	GLY	conflict	UNP P51159
P	56	LYS	GLN	conflict	UNP P51159
P	59	LYS	HIS	conflict	UNP P51159
P	68	LEU	GLN	conflict	UNP P51159
P	95	GLU	GLN	conflict	UNP P51159
P	108	LYS	GLN	conflict	UNP P51159
P	109	THR	MET	conflict	UNP P51159
P	113	SER	CYS	conflict	UNP P51159
P	130	GLU	GLN	conflict	UNP P51159
P	134	ALA	LYS	conflict	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
P	135	ALA	GLU	conflict	UNP P51159
P	136	ALA	GLU	conflict	UNP P51159
P	139	ARG	ILE	conflict	UNP P51159
P	140	GLN	ALA	conflict	UNP P51159
P	144	HIS	LYS	conflict	UNP P51159
P	178	SER	CYS	conflict	UNP P51159
F	1	GLY	-	expression tag	UNP P51159
F	?	-	ARG	deletion	UNP P51159
F	50	THR	VAL	conflict	UNP P51159
F	51	ILE	VAL	conflict	UNP P51159
F	?	-	ALA	deletion	UNP P51159
F	?	-	SER	deletion	UNP P51159
F	?	-	GLY	deletion	UNP P51159
F	?	-	PRO	deletion	UNP P51159
F	?	-	ASP	deletion	UNP P51159
F	?	-	GLY	deletion	UNP P51159
F	?	-	ALA	deletion	UNP P51159
F	?	-	THR	deletion	UNP P51159
F	?	-	GLY	deletion	UNP P51159
F	54	ASN	ARG	conflict	UNP P51159
F	55	ASP	GLY	conflict	UNP P51159
F	56	LYS	GLN	conflict	UNP P51159
F	59	LYS	HIS	conflict	UNP P51159
F	68	LEU	GLN	conflict	UNP P51159
F	95	GLU	GLN	conflict	UNP P51159
F	108	LYS	GLN	conflict	UNP P51159
F	109	THR	MET	conflict	UNP P51159
F	113	SER	CYS	conflict	UNP P51159
F	130	GLU	GLN	conflict	UNP P51159
F	134	ALA	LYS	conflict	UNP P51159
F	135	ALA	GLU	conflict	UNP P51159
F	136	ALA	GLU	conflict	UNP P51159
F	139	ARG	ILE	conflict	UNP P51159
F	140	GLN	ALA	conflict	UNP P51159
F	144	HIS	LYS	conflict	UNP P51159
F	178	SER	CYS	conflict	UNP P51159
J	1	GLY	-	expression tag	UNP P51159
J	?	-	ARG	deletion	UNP P51159
J	50	THR	VAL	conflict	UNP P51159
J	51	ILE	VAL	conflict	UNP P51159
J	?	-	ALA	deletion	UNP P51159
J	?	-	SER	deletion	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
J	?	-	GLY	deletion	UNP P51159
J	?	-	PRO	deletion	UNP P51159
J	?	-	ASP	deletion	UNP P51159
J	?	-	GLY	deletion	UNP P51159
J	?	-	ALA	deletion	UNP P51159
J	?	-	THR	deletion	UNP P51159
J	?	-	GLY	deletion	UNP P51159
J	54	ASN	ARG	conflict	UNP P51159
J	55	ASP	GLY	conflict	UNP P51159
J	56	LYS	GLN	conflict	UNP P51159
J	59	LYS	HIS	conflict	UNP P51159
J	68	LEU	GLN	conflict	UNP P51159
J	95	GLU	GLN	conflict	UNP P51159
J	108	LYS	GLN	conflict	UNP P51159
J	109	THR	MET	conflict	UNP P51159
J	113	SER	CYS	conflict	UNP P51159
J	130	GLU	GLN	conflict	UNP P51159
J	134	ALA	LYS	conflict	UNP P51159
J	135	ALA	GLU	conflict	UNP P51159
J	136	ALA	GLU	conflict	UNP P51159
J	139	ARG	ILE	conflict	UNP P51159
J	140	GLN	ALA	conflict	UNP P51159
J	144	HIS	LYS	conflict	UNP P51159
J	178	SER	CYS	conflict	UNP P51159
G	1	GLY	-	expression tag	UNP P51159
G	?	-	ARG	deletion	UNP P51159
G	50	THR	VAL	conflict	UNP P51159
G	51	ILE	VAL	conflict	UNP P51159
G	?	-	ALA	deletion	UNP P51159
G	?	-	SER	deletion	UNP P51159
G	?	-	GLY	deletion	UNP P51159
G	?	-	PRO	deletion	UNP P51159
G	?	-	ASP	deletion	UNP P51159
G	?	-	GLY	deletion	UNP P51159
G	?	-	ALA	deletion	UNP P51159
G	?	-	THR	deletion	UNP P51159
G	?	-	GLY	deletion	UNP P51159
G	54	ASN	ARG	conflict	UNP P51159
G	55	ASP	GLY	conflict	UNP P51159
G	56	LYS	GLN	conflict	UNP P51159
G	59	LYS	HIS	conflict	UNP P51159
G	68	LEU	GLN	conflict	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
G	95	GLU	GLN	conflict	UNP P51159
G	108	LYS	GLN	conflict	UNP P51159
G	109	THR	MET	conflict	UNP P51159
G	113	SER	CYS	conflict	UNP P51159
G	130	GLU	GLN	conflict	UNP P51159
G	134	ALA	LYS	conflict	UNP P51159
G	135	ALA	GLU	conflict	UNP P51159
G	136	ALA	GLU	conflict	UNP P51159
G	139	ARG	ILE	conflict	UNP P51159
G	140	GLN	ALA	conflict	UNP P51159
G	144	HIS	LYS	conflict	UNP P51159
G	178	SER	CYS	conflict	UNP P51159
I	1	GLY	-	expression tag	UNP P51159
I	?	-	ARG	deletion	UNP P51159
I	50	THR	VAL	conflict	UNP P51159
I	51	ILE	VAL	conflict	UNP P51159
I	?	-	ALA	deletion	UNP P51159
I	?	-	SER	deletion	UNP P51159
I	?	-	GLY	deletion	UNP P51159
I	?	-	PRO	deletion	UNP P51159
I	?	-	ASP	deletion	UNP P51159
I	?	-	GLY	deletion	UNP P51159
I	?	-	ALA	deletion	UNP P51159
I	?	-	THR	deletion	UNP P51159
I	?	-	GLY	deletion	UNP P51159
I	54	ASN	ARG	conflict	UNP P51159
I	55	ASP	GLY	conflict	UNP P51159
I	56	LYS	GLN	conflict	UNP P51159
I	59	LYS	HIS	conflict	UNP P51159
I	68	LEU	GLN	conflict	UNP P51159
I	95	GLU	GLN	conflict	UNP P51159
I	108	LYS	GLN	conflict	UNP P51159
I	109	THR	MET	conflict	UNP P51159
I	113	SER	CYS	conflict	UNP P51159
I	130	GLU	GLN	conflict	UNP P51159
I	134	ALA	LYS	conflict	UNP P51159
I	135	ALA	GLU	conflict	UNP P51159
I	136	ALA	GLU	conflict	UNP P51159
I	139	ARG	ILE	conflict	UNP P51159
I	140	GLN	ALA	conflict	UNP P51159
I	144	HIS	LYS	conflict	UNP P51159
I	178	SER	CYS	conflict	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLY	-	expression tag	UNP P51159
H	?	-	ARG	deletion	UNP P51159
H	50	THR	VAL	conflict	UNP P51159
H	51	ILE	VAL	conflict	UNP P51159
H	?	-	ALA	deletion	UNP P51159
H	?	-	SER	deletion	UNP P51159
H	?	-	GLY	deletion	UNP P51159
H	?	-	PRO	deletion	UNP P51159
H	?	-	ASP	deletion	UNP P51159
H	?	-	GLY	deletion	UNP P51159
H	?	-	ALA	deletion	UNP P51159
H	?	-	THR	deletion	UNP P51159
H	?	-	GLY	deletion	UNP P51159
H	54	ASN	ARG	conflict	UNP P51159
H	55	ASP	GLY	conflict	UNP P51159
H	56	LYS	GLN	conflict	UNP P51159
H	59	LYS	HIS	conflict	UNP P51159
H	68	LEU	GLN	conflict	UNP P51159
H	95	GLU	GLN	conflict	UNP P51159
H	108	LYS	GLN	conflict	UNP P51159
H	109	THR	MET	conflict	UNP P51159
H	113	SER	CYS	conflict	UNP P51159
H	130	GLU	GLN	conflict	UNP P51159
H	134	ALA	LYS	conflict	UNP P51159
H	135	ALA	GLU	conflict	UNP P51159
H	136	ALA	GLU	conflict	UNP P51159
H	139	ARG	ILE	conflict	UNP P51159
H	140	GLN	ALA	conflict	UNP P51159
H	144	HIS	LYS	conflict	UNP P51159
H	178	SER	CYS	conflict	UNP P51159
L	1	GLY	-	expression tag	UNP P51159
L	?	-	ARG	deletion	UNP P51159
L	50	THR	VAL	conflict	UNP P51159
L	51	ILE	VAL	conflict	UNP P51159
L	?	-	ALA	deletion	UNP P51159
L	?	-	SER	deletion	UNP P51159
L	?	-	GLY	deletion	UNP P51159
L	?	-	PRO	deletion	UNP P51159
L	?	-	ASP	deletion	UNP P51159
L	?	-	GLY	deletion	UNP P51159
L	?	-	ALA	deletion	UNP P51159
L	?	-	THR	deletion	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	GLY	deletion	UNP P51159
L	54	ASN	ARG	conflict	UNP P51159
L	55	ASP	GLY	conflict	UNP P51159
L	56	LYS	GLN	conflict	UNP P51159
L	59	LYS	HIS	conflict	UNP P51159
L	68	LEU	GLN	conflict	UNP P51159
L	95	GLU	GLN	conflict	UNP P51159
L	108	LYS	GLN	conflict	UNP P51159
L	109	THR	MET	conflict	UNP P51159
L	113	SER	CYS	conflict	UNP P51159
L	130	GLU	GLN	conflict	UNP P51159
L	134	ALA	LYS	conflict	UNP P51159
L	135	ALA	GLU	conflict	UNP P51159
L	136	ALA	GLU	conflict	UNP P51159
L	139	ARG	ILE	conflict	UNP P51159
L	140	GLN	ALA	conflict	UNP P51159
L	144	HIS	LYS	conflict	UNP P51159
L	178	SER	CYS	conflict	UNP P51159

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

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

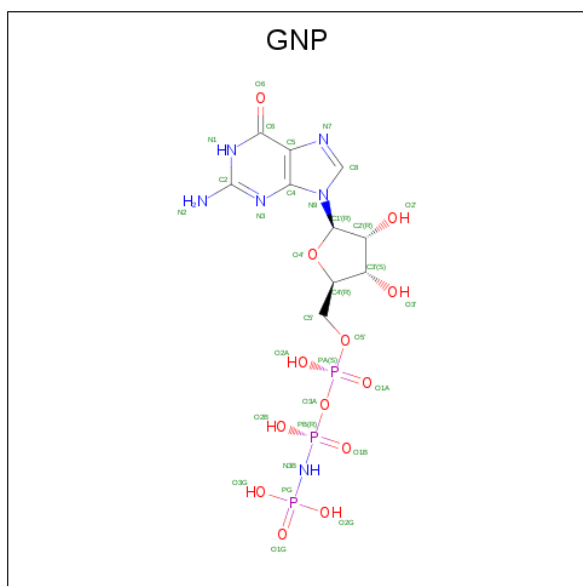
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	N	1	Total	Mg	0	0
			1	1		
2	O	1	Total	Mg	0	0
			1	1		
2	L	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		
2	M	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	O	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	N	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	K	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	M	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	P	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	J	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	G	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	I	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	H	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	L	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

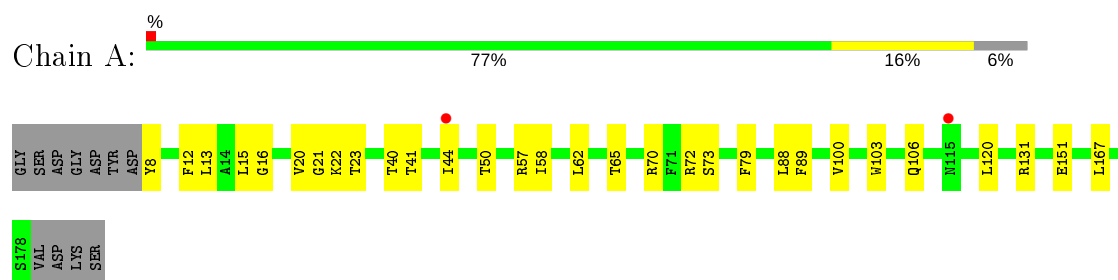
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	G	1	Total	O	0	0
			1	1		

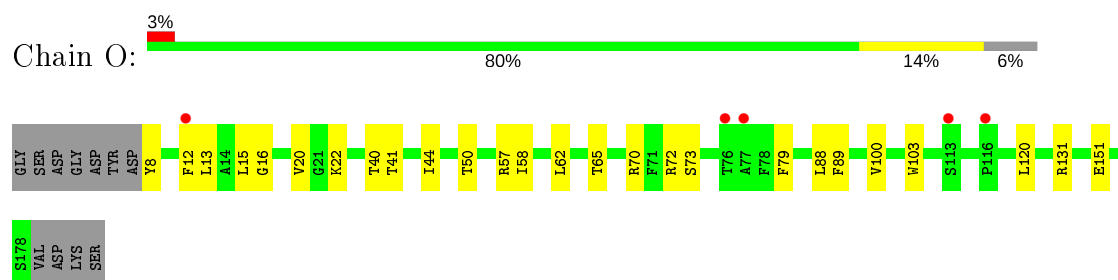
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

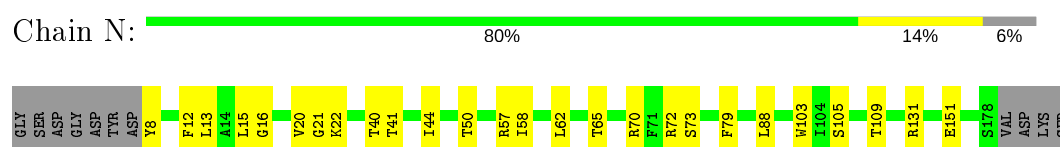
- Molecule 1: Ras-related protein Rab-27A



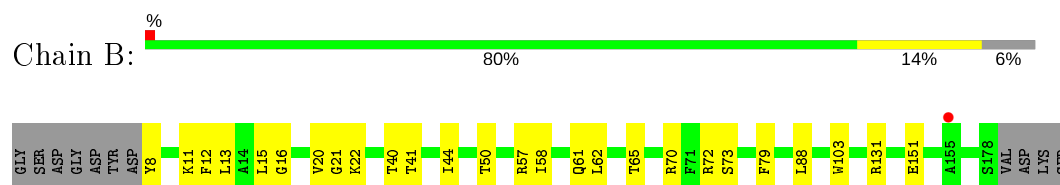
- Molecule 1: Ras-related protein Rab-27A



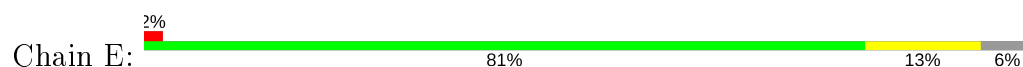
- Molecule 1: Ras-related protein Rab-27A

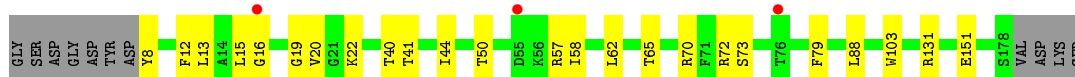


- Molecule 1: Ras-related protein Rab-27A

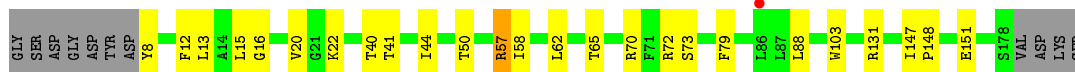
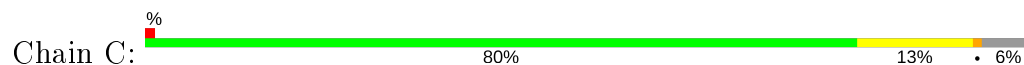


- Molecule 1: Ras-related protein Rab-27A

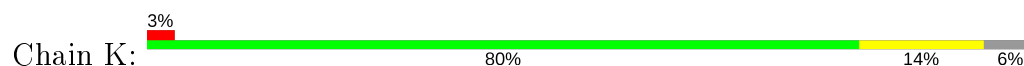




- Molecule 1: Ras-related protein Rab-27A

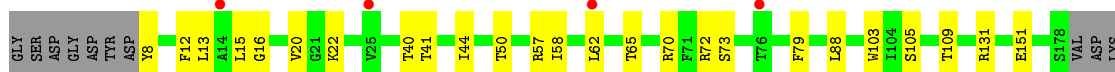
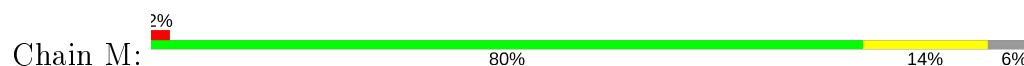


- Molecule 1: Ras-related protein Rab-27A



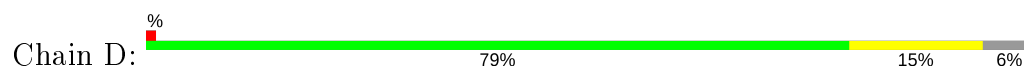
ASP  
LYS  
SER

- Molecule 1: Ras-related protein Rab-27A



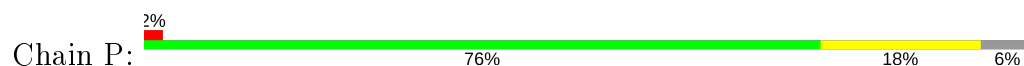
SER

- Molecule 1: Ras-related protein Rab-27A



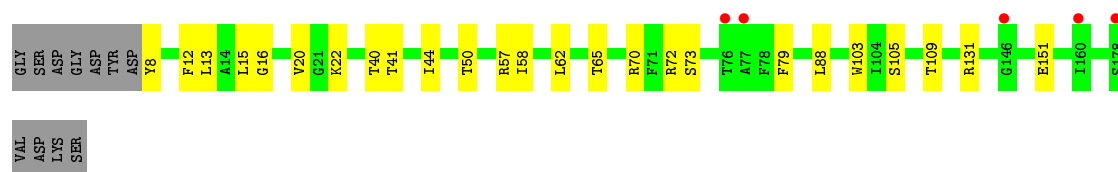
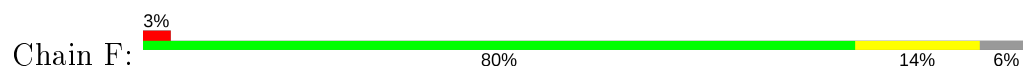
VAL  
ASP  
LYS  
SER

- Molecule 1: Ras-related protein Rab-27A

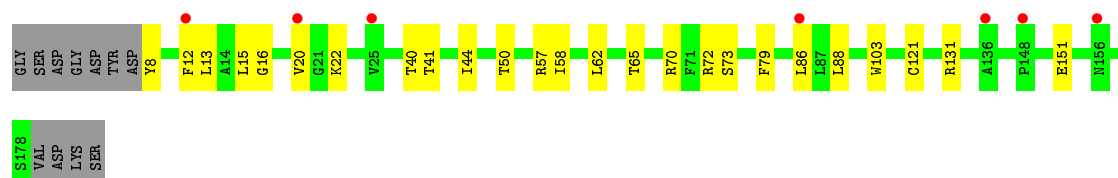
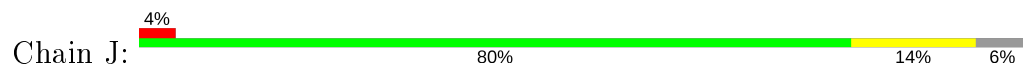


S105  
T109  
R131  
E151  
S178  
VAL  
ASP  
LYS  
SER

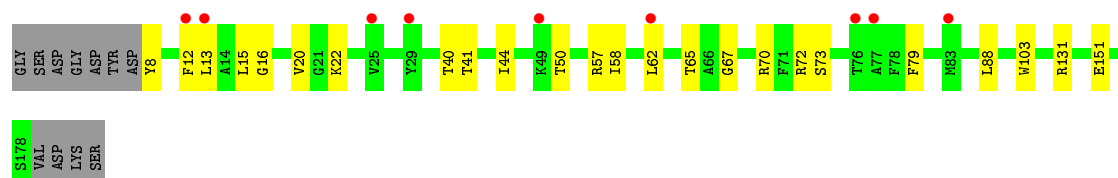
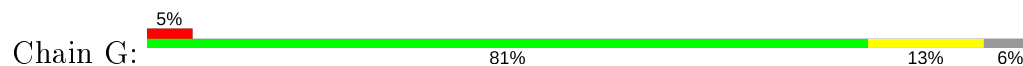
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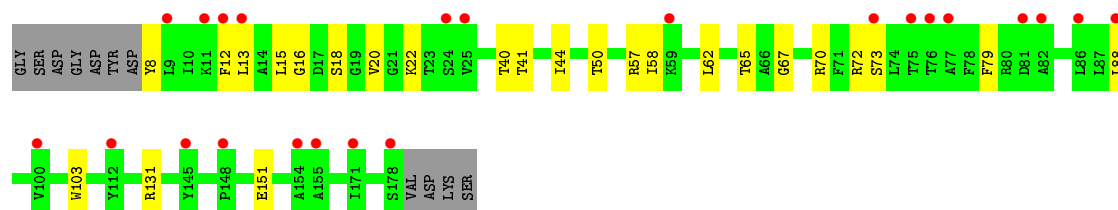
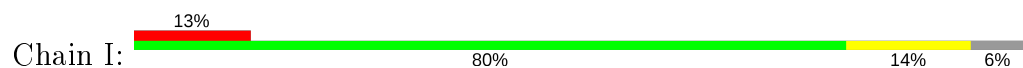
- Molecule 1: Ras-related protein Rab-27A



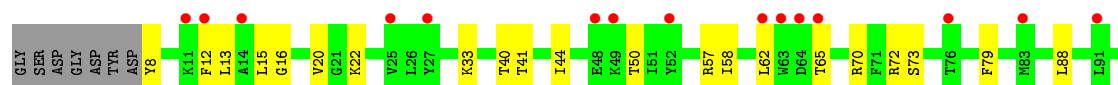
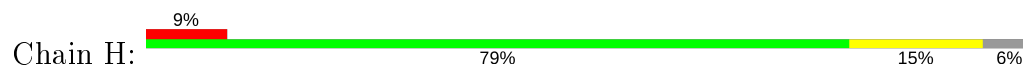
- Molecule 1: Ras-related protein Rab-27A



- Molecule 1: Ras-related protein Rab-27A

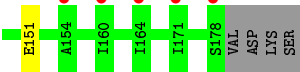
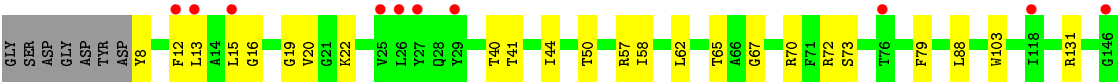
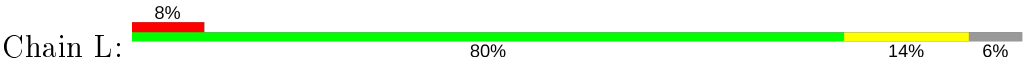


- Molecule 1: Ras-related protein Rab-27A





● Molecule 1: Ras-related protein Rab-27A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.42Å 132.41Å 230.59Å 90.00° 103.57° 90.00°	Depositor
Resolution (Å)	80.15 – 2.82 80.15 – 2.82	Depositor EDS
% Data completeness (in resolution range)	75.8 (80.15-2.82) 75.8 (80.15-2.82)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.312 , 0.342 0.311 , 0.339	Depositor DCC
$R_{free}$ test set	3513 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.965	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2444e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.71	0/1176	0.83	0/1610
1	B	0.71	0/1169	0.83	0/1601
1	C	0.72	0/1170	0.83	0/1602
1	D	0.71	0/1173	0.82	0/1606
1	E	0.73	0/1166	0.83	0/1597
1	F	0.71	0/1173	0.82	0/1606
1	G	0.72	0/1169	0.82	0/1601
1	H	0.72	0/1166	0.82	0/1597
1	I	0.72	0/1166	0.82	0/1597
1	J	0.72	0/1173	0.82	0/1606
1	K	0.73	0/1179	0.82	0/1614
1	L	0.72	0/1166	0.82	0/1597
1	M	0.71	0/1166	0.82	0/1597
1	N	0.72	0/1166	0.84	0/1597
1	O	0.73	0/1169	0.84	0/1601
1	P	0.71	0/1173	0.84	0/1606
All	All	0.72	0/18720	0.83	0/25635

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
All	All	0	16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	TYR	Peptide
1	B	8	TYR	Peptide
1	E	8	TYR	Peptide
1	N	8	TYR	Peptide
1	O	8	TYR	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1159	0	962	29	0
1	B	1152	0	947	22	0
1	C	1153	0	943	22	0
1	D	1155	0	945	26	0
1	E	1149	0	939	21	0
1	F	1155	0	945	21	0
1	G	1152	0	942	22	0
1	H	1149	0	938	24	0
1	I	1149	0	938	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1155	0	946	22	0
1	K	1161	0	964	23	0
1	L	1149	0	938	23	0
1	M	1149	0	938	21	0
1	N	1149	0	938	23	0
1	O	1152	0	947	24	0
1	P	1155	0	946	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	32	0	13	2	0
3	B	32	0	13	1	0
3	C	32	0	13	0	0
3	D	32	0	13	3	0
3	E	32	0	13	1	0
3	F	32	0	13	0	0
3	G	32	0	13	2	0
3	H	32	0	13	0	0
3	I	32	0	13	2	0
3	J	32	0	13	0	0
3	K	32	0	13	0	0
3	L	32	0	13	2	0
3	M	32	0	13	0	0
3	N	32	0	13	2	0
3	O	32	0	13	0	0
3	P	32	0	13	3	0
4	A	5	0	0	1	0
4	G	1	0	0	0	0
All	All	18977	0	15324	367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 367 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:O:89:PHE:HE1	1:O:120:LEU:HD21	1.30	0.96
1:A:89:PHE:HE1	1:A:120:LEU:HD21	1.32	0.92
1:A:89:PHE:CE1	1:A:120:LEU:HD21	2.13	0.83
1:O:89:PHE:CE1	1:O:120:LEU:HD21	2.13	0.82
1:J:86:LEU:HD11	1:J:121:CYS:SG	2.21	0.81

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/182 (93%)	155 (92%)	12 (7%)	2 (1%)	13	37
1	B	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
1	C	169/182 (93%)	153 (90%)	14 (8%)	2 (1%)	13	37
1	D	169/182 (93%)	155 (92%)	13 (8%)	1 (1%)	25	54
1	E	169/182 (93%)	153 (90%)	14 (8%)	2 (1%)	13	37
1	F	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
1	G	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
1	H	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
1	I	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
1	J	169/182 (93%)	153 (90%)	14 (8%)	2 (1%)	13	37
1	K	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
1	L	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	169/182 (93%)	155 (92%)	12 (7%)	2 (1%)	13	37
1	N	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
1	O	169/182 (93%)	153 (90%)	14 (8%)	2 (1%)	13	37
1	P	169/182 (93%)	154 (91%)	13 (8%)	2 (1%)	13	37
All	All	2704/2912 (93%)	2463 (91%)	210 (8%)	31 (1%)	14	39

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	40	THR
1	P	40	THR
1	A	40	THR
1	O	40	THR
1	N	40	THR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/157 (59%)	92 (100%)	0	100	100
1	B	90/157 (57%)	90 (100%)	0	100	100
1	C	90/157 (57%)	89 (99%)	1 (1%)	73	91
1	D	90/157 (57%)	90 (100%)	0	100	100
1	E	89/157 (57%)	89 (100%)	0	100	100
1	F	90/157 (57%)	90 (100%)	0	100	100
1	G	90/157 (57%)	90 (100%)	0	100	100
1	H	89/157 (57%)	89 (100%)	0	100	100
1	I	89/157 (57%)	89 (100%)	0	100	100
1	J	90/157 (57%)	90 (100%)	0	100	100
1	K	92/157 (59%)	92 (100%)	0	100	100
1	L	89/157 (57%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	89/157 (57%)	89 (100%)	0	100	100
1	N	89/157 (57%)	89 (100%)	0	100	100
1	O	90/157 (57%)	90 (100%)	0	100	100
1	P	90/157 (57%)	90 (100%)	0	100	100
All	All	1438/2512 (57%)	1437 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	156	ASN
1	D	156	ASN
1	G	156	ASN
1	K	156	ASN
1	I	156	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GNP	C	202	2	28,34,34	2.45	7 (25%)	30,54,54	2.40	7 (23%)
3	GNP	L	202	2	28,34,34	2.37	7 (25%)	30,54,54	2.58	9 (30%)
3	GNP	I	202	2	28,34,34	2.34	8 (28%)	30,54,54	2.12	5 (16%)
3	GNP	J	202	2	28,34,34	2.58	9 (32%)	30,54,54	2.34	7 (23%)
3	GNP	O	202	2	28,34,34	2.61	8 (28%)	30,54,54	2.44	8 (26%)
3	GNP	H	202	2	28,34,34	2.51	10 (35%)	30,54,54	2.08	5 (16%)
3	GNP	K	202	2	28,34,34	2.45	9 (32%)	30,54,54	2.82	10 (33%)
3	GNP	P	202	2	28,34,34	2.53	8 (28%)	30,54,54	2.35	8 (26%)
3	GNP	E	202	2	28,34,34	2.28	10 (35%)	30,54,54	2.14	8 (26%)
3	GNP	F	202	2	28,34,34	2.36	8 (28%)	30,54,54	2.28	8 (26%)
3	GNP	D	202	2	28,34,34	2.53	8 (28%)	30,54,54	2.17	6 (20%)
3	GNP	A	202	2	28,34,34	2.70	8 (28%)	30,54,54	2.21	7 (23%)
3	GNP	B	202	2	28,34,34	2.49	10 (35%)	30,54,54	2.31	6 (20%)
3	GNP	G	202	2	28,34,34	2.40	9 (32%)	30,54,54	2.52	7 (23%)
3	GNP	M	202	2	28,34,34	2.30	8 (28%)	30,54,54	2.25	7 (23%)
3	GNP	N	202	2	28,34,34	2.41	8 (28%)	30,54,54	2.21	6 (20%)

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	GNP	C	202	2	-	4/17/38/38	0/3/3/3
3	GNP	L	202	2	-	4/17/38/38	0/3/3/3
3	GNP	I	202	2	-	3/17/38/38	0/3/3/3
3	GNP	J	202	2	-	9/17/38/38	0/3/3/3
3	GNP	O	202	2	-	4/17/38/38	0/3/3/3
3	GNP	H	202	2	-	7/17/38/38	0/3/3/3
3	GNP	K	202	2	-	4/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	P	202	2	-	7/17/38/38	0/3/3/3
3	GNP	E	202	2	-	4/17/38/38	0/3/3/3
3	GNP	F	202	2	-	4/17/38/38	0/3/3/3
3	GNP	D	202	2	-	7/17/38/38	0/3/3/3
3	GNP	A	202	2	-	6/17/38/38	0/3/3/3
3	GNP	B	202	2	-	4/17/38/38	0/3/3/3
3	GNP	G	202	2	-	6/17/38/38	0/3/3/3
3	GNP	M	202	2	-	6/17/38/38	0/3/3/3
3	GNP	N	202	2	-	4/17/38/38	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)
3	D	202	GNP	C4-N9	-8.19	1.36	1.47
3	O	202	GNP	C4-N9	-8.19	1.36	1.47
3	B	202	GNP	C4-N9	-7.84	1.37	1.47
3	J	202	GNP	C4-N9	-7.78	1.37	1.47
3	C	202	GNP	C4-N9	-7.69	1.37	1.47

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	202	GNP	O1B-PB-N3B	-7.89	100.15	111.77
3	A	202	GNP	C4-C5-N7	6.89	111.59	102.46
3	O	202	GNP	C4-C5-N7	6.71	111.36	102.46
3	L	202	GNP	C4-C5-N7	6.53	111.11	102.46
3	G	202	GNP	C4-C5-N7	6.49	111.07	102.46

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	202	GNP	PB-N3B-PG-O1G
3	F	202	GNP	PG-N3B-PB-O1B
3	F	202	GNP	PG-N3B-PB-O3A
3	F	202	GNP	C2'-C1'-N9-C4
3	A	202	GNP	PG-N3B-PB-O1B

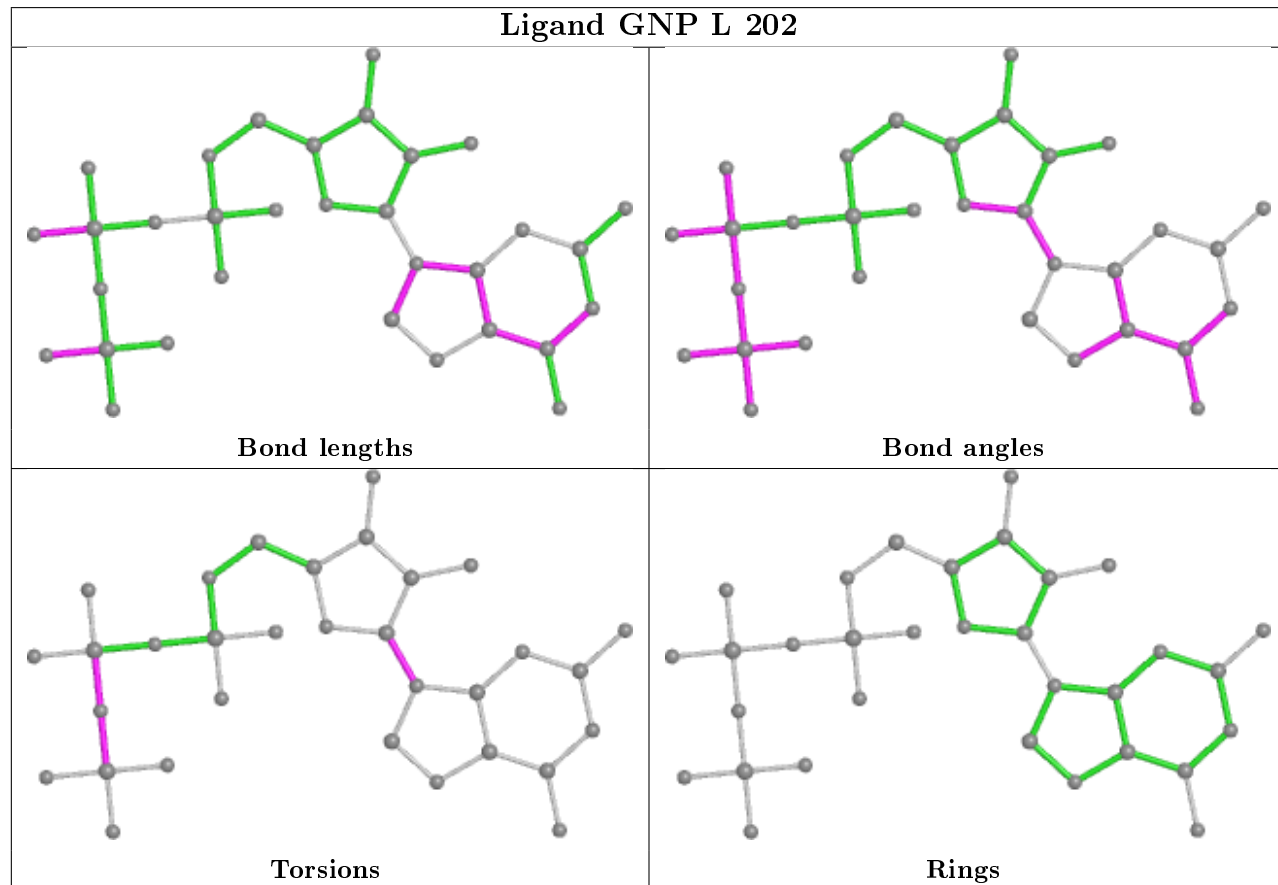
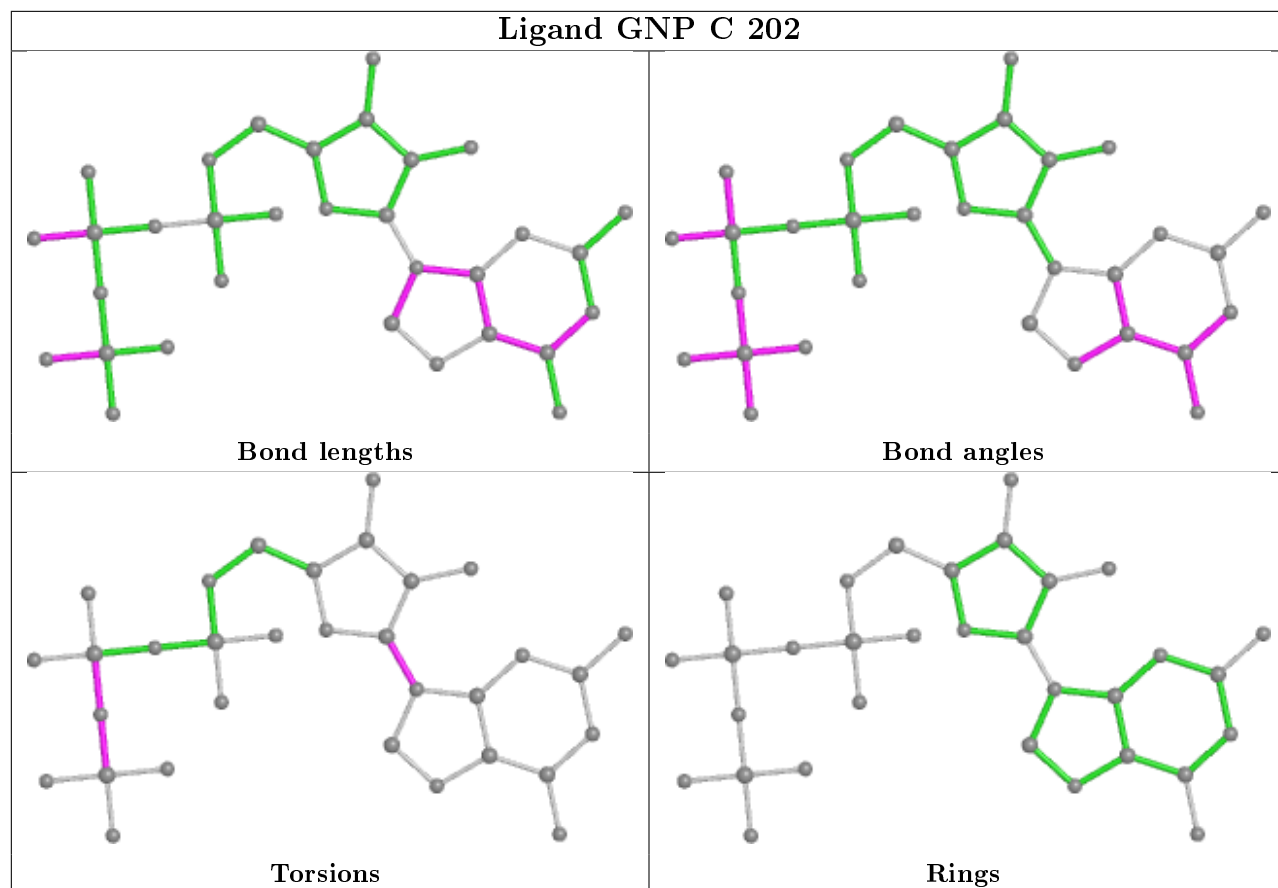
There are no ring outliers.

9 monomers are involved in 18 short contacts:

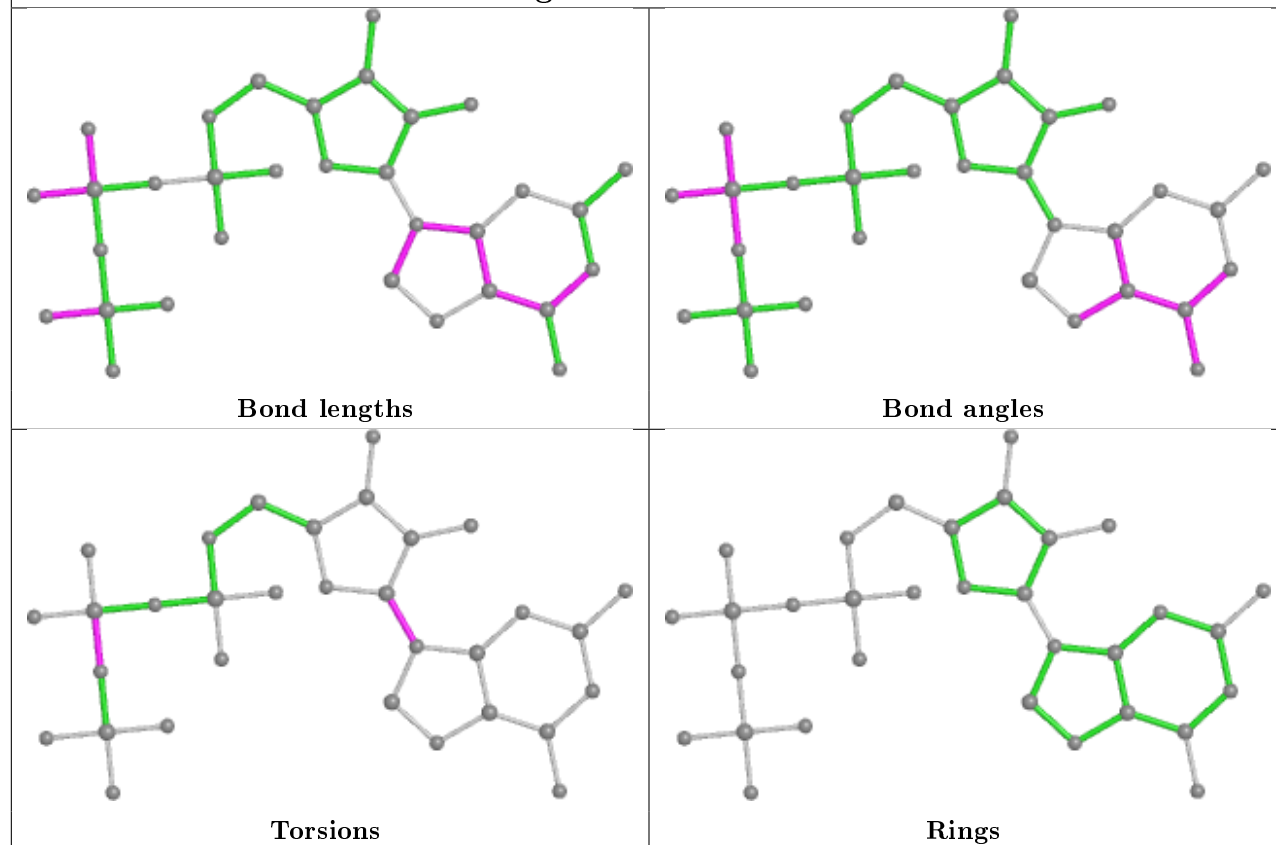
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	202	GNP	2	0
3	I	202	GNP	2	0
3	P	202	GNP	3	0
3	E	202	GNP	1	0
3	D	202	GNP	3	0
3	A	202	GNP	2	0
3	B	202	GNP	1	0
3	G	202	GNP	2	0
3	N	202	GNP	2	0

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

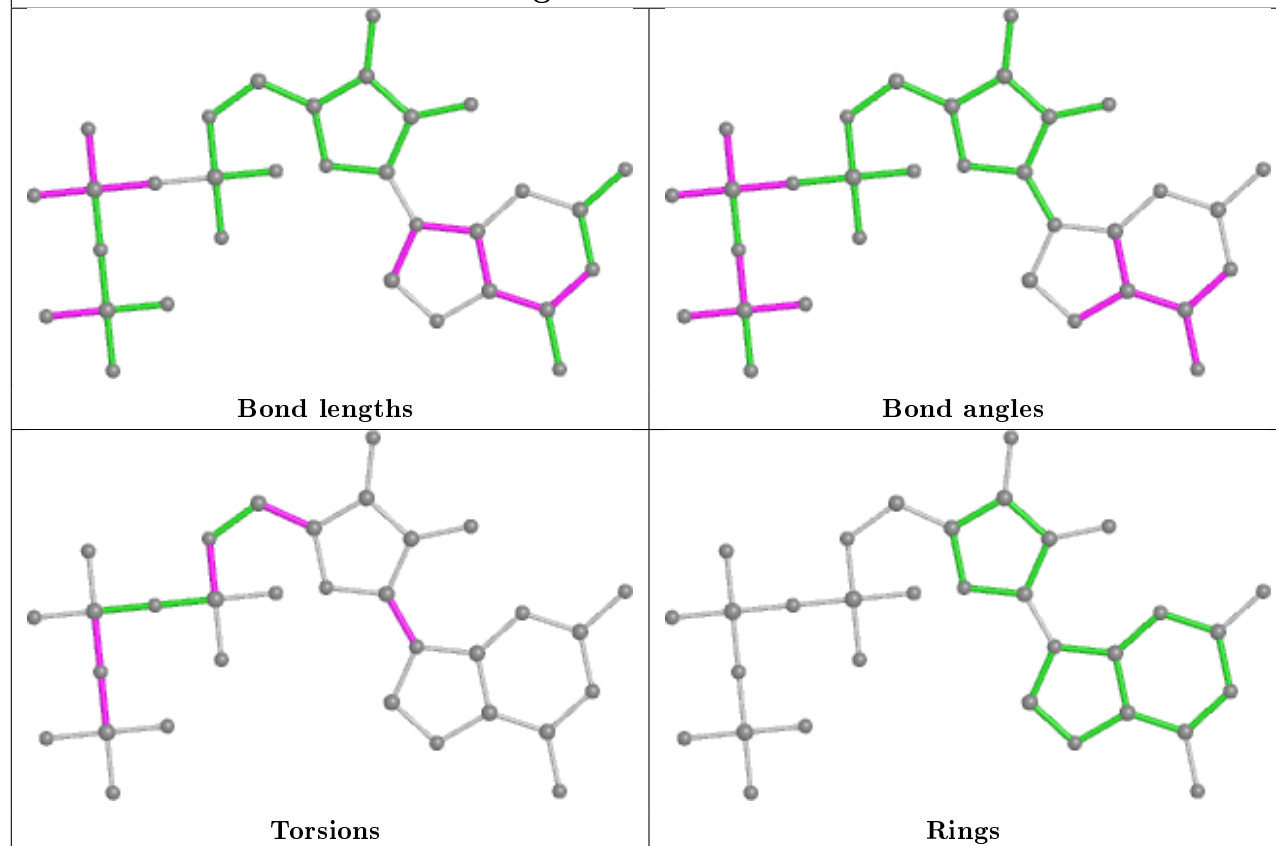


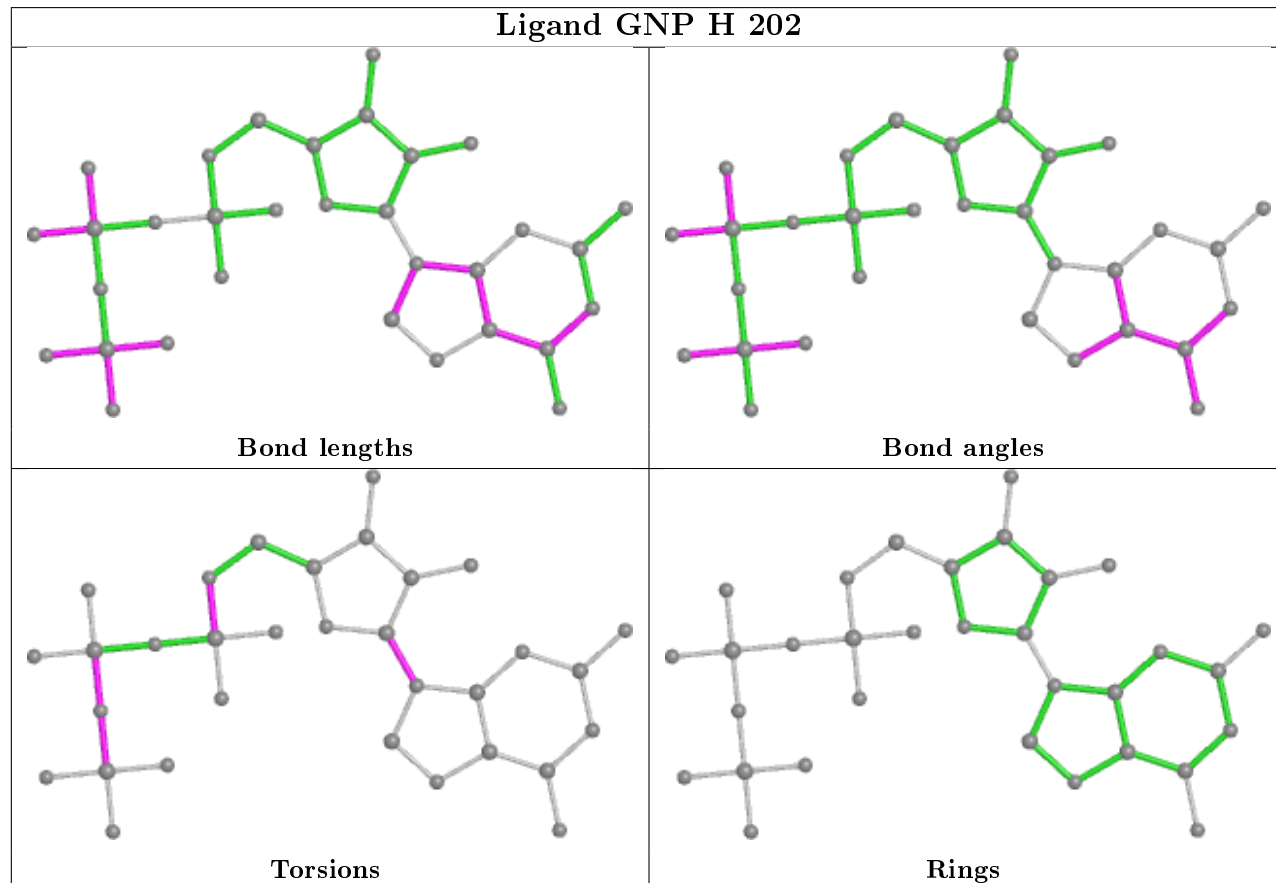
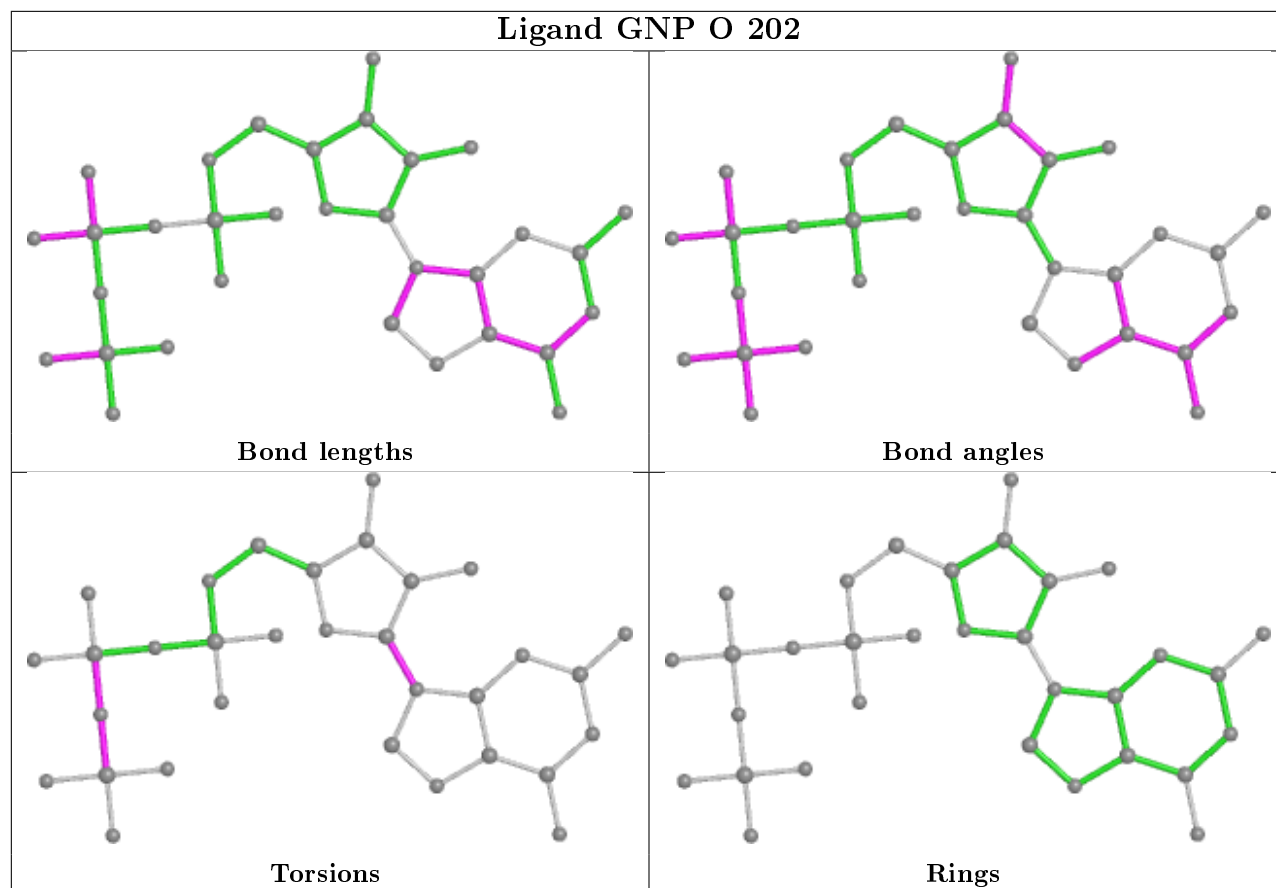


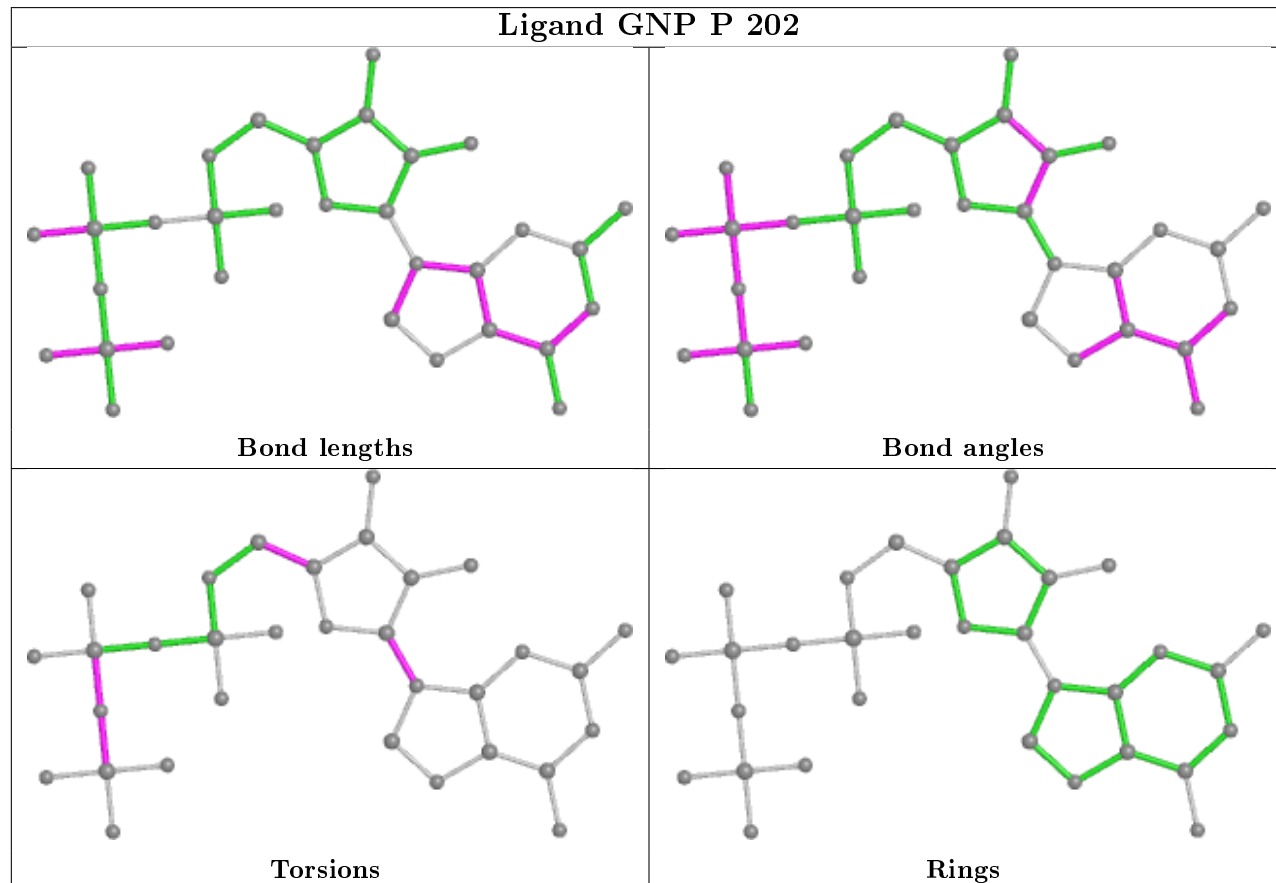
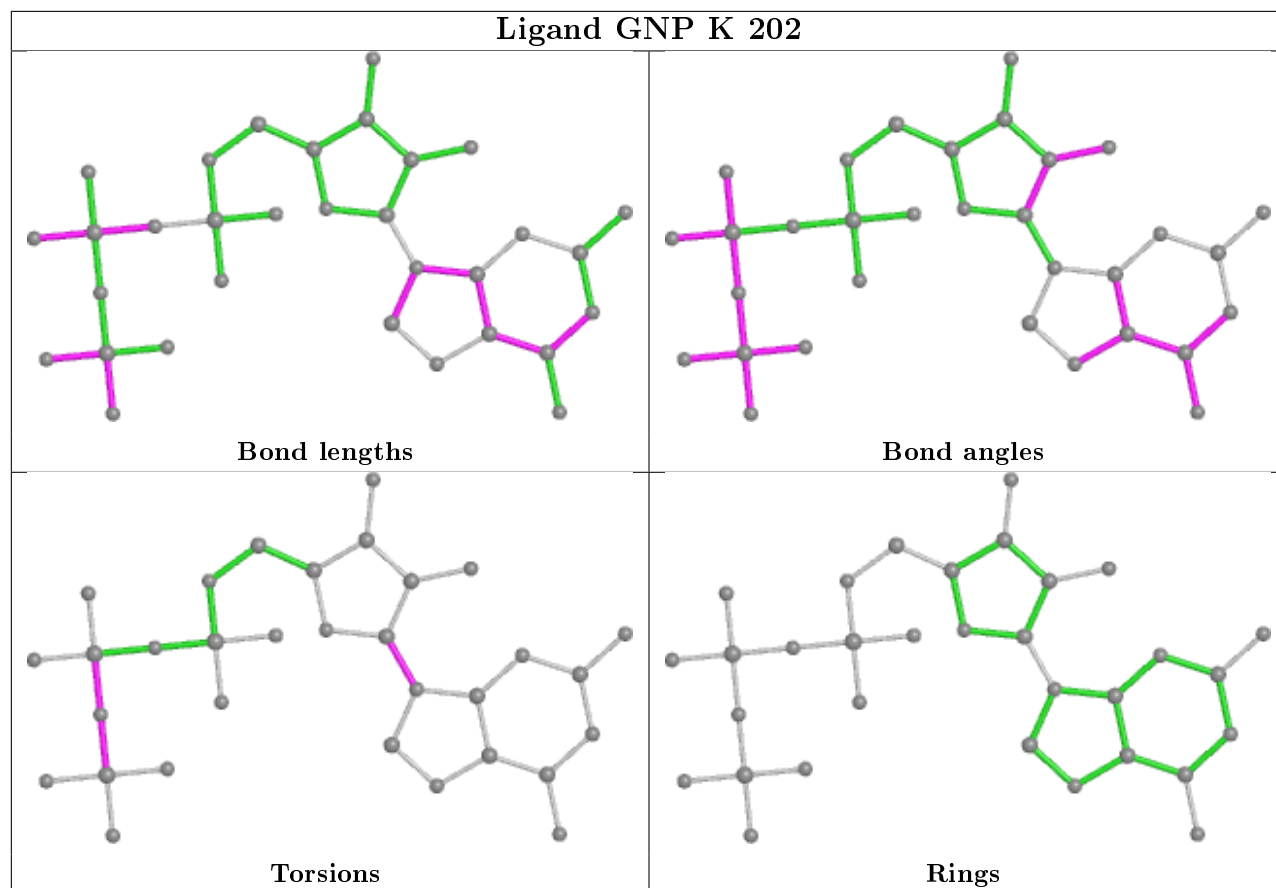
## Ligand GNP I 202



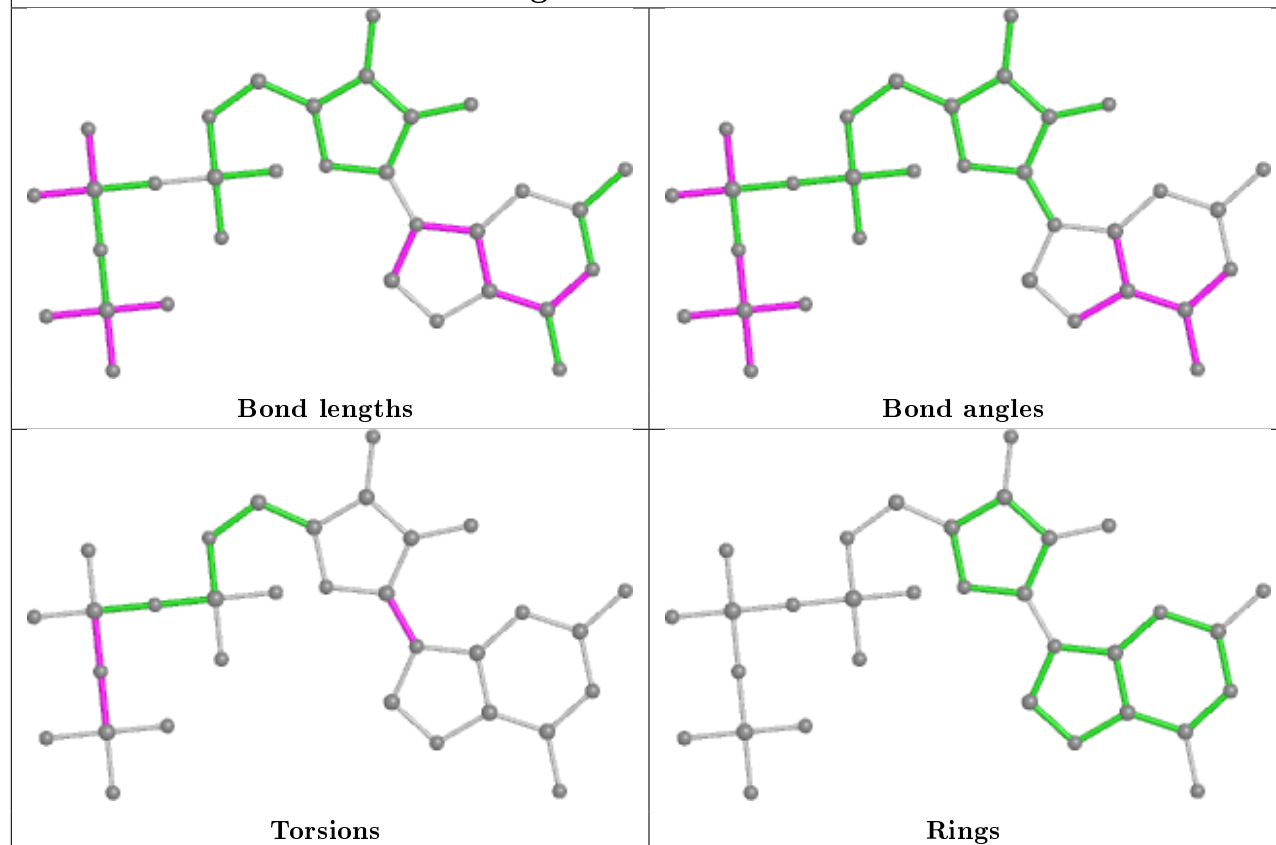
## Ligand GNP J 202



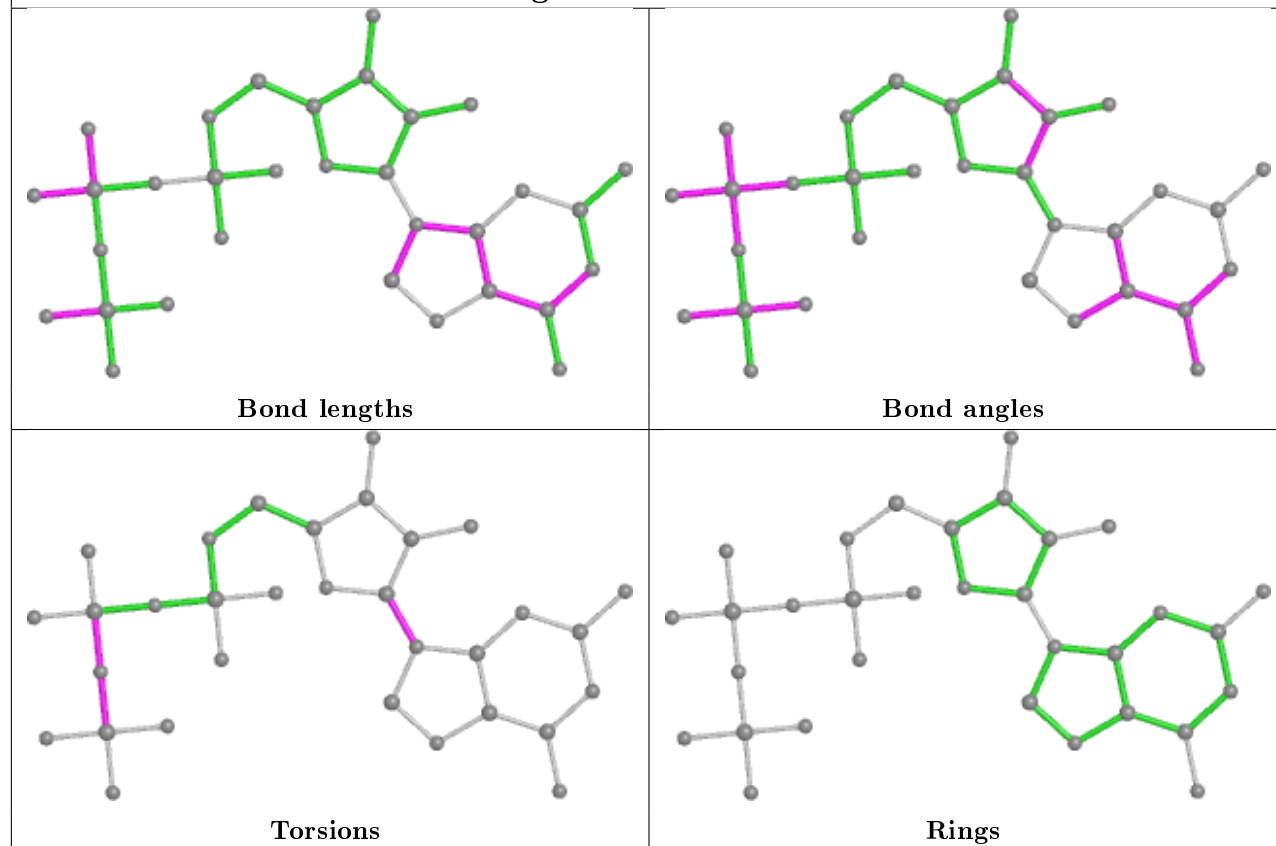


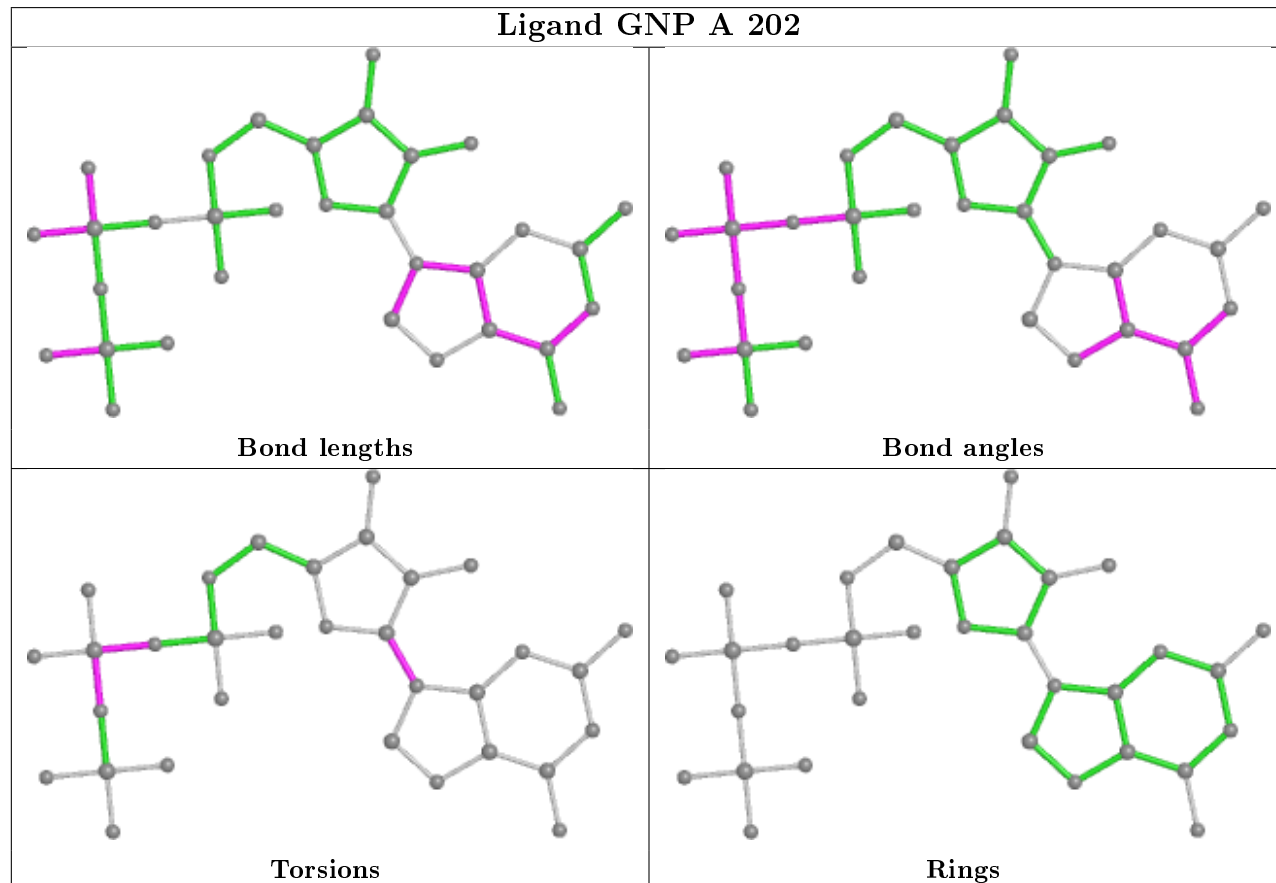
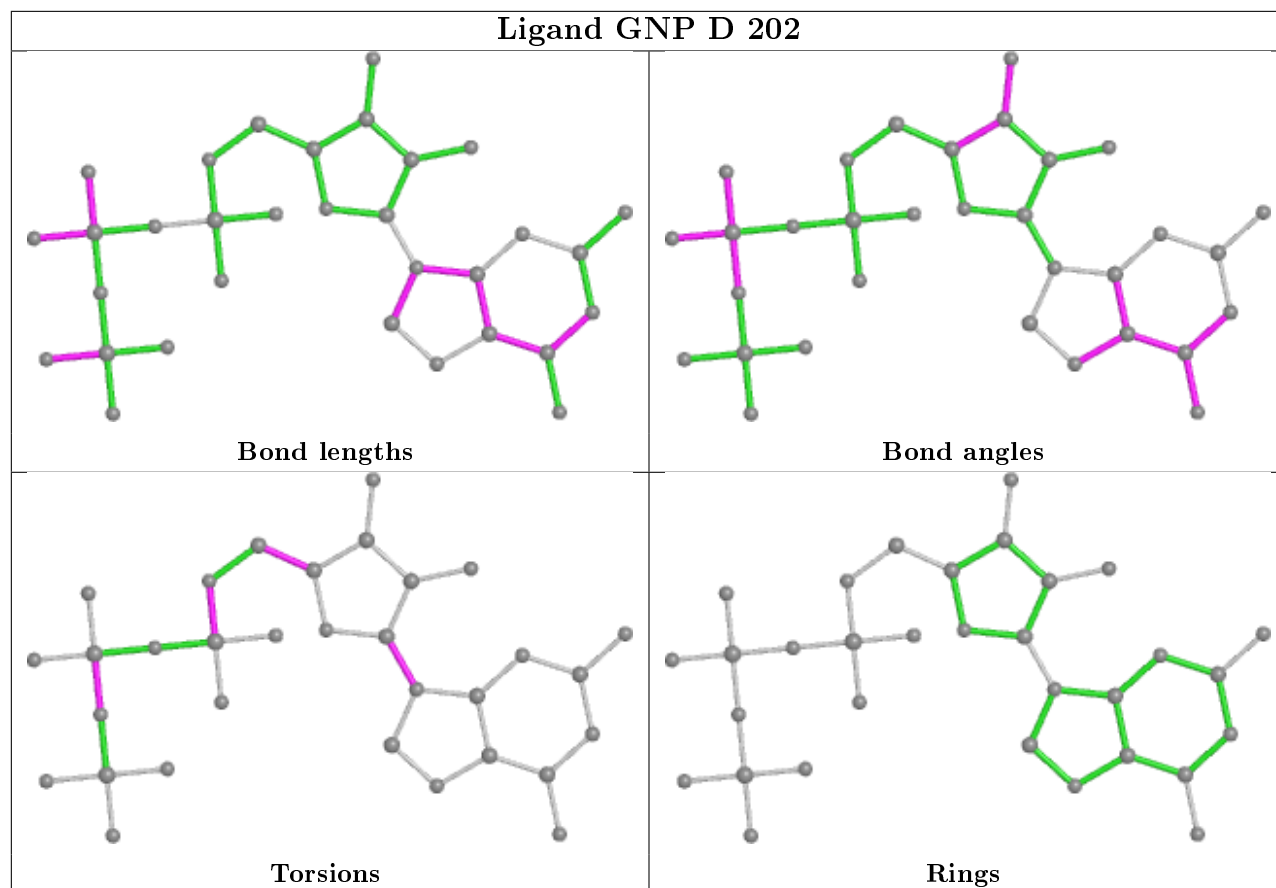


## Ligand GNP E 202

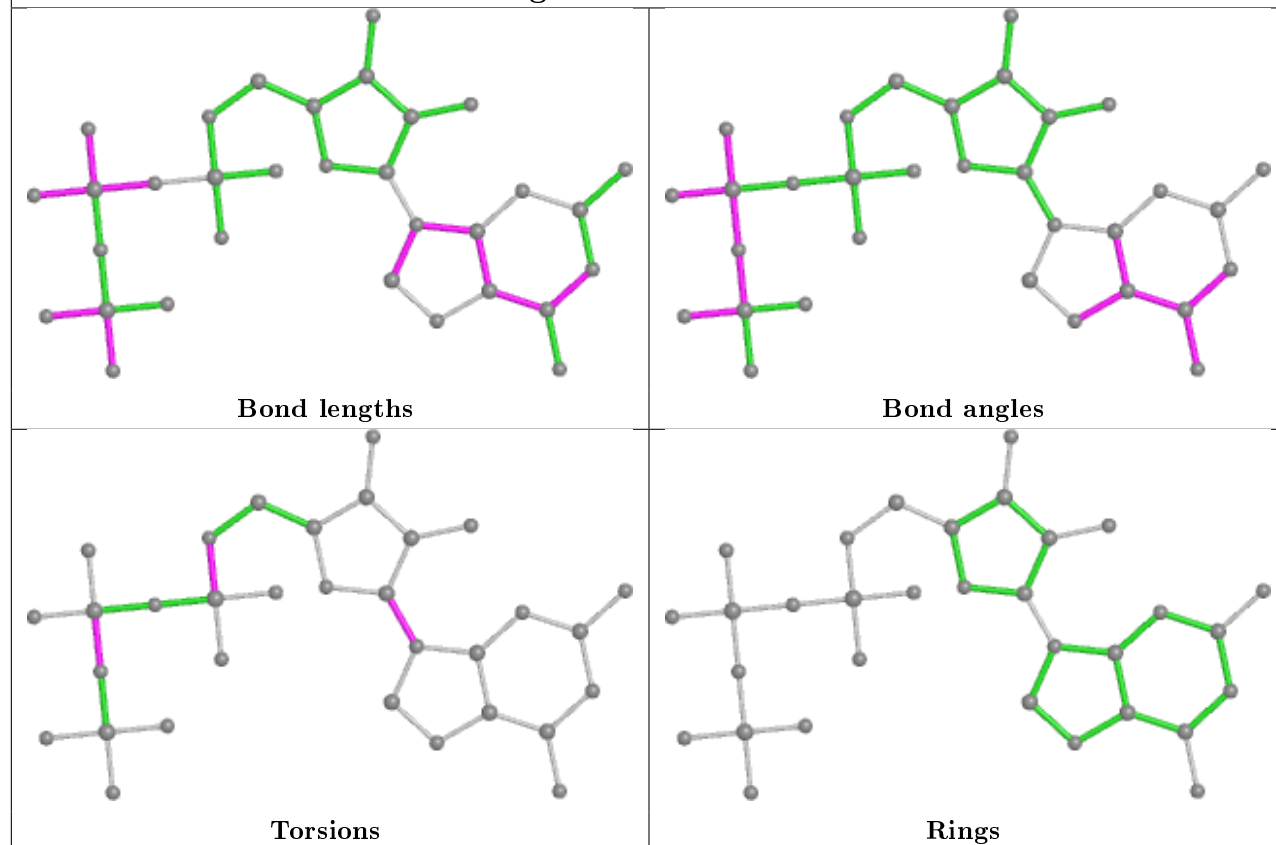


## Ligand GNP F 202

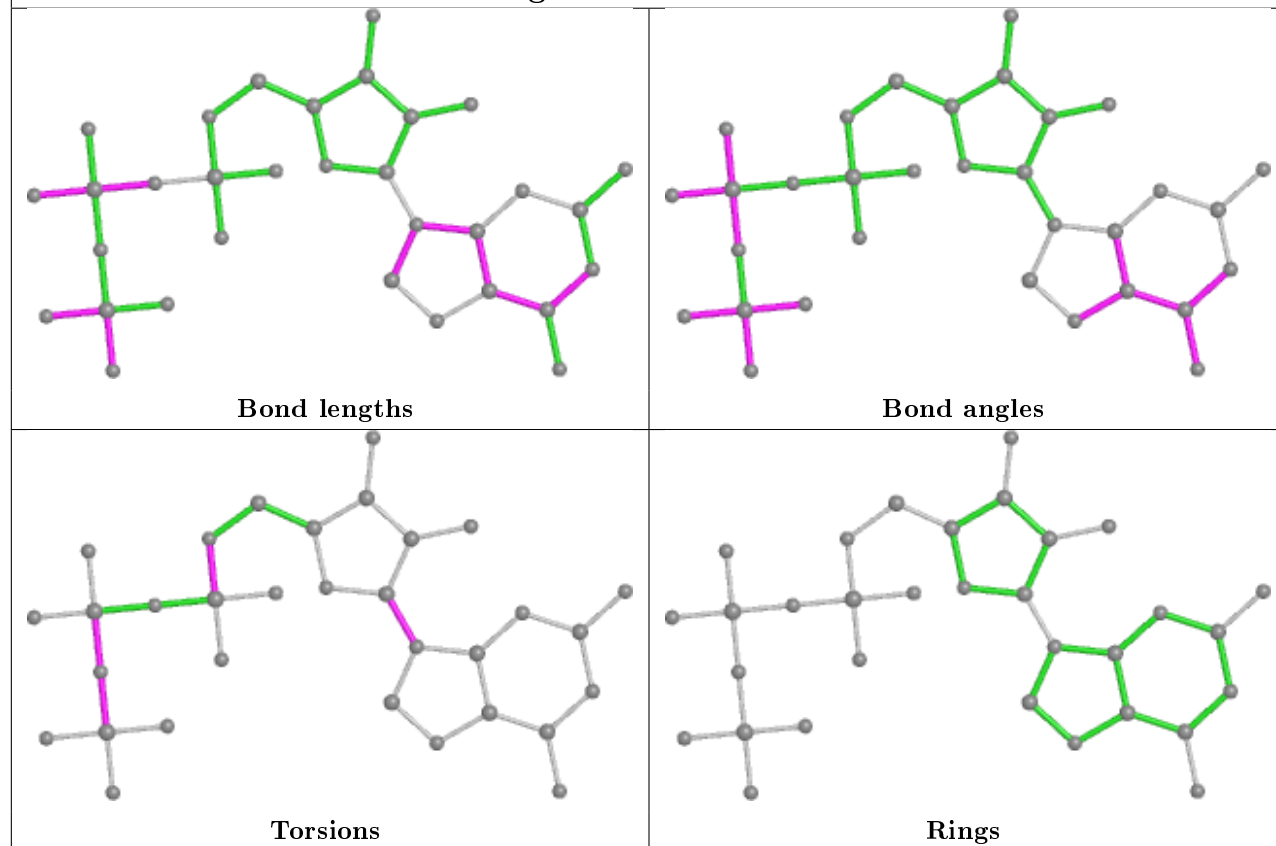




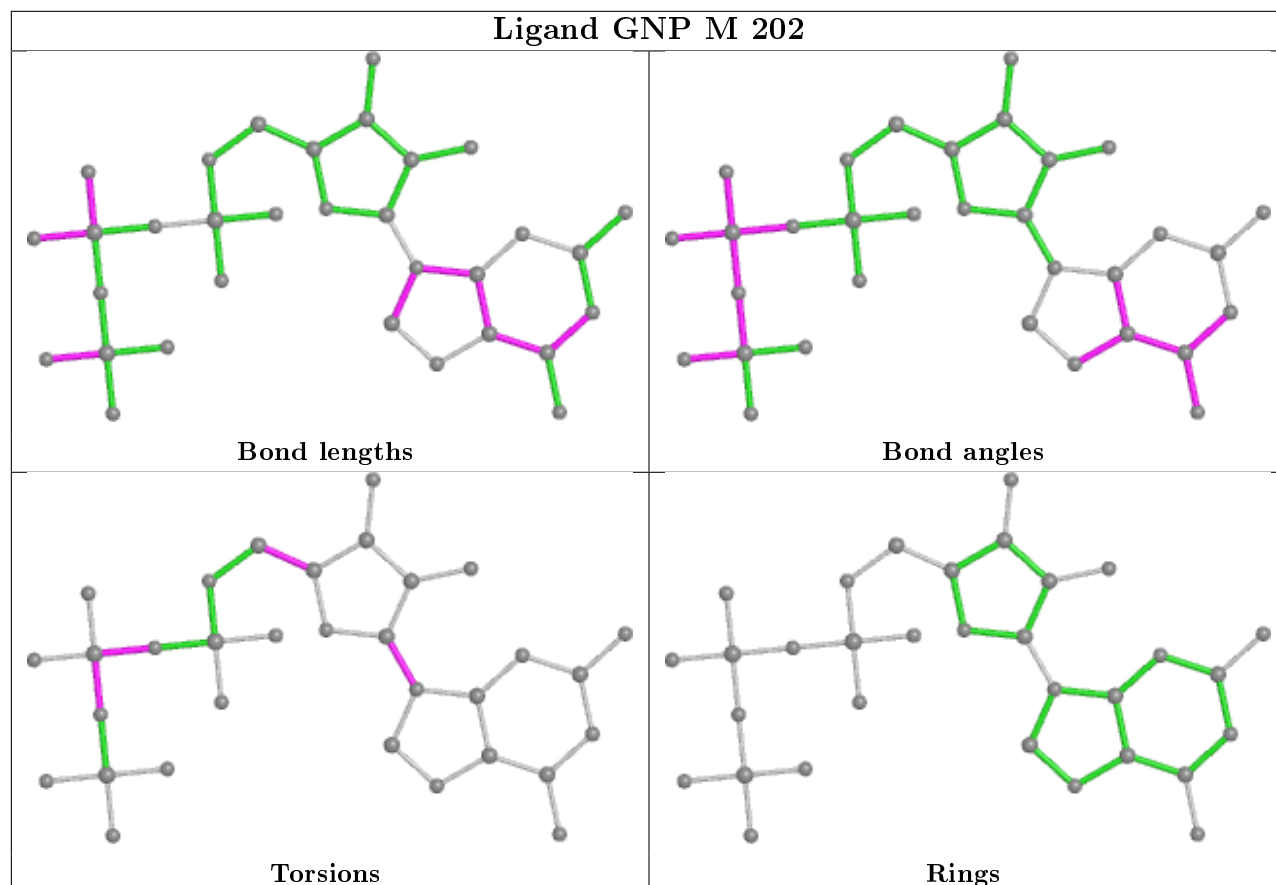
## Ligand GNP B 202



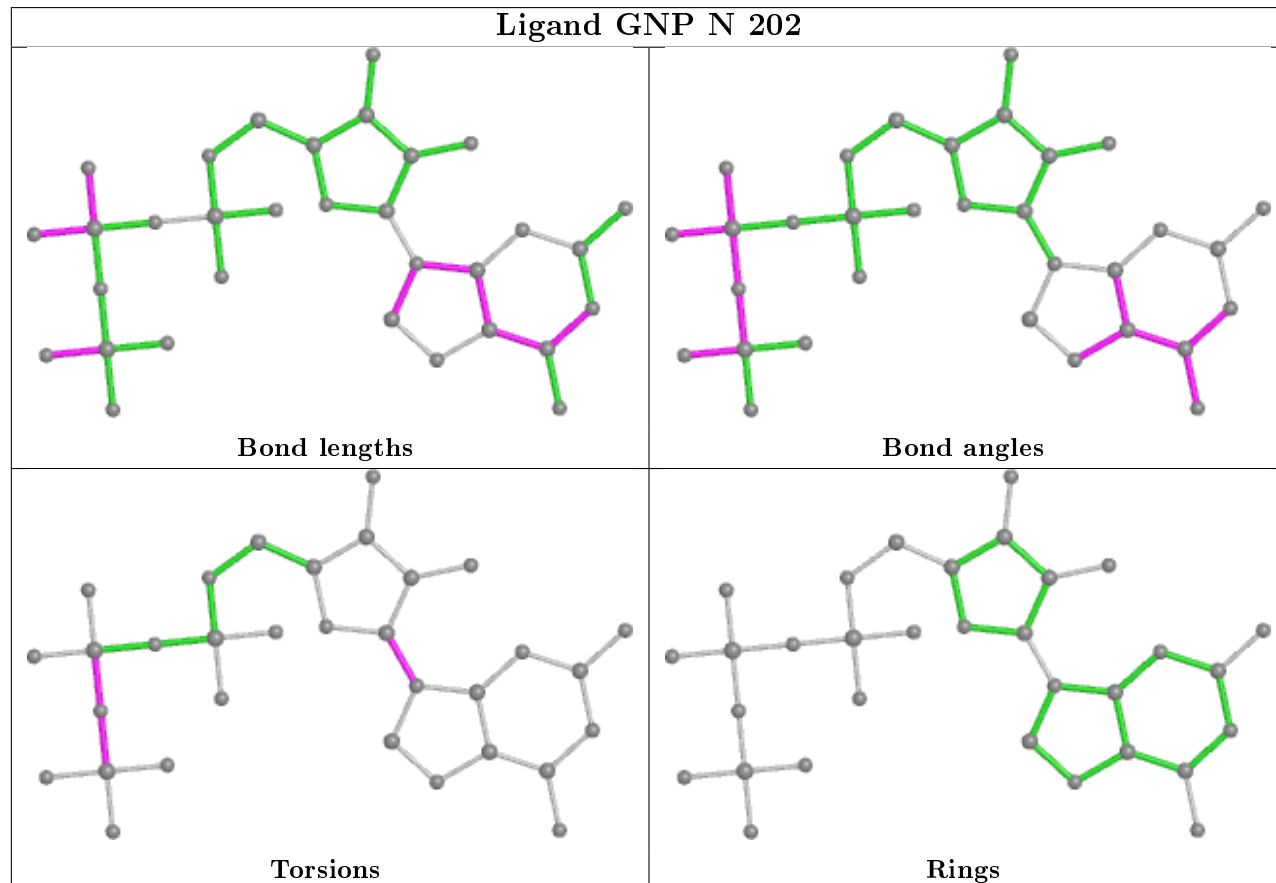
## Ligand GNP G 202



## Ligand GNP M 202



## Ligand GNP N 202





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	171/182 (93%)	-0.10	2 (1%) 79 73	39, 68, 122, 160	0
1	B	171/182 (93%)	-0.30	1 (0%) 89 86	49, 74, 108, 137	0
1	C	171/182 (93%)	-0.17	1 (0%) 89 86	54, 84, 123, 169	0
1	D	171/182 (93%)	-0.19	2 (1%) 79 73	49, 86, 127, 141	0
1	E	171/182 (93%)	-0.12	3 (1%) 68 61	45, 68, 124, 153	0
1	F	171/182 (93%)	-0.12	5 (2%) 51 41	56, 88, 138, 164	0
1	G	171/182 (93%)	0.06	9 (5%) 26 18	58, 91, 138, 168	0
1	H	171/182 (93%)	0.39	16 (9%) 8 4	60, 94, 166, 211	0
1	I	171/182 (93%)	0.47	23 (13%) 3 2	63, 95, 148, 209	0
1	J	171/182 (93%)	-0.02	7 (4%) 37 27	53, 88, 131, 167	0
1	K	171/182 (93%)	-0.01	6 (3%) 44 34	41, 68, 121, 171	0
1	L	171/182 (93%)	0.16	15 (8%) 10 5	58, 95, 142, 200	0
1	M	171/182 (93%)	-0.18	4 (2%) 60 50	49, 79, 111, 164	0
1	N	171/182 (93%)	-0.27	0 100 100	45, 68, 113, 134	0
1	O	171/182 (93%)	-0.10	5 (2%) 51 41	37, 64, 116, 152	0
1	P	171/182 (93%)	-0.19	3 (1%) 68 61	46, 77, 116, 165	0
All	All	2736/2912 (93%)	-0.04	102 (3%) 41 31	37, 81, 134, 211	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	76	THR	10.4
1	H	12	PHE	9.2
1	H	52	TYR	8.4
1	H	62	LEU	8.0
1	L	12	PHE	7.9

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	I	201	1/1	0.85	0.14	68,68,68,68	0
3	GNP	I	202	32/32	0.92	0.15	54,75,96,98	0
3	GNP	C	202	32/32	0.94	0.14	47,57,73,80	0
3	GNP	E	202	32/32	0.94	0.17	33,44,61,67	0
3	GNP	N	202	32/32	0.95	0.16	46,57,65,73	0
3	GNP	G	202	32/32	0.95	0.13	51,67,77,94	0
3	GNP	H	202	32/32	0.95	0.16	46,60,72,78	0
2	MG	G	201	1/1	0.95	0.21	36,36,36,36	0
3	GNP	J	202	32/32	0.95	0.16	40,53,82,87	0
3	GNP	K	202	32/32	0.95	0.16	34,44,55,58	0
3	GNP	P	202	32/32	0.95	0.14	40,53,67,83	0
2	MG	P	201	1/1	0.95	0.15	41,41,41,41	0
2	MG	K	201	1/1	0.96	0.25	34,34,34,34	0
2	MG	E	201	1/1	0.96	0.15	38,38,38,38	0
2	MG	C	201	1/1	0.96	0.11	43,43,43,43	0
3	GNP	M	202	32/32	0.96	0.14	42,60,68,69	0
3	GNP	D	202	32/32	0.96	0.12	38,52,69,73	0
3	GNP	B	202	32/32	0.96	0.13	44,58,65,75	0
2	MG	D	201	1/1	0.97	0.17	39,39,39,39	0
2	MG	L	201	1/1	0.97	0.16	45,45,45,45	0
3	GNP	F	202	32/32	0.97	0.13	42,60,70,71	0
3	GNP	L	202	32/32	0.97	0.13	46,58,65,69	0
3	GNP	O	202	32/32	0.97	0.15	38,46,55,61	0
2	MG	F	201	1/1	0.97	0.17	39,39,39,39	0
2	MG	H	201	1/1	0.98	0.21	45,45,45,45	0
2	MG	M	201	1/1	0.98	0.20	34,34,34,34	0
3	GNP	A	202	32/32	0.98	0.13	39,47,56,60	0

*Continued on next page...*

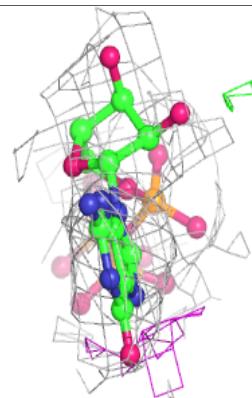
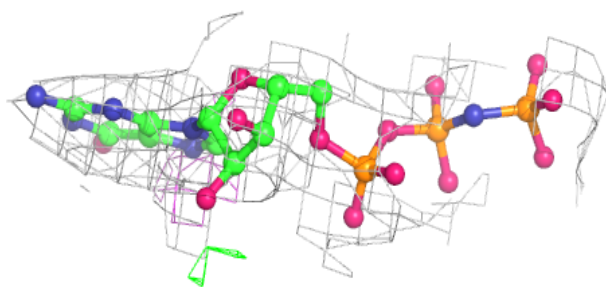
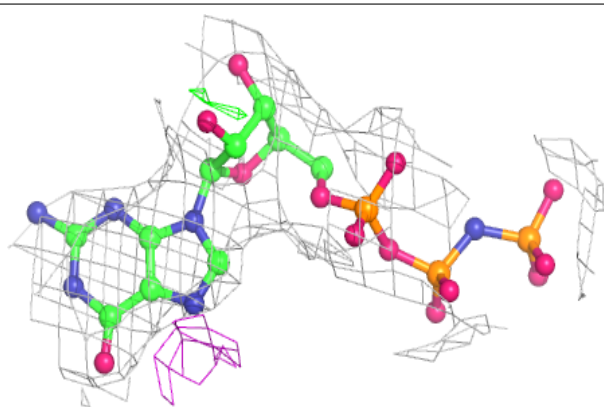
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	N	201	1/1	0.98	0.20	34,34,34,34	0
2	MG	J	201	1/1	0.98	0.17	44,44,44,44	0
2	MG	B	201	1/1	0.99	0.20	35,35,35,35	0
2	MG	O	201	1/1	0.99	0.17	28,28,28,28	0
2	MG	A	201	1/1	0.99	0.20	29,29,29,29	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.

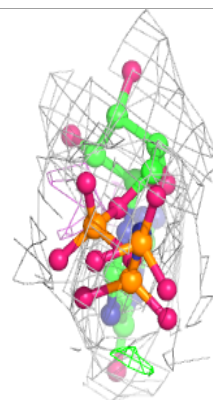
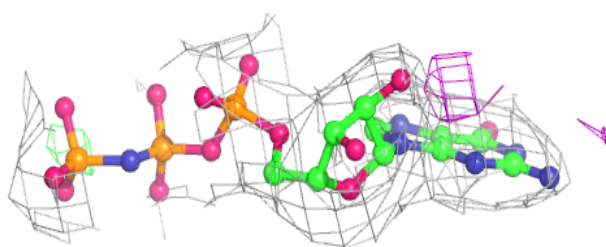
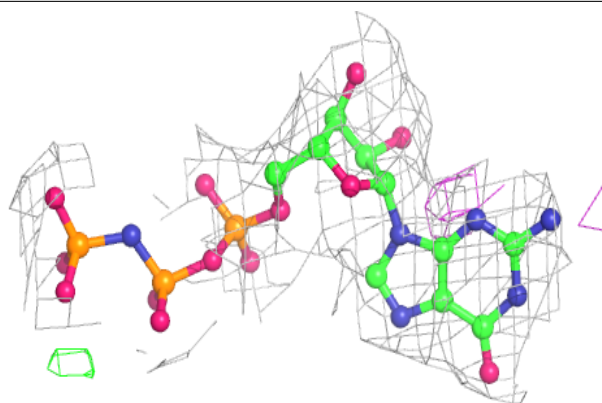
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mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

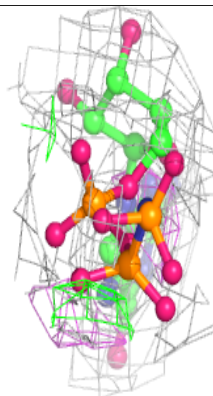
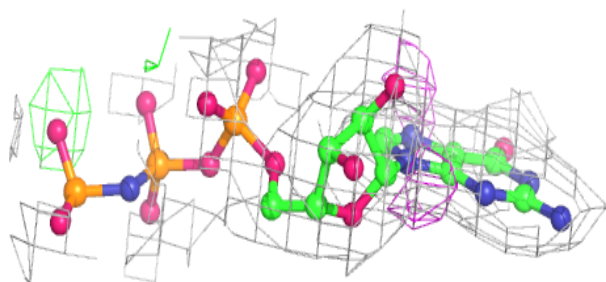
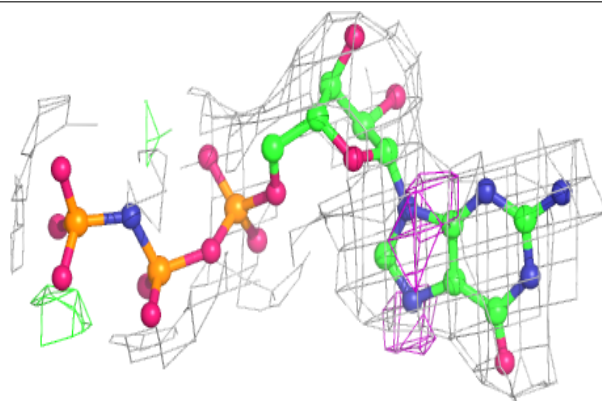


**Electron density around GNP C 202:**

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

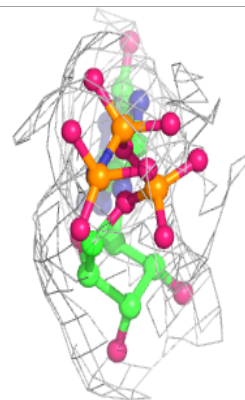
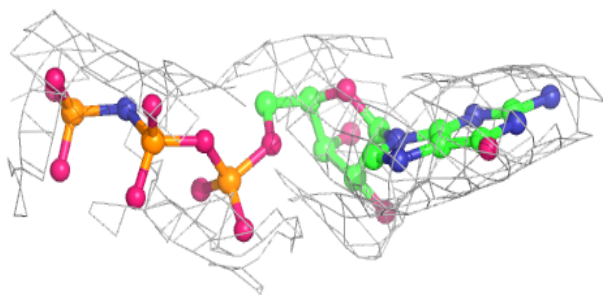
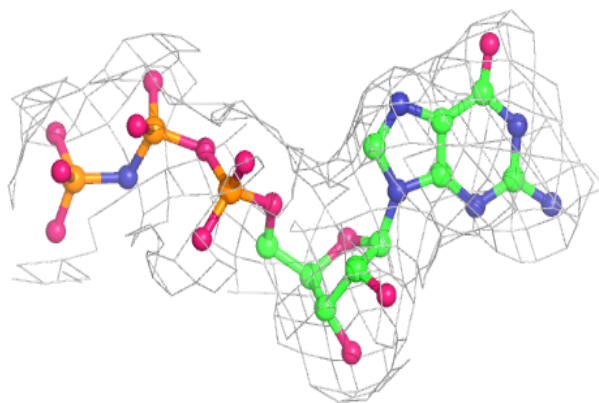
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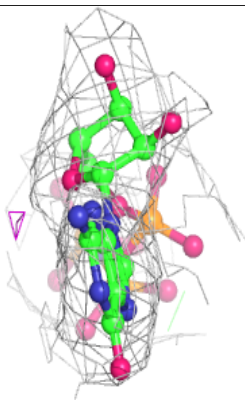
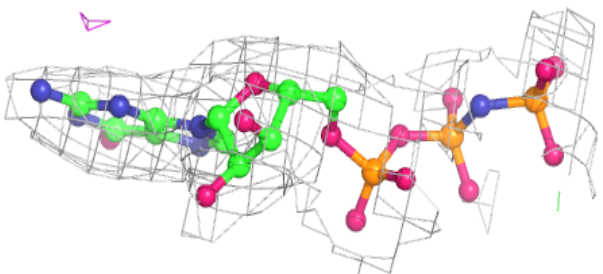
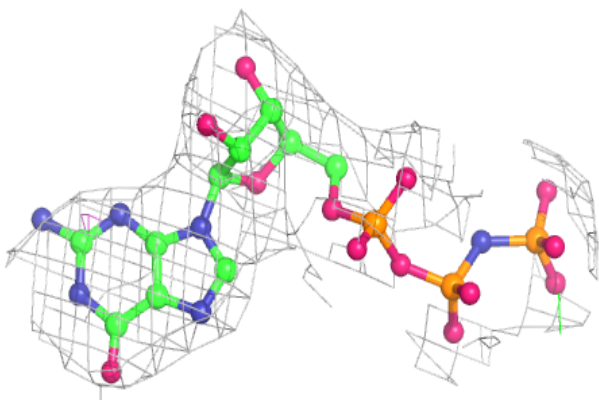


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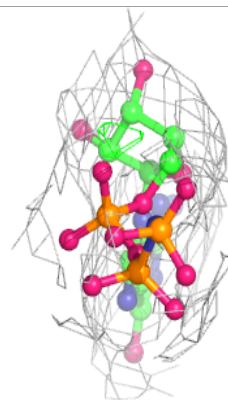
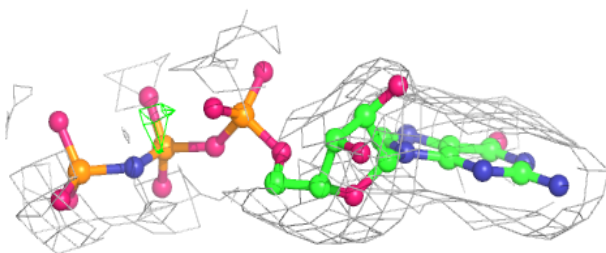
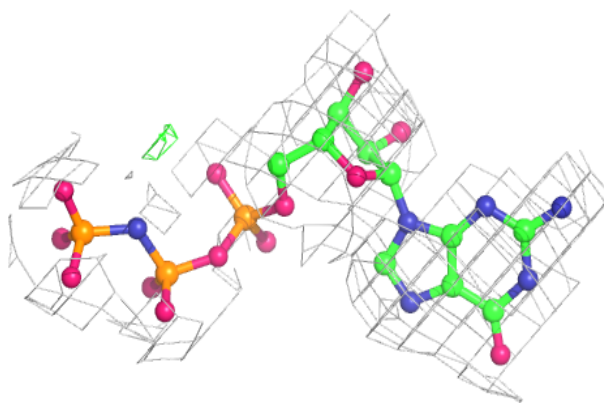
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and green (positive)

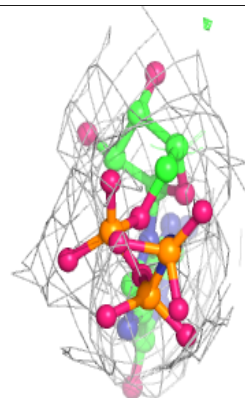
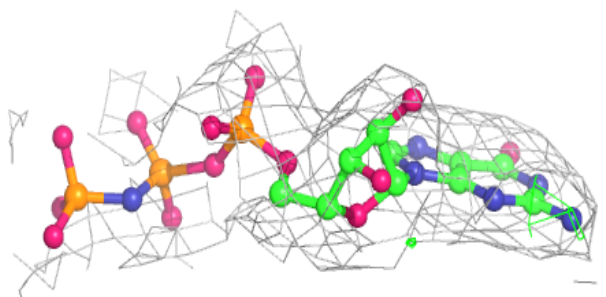
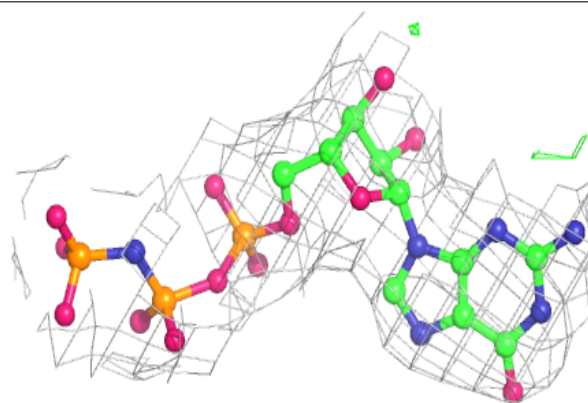


**Electron density around GNP H 202:**

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and green (positive)

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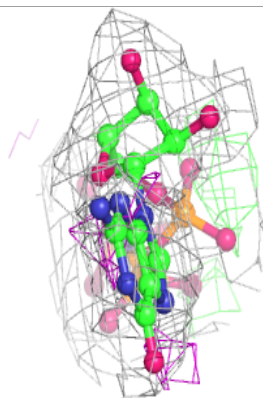
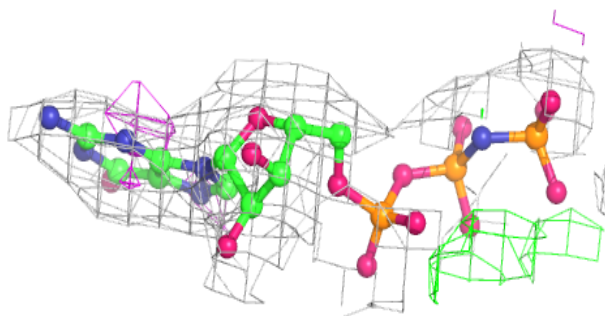
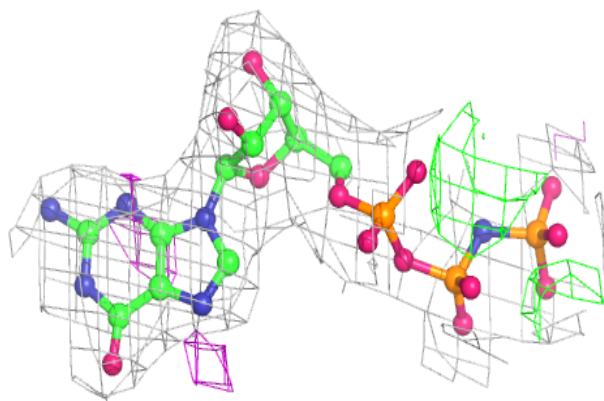
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



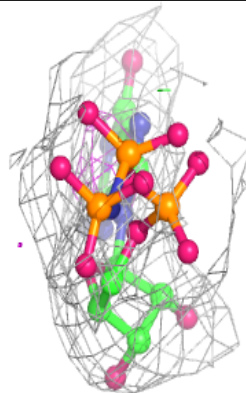
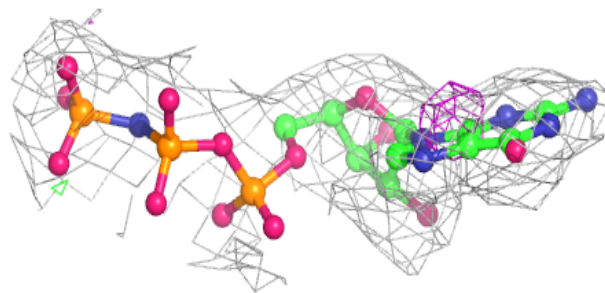
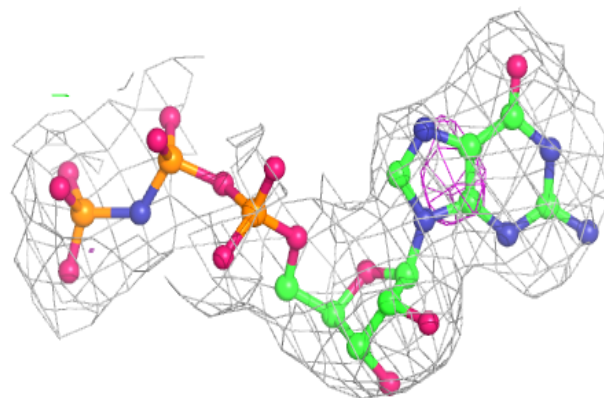


**Electron density around GNP K 202:**

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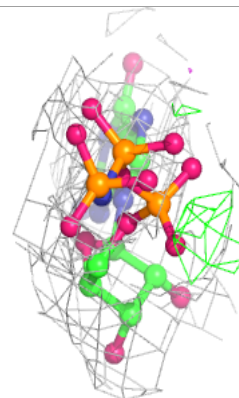
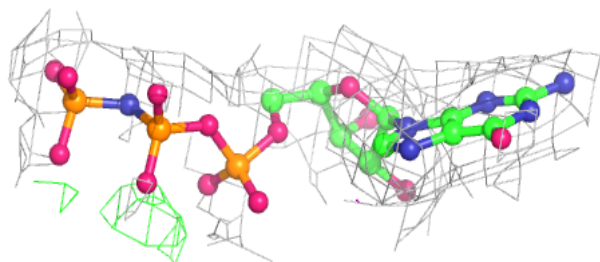
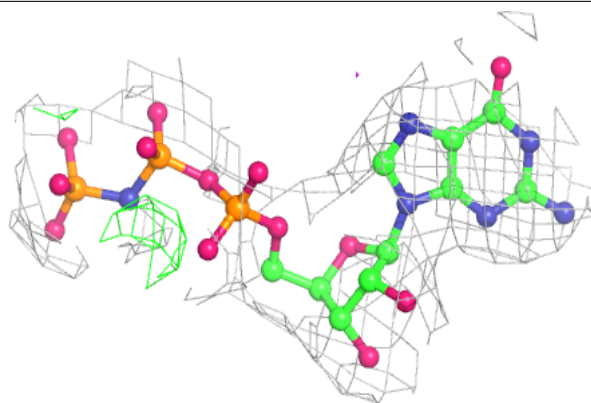
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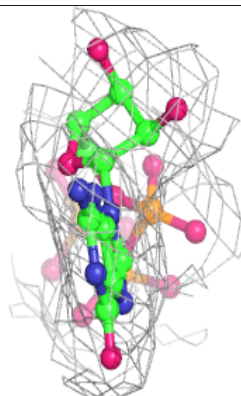
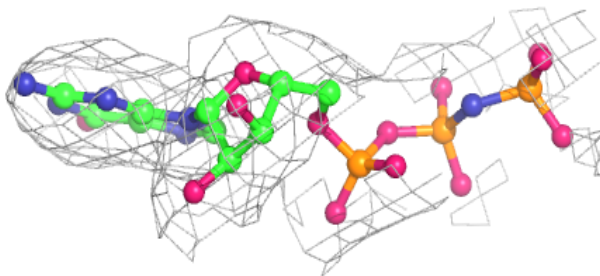
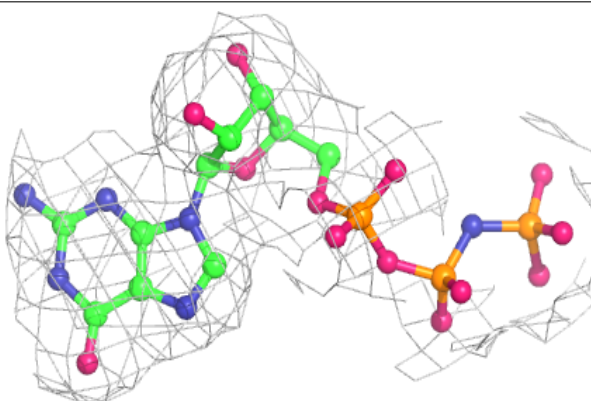


**Electron density around GNP M 202:**

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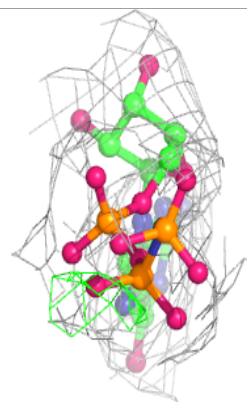
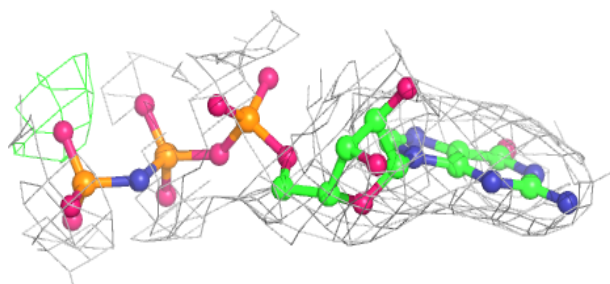
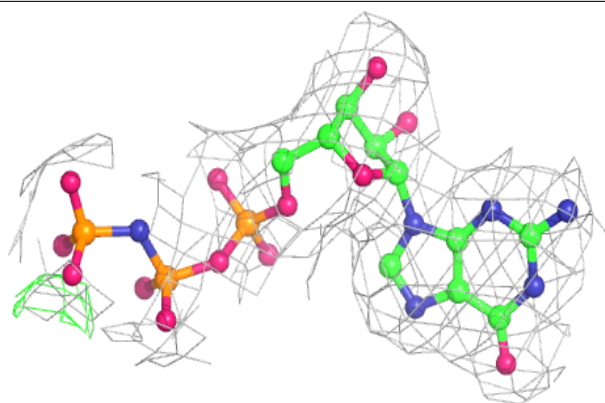
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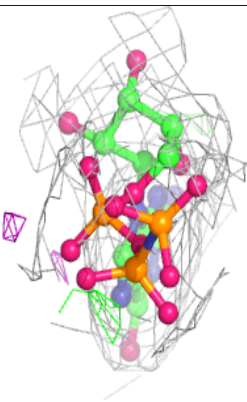
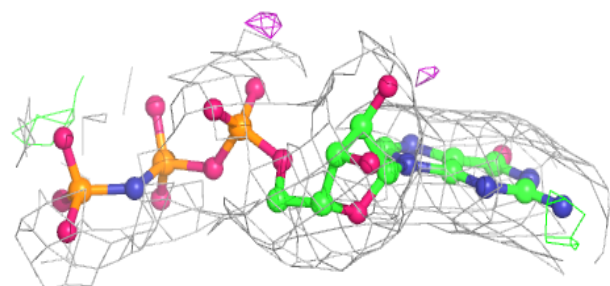
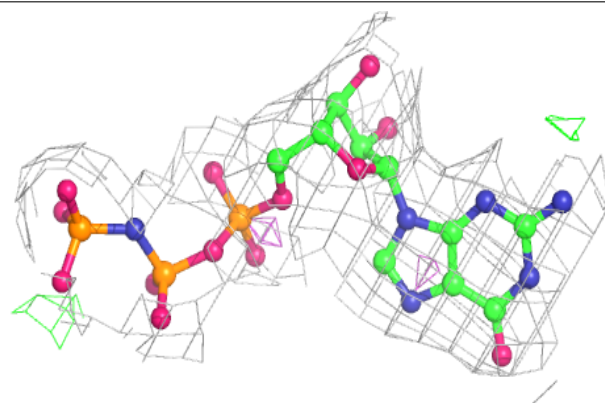


**Electron density around GNP B 202:**

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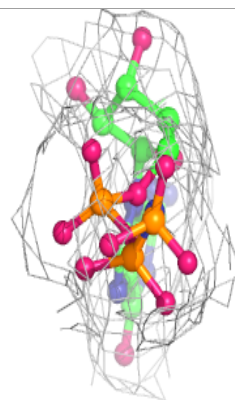
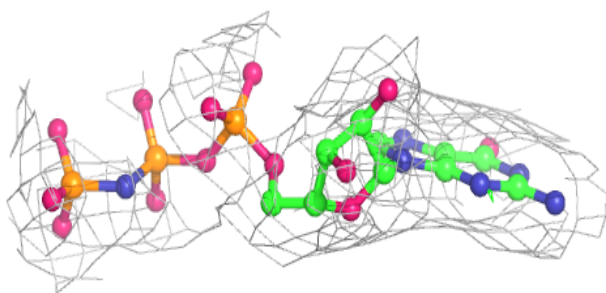
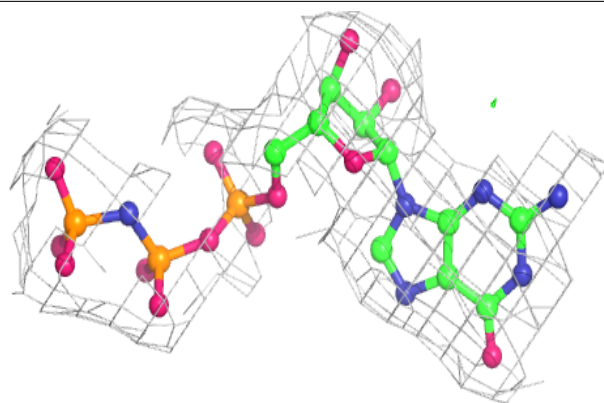
**Electron density around GNP F 202:**

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and green (positive)

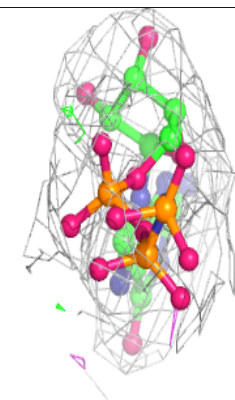
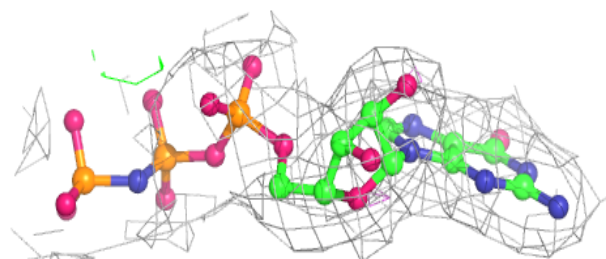
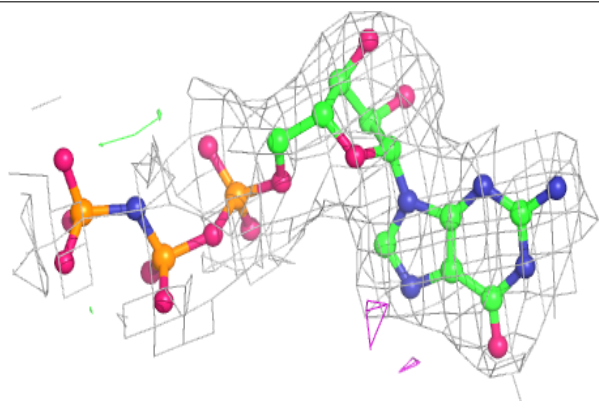


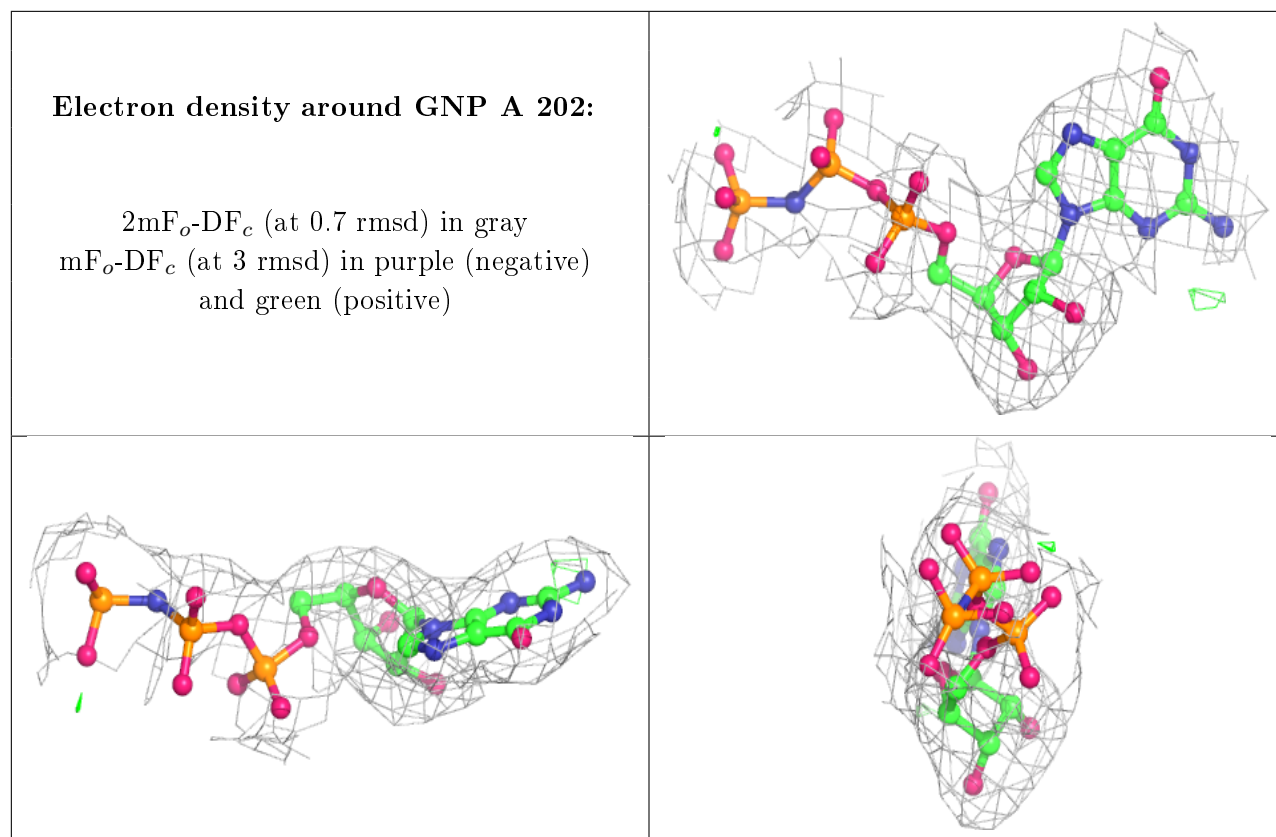
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and green (positive)

**Electron density around GNP O 202:**

$2mF_o-DF_c$  (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.