



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:40 am BST

PDB ID : 4UJ3
Title : Crystal structure of human Rab11-Rabin8-FIP3
Authors : Vetter, M.; Lorentzen, E.
Deposited on : 2015-04-08
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

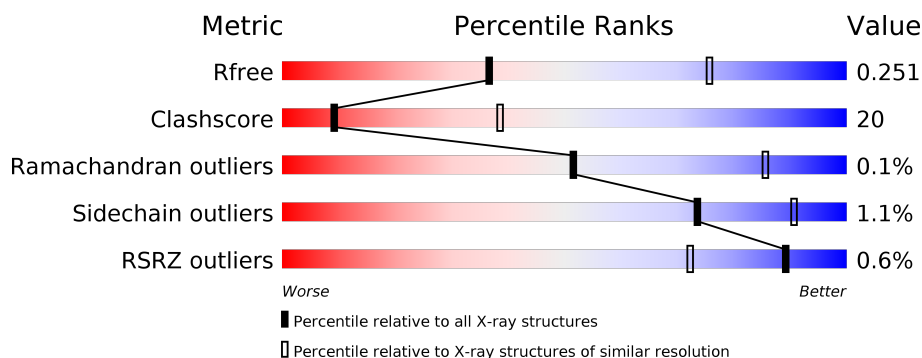
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	187	<div> <div>70%</div> <div>24%</div> <div>• 6%</div> </div>
1	D	187	<div> <div>66%</div> <div>28%</div> <div>6%</div> </div>
1	G	187	<div> <div>64%</div> <div>28%</div> <div>• 6%</div> </div>
1	J	187	<div> <div>57%</div> <div>35%</div> <div>• 7%</div> </div>
1	M	187	<div> <div>63%</div> <div>30%</div> <div>7%</div> </div>
1	P	187	<div> <div>%</div> <div>63%</div> <div>28%</div> <div>• 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	187	
1	V	187	
2	B	195	
2	E	195	
2	H	195	
2	K	195	
2	N	195	
2	Q	195	
2	T	195	
2	W	195	
3	C	66	
3	F	66	
3	I	66	
3	L	66	
3	O	66	
3	R	66	
3	U	66	
3	X	66	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PG4	V	300	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23392 atoms, of which 18 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-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1365	862	232	270	1			
1	D	175	Total	C	N	O	S	0	2	0
			1368	864	233	270	1			
1	G	175	Total	C	N	O	S	0	2	0
			1370	865	233	271	1			
1	J	174	Total	C	N	O	S	0	0	0
			1336	847	225	263	1			
1	M	174	Total	C	N	O	S	0	0	0
			1331	847	223	260	1			
1	P	171	Total	C	N	O	S	0	0	0
			1300	825	219	255	1			
1	S	171	Total	C	N	O	S	0	0	0
			1318	835	225	257	1			
1	V	169	Total	C	N	O	S	0	0	0
			1299	825	222	251	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P62491
A	1	ALA	-	expression tag	UNP P62491
A	2	ALA	-	expression tag	UNP P62491
A	3	SER	-	expression tag	UNP P62491
A	70	LEU	GLN	engineered mutation	UNP P62491
D	0	GLY	-	expression tag	UNP P62491
D	1	ALA	-	expression tag	UNP P62491
D	2	ALA	-	expression tag	UNP P62491
D	3	SER	-	expression tag	UNP P62491
D	70	LEU	GLN	engineered mutation	UNP P62491
G	0	GLY	-	expression tag	UNP P62491
G	1	ALA	-	expression tag	UNP P62491
G	2	ALA	-	expression tag	UNP P62491

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Chain	Residue	Modelled	Actual	Comment	Reference
G	3	SER	-	expression tag	UNP P62491
G	70	LEU	GLN	engineered mutation	UNP P62491
J	0	GLY	-	expression tag	UNP P62491
J	1	ALA	-	expression tag	UNP P62491
J	2	ALA	-	expression tag	UNP P62491
J	3	SER	-	expression tag	UNP P62491
J	70	LEU	GLN	engineered mutation	UNP P62491
M	0	GLY	-	expression tag	UNP P62491
M	1	ALA	-	expression tag	UNP P62491
M	2	ALA	-	expression tag	UNP P62491
M	3	SER	-	expression tag	UNP P62491
M	70	LEU	GLN	engineered mutation	UNP P62491
P	0	GLY	-	expression tag	UNP P62491
P	1	ALA	-	expression tag	UNP P62491
P	2	ALA	-	expression tag	UNP P62491
P	3	SER	-	expression tag	UNP P62491
P	70	LEU	GLN	engineered mutation	UNP P62491
S	0	GLY	-	expression tag	UNP P62491
S	1	ALA	-	expression tag	UNP P62491
S	2	ALA	-	expression tag	UNP P62491
S	3	SER	-	expression tag	UNP P62491
S	70	LEU	GLN	engineered mutation	UNP P62491
V	0	GLY	-	expression tag	UNP P62491
V	1	ALA	-	expression tag	UNP P62491
V	2	ALA	-	expression tag	UNP P62491
V	3	SER	-	expression tag	UNP P62491
V	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 2 is a protein called RAB-3A-INTERACTING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	0	0	0
			1288	822	211	243	12			
2	E	162	Total	C	N	O	S	0	0	0
			1268	811	207	238	12			
2	H	155	Total	C	N	O	S	0	2	0
			1263	810	208	233	12			
2	K	159	Total	C	N	O	S	0	1	0
			1259	804	204	239	12			
2	N	164	Total	C	N	O	S	0	0	0
			1293	824	211	246	12			
2	Q	161	Total	C	N	O	S	0	1	0
			1281	818	208	243	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	164	Total	C	N	O	S	0	1	0
			1291	827	208	245	11			
2	W	155	Total	C	N	O	S	0	1	0
			1251	798	203	238	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	266	GLY	-	expression tag	UNP Q96QF0
B	267	ALA	-	expression tag	UNP Q96QF0
B	268	ALA	-	expression tag	UNP Q96QF0
B	269	SER	-	expression tag	UNP Q96QF0
E	266	GLY	-	expression tag	UNP Q96QF0
E	267	ALA	-	expression tag	UNP Q96QF0
E	268	ALA	-	expression tag	UNP Q96QF0
E	269	SER	-	expression tag	UNP Q96QF0
H	266	GLY	-	expression tag	UNP Q96QF0
H	267	ALA	-	expression tag	UNP Q96QF0
H	268	ALA	-	expression tag	UNP Q96QF0
H	269	SER	-	expression tag	UNP Q96QF0
K	266	GLY	-	expression tag	UNP Q96QF0
K	267	ALA	-	expression tag	UNP Q96QF0
K	268	ALA	-	expression tag	UNP Q96QF0
K	269	SER	-	expression tag	UNP Q96QF0
N	266	GLY	-	expression tag	UNP Q96QF0
N	267	ALA	-	expression tag	UNP Q96QF0
N	268	ALA	-	expression tag	UNP Q96QF0
N	269	SER	-	expression tag	UNP Q96QF0
Q	266	GLY	-	expression tag	UNP Q96QF0
Q	267	ALA	-	expression tag	UNP Q96QF0
Q	268	ALA	-	expression tag	UNP Q96QF0
Q	269	SER	-	expression tag	UNP Q96QF0
T	266	GLY	-	expression tag	UNP Q96QF0
T	267	ALA	-	expression tag	UNP Q96QF0
T	268	ALA	-	expression tag	UNP Q96QF0
T	269	SER	-	expression tag	UNP Q96QF0
W	266	GLY	-	expression tag	UNP Q96QF0
W	267	ALA	-	expression tag	UNP Q96QF0
W	268	ALA	-	expression tag	UNP Q96QF0
W	269	SER	-	expression tag	UNP Q96QF0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	36	Total	C	N	O	S	0	0	0
			265	169	46	48	2			
3	F	37	Total	C	N	O	S	0	0	0
			251	163	40	46	2			
3	I	41	Total	C	N	O	S	0	0	0
			287	184	47	54	2			
3	L	38	Total	C	N	O	S	0	0	0
			265	172	44	47	2			
3	O	37	Total	C	N	O	S	0	0	0
			254	162	43	48	1			
3	R	37	Total	C	N	O	S	0	0	0
			255	164	41	49	1			
3	U	37	Total	C	N	O	S	0	0	0
			269	175	46	46	2			
3	X	36	Total	C	N	O	S	0	0	0
			257	163	43	50	1			

There are 32 discrepancies between the modelled and reference sequences:

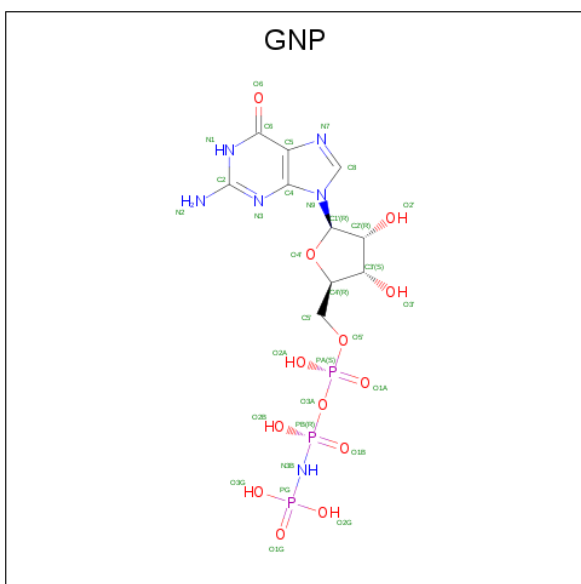
Chain	Residue	Modelled	Actual	Comment	Reference
C	691	GLY	-	expression tag	UNP O75154
C	692	ALA	-	expression tag	UNP O75154
C	693	ALA	-	expression tag	UNP O75154
C	694	SER	-	expression tag	UNP O75154
F	691	GLY	-	expression tag	UNP O75154
F	692	ALA	-	expression tag	UNP O75154
F	693	ALA	-	expression tag	UNP O75154
F	694	SER	-	expression tag	UNP O75154
I	691	GLY	-	expression tag	UNP O75154
I	692	ALA	-	expression tag	UNP O75154
I	693	ALA	-	expression tag	UNP O75154
I	694	SER	-	expression tag	UNP O75154
L	691	GLY	-	expression tag	UNP O75154
L	692	ALA	-	expression tag	UNP O75154
L	693	ALA	-	expression tag	UNP O75154
L	694	SER	-	expression tag	UNP O75154
O	691	GLY	-	expression tag	UNP O75154
O	692	ALA	-	expression tag	UNP O75154
O	693	ALA	-	expression tag	UNP O75154
O	694	SER	-	expression tag	UNP O75154
R	691	GLY	-	expression tag	UNP O75154
R	692	ALA	-	expression tag	UNP O75154
R	693	ALA	-	expression tag	UNP O75154
R	694	SER	-	expression tag	UNP O75154

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Chain	Residue	Modelled	Actual	Comment	Reference
U	691	GLY	-	expression tag	UNP O75154
U	692	ALA	-	expression tag	UNP O75154
U	693	ALA	-	expression tag	UNP O75154
U	694	SER	-	expression tag	UNP O75154
X	691	GLY	-	expression tag	UNP O75154
X	692	ALA	-	expression tag	UNP O75154
X	693	ALA	-	expression tag	UNP O75154
X	694	SER	-	expression tag	UNP O75154

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	G	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	J	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	M	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	P	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	S	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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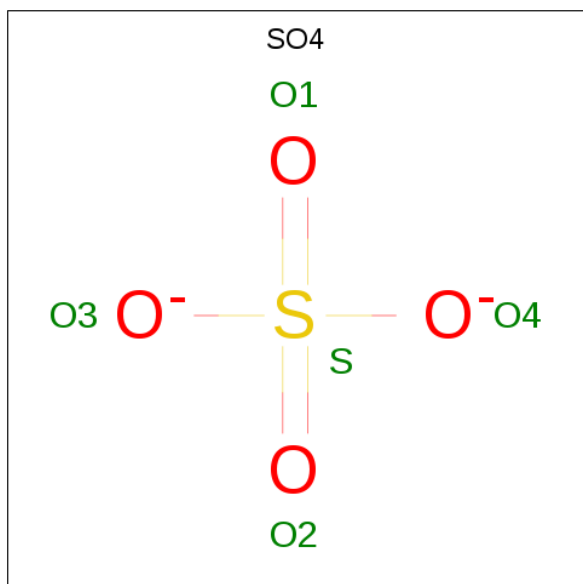
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	V	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

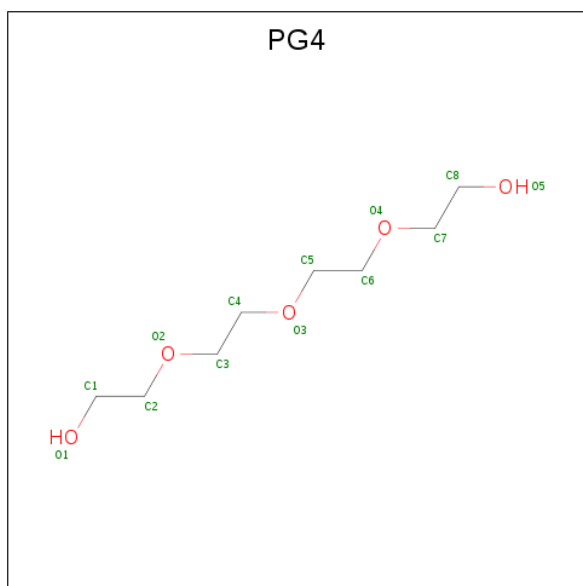
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	V	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	S	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	V	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	13	Total	O	0	0
			13	13		
8	B	6	Total	O	0	0
			6	6		
8	C	1	Total	O	0	0
			1	1		
8	D	9	Total	O	0	0
			9	9		
8	E	1	Total	O	0	0
			1	1		
8	F	1	Total	O	0	0
			1	1		
8	G	13	Total	O	0	0
			13	13		
8	H	10	Total	O	0	0
			10	10		

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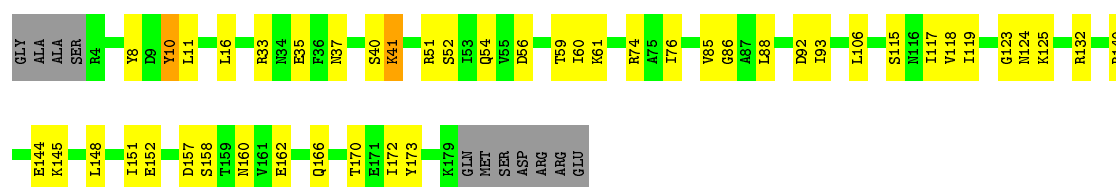
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	8	Total 8	O 8	0	0
8	K	1	Total 1	O 1	0	0
8	N	9	Total 9	O 9	0	0
8	P	9	Total 9	O 9	0	0
8	Q	5	Total 5	O 5	0	0
8	R	1	Total 1	O 1	0	0
8	S	4	Total 4	O 4	0	0
8	T	3	Total 3	O 3	0	0
8	U	1	Total 1	O 1	0	0
8	V	6	Total 6	O 6	0	0
8	W	7	Total 7	O 7	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

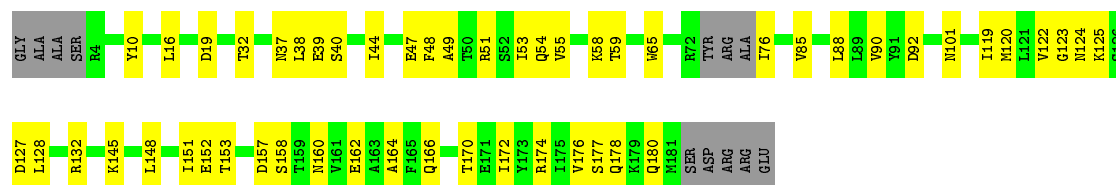
• Molecule 1: RAS-RELATED PROTEIN RAB-11A

Chain A: 



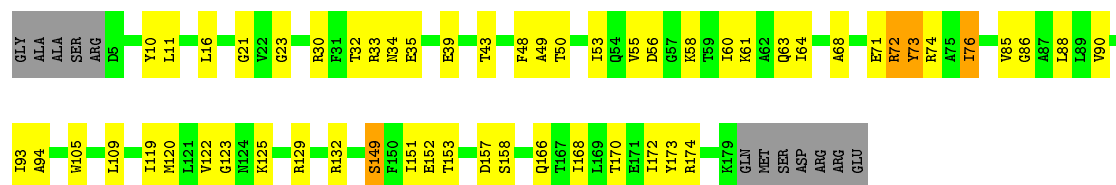
• Molecule 1: RAS-RELATED PROTEIN RAB-11A

Chain D: 



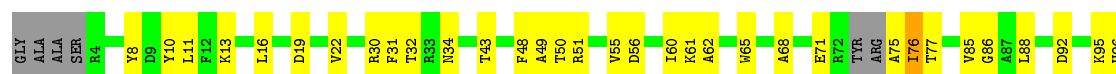
• Molecule 1: RAS-RELATED PROTEIN RAB-11A

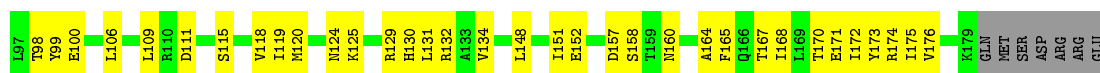
Chain G: 



• Molecule 1: RAS-RELATED PROTEIN RAB-11A

Chain J: 





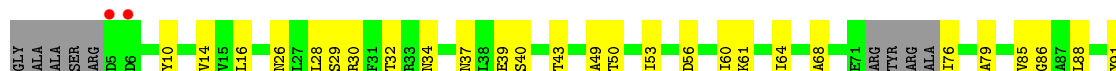
• Molecule 1: RAS-RELATED PROTEIN RAB-11A

Chain M: 63% 30% 7%



• Molecule 1: RAS-RELATED PROTEIN RAB-11A

Chain P: 63% 28% 9%



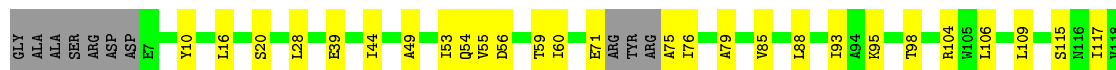
• Molecule 1: RAS-RELATED PROTEIN RAB-11A

Chain S: 57% 34% 9%



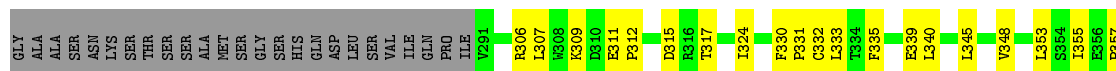
• Molecule 1: RAS-RELATED PROTEIN RAB-11A

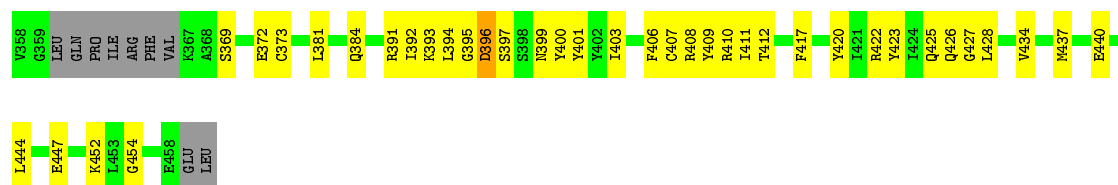
Chain V: 66% 25% 10%



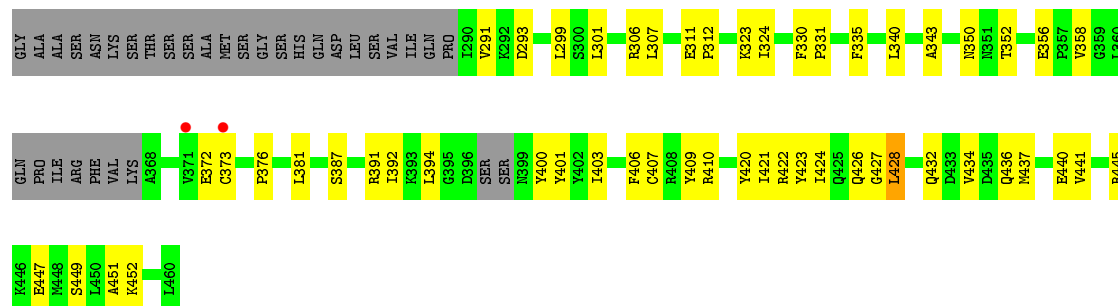
• Molecule 2: RAB-3A-INTERACTING PROTEIN

Chain B: 53% 29% 17%

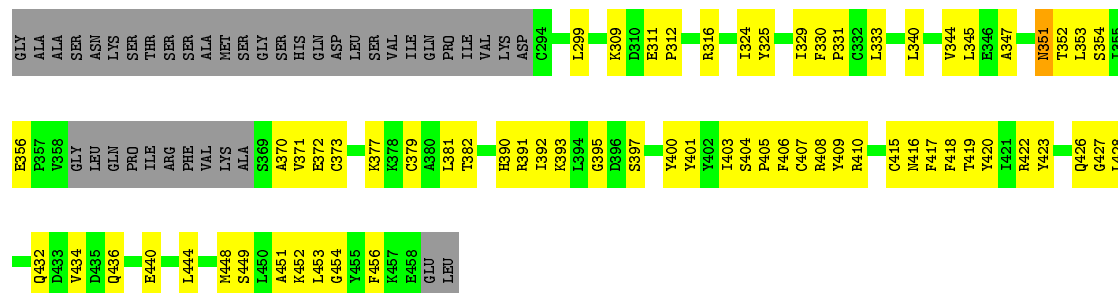




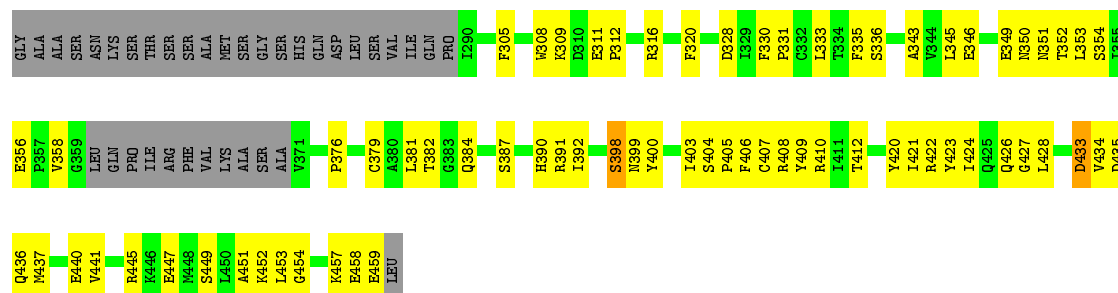
• Molecule 2: RAB-3A-INTERACTING PROTEIN



• Molecule 2: RAB-3A-INTERACTING PROTEIN



• Molecule 2: RAB-3A-INTERACTING PROTEIN

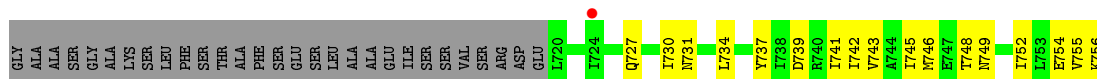
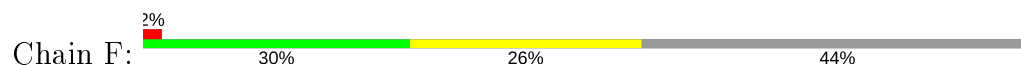


• Molecule 2: RAB-3A-INTERACTING PROTEIN

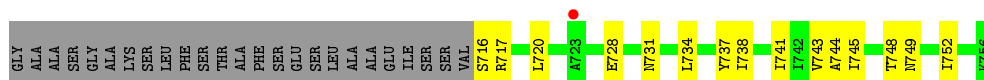




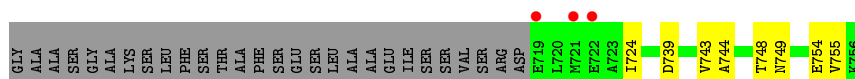
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



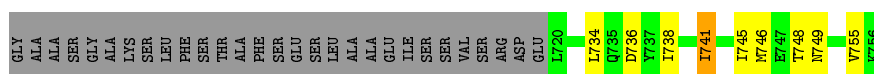
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



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GLY	ALA	ALA	SER	GLY	ALA	LYS	SER	PHE	SER	THR	ALA	PHE	SER	SER	SER	LEU	ALA	ALA	GLU	ILE	SER	SER	VAL	SER	ARG	ASP	GLU	LEU	K721

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.50Å 165.37Å 218.69Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	48.54 – 3.00 48.54 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.54-3.00) 87.3 (48.54-2.77)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1647)	Depositor
R, R_{free}	0.198 , 0.250 0.199 , 0.251	Depositor DCC
R_{free} test set	5320 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23392	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PG4, MG, GNP, SO4

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	0.32	0/1386	0.51	0/1878
1	D	0.32	0/1394	0.53	0/1889
1	G	0.35	0/1397	0.58	0/1893
1	J	0.31	0/1356	0.52	0/1839
1	M	0.31	0/1351	0.50	0/1833
1	P	0.27	0/1320	0.48	0/1793
1	S	0.27	0/1338	0.48	0/1814
1	V	0.28	0/1319	0.49	0/1789
2	B	0.32	0/1315	0.53	0/1772
2	E	0.29	0/1294	0.50	0/1748
2	H	0.34	0/1296	0.57	0/1746
2	K	0.28	0/1289	0.53	0/1742
2	N	0.30	0/1320	0.51	0/1784
2	Q	0.28	0/1311	0.51	0/1769
2	T	0.28	0/1323	0.49	0/1790
2	W	0.32	0/1281	0.55	0/1728
3	C	0.29	0/266	0.47	0/362
3	F	0.28	0/252	0.50	0/346
3	I	0.27	0/288	0.49	0/394
3	L	0.29	0/266	0.50	0/364
3	O	0.26	0/255	0.49	0/350
3	R	0.22	0/256	0.41	0/352
3	U	0.27	0/271	0.47	0/369
3	X	0.24	0/258	0.46	0/353
All	All	0.30	0/23402	0.51	0/31697

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	G	0	3
2	B	0	1
2	K	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	396	ASP	Peptide
1	G	72	ARG	Peptide
1	G	73	TYR	Peptide
1	G	74	ARG	Peptide
2	K	398	SER	Peptide

5.2 Too-close contacts [i](#)

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	1365	0	1322	39	0
1	D	1368	0	1322	46	0
1	G	1370	0	1328	46	0
1	J	1336	0	1290	58	0
1	M	1331	0	1290	54	0
1	P	1300	0	1242	44	0
1	S	1318	0	1277	66	0
1	V	1299	0	1260	51	0
2	B	1288	0	1249	65	0
2	E	1268	0	1197	50	0
2	H	1263	0	1244	67	0
2	K	1259	0	1185	64	0
2	N	1293	0	1229	52	0
2	Q	1281	0	1230	54	0
2	T	1291	0	1216	61	0
2	W	1251	0	1201	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	265	0	255	11	0
3	F	251	0	227	22	0
3	I	287	0	261	16	0
3	L	265	0	249	5	0
3	O	254	0	224	6	0
3	R	255	0	228	10	0
3	U	269	0	256	16	0
3	X	257	0	232	11	0
4	A	32	0	13	0	0
4	D	32	0	13	2	0
4	G	32	0	13	6	0
4	J	32	0	13	2	0
4	M	32	0	13	2	0
4	P	32	0	13	1	0
4	S	32	0	13	1	0
4	V	32	0	13	4	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
5	M	1	0	0	0	0
5	P	1	0	0	0	0
5	S	1	0	0	0	0
5	V	1	0	0	0	0
6	M	5	0	0	0	0
7	V	13	18	18	1	0
8	A	13	0	0	1	0
8	B	6	0	0	1	0
8	C	1	0	0	0	0
8	D	9	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	13	0	0	0	0
8	H	10	0	0	0	0
8	J	8	0	0	1	0
8	K	1	0	0	0	0
8	N	9	0	0	3	0
8	P	9	0	0	0	0
8	Q	5	0	0	0	0
8	R	1	0	0	1	0
8	S	4	0	0	0	0
8	T	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	U	1	0	0	0	0
8	V	6	0	0	0	0
8	W	7	0	0	0	0
All	All	23374	18	22136	905	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 20.

The worst 5 of 905 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:P:132:ARG:HD2	2:Q:356:GLU:HG2	1.36	1.06
2:Q:368:ALA:HB3	2:Q:369:SER:HA	1.34	1.06
2:B:391:ARG:HD3	2:B:400:TYR:HB3	1.35	1.05
1:P:10:TYR:HB2	1:P:60:ILE:HD12	1.40	1.02
2:B:393:LYS:HE2	2:B:397:SER:HB3	1.43	0.99

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	174/187 (93%)	168 (97%)	6 (3%)	0	100	100
1	D	173/187 (92%)	169 (98%)	4 (2%)	0	100	100
1	G	175/187 (94%)	168 (96%)	5 (3%)	2 (1%)	14	50
1	J	170/187 (91%)	165 (97%)	5 (3%)	0	100	100
1	M	170/187 (91%)	165 (97%)	5 (3%)	0	100	100
1	P	167/187 (89%)	161 (96%)	6 (4%)	0	100	100
1	S	167/187 (89%)	164 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	165/187 (88%)	161 (98%)	4 (2%)	0	100	100
2	B	157/195 (80%)	152 (97%)	5 (3%)	0	100	100
2	E	156/195 (80%)	151 (97%)	5 (3%)	0	100	100
2	H	153/195 (78%)	150 (98%)	3 (2%)	0	100	100
2	K	156/195 (80%)	148 (95%)	8 (5%)	0	100	100
2	N	160/195 (82%)	152 (95%)	8 (5%)	0	100	100
2	Q	158/195 (81%)	155 (98%)	3 (2%)	0	100	100
2	T	161/195 (83%)	156 (97%)	5 (3%)	0	100	100
2	W	152/195 (78%)	148 (97%)	4 (3%)	0	100	100
3	C	34/66 (52%)	33 (97%)	1 (3%)	0	100	100
3	F	35/66 (53%)	33 (94%)	2 (6%)	0	100	100
3	I	39/66 (59%)	36 (92%)	3 (8%)	0	100	100
3	L	36/66 (54%)	35 (97%)	1 (3%)	0	100	100
3	O	35/66 (53%)	33 (94%)	2 (6%)	0	100	100
3	R	35/66 (53%)	34 (97%)	1 (3%)	0	100	100
3	U	35/66 (53%)	34 (97%)	1 (3%)	0	100	100
3	X	34/66 (52%)	32 (94%)	2 (6%)	0	100	100
All	All	2897/3584 (81%)	2803 (97%)	92 (3%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	76	ILE
1	G	73	TYR

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	142/158 (90%)	140 (99%)	2 (1%)	67	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	143/158 (90%)	142 (99%)	1 (1%)	84	94
1	G	143/158 (90%)	141 (99%)	2 (1%)	67	88
1	J	138/158 (87%)	136 (99%)	2 (1%)	67	88
1	M	137/158 (87%)	137 (100%)	0	100	100
1	P	132/158 (84%)	131 (99%)	1 (1%)	81	93
1	S	136/158 (86%)	135 (99%)	1 (1%)	84	94
1	V	133/158 (84%)	132 (99%)	1 (1%)	81	93
2	B	141/175 (81%)	139 (99%)	2 (1%)	67	88
2	E	133/175 (76%)	131 (98%)	2 (2%)	65	87
2	H	140/175 (80%)	139 (99%)	1 (1%)	84	94
2	K	134/175 (77%)	132 (98%)	2 (2%)	65	87
2	N	139/175 (79%)	137 (99%)	2 (1%)	67	88
2	Q	139/175 (79%)	139 (100%)	0	100	100
2	T	137/175 (78%)	134 (98%)	3 (2%)	52	81
2	W	138/175 (79%)	136 (99%)	2 (1%)	67	88
3	C	25/56 (45%)	25 (100%)	0	100	100
3	F	21/56 (38%)	21 (100%)	0	100	100
3	I	25/56 (45%)	25 (100%)	0	100	100
3	L	23/56 (41%)	22 (96%)	1 (4%)	29	66
3	O	21/56 (38%)	19 (90%)	2 (10%)	8	32
3	R	22/56 (39%)	22 (100%)	0	100	100
3	U	24/56 (43%)	24 (100%)	0	100	100
3	X	23/56 (41%)	23 (100%)	0	100	100
All	All	2389/3112 (77%)	2362 (99%)	27 (1%)	73	90

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	433[A]	ASP
2	N	332	CYS
1	V	39	GLU
2	K	433[B]	ASP
1	D	39	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	351	ASN
2	W	390	HIS
3	I	727	GLN
1	D	54	GLN
1	M	54	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GNP	J	200	5	28,34,34	2.61	8 (28%)	30,54,54	2.29	7 (23%)
6	SO4	M	1182	-	4,4,4	0.16	0	6,6,6	0.10	0
4	GNP	A	200	5	28,34,34	2.56	9 (32%)	30,54,54	2.11	6 (20%)
7	PG4	V	300	-	12,12,12	0.65	0	11,11,11	0.36	0
4	GNP	P	200	5	28,34,34	2.56	10 (35%)	30,54,54	2.29	10 (33%)
4	GNP	S	200	5	28,34,34	2.55	8 (28%)	30,54,54	2.28	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GNP	V	200	5	28,34,34	2.53	8 (28%)	30,54,54	2.16	8 (26%)
4	GNP	M	200	5	28,34,34	2.72	8 (28%)	30,54,54	2.24	8 (26%)
4	GNP	D	200	5	28,34,34	2.58	9 (32%)	30,54,54	2.19	8 (26%)
4	GNP	G	200	5	28,34,34	2.71	9 (32%)	30,54,54	2.26	8 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GNP	J	200	5	-	3/17/38/38	0/3/3/3
4	GNP	A	200	5	-	3/17/38/38	0/3/3/3
7	PG4	V	300	-	-	2/10/10/10	-
4	GNP	P	200	5	-	8/17/38/38	0/3/3/3
4	GNP	S	200	5	-	7/17/38/38	0/3/3/3
4	GNP	V	200	5	-	5/17/38/38	0/3/3/3
4	GNP	M	200	5	-	4/17/38/38	0/3/3/3
4	GNP	D	200	5	-	6/17/38/38	0/3/3/3
4	GNP	G	200	5	-	6/17/38/38	0/3/3/3

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	200	GNP	C4-N9	-8.13	1.36	1.47
4	J	200	GNP	C4-N9	-8.00	1.37	1.47
4	M	200	GNP	C4-N9	-7.88	1.37	1.47
4	S	200	GNP	C4-N9	-7.55	1.37	1.47
4	A	200	GNP	C4-N9	-7.52	1.37	1.47

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	200	GNP	C4-C5-N7	6.73	111.38	102.46
4	G	200	GNP	C4-C5-N7	6.50	111.08	102.46
4	D	200	GNP	C4-C5-N7	6.49	111.07	102.46
4	J	200	GNP	C4-C5-N7	6.49	111.06	102.46
4	P	200	GNP	C4-C5-N7	6.48	111.05	102.46

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	200	GNP	PG-N3B-PB-O1B
4	J	200	GNP	C2'-C1'-N9-C4
4	A	200	GNP	PG-N3B-PB-O1B
4	A	200	GNP	PG-N3B-PB-O3A
4	A	200	GNP	C2'-C1'-N9-C4

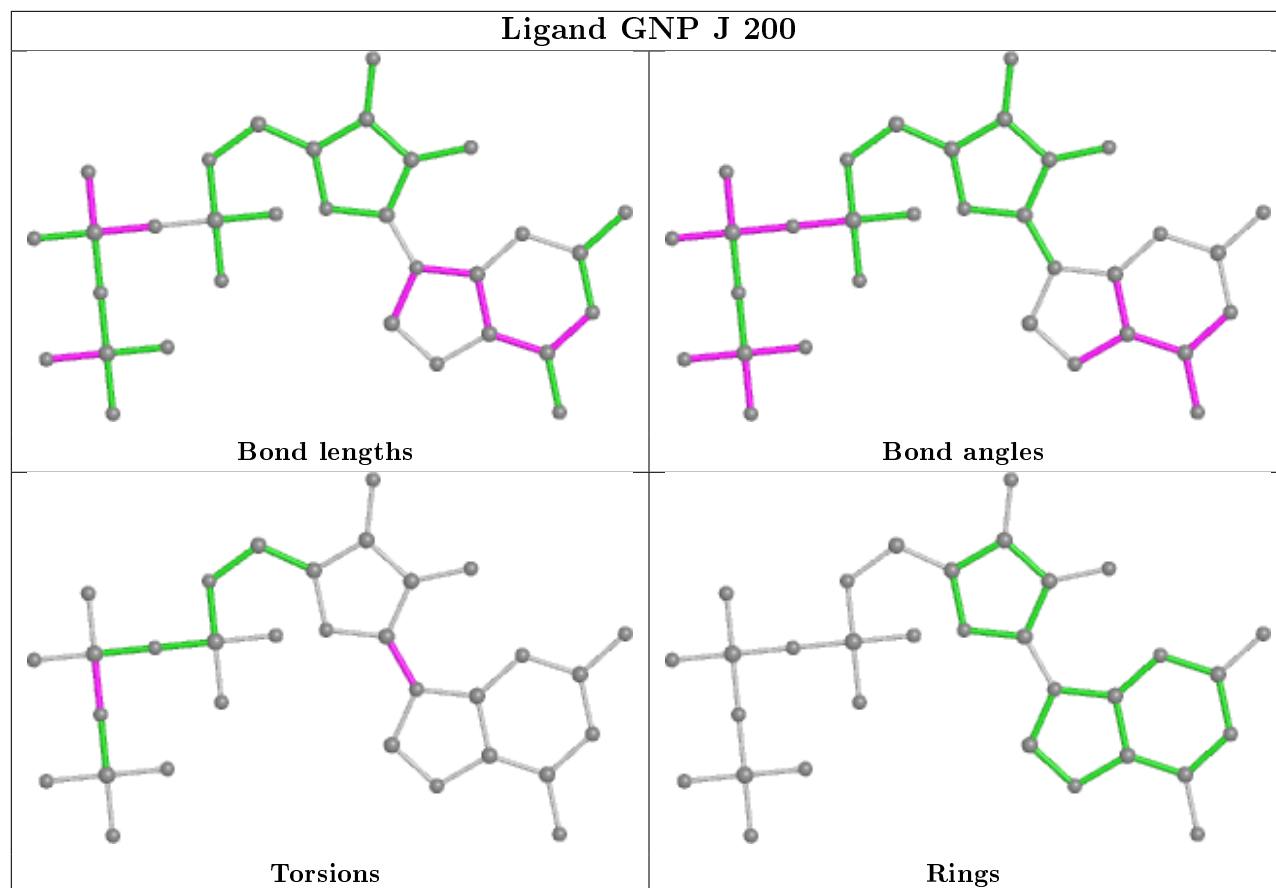
There are no ring outliers.

8 monomers are involved in 18 short contacts:

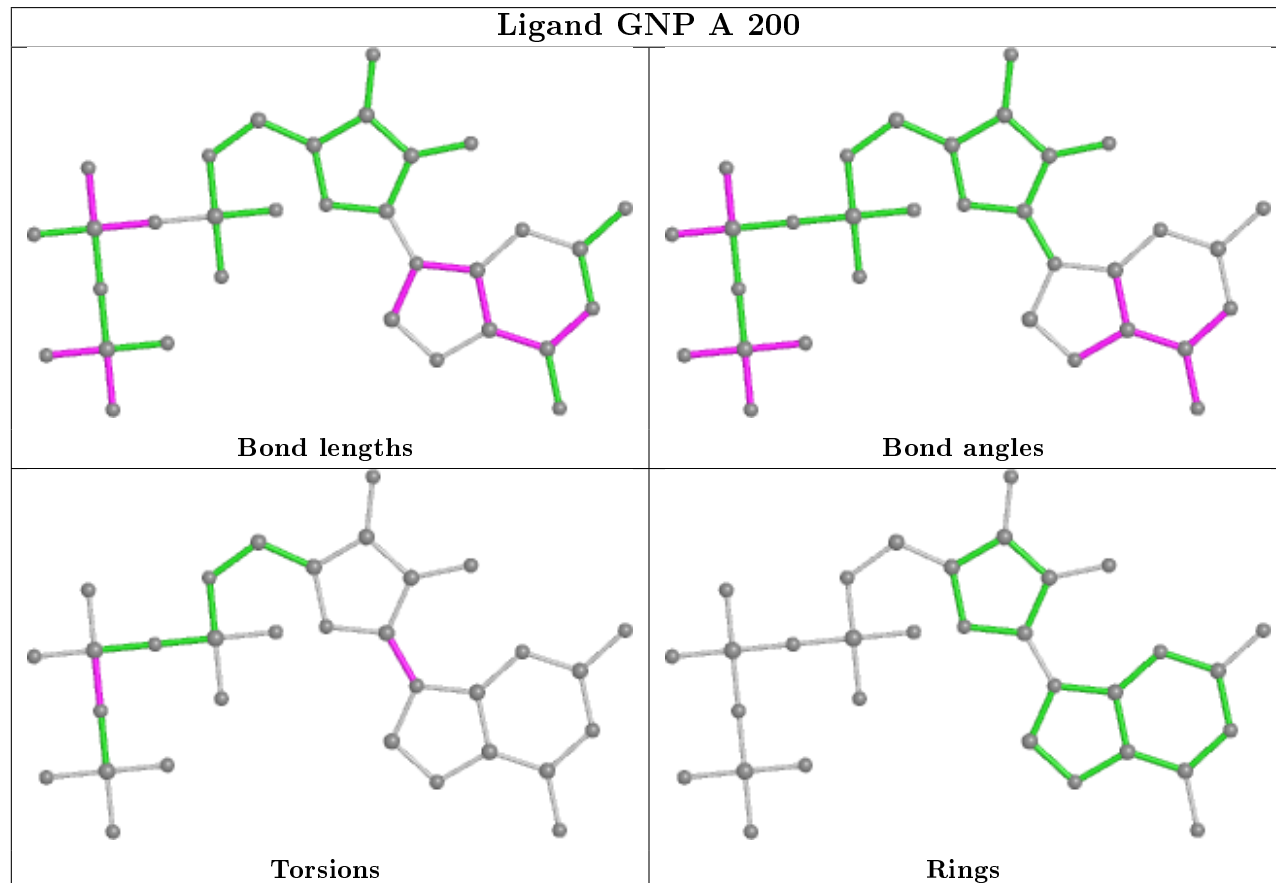
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	200	GNP	2	0
7	V	300	PG4	1	0
4	P	200	GNP	1	0
4	S	200	GNP	1	0
4	V	200	GNP	4	0
4	M	200	GNP	2	0
4	D	200	GNP	2	0
4	G	200	GNP	6	0

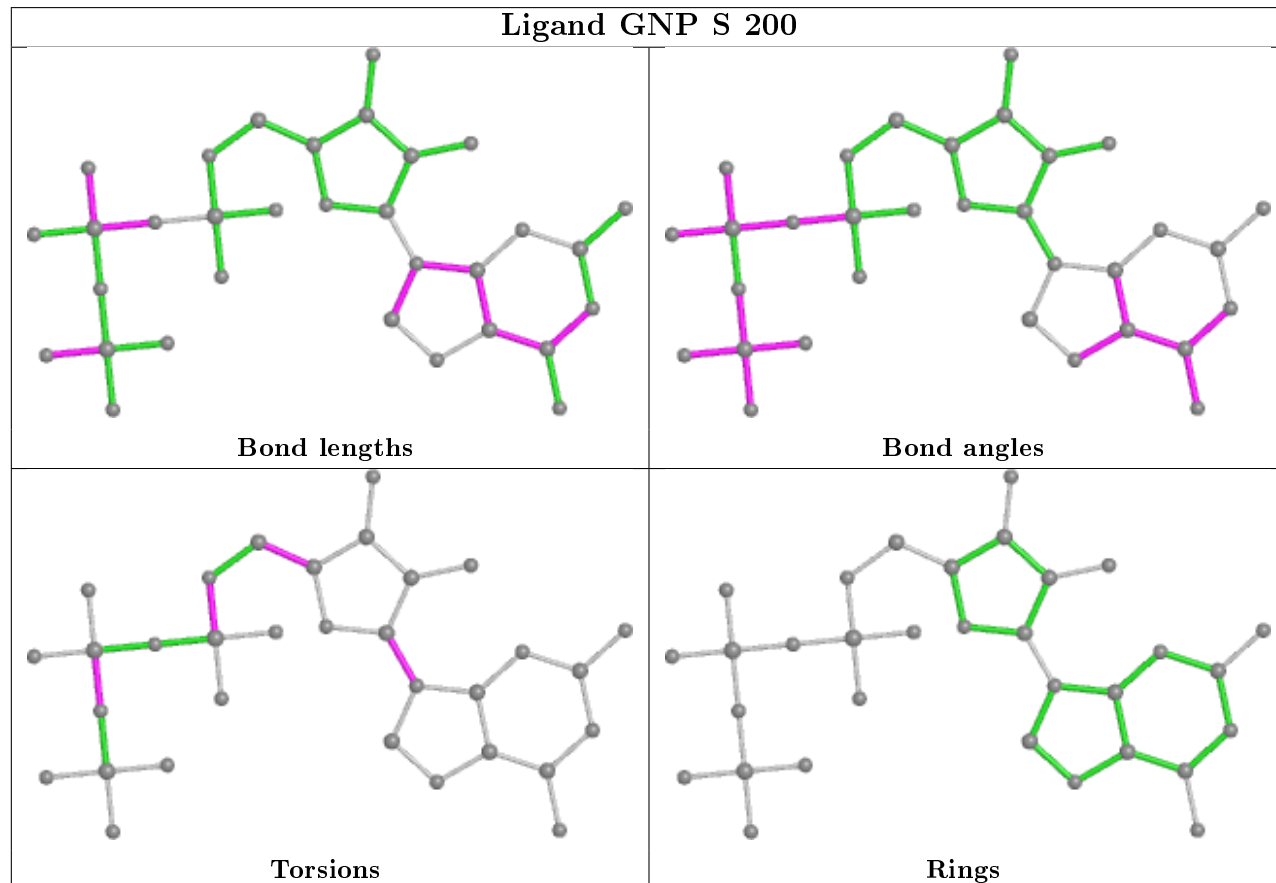
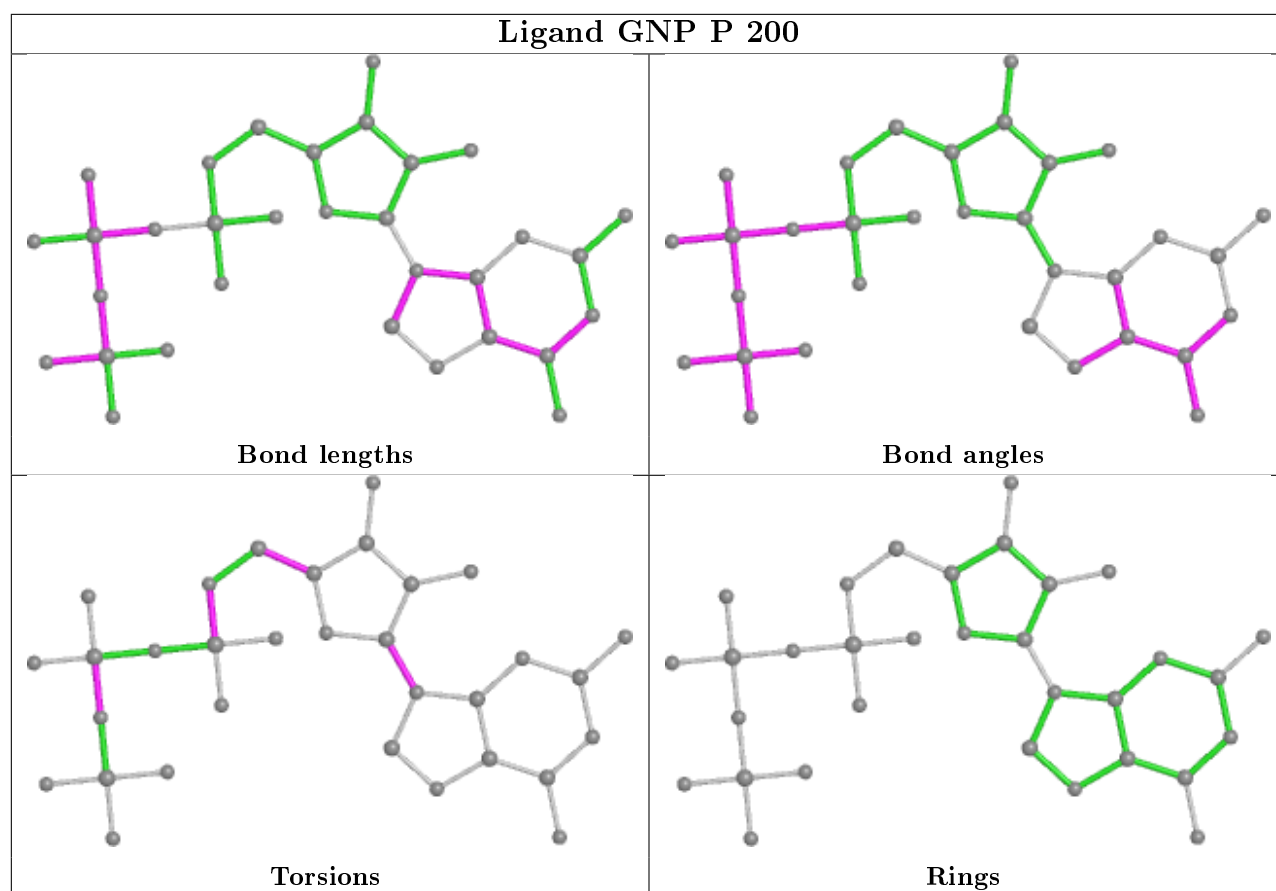
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

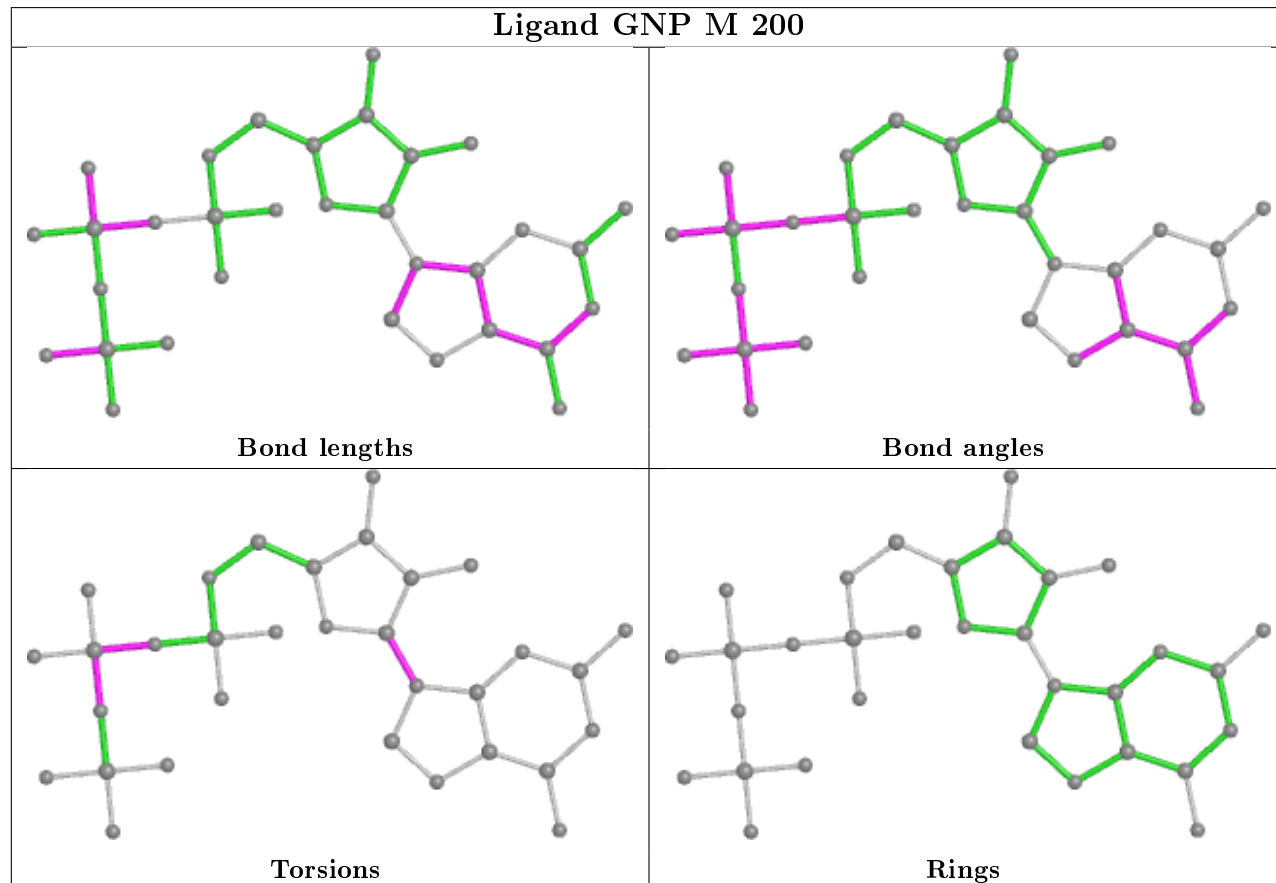
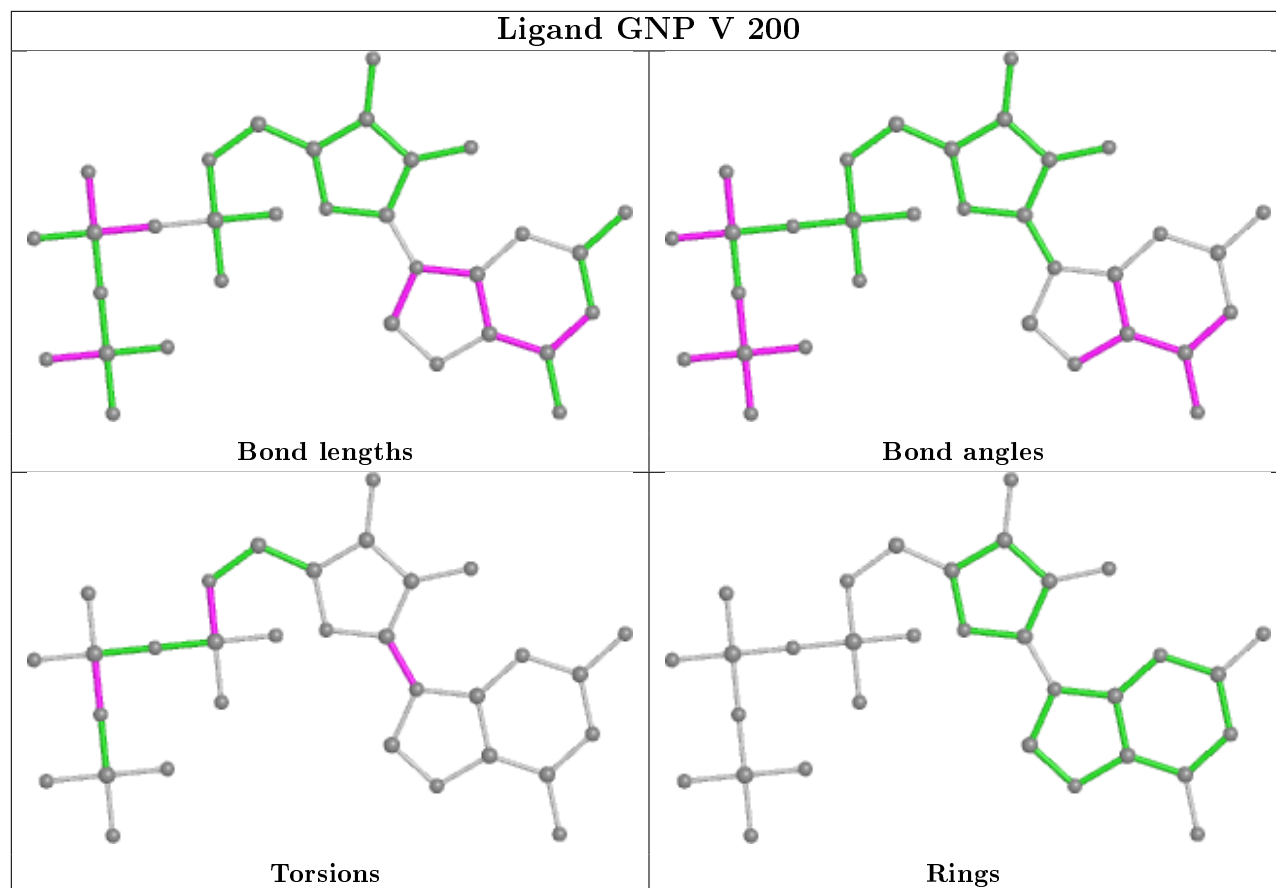
Ligand GNP J 200

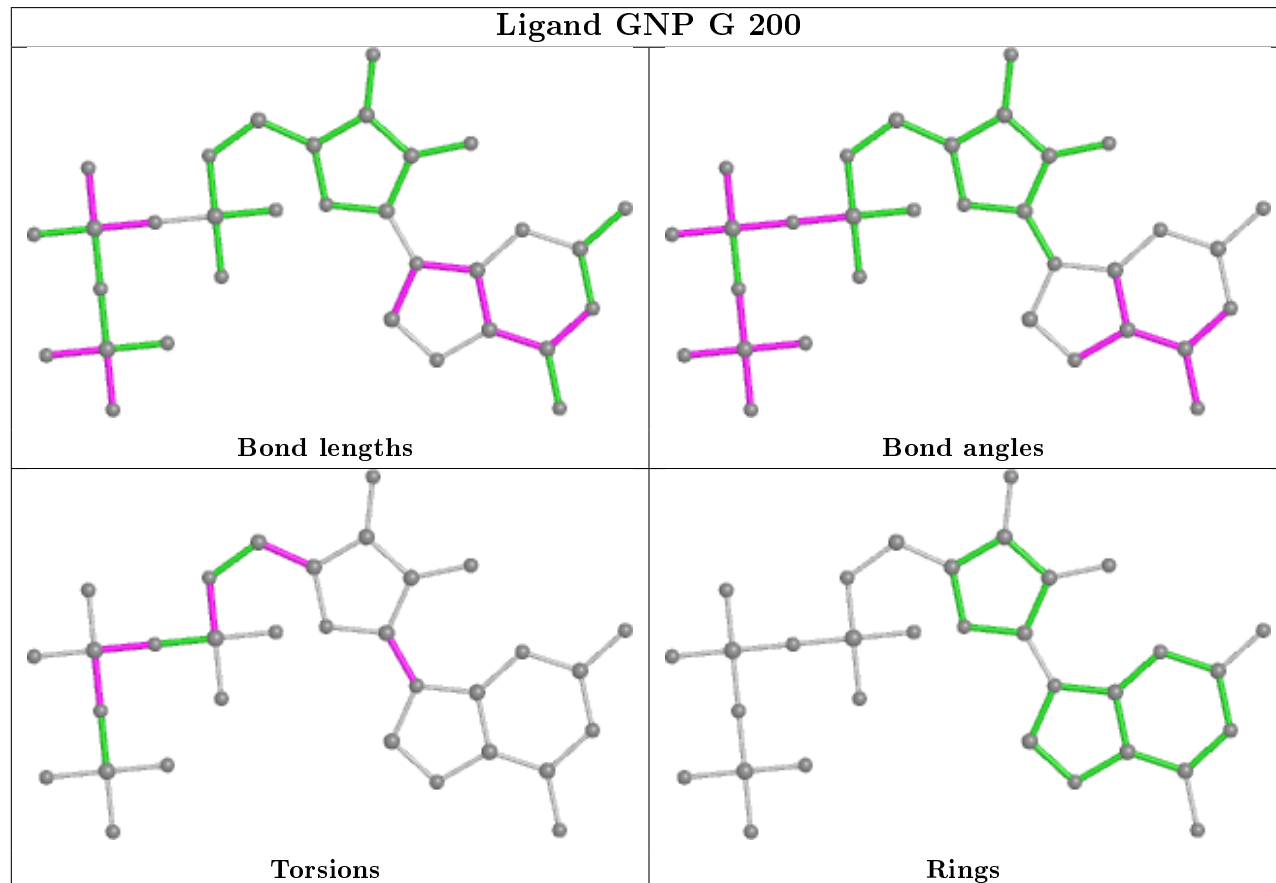
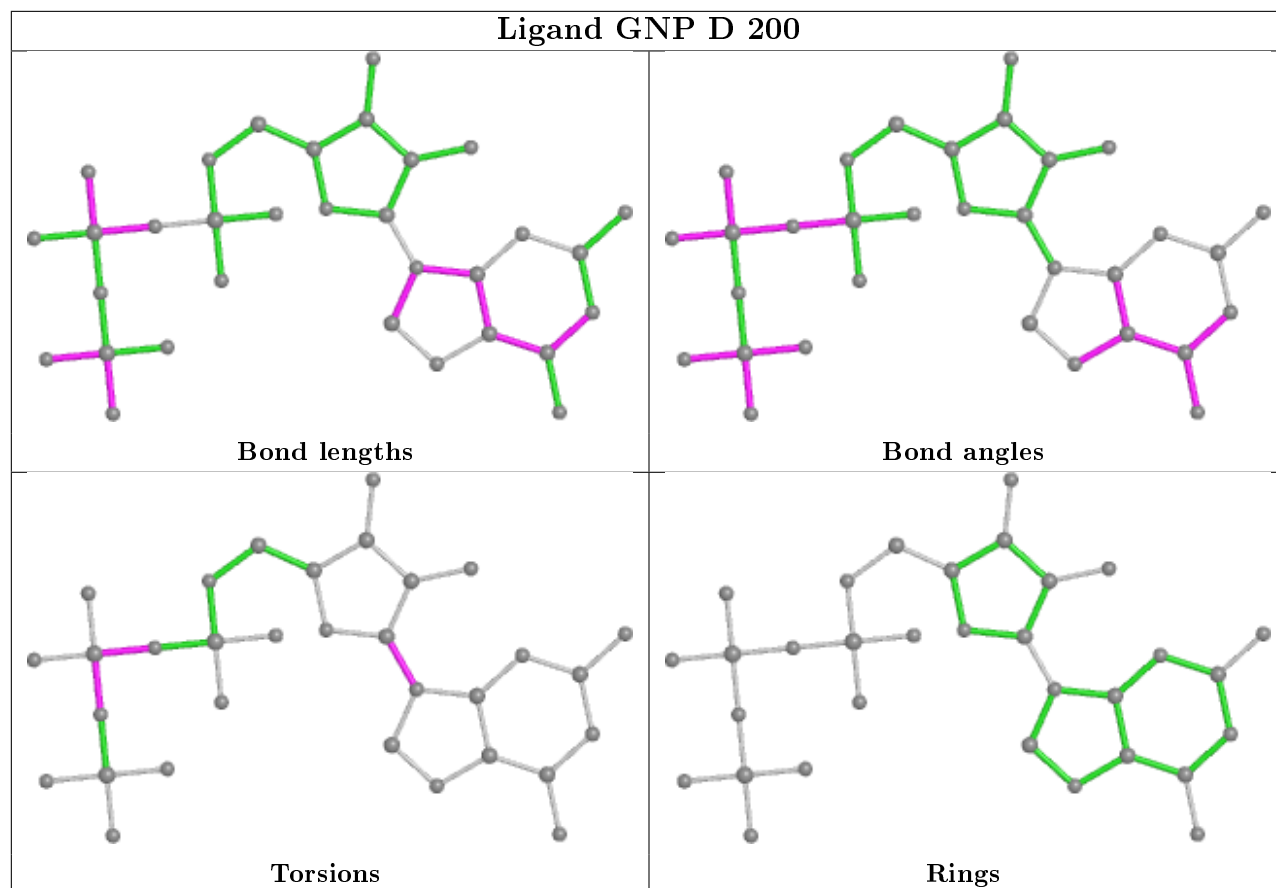


Ligand GNP A 200









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, 95th 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	176/187 (94%)	-0.56	0 100 100	51, 69, 109, 153	0
1	D	175/187 (93%)	-0.62	0 100 100	52, 68, 102, 125	0
1	G	175/187 (93%)	-0.60	0 100 100	47, 63, 101, 150	0
1	J	174/187 (93%)	-0.59	0 100 100	51, 73, 102, 117	0
1	M	174/187 (93%)	-0.43	0 100 100	53, 77, 121, 144	0
1	P	171/187 (91%)	-0.41	2 (1%) 79 54	71, 101, 154, 172	0
1	S	171/187 (91%)	-0.42	2 (1%) 79 54	65, 97, 132, 149	0
1	V	169/187 (90%)	-0.53	0 100 100	56, 86, 128, 140	0
2	B	161/195 (82%)	-0.44	0 100 100	48, 79, 141, 187	0
2	E	162/195 (83%)	-0.18	2 (1%) 79 54	65, 99, 137, 169	0
2	H	155/195 (79%)	-0.48	0 100 100	48, 67, 94, 128	0
2	K	159/195 (81%)	-0.40	0 100 100	65, 100, 130, 147	0
2	N	164/195 (84%)	-0.45	0 100 100	57, 84, 122, 151	0
2	Q	161/195 (82%)	-0.44	0 100 100	68, 90, 119, 146	0
2	T	164/195 (84%)	-0.27	5 (3%) 50 22	70, 106, 141, 163	0
2	W	155/195 (79%)	-0.27	0 100 100	54, 73, 102, 117	0
3	C	36/66 (54%)	-0.53	1 (2%) 53 25	59, 80, 147, 160	0
3	F	37/66 (56%)	-0.23	1 (2%) 54 26	62, 81, 161, 167	0
3	I	41/66 (62%)	-0.10	1 (2%) 59 30	65, 84, 164, 172	0
3	L	38/66 (57%)	0.05	3 (7%) 12 4	60, 84, 167, 168	0
3	O	37/66 (56%)	-0.09	0 100 100	77, 96, 148, 157	0
3	R	37/66 (56%)	-0.25	1 (2%) 54 26	96, 108, 167, 179	0
3	U	37/66 (56%)	-0.18	0 100 100	81, 105, 167, 176	0
3	X	36/66 (54%)	-0.39	0 100 100	87, 115, 159, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2965/3584 (82%)	-0.42	18 (0%) 89 72	47, 85, 134, 187	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	5	ASP	3.2
3	L	721	MET	3.0
1	S	137	ASP	3.0
3	C	721	MET	2.7
1	P	6	ASP	2.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

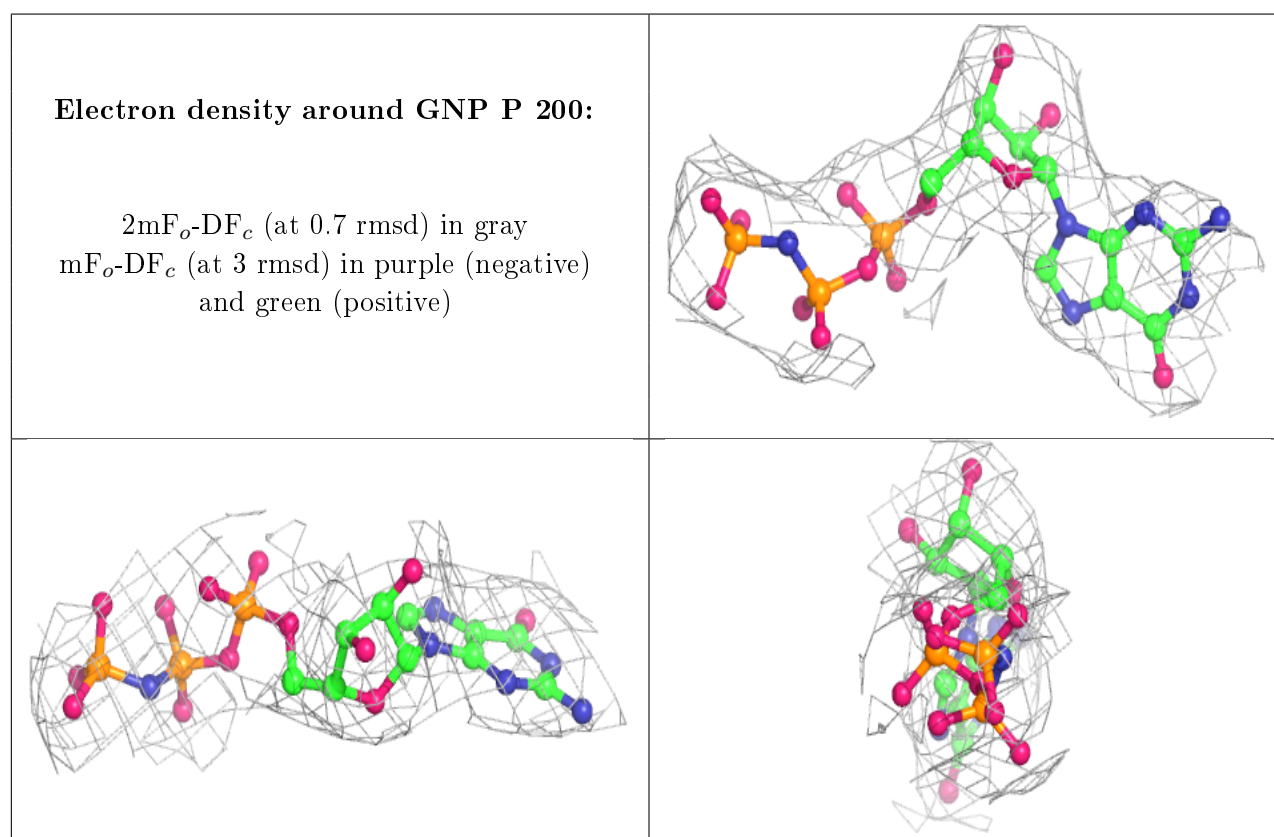
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PG4	V	300	13/13	0.69	0.45	84,107,125,130	0
6	SO4	M	1182	5/5	0.90	0.22	127,130,141,167	0
5	MG	G	201	1/1	0.92	0.17	50,50,50,50	0
5	MG	A	201	1/1	0.96	0.19	62,62,62,62	0
5	MG	J	201	1/1	0.96	0.12	70,70,70,70	0
5	MG	V	201	1/1	0.97	0.17	68,68,68,68	0
4	GNP	P	200	32/32	0.98	0.13	68,82,92,101	0
4	GNP	S	200	32/32	0.98	0.13	61,80,91,93	0
4	GNP	V	200	32/32	0.98	0.14	51,63,80,93	0
4	GNP	A	200	32/32	0.98	0.17	46,61,75,77	0
4	GNP	M	200	32/32	0.98	0.15	44,61,69,84	0
5	MG	D	201	1/1	0.98	0.13	63,63,63,63	0
4	GNP	J	200	32/32	0.98	0.15	50,64,79,85	0

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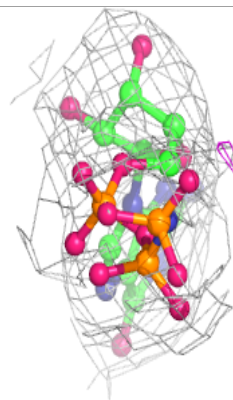
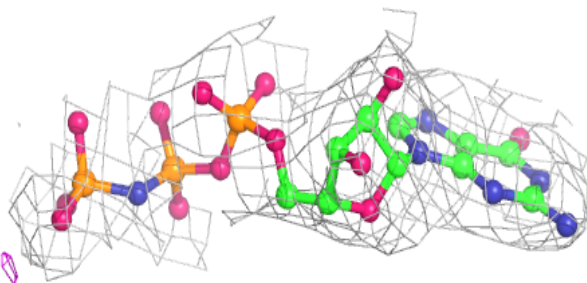
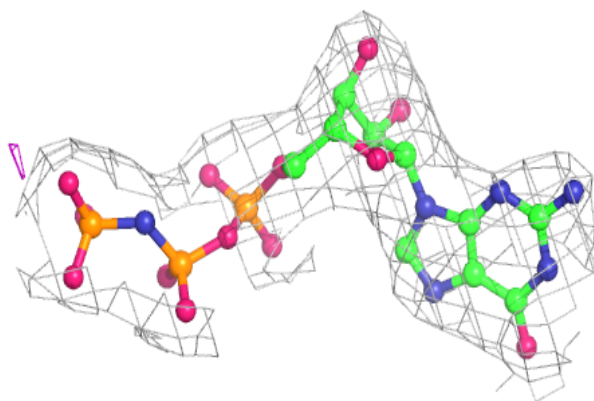
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GNP	D	200	32/32	0.98	0.14	49,63,72,79	0
4	GNP	G	200	32/32	0.98	0.16	35,51,65,84	0
5	MG	P	201	1/1	0.99	0.14	76,76,76,76	0
5	MG	S	201	1/1	0.99	0.13	61,61,61,61	0
5	MG	M	201	1/1	0.99	0.12	58,58,58,58	0

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

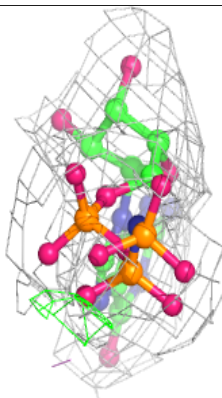
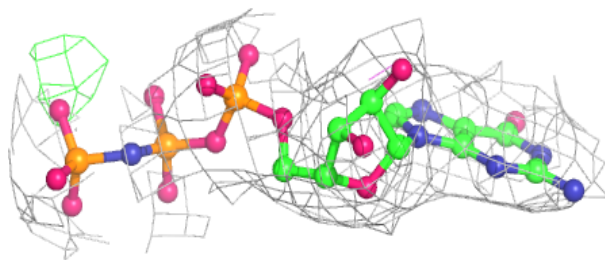
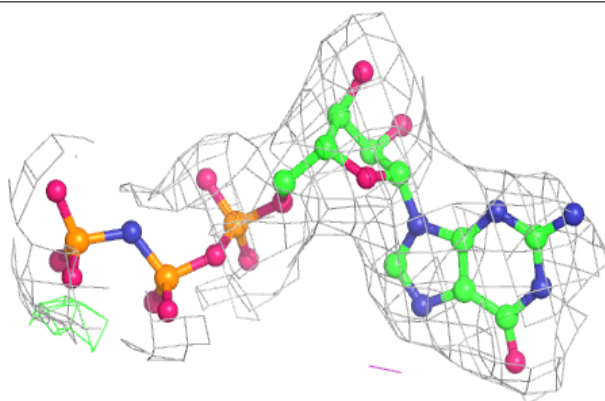


Electron density around GNP S 200:

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

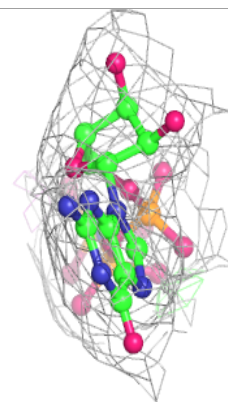
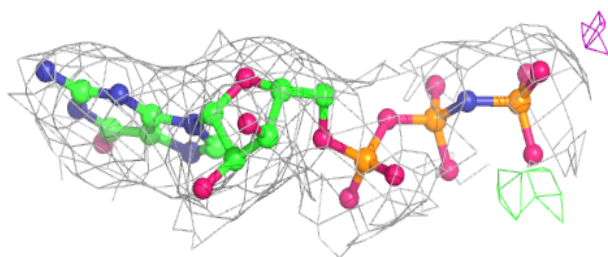
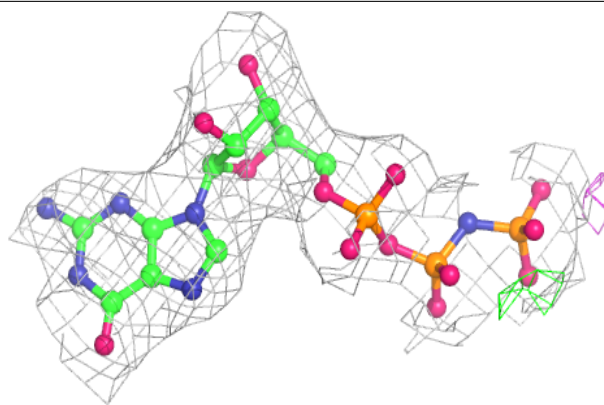
**Electron density around GNP V 200:**

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

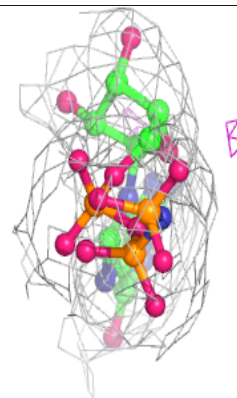
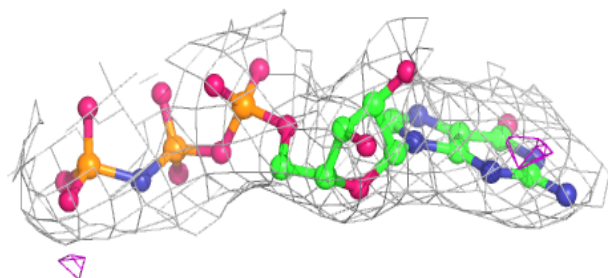
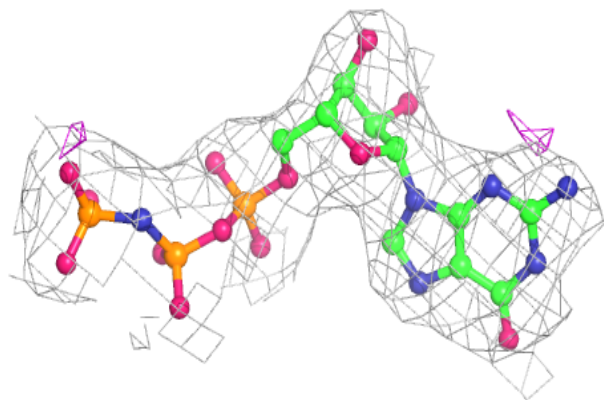


Electron density around GNP A 200:

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

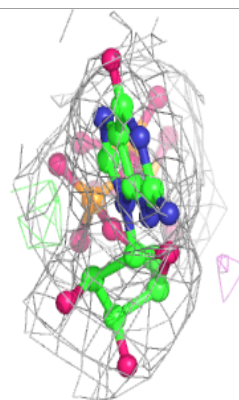
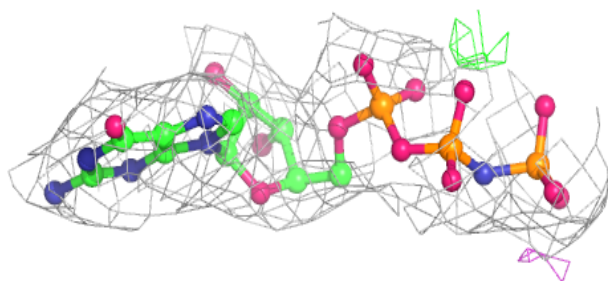
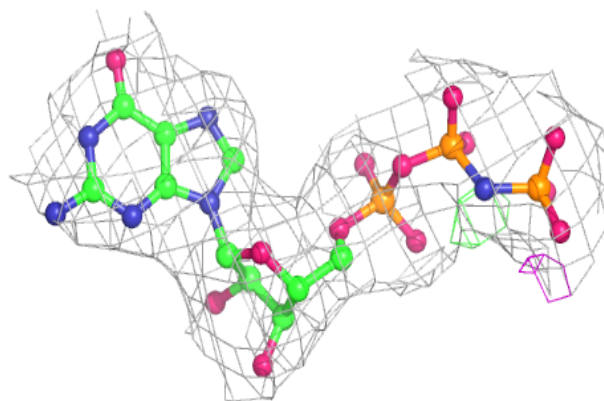
**Electron density around GNP M 200:**

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

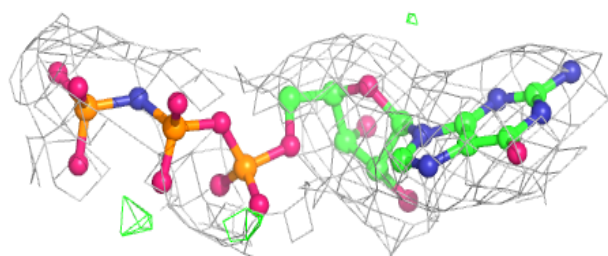
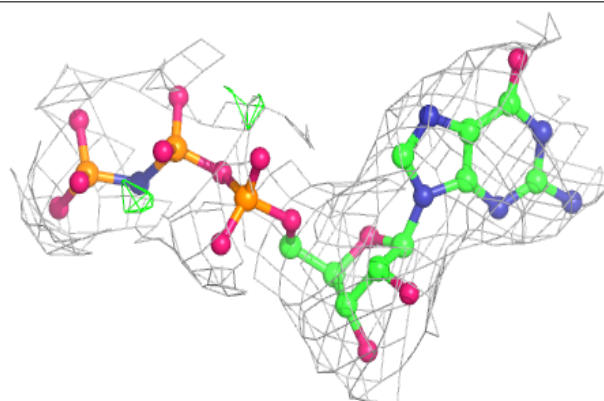


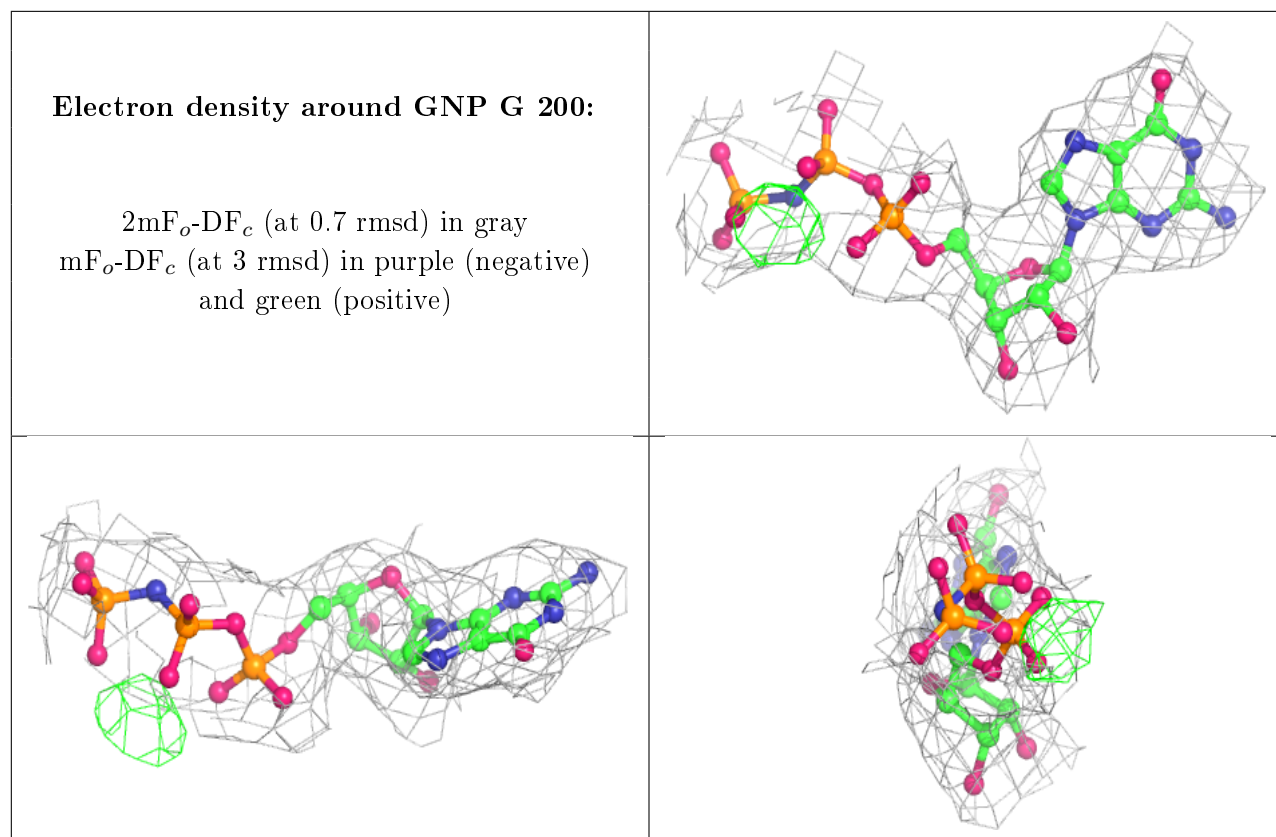
Electron density around GNP J 200:

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

**Electron density around GNP D 200:**

$2mF_o-DF_c$ (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.