



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:35 pm BST

PDB ID : 5L3S
Title : Structure of the GTPase heterodimer of crenarchaeal SRP54 and FtsY
Authors : Bange, G.; Wild, K.; Sinning, I.
Deposited on : 2016-05-24
Resolution : 1.90 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

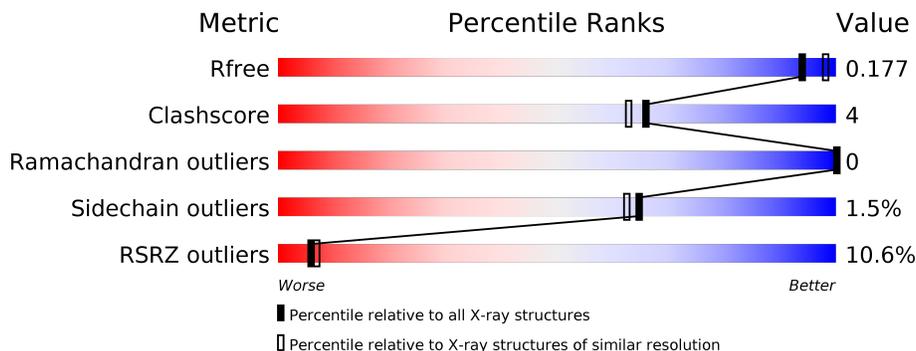
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	298	 7% 83% 9% 8%
1	C	298	 19% 78% 12% 9%
1	E	298	 11% 83% 7% 9%
1	G	298	 5% 83% 10% 7%
2	B	296	 6% 87% 9% 9%
2	D	296	 13% 82% 9% 8%

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Mol	Chain	Length	Quality of chain
2	F	296	
2	H	296	

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
5	G	A	303	-	-	-	X
6	GOL	H	404	-	-	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 19033 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 Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	Total 2142	C 1380	N 353	O 404	S 5	0	2	0
1	C	270	Total 2110	C 1360	N 346	O 399	S 5	0	2	0
1	E	271	Total 2115	C 1362	N 349	O 399	S 5	0	1	0
1	G	277	Total 2150	C 1383	N 355	O 407	S 5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q97ZE7
A	-4	HIS	-	expression tag	UNP Q97ZE7
A	-3	HIS	-	expression tag	UNP Q97ZE7
A	-2	HIS	-	expression tag	UNP Q97ZE7
A	-1	HIS	-	expression tag	UNP Q97ZE7
A	0	HIS	-	expression tag	UNP Q97ZE7
C	-5	HIS	-	expression tag	UNP Q97ZE7
C	-4	HIS	-	expression tag	UNP Q97ZE7
C	-3	HIS	-	expression tag	UNP Q97ZE7
C	-2	HIS	-	expression tag	UNP Q97ZE7
C	-1	HIS	-	expression tag	UNP Q97ZE7
C	0	HIS	-	expression tag	UNP Q97ZE7
E	-5	HIS	-	expression tag	UNP Q97ZE7
E	-4	HIS	-	expression tag	UNP Q97ZE7
E	-3	HIS	-	expression tag	UNP Q97ZE7
E	-2	HIS	-	expression tag	UNP Q97ZE7
E	-1	HIS	-	expression tag	UNP Q97ZE7
E	0	HIS	-	expression tag	UNP Q97ZE7
G	-5	HIS	-	expression tag	UNP Q97ZE7
G	-4	HIS	-	expression tag	UNP Q97ZE7
G	-3	HIS	-	expression tag	UNP Q97ZE7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	HIS	-	expression tag	UNP Q97ZE7
G	-1	HIS	-	expression tag	UNP Q97ZE7
G	0	HIS	-	expression tag	UNP Q97ZE7

- Molecule 2 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	283	Total	C	N	O	S	0	1	0
			2235	1429	374	429	3			
2	D	271	Total	C	N	O	S	0	1	0
			2128	1361	352	412	3			
2	F	283	Total	C	N	O	S	0	0	0
			2228	1426	371	428	3			
2	H	278	Total	C	N	O	S	0	2	0
			2198	1406	367	422	3			

There are 28 discrepancies between the modelled and reference sequences:

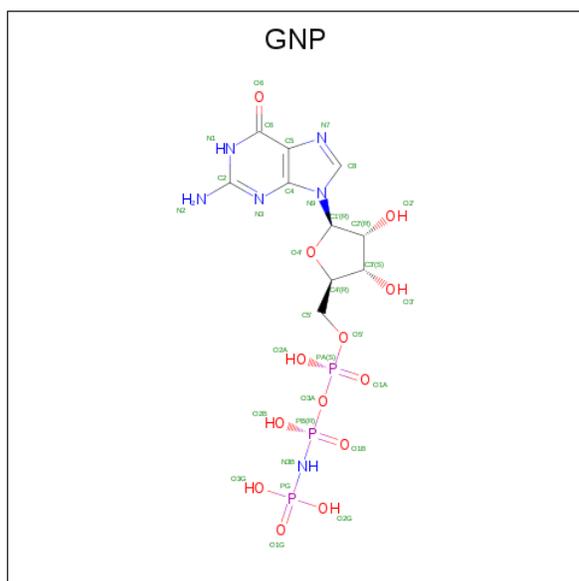
Chain	Residue	Modelled	Actual	Comment	Reference
B	73	HIS	-	expression tag	UNP P27414
B	74	HIS	-	expression tag	UNP P27414
B	75	HIS	-	expression tag	UNP P27414
B	76	HIS	-	expression tag	UNP P27414
B	77	HIS	-	expression tag	UNP P27414
B	78	HIS	-	expression tag	UNP P27414
B	279	LYS	ARG	conflict	UNP P27414
D	73	HIS	-	expression tag	UNP P27414
D	74	HIS	-	expression tag	UNP P27414
D	75	HIS	-	expression tag	UNP P27414
D	76	HIS	-	expression tag	UNP P27414
D	77	HIS	-	expression tag	UNP P27414
D	78	HIS	-	expression tag	UNP P27414
D	279	LYS	ARG	conflict	UNP P27414
F	73	HIS	-	expression tag	UNP P27414
F	74	HIS	-	expression tag	UNP P27414
F	75	HIS	-	expression tag	UNP P27414
F	76	HIS	-	expression tag	UNP P27414
F	77	HIS	-	expression tag	UNP P27414
F	78	HIS	-	expression tag	UNP P27414
F	279	LYS	ARG	conflict	UNP P27414
H	73	HIS	-	expression tag	UNP P27414
H	74	HIS	-	expression tag	UNP P27414

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Chain	Residue	Modelled	Actual	Comment	Reference
H	75	HIS	-	expression tag	UNP P27414
H	76	HIS	-	expression tag	UNP P27414
H	77	HIS	-	expression tag	UNP P27414
H	78	HIS	-	expression tag	UNP P27414
H	279	LYS	ARG	conflict	UNP P27414

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

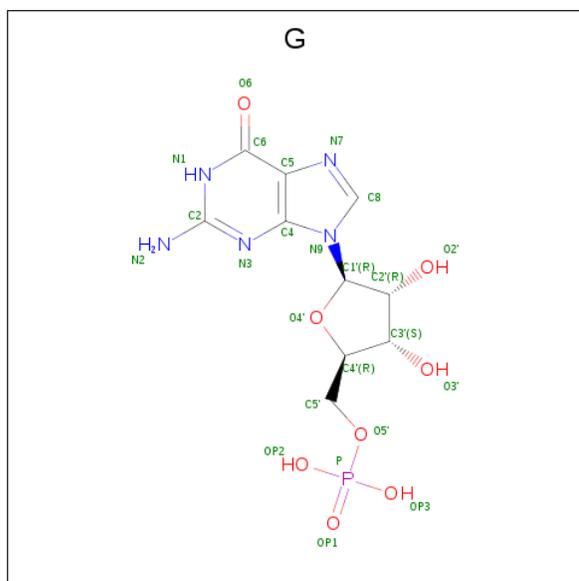


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	F	1	Total	C	N	O	P	0	0
		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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: C₁₀H₁₄N₅O₈P).



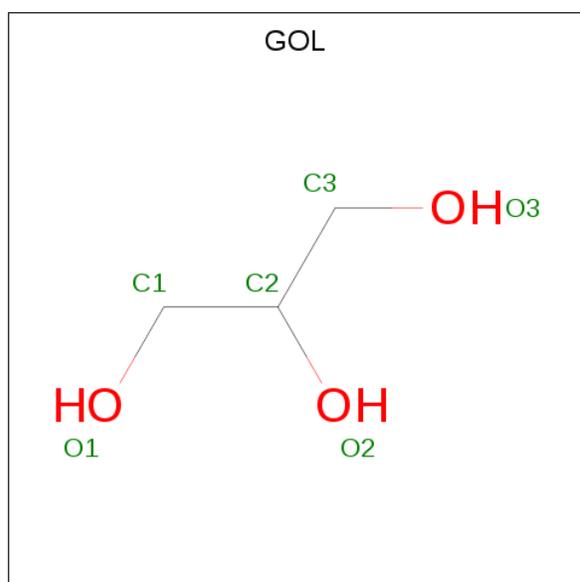
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 24 10 5 8 1	0	0
5	C	1	Total C N O P 24 10 5 8 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
5	G	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



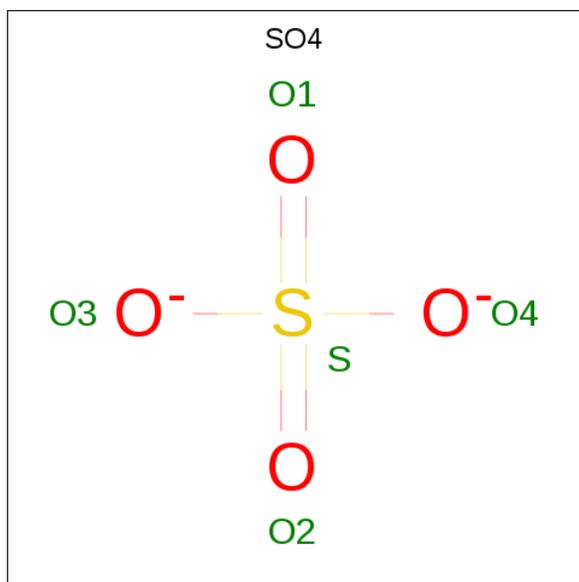
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			6	3 3		
6	A	1	Total	C O	0	0
			6	3 3		
6	A	1	Total	C O	0	0
			6	3 3		
6	B	1	Total	C O	0	0
			6	3 3		
6	B	1	Total	C O	0	0
			6	3 3		
6	B	1	Total	C O	0	0
			6	3 3		
6	B	1	Total	C O	0	0
			6	3 3		
6	C	1	Total	C O	0	0
			6	3 3		
6	C	1	Total	C O	0	0
			6	3 3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0
7	C	1	Total 5	O 4	S 1	0	0
7	E	1	Total 5	O 4	S 1	0	0
7	G	1	Total 5	O 4	S 1	0	0
7	H	1	Total 5	O 4	S 1	0	0

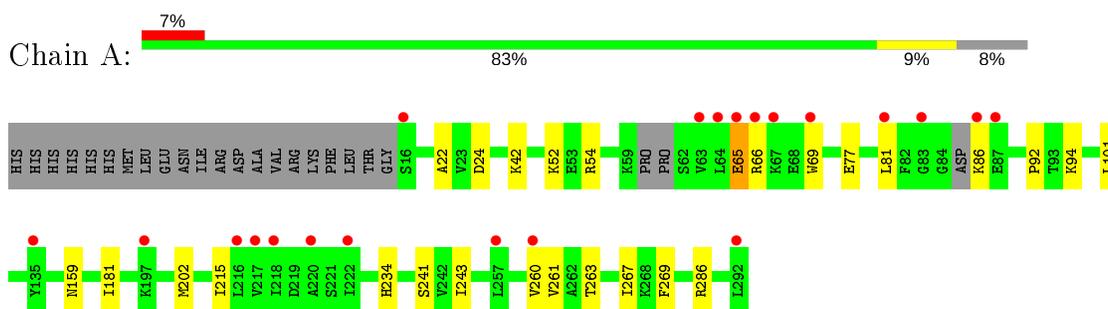
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	193	Total 193	O 193	0	0
8	B	190	Total 190	O 190	0	0
8	C	128	Total 128	O 128	0	0
8	D	135	Total 135	O 135	0	0
8	E	141	Total 141	O 141	0	0
8	F	106	Total 106	O 106	0	0
8	G	168	Total 168	O 168	0	0
8	H	153	Total 153	O 153	0	0

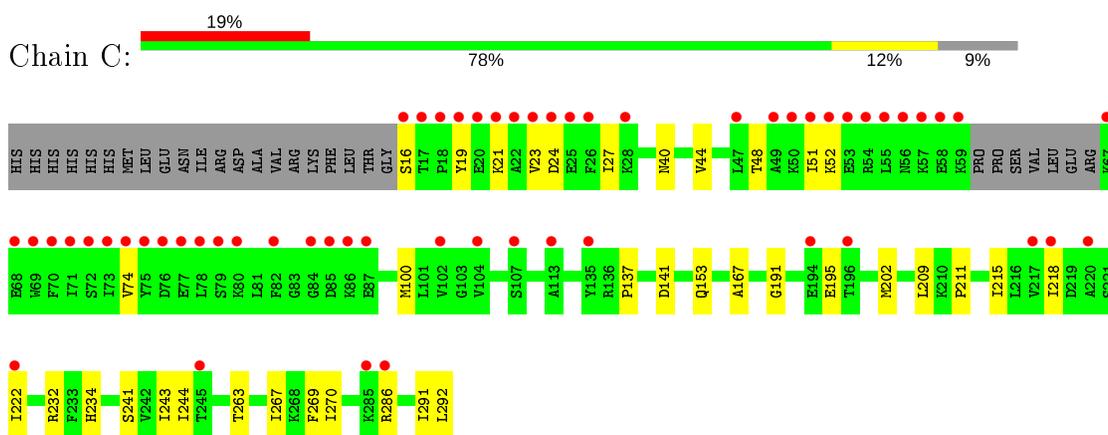
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

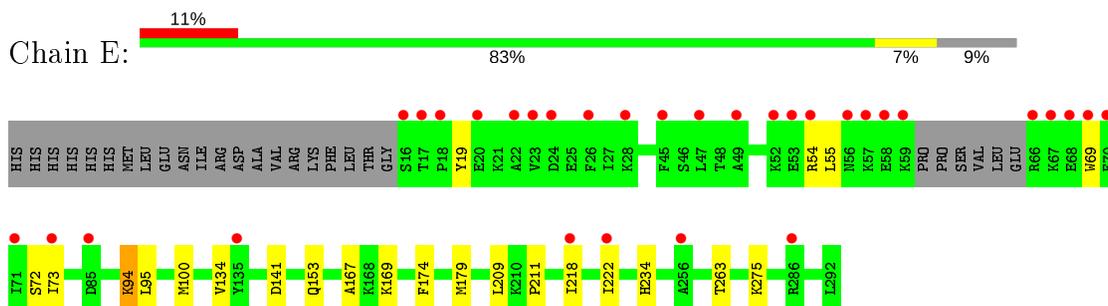
- Molecule 1: Signal recognition particle 54 kDa protein



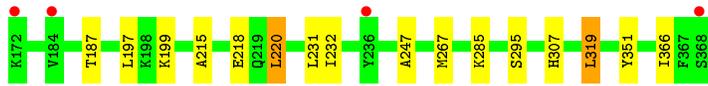
- Molecule 1: Signal recognition particle 54 kDa protein



- Molecule 1: Signal recognition particle 54 kDa protein



- Molecule 1: Signal recognition particle 54 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.20Å 199.67Å 124.87Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	37.87 – 1.90 37.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (37.87-1.90) 89.8 (37.87-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.173 , 0.216 0.175 , 0.177	Depositor DCC
R_{free} test set	3836 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtrriage
Anisotropy	0.691	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19033	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: GOL, 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	0.37	0/2181	0.52	0/2934
1	C	0.33	0/2150	0.47	0/2894
1	E	0.34	0/2152	0.48	0/2896
1	G	0.35	0/2186	0.49	0/2946
2	B	0.37	0/2268	0.51	0/3059
2	D	0.33	0/2159	0.48	0/2915
2	F	0.32	0/2257	0.49	0/3043
2	H	0.37	0/2233	0.50	0/3010
All	All	0.35	0/17586	0.49	0/23697

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2142	0	2217	17	0
1	C	2110	0	2180	22	0
1	E	2115	0	2185	14	0
1	G	2150	0	2222	20	0
2	B	2235	0	2310	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2128	0	2184	15	0
2	F	2228	0	2300	21	0
2	H	2198	0	2268	18	0
3	A	32	0	13	0	0
3	B	32	0	13	0	0
3	C	32	0	13	0	0
3	D	32	0	13	0	0
3	E	32	0	13	0	0
3	F	32	0	13	0	0
3	G	32	0	13	0	0
3	H	32	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	24	0	12	0	0
5	C	24	0	12	1	0
5	E	24	0	12	0	0
5	G	24	0	12	1	0
6	A	18	0	24	3	0
6	B	24	0	32	1	0
6	C	12	0	16	3	0
6	D	6	0	8	0	0
6	E	12	0	16	0	0
6	F	6	0	8	0	0
6	G	18	0	24	2	0
6	H	12	0	16	1	0
7	A	15	0	0	0	0
7	B	10	0	0	0	0
7	C	5	0	0	1	0
7	E	5	0	0	0	0
7	G	5	0	0	0	0
7	H	5	0	0	0	0
8	A	193	0	0	4	0
8	B	190	0	0	5	3
8	C	128	0	0	3	0
8	D	135	0	0	2	0
8	E	141	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	106	0	0	2	3
8	G	168	0	0	6	0
8	H	153	0	0	6	0
All	All	19033	0	18162	145	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 145 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:SD	8:A:567:HOH:O	2.33	0.86
1:C:153[B]:GLN:NE2	1:E:153:GLN:OE1	2.18	0.76
2:B:91:LYS:NZ	8:B:502:HOH:O	2.18	0.75
2:F:88:LYS:HG3	2:F:135:ARG:HB2	1.70	0.73
1:A:286:ARG:NH1	6:A:305:GOL:O2	2.23	0.72

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:501:HOH:O	8:F:534:HOH:O[2_546]	2.13	0.07
8:B:502:HOH:O	8:F:599:HOH:O[2_546]	2.13	0.07
8:B:649:HOH:O	8:F:593:HOH:O[2_546]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/298 (91%)	267 (99%)	3 (1%)	0	100	100
1	C	268/298 (90%)	267 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	268/298 (90%)	268 (100%)	0	0	100	100
1	G	275/298 (92%)	273 (99%)	2 (1%)	0	100	100
2	B	282/296 (95%)	276 (98%)	6 (2%)	0	100	100
2	D	268/296 (90%)	262 (98%)	6 (2%)	0	100	100
2	F	279/296 (94%)	273 (98%)	6 (2%)	0	100	100
2	H	276/296 (93%)	270 (98%)	6 (2%)	0	100	100
All	All	2186/2376 (92%)	2156 (99%)	30 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/252 (92%)	230 (99%)	2 (1%)	78	79
1	C	228/252 (90%)	227 (100%)	1 (0%)	91	91
1	E	228/252 (90%)	225 (99%)	3 (1%)	69	68
1	G	233/252 (92%)	230 (99%)	3 (1%)	69	68
2	B	247/259 (95%)	246 (100%)	1 (0%)	91	91
2	D	235/259 (91%)	233 (99%)	2 (1%)	78	79
2	F	246/259 (95%)	239 (97%)	7 (3%)	43	36
2	H	243/259 (94%)	234 (96%)	9 (4%)	34	25
All	All	1892/2044 (93%)	1864 (98%)	28 (2%)	65	62

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	231	LEU
2	F	366	ILE
2	H	307	HIS
2	F	235	LYS

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Mol	Chain	Res	Type
2	F	338	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	157	ASN
1	E	177	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 47 ligands modelled in this entry, 8 are monoatomic - leaving 39 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	$\# Z > 2$
7	SO4	A	309	-	4,4,4	0.15	0	6,6,6	0.13	0
6	GOL	B	404	-	5,5,5	0.30	0	5,5,5	0.37	0
6	GOL	G	304	-	5,5,5	0.35	0	5,5,5	0.97	0
6	GOL	A	305	-	5,5,5	0.36	0	5,5,5	0.50	0
6	GOL	H	404	-	5,5,5	0.37	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GNP	B	401	4	28,34,34	2.67	8 (28%)	30,54,54	1.82	4 (13%)
7	SO4	B	407	-	4,4,4	0.16	0	6,6,6	0.13	0
7	SO4	A	308	-	4,4,4	0.13	0	6,6,6	0.13	0
3	GNP	D	401	4	28,34,34	2.55	8 (28%)	30,54,54	1.98	6 (20%)
7	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	B	403	-	5,5,5	0.40	0	5,5,5	0.47	0
7	SO4	E	306	-	4,4,4	0.14	0	6,6,6	0.05	0
7	SO4	C	306	-	4,4,4	0.15	0	6,6,6	0.05	0
7	SO4	A	307	-	4,4,4	0.14	0	6,6,6	0.05	0
7	SO4	H	405	-	4,4,4	0.16	0	6,6,6	0.14	0
6	GOL	E	305	-	5,5,5	0.35	0	5,5,5	0.55	0
6	GOL	G	305	-	5,5,5	0.40	0	5,5,5	0.51	0
3	GNP	A	301	4	28,34,34	2.57	9 (32%)	30,54,54	2.33	10 (33%)
3	GNP	G	301	4	28,34,34	2.48	10 (35%)	30,54,54	2.24	10 (33%)
6	GOL	H	403	-	5,5,5	0.51	0	5,5,5	0.54	0
6	GOL	C	305	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	B	405	-	5,5,5	0.43	0	5,5,5	0.29	0
3	GNP	F	401	4	28,34,34	2.62	9 (32%)	30,54,54	2.06	6 (20%)
6	GOL	D	403	-	5,5,5	0.43	0	5,5,5	0.48	0
6	GOL	A	304	-	5,5,5	0.34	0	5,5,5	0.28	0
6	GOL	C	304	-	5,5,5	0.31	0	5,5,5	0.30	0
6	GOL	E	304	-	5,5,5	0.34	0	5,5,5	0.30	0
7	SO4	G	307	-	4,4,4	0.14	0	6,6,6	0.07	0
6	GOL	G	306	-	5,5,5	0.35	0	5,5,5	0.32	0
3	GNP	E	301	4	28,34,34	2.61	11 (39%)	30,54,54	2.27	10 (33%)
6	GOL	A	306	-	5,5,5	0.35	0	5,5,5	0.32	0
6	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.39	0
3	GNP	C	301	4	28,34,34	2.63	10 (35%)	30,54,54	2.28	10 (33%)
3	GNP	H	401	4	28,34,34	2.34	9 (32%)	30,54,54	1.89	5 (16%)
6	GOL	F	403	-	5,5,5	0.40	0	5,5,5	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	404	-	-	0/4/4/4	-
6	GOL	G	304	-	-	2/4/4/4	-
6	GOL	A	305	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	H	404	-	-	2/4/4/4	-
3	GNP	B	401	4	-	4/17/38/38	0/3/3/3
3	GNP	D	401	4	-	4/17/38/38	0/3/3/3
6	GOL	B	403	-	-	2/4/4/4	-
6	GOL	E	305	-	-	2/4/4/4	-
6	GOL	G	305	-	-	0/4/4/4	-
3	GNP	A	301	4	-	3/17/38/38	0/3/3/3
3	GNP	G	301	4	-	3/17/38/38	0/3/3/3
6	GOL	H	403	-	-	3/4/4/4	-
6	GOL	C	305	-	-	0/4/4/4	-
6	GOL	B	405	-	-	0/4/4/4	-
3	GNP	F	401	4	-	4/17/38/38	0/3/3/3
6	GOL	D	403	-	-	2/4/4/4	-
6	GOL	A	304	-	-	4/4/4/4	-
6	GOL	C	304	-	-	2/4/4/4	-
6	GOL	E	304	-	-	4/4/4/4	-
6	GOL	G	306	-	-	4/4/4/4	-
3	GNP	E	301	4	-	3/17/38/38	0/3/3/3
6	GOL	A	306	-	-	2/4/4/4	-
6	GOL	B	406	-	-	2/4/4/4	-
3	GNP	C	301	4	-	3/17/38/38	0/3/3/3
3	GNP	H	401	4	-	4/17/38/38	0/3/3/3
6	GOL	F	403	-	-	2/4/4/4	-

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	GNP	C4-N9	-7.80	1.37	1.47
3	A	301	GNP	C4-N9	-7.70	1.37	1.47
3	C	301	GNP	C4-N9	-7.60	1.37	1.47
3	D	401	GNP	C4-N9	-7.54	1.37	1.47
3	B	401	GNP	C4-N9	-7.51	1.37	1.47

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	GNP	C4-C5-N7	6.54	111.13	102.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	GNP	C4-C5-N7	6.47	111.03	102.46
3	D	401	GNP	C4-C5-N7	5.86	110.22	102.46
3	E	301	GNP	C4-C5-N7	5.80	110.15	102.46
3	C	301	GNP	C4-C5-N7	5.76	110.10	102.46

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

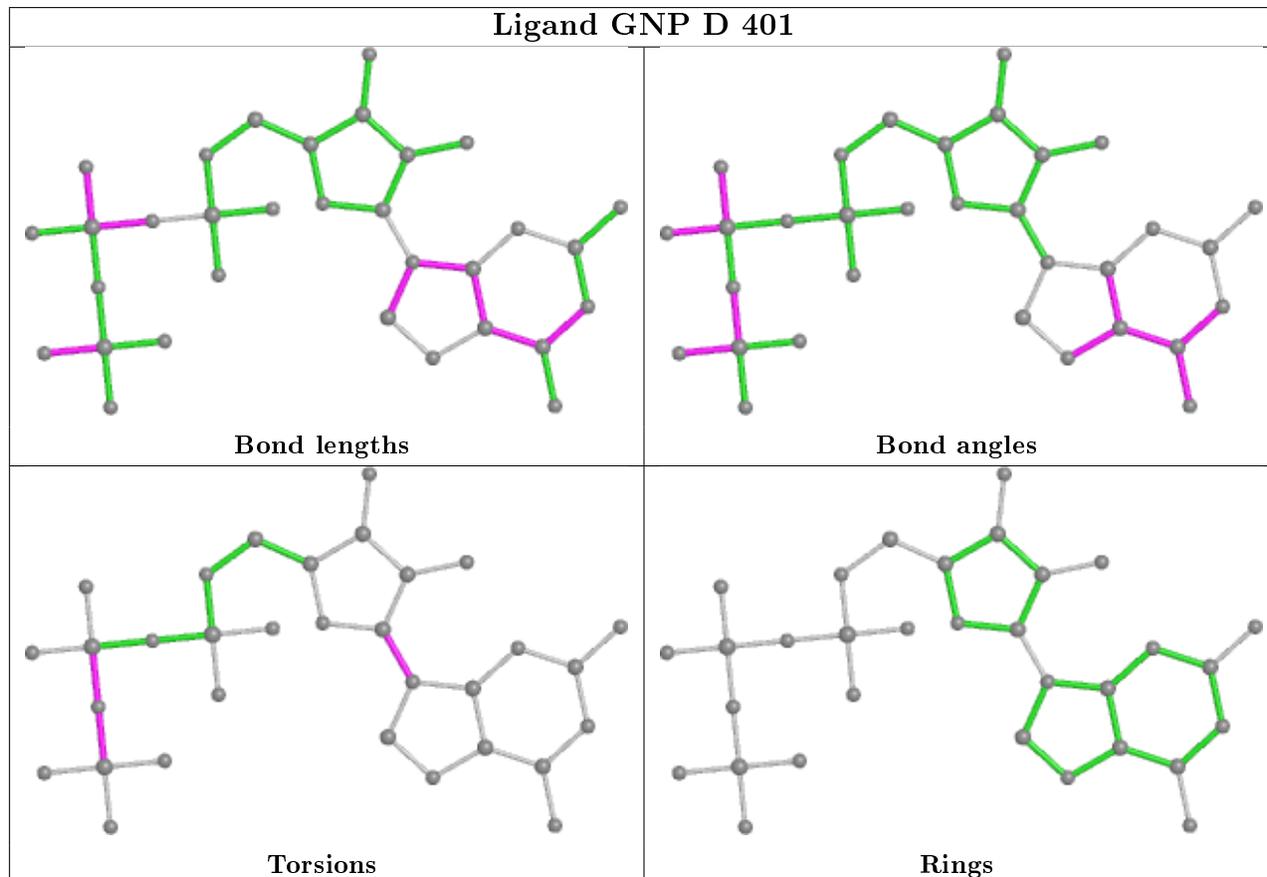
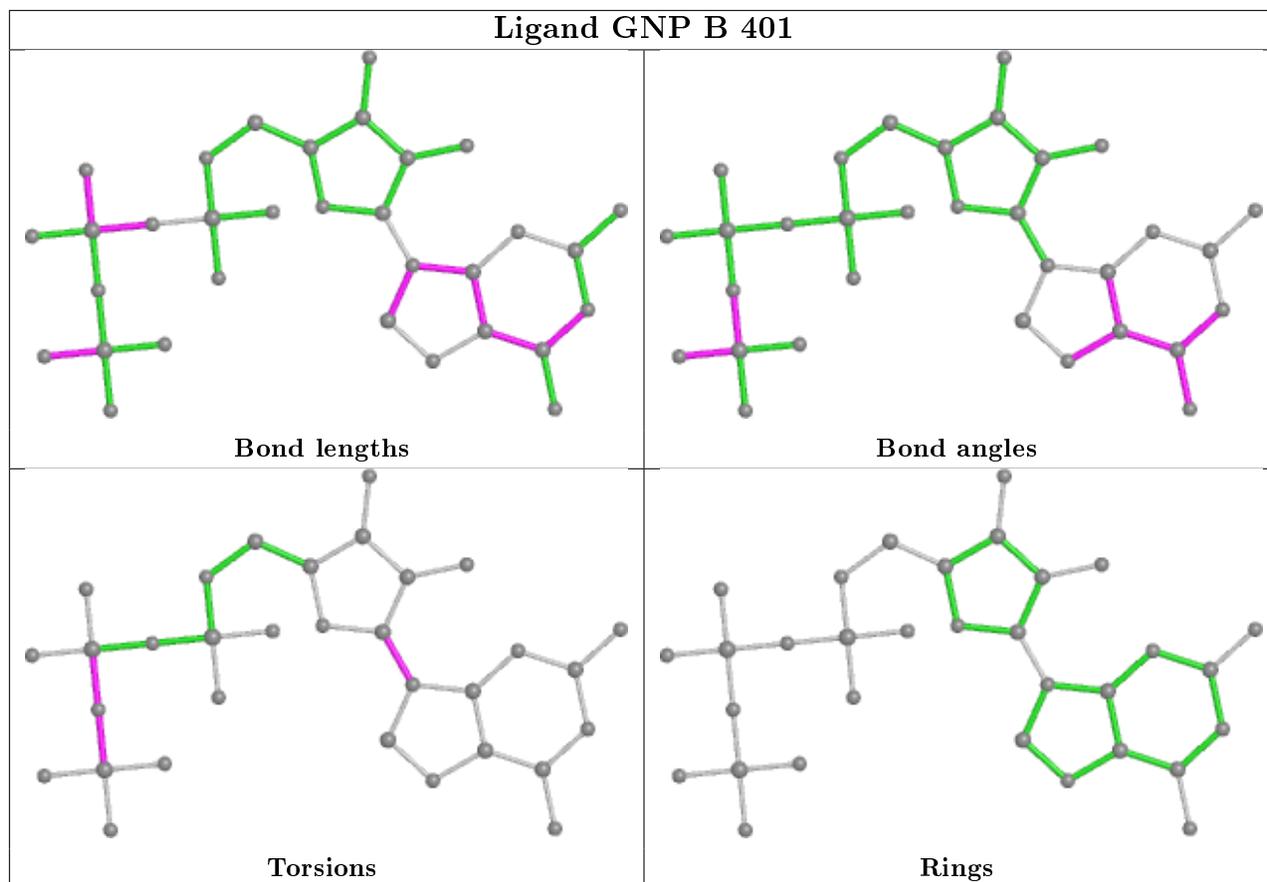
Mol	Chain	Res	Type	Atoms
6	G	304	GOL	C1-C2-C3-O3
6	H	404	GOL	O1-C1-C2-C3
3	B	401	GNP	PB-N3B-PG-O1G
3	B	401	GNP	PG-N3B-PB-O1B
3	B	401	GNP	PG-N3B-PB-O3A

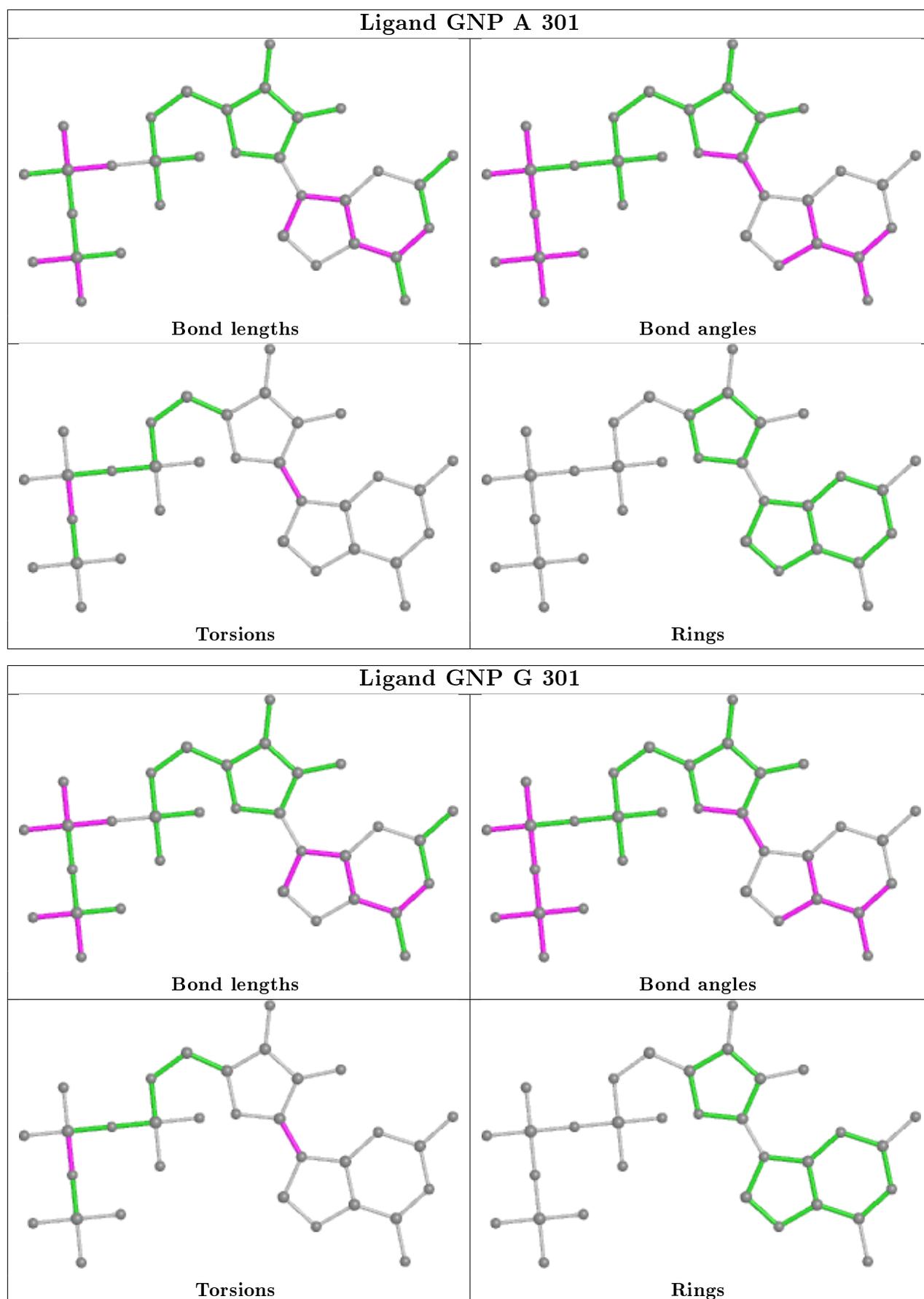
There are no ring outliers.

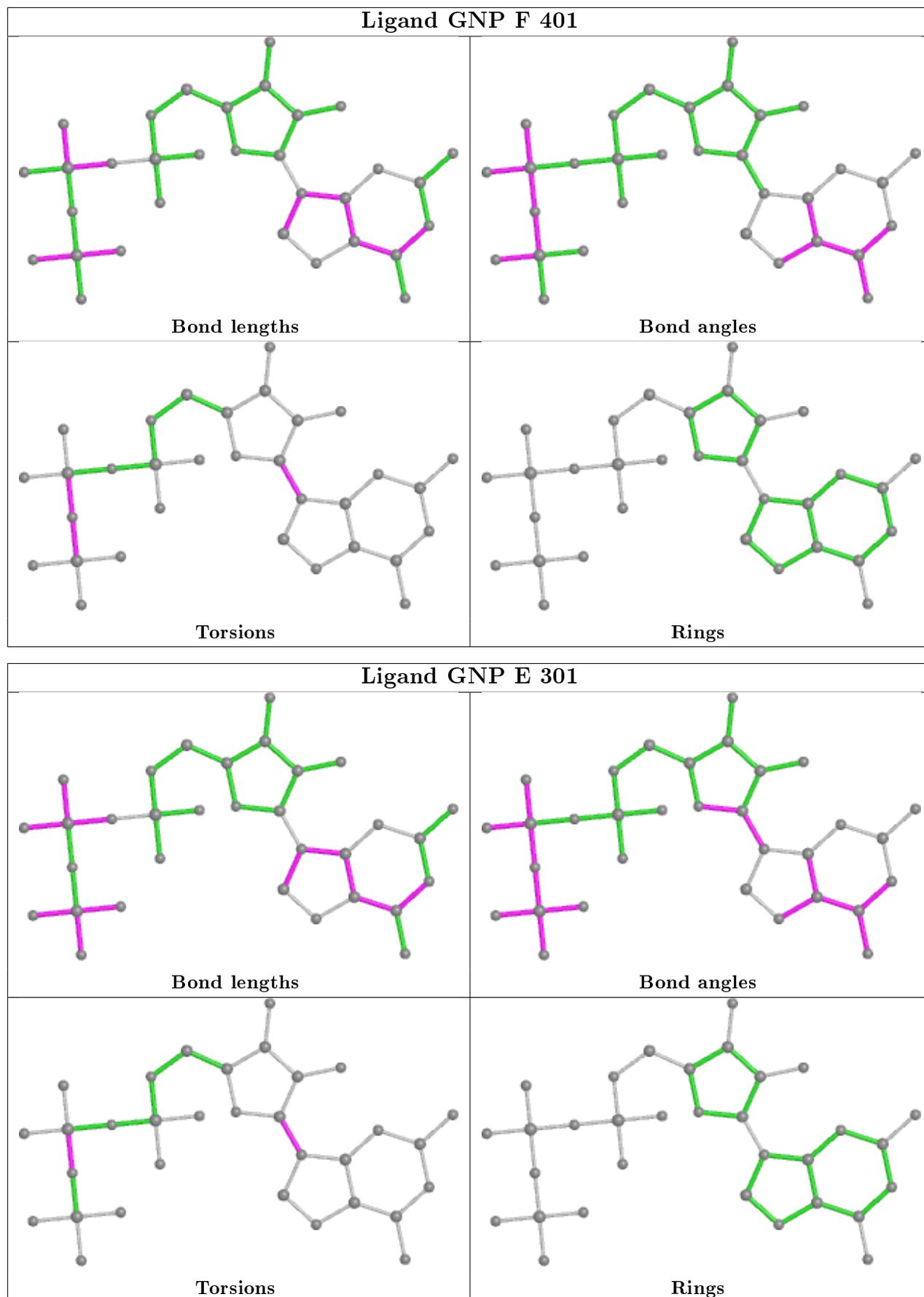
9 monomers are involved in 11 short contacts:

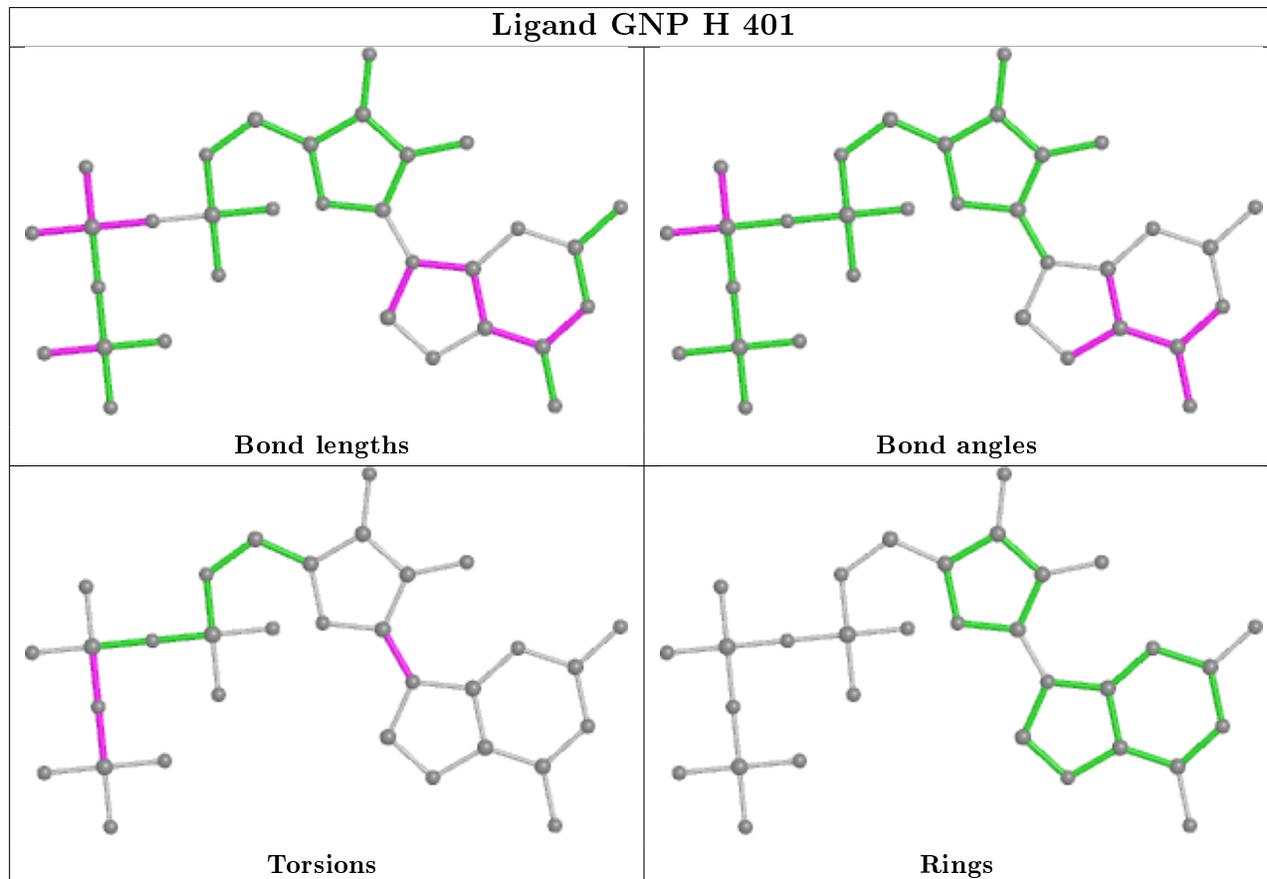
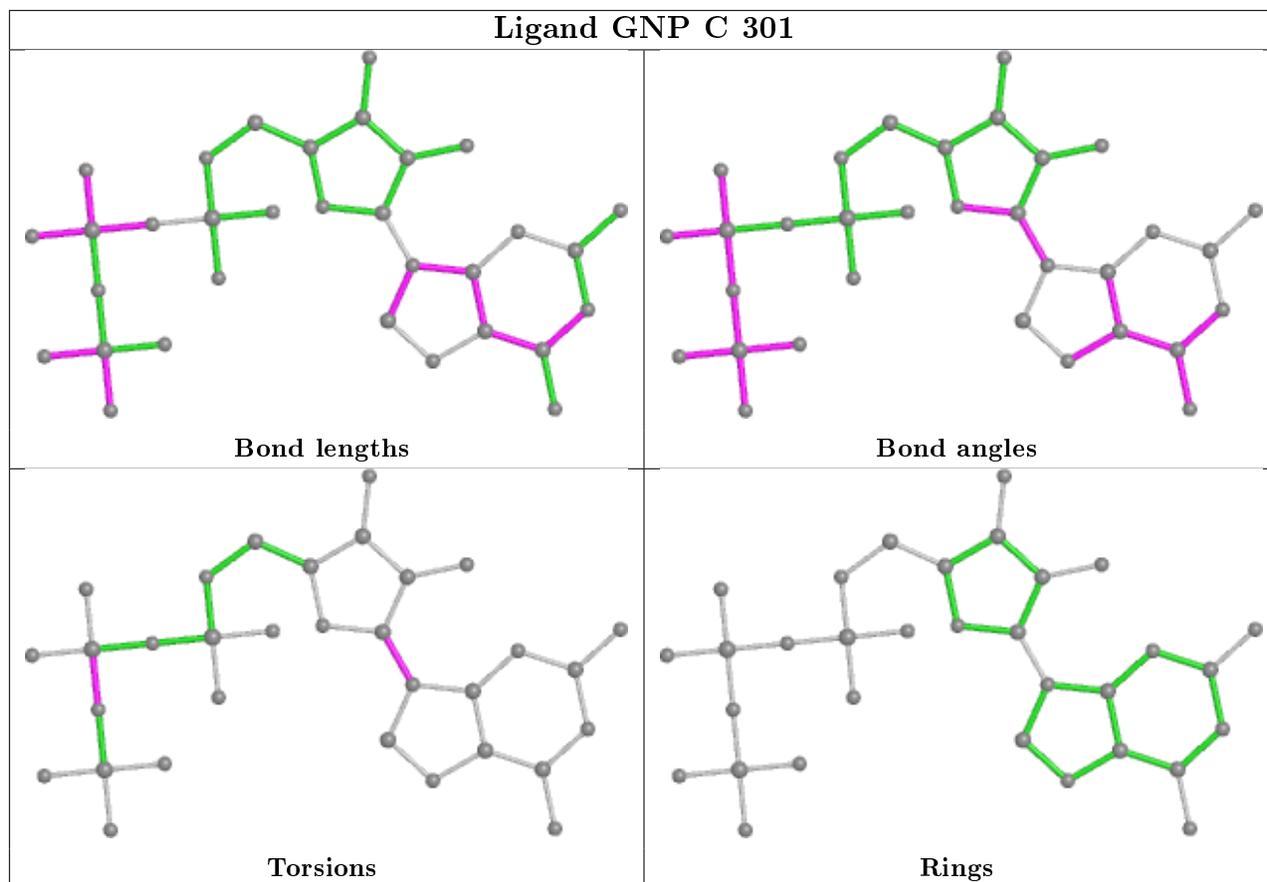
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	305	GOL	1	0
7	C	306	SO4	1	0
6	H	403	GOL	1	0
6	C	305	GOL	1	0
6	B	405	GOL	1	0
6	A	304	GOL	1	0
6	C	304	GOL	2	0
6	G	306	GOL	2	0
6	A	306	GOL	1	0

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.









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	274/298 (91%)	0.41	21 (7%) 13 15	18, 34, 73, 113	0
1	C	270/298 (90%)	1.17	57 (21%) 1 0	22, 44, 106, 135	0
1	E	271/298 (90%)	0.48	32 (11%) 4 5	22, 39, 97, 126	0
1	G	277/298 (92%)	0.27	15 (5%) 25 29	18, 38, 70, 112	0
2	B	283/296 (95%)	0.29	17 (6%) 21 24	19, 33, 64, 107	0
2	D	271/296 (91%)	0.73	37 (13%) 3 3	23, 44, 100, 120	0
2	F	283/296 (95%)	0.60	23 (8%) 12 13	23, 46, 79, 123	0
2	H	278/296 (93%)	0.50	32 (11%) 4 5	19, 36, 90, 117	0
All	All	2207/2376 (92%)	0.55	234 (10%) 6 7	18, 39, 89, 135	0

The worst 5 of 234 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	236	TYR	9.8
1	G	63	VAL	9.4
1	C	19	TYR	8.9
2	H	368	SER	8.7
2	H	132	VAL	8.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

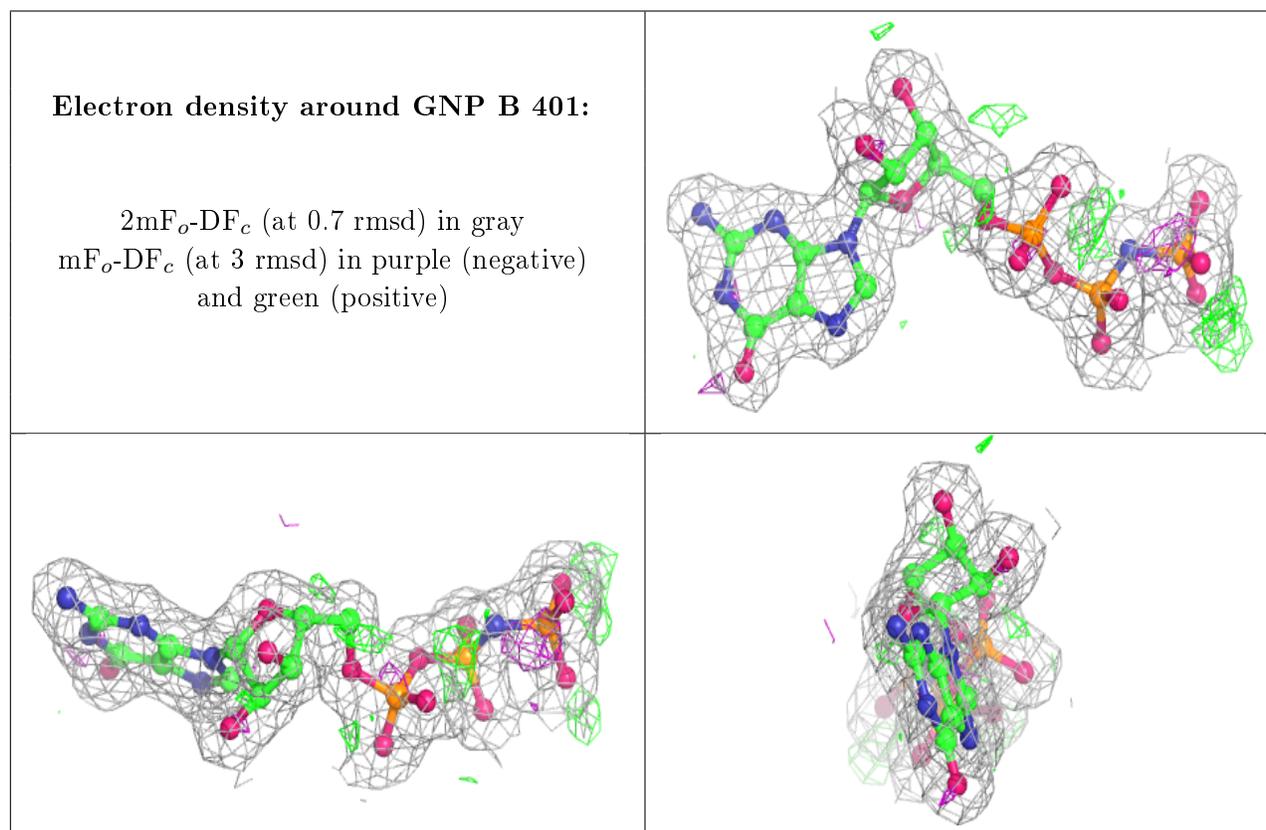
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	H	404	6/6	0.49	0.45	74,84,86,87	0
5	G	A	303	24/24	0.55	0.43	84,97,107,109	24
6	GOL	A	304	6/6	0.60	0.24	54,63,71,73	0
6	GOL	C	305	6/6	0.62	0.29	67,76,78,79	0
5	G	E	303	24/24	0.70	0.36	58,83,95,99	24
6	GOL	B	403	6/6	0.78	0.21	45,47,52,52	0
6	GOL	B	406	6/6	0.80	0.27	65,72,74,77	0
6	GOL	F	403	6/6	0.80	0.20	50,55,58,58	0
7	SO4	C	306	5/5	0.81	0.29	108,109,110,111	0
7	SO4	G	307	5/5	0.81	0.35	103,104,104,107	0
5	G	C	303	24/24	0.82	0.30	53,83,110,112	0
6	GOL	C	304	6/6	0.82	0.16	46,51,56,59	0
6	GOL	G	306	6/6	0.83	0.14	39,52,53,56	0
7	SO4	E	306	5/5	0.83	0.27	134,135,136,137	0
7	SO4	B	408	5/5	0.84	0.25	119,121,122,122	0
6	GOL	B	404	6/6	0.84	0.17	46,58,60,61	0
5	G	G	303	24/24	0.85	0.29	35,80,100,105	24
6	GOL	B	405	6/6	0.86	0.17	40,45,52,54	0
6	GOL	A	306	6/6	0.87	0.20	56,59,63,64	0
6	GOL	G	305	6/6	0.88	0.18	45,54,60,60	0
6	GOL	A	305	6/6	0.88	0.15	29,35,43,45	0
6	GOL	E	304	6/6	0.88	0.13	45,46,55,63	0
6	GOL	D	403	6/6	0.90	0.16	40,43,47,48	0
6	GOL	G	304	6/6	0.90	0.14	30,37,51,61	0
6	GOL	H	403	6/6	0.91	0.13	35,40,43,45	0
6	GOL	E	305	6/6	0.91	0.25	41,55,59,63	0
7	SO4	A	309	5/5	0.94	0.23	52,66,81,84	0
7	SO4	A	307	5/5	0.95	0.27	59,67,71,72	0
7	SO4	A	308	5/5	0.95	0.16	56,58,62,71	0
7	SO4	B	407	5/5	0.95	0.15	38,44,60,65	0
4	MG	H	402	1/1	0.97	0.06	21,21,21,21	0
4	MG	B	402	1/1	0.97	0.12	19,19,19,19	0
3	GNP	B	401	32/32	0.98	0.14	12,18,23,24	0
4	MG	C	302	1/1	0.98	0.09	25,25,25,25	0
4	MG	G	302	1/1	0.98	0.09	22,22,22,22	0
3	GNP	E	301	32/32	0.98	0.10	16,23,30,31	0
3	GNP	F	401	32/32	0.98	0.12	18,22,27,30	0

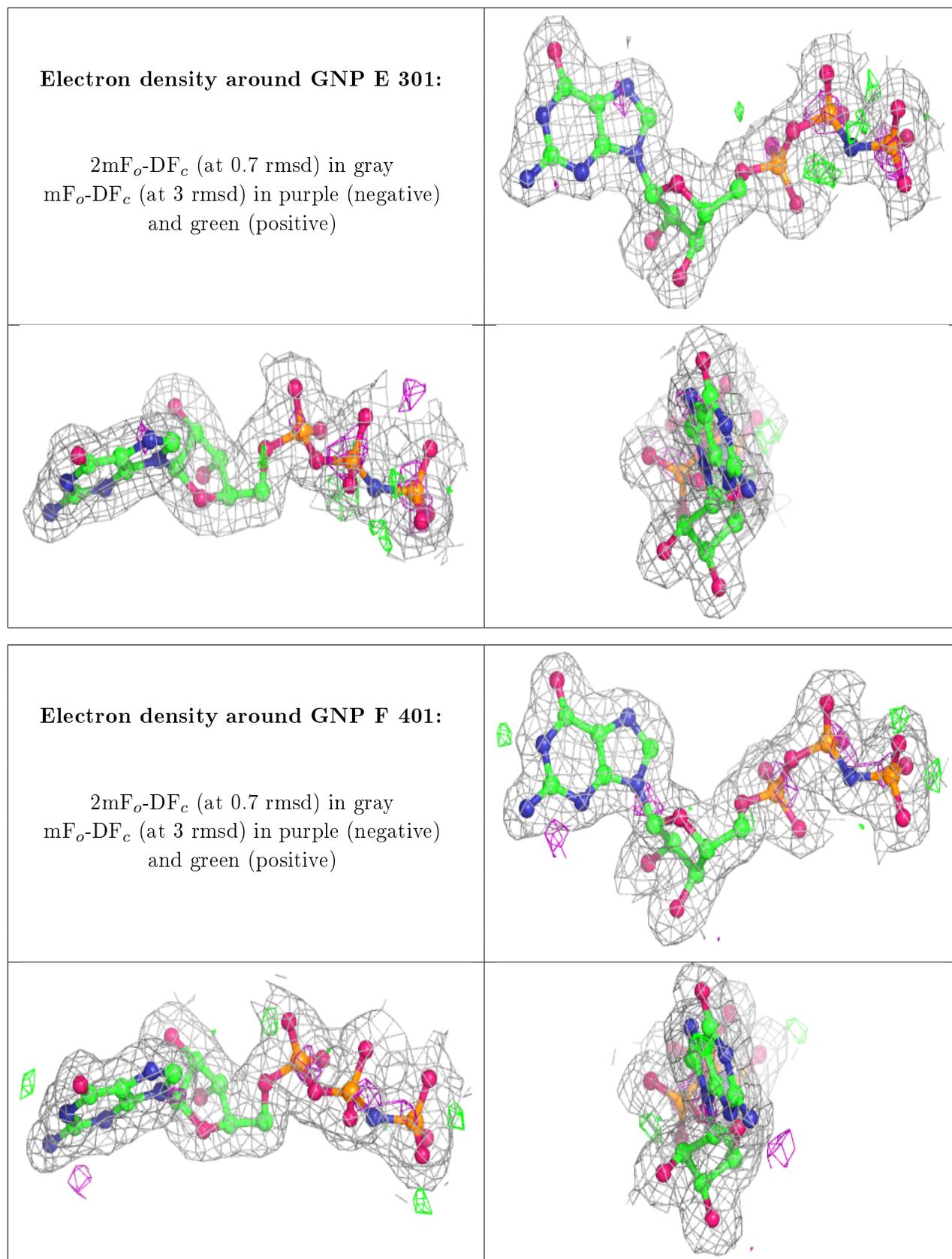
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GNP	A	301	32/32	0.98	0.14	13,20,23,24	0
7	SO4	H	405	5/5	0.98	0.16	58,60,68,70	0
4	MG	D	402	1/1	0.98	0.08	22,22,22,22	0
3	GNP	D	401	32/32	0.98	0.12	17,23,29,31	0
4	MG	F	402	1/1	0.99	0.08	24,24,24,24	0
3	GNP	G	301	32/32	0.99	0.10	14,20,24,27	0
3	GNP	C	301	32/32	0.99	0.15	17,24,28,28	0
3	GNP	H	401	32/32	0.99	0.12	16,22,25,26	0
4	MG	E	302	1/1	0.99	0.04	25,25,25,25	0
4	MG	A	302	1/1	0.99	0.12	20,20,20,20	0

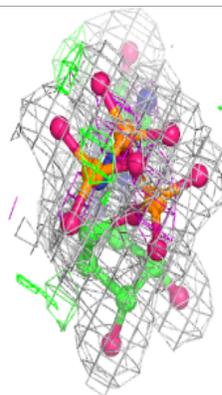
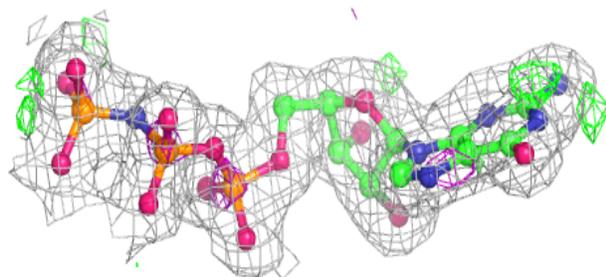
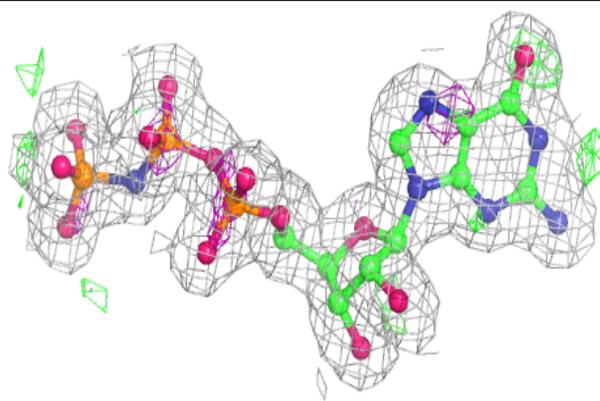
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



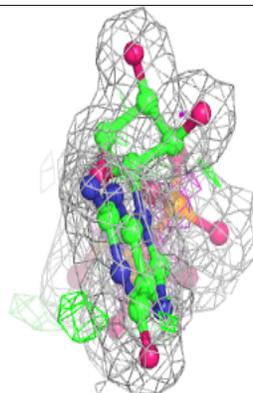
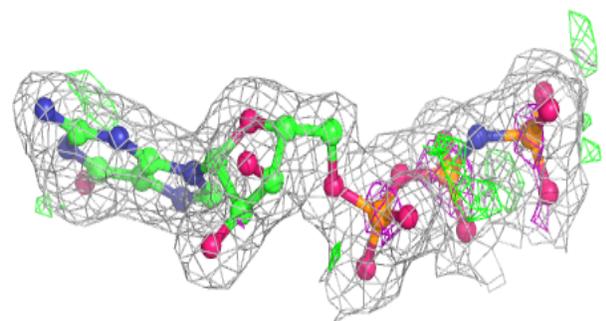
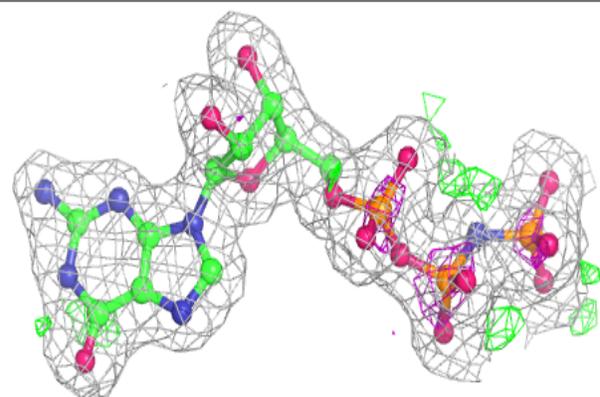


Electron density around GNP A 301:

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

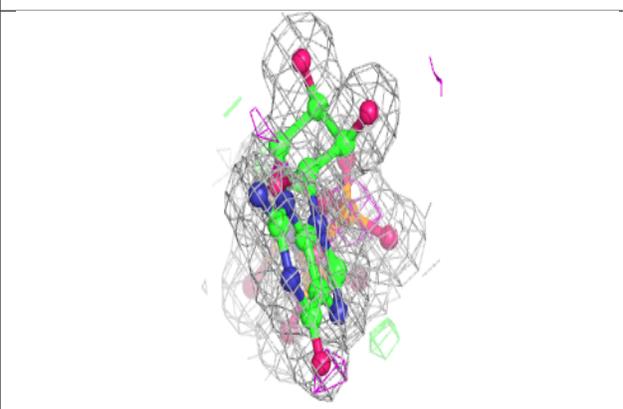
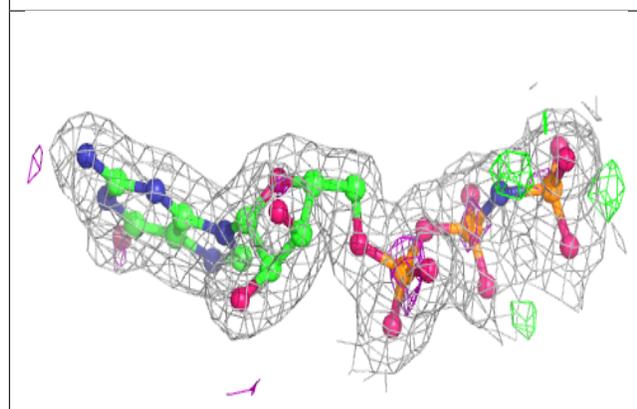
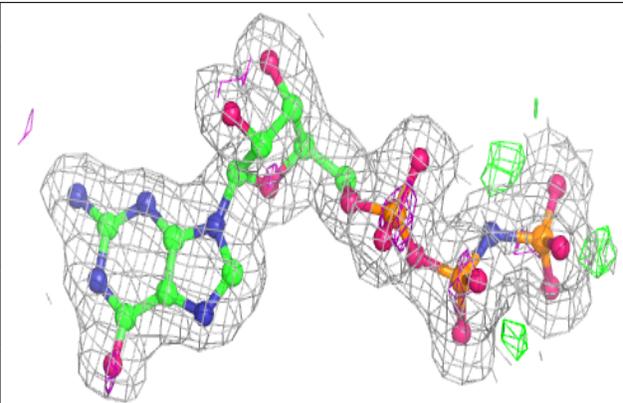
**Electron density around GNP D 401:**

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

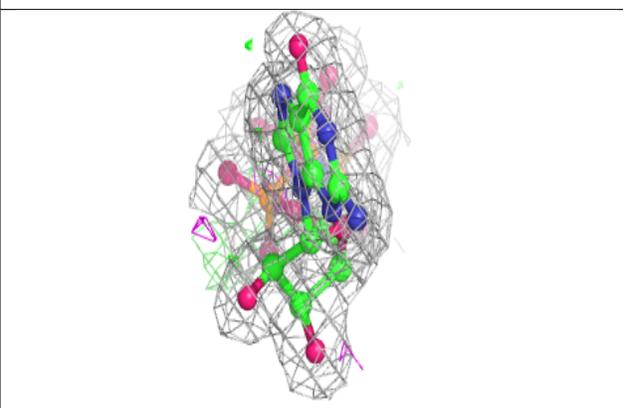
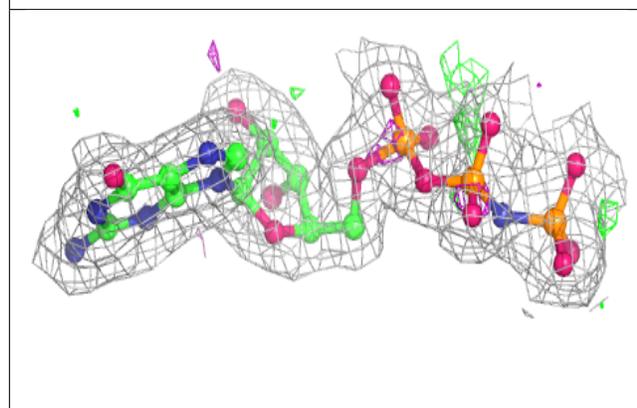
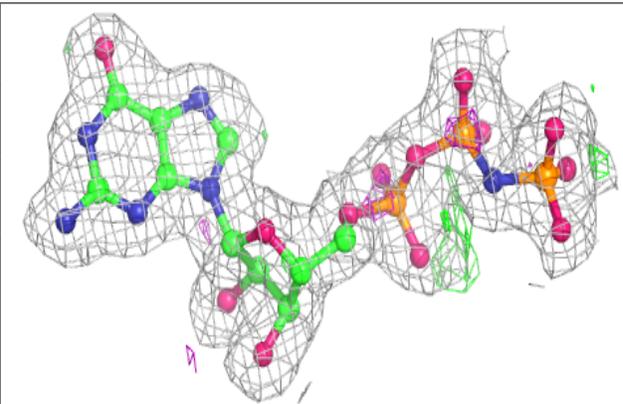


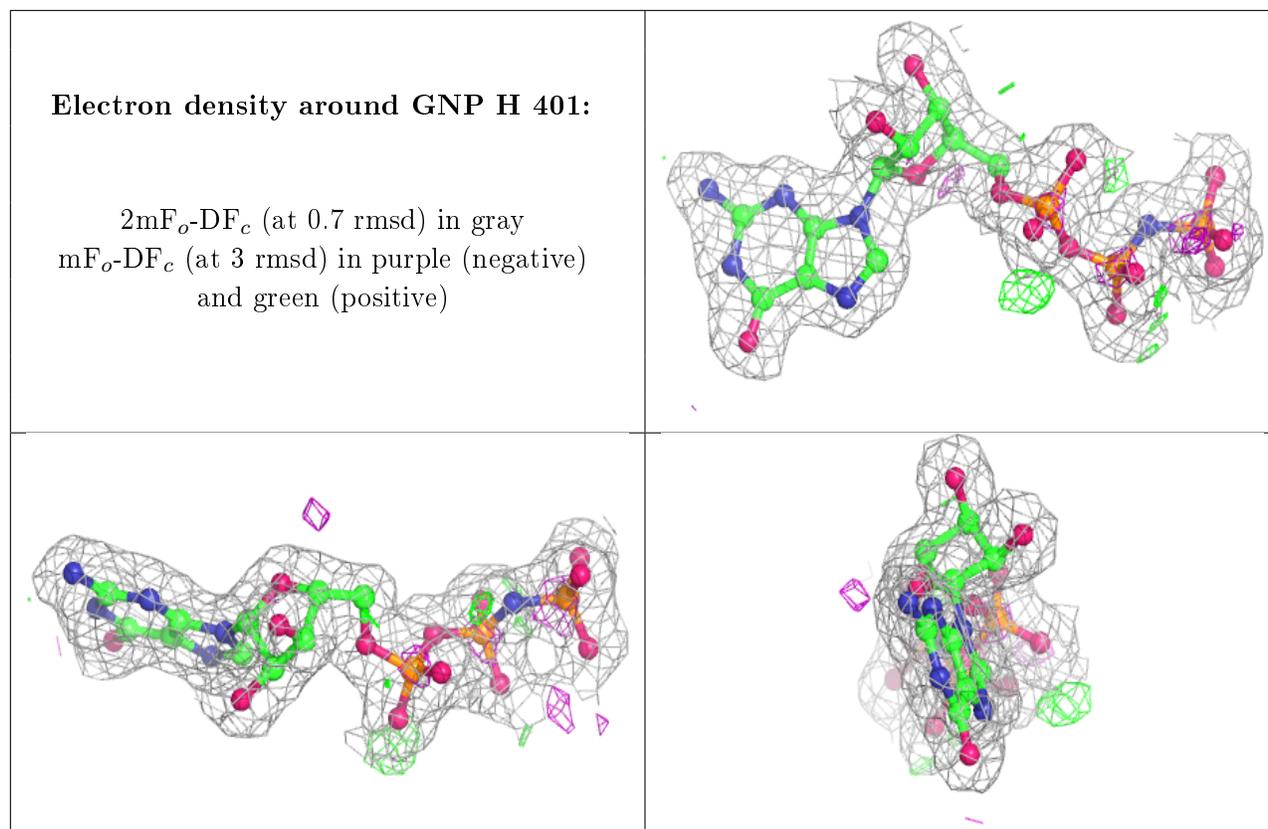
Electron density around GNP G 301:

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

**Electron density around GNP C 301:**

$2mF_o-DF_c$ (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.