



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2026 – 11:20 am BST

PDB ID : 5L3S / pdb_00005l3s
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

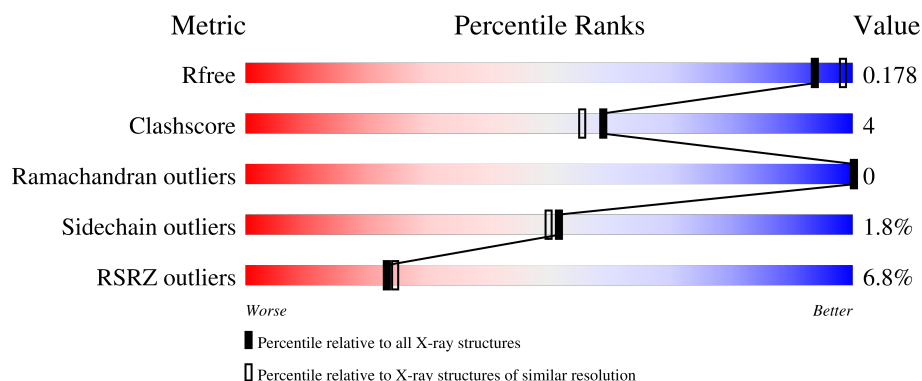
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 82% 9% 8%
1	C	298	9% 78% 12% 9%
1	E	298	8% 84% 7% 9%
1	G	298	3% 83% 10% 7%
2	B	296	3% 85% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	296	9% 80% 11% 8%
2	F	296	7% 81% 12%
2	H	296	6% 85% 7% 6%

2 Entry composition

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

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

Continued on next page...

Continued from previous page...

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:

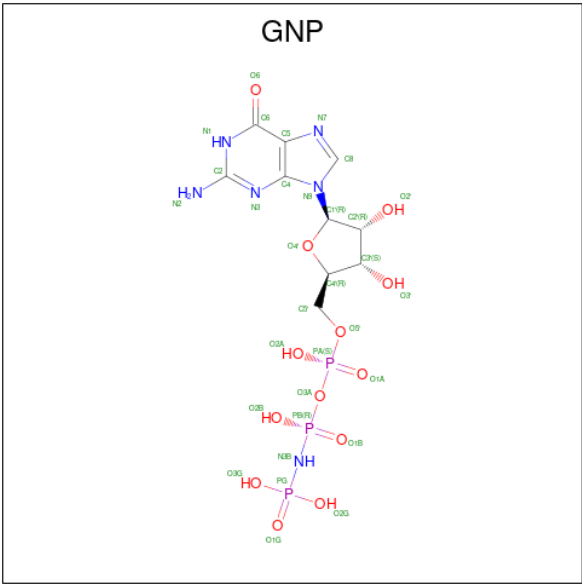
Chain	Residue	Modelled	Actual	Comment	Reference
B	73	HIS	-	expression tag	UNP P27414
B	74	HIS	-	expression tag	UNP P27414
B	75	HIS	-	expression tag	UNP P27414
B	76	HIS	-	expression tag	UNP P27414
B	77	HIS	-	expression tag	UNP P27414
B	78	HIS	-	expression tag	UNP P27414
B	279	LYS	ARG	conflict	UNP P27414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

Continued on next page...

Continued from previous page...

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 (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

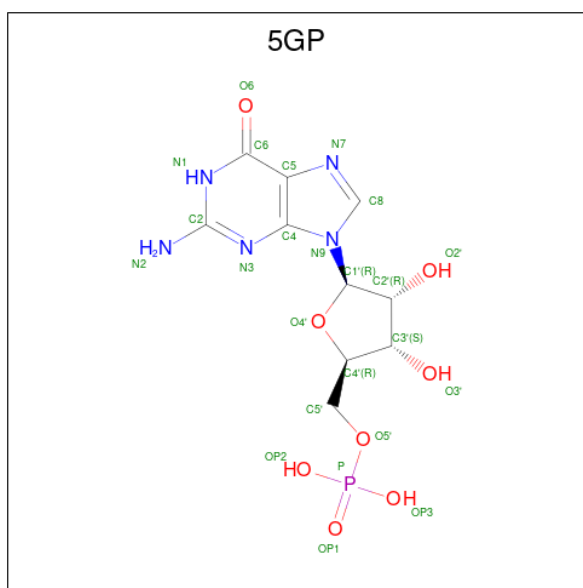


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	G	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 (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



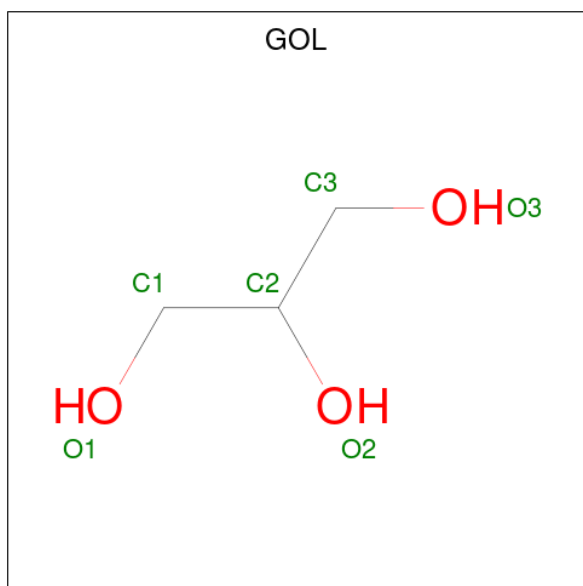
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
5	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
5	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



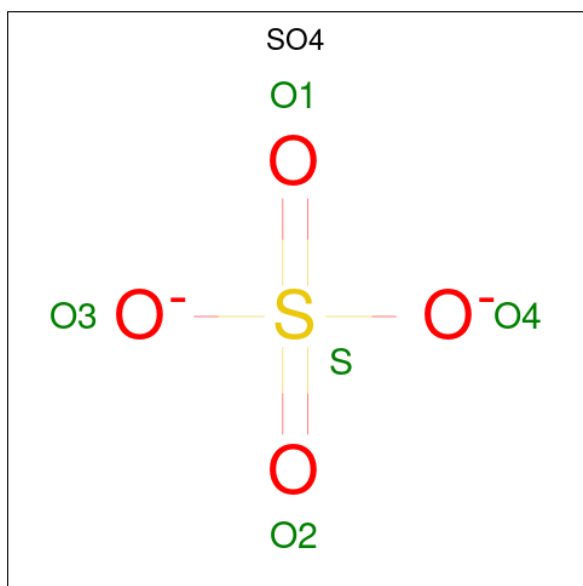
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 (CCD ID: 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		
7	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

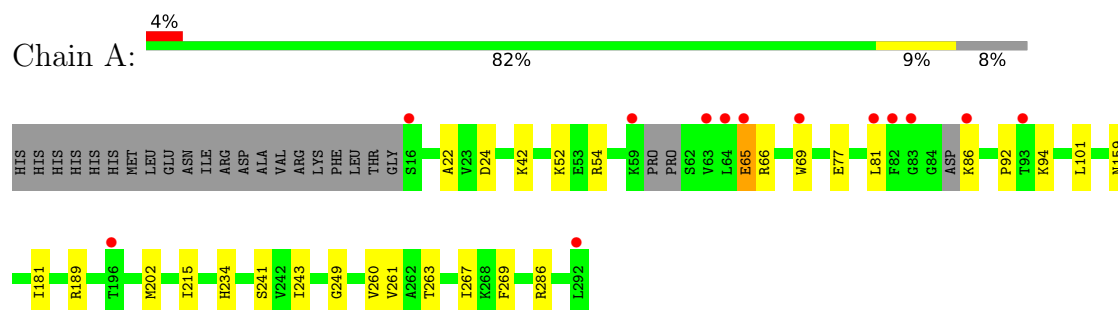
- Molecule 8 is water.

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

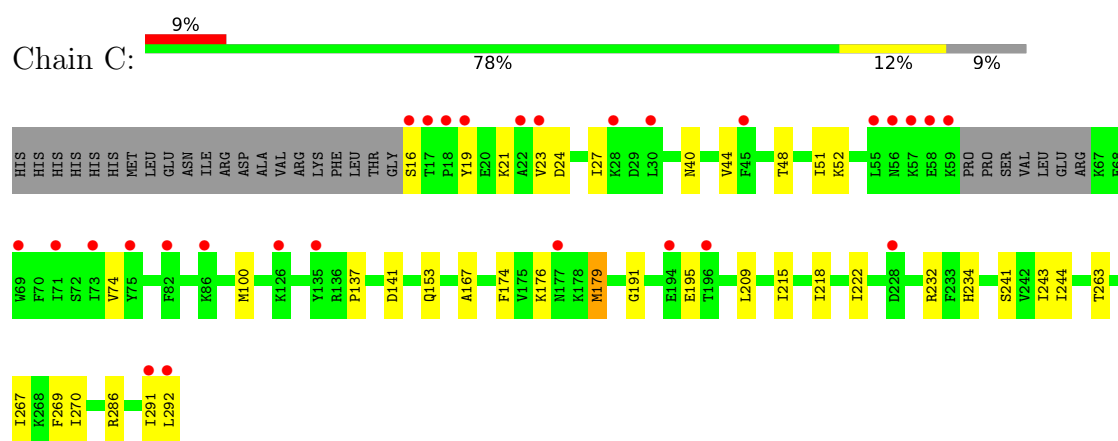
3 Residue-property plots [i](#)

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

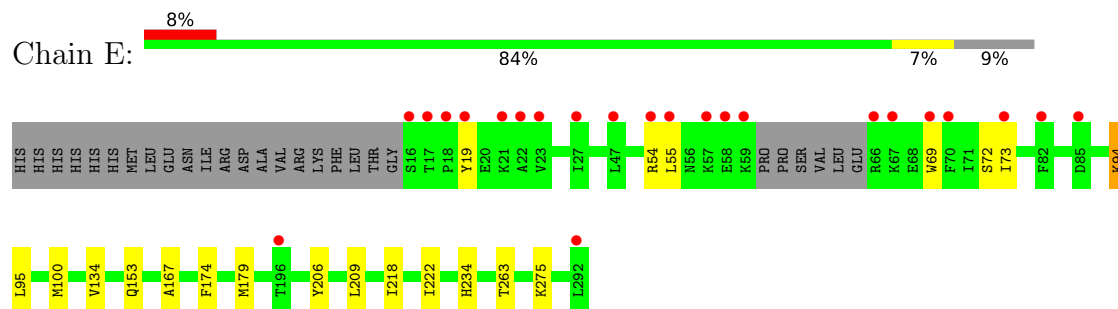
- Molecule 1: Signal recognition particle 54 kDa protein



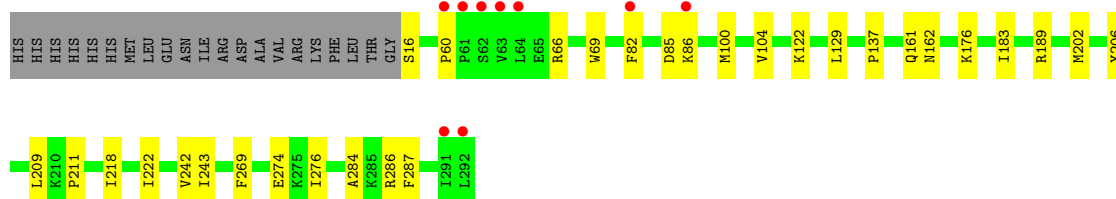
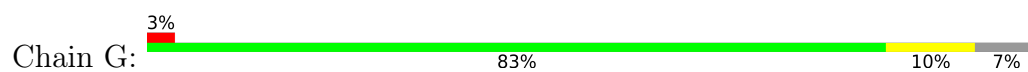
- Molecule 1: Signal recognition particle 54 kDa protein



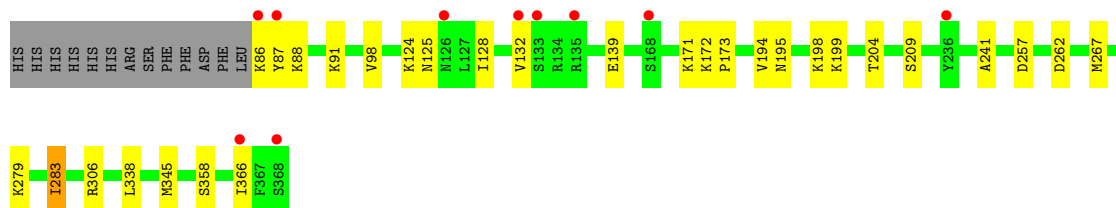
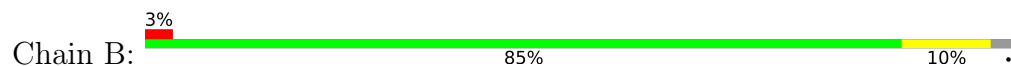
- Molecule 1: Signal recognition particle 54 kDa protein



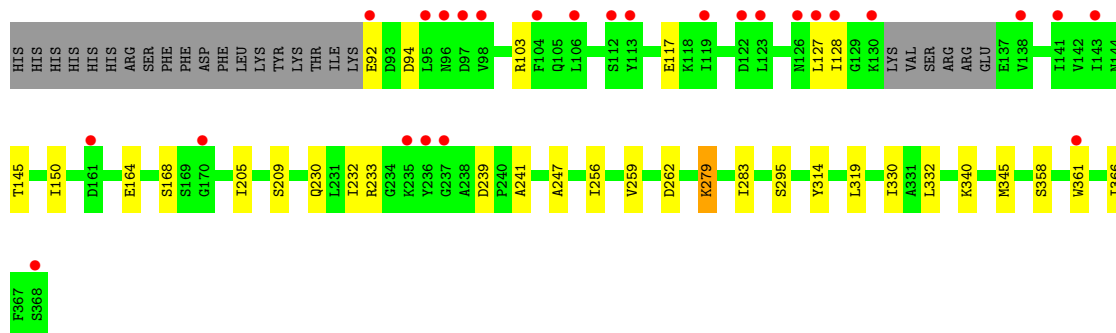
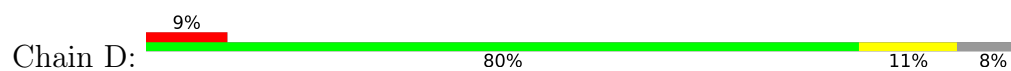
- Molecule 1: Signal recognition particle 54 kDa protein



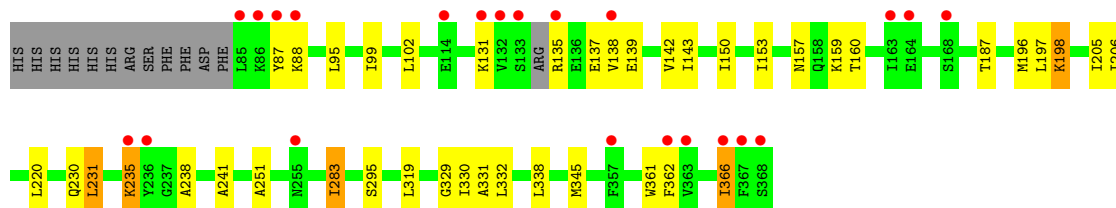
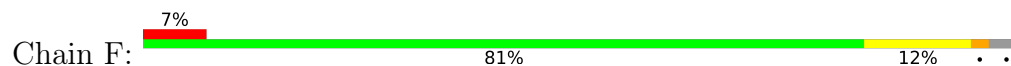
- Molecule 2: Signal recognition particle receptor FtsY



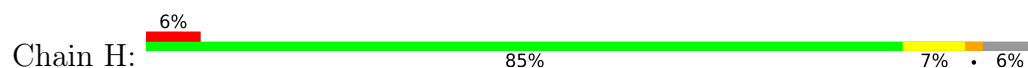
- Molecule 2: Signal recognition particle receptor FtsY

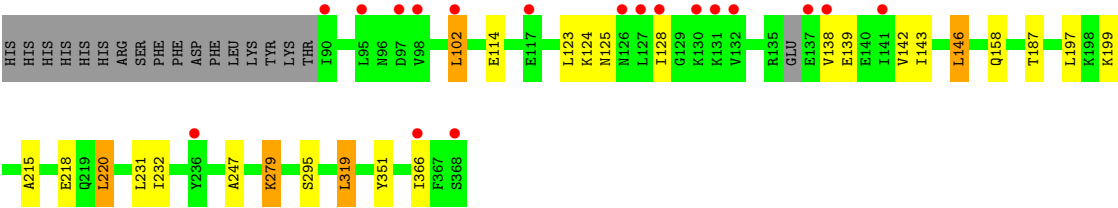


- Molecule 2: Signal recognition particle receptor FtsY



- Molecule 2: Signal recognition particle receptor FtsY





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) 90.1 (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)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.173 , 0.216 0.175 , 0.178	Depositor DCC
R_{free} test set	3836 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
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

Xtriage'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: SO4, MG, GOL, 5GP, GNP

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	0.47	0/2181	0.76	0/2934
1	C	0.41	0/2150	0.72	0/2894
1	E	0.43	0/2152	0.76	0/2896
1	G	0.45	0/2186	0.77	0/2946
2	B	0.48	0/2268	0.74	0/3059
2	D	0.40	0/2159	0.74	2/2915 (0.1%)
2	F	0.41	0/2257	0.70	0/3043
2	H	0.46	0/2233	0.73	0/3010
All	All	0.44	0/17586	0.74	2/23697 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	358	SER	CA-C-N	5.63	125.09	119.24
2	D	358	SER	C-N-CA	5.63	125.09	119.24

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	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2110	0	2180	23	0
1	E	2115	0	2185	12	0
1	G	2150	0	2222	24	0
2	B	2235	0	2310	20	0
2	D	2128	0	2184	17	0
2	F	2228	0	2300	24	0
2	H	2198	0	2268	17	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	2	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	190	0	0	6	3
8	C	128	0	0	4	0
8	D	135	0	0	3	0
8	E	141	0	0	1	0
8	F	106	0	0	2	3
8	G	168	0	0	6	0
8	H	153	0	0	5	0
All	All	19033	0	18162	158	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.

All (158) 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:G:100:MET:HE2	1:G:209:LEU:HD12	1.52	0.91
1:A:202:MET:SD	8:A:567:HOH:O	2.33	0.86
1:E:100:MET:HE2	1:E:209:LEU:HD12	1.60	0.83
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:D:279:LYS:NZ	8:D:501:HOH:O	2.21	0.73
2:F:88:LYS:HG3	2:F:135:ARG:HB2	1.70	0.73
1:C:100:MET:HE2	1:C:209:LEU:HD12	1.69	0.72
1:A:286:ARG:NH1	6:A:305:GOL:O2	2.23	0.72
2:H:114:GLU:OE2	8:H:501:HOH:O	2.09	0.69
1:G:162:ASN:OD1	8:G:401:HOH:O	2.11	0.68
1:G:100:MET:HE1	1:G:206:TYR:HA	1.76	0.67
1:G:189:ARG:HD2	1:G:202:MET:HE3	1.77	0.65
2:H:279:LYS:NZ	8:H:502:HOH:O	2.18	0.65
1:A:159[A]:ASN:OD1	8:A:401:HOH:O	2.14	0.65
2:B:125:ASN:OD1	8:B:501:HOH:O	2.13	0.65
2:F:196:MET:SD	8:F:603:HOH:O	2.54	0.65
2:D:103:ARG:NH1	2:D:117:GLU:OE1	2.29	0.64
2:D:205:ILE:HG22	2:D:230:GLN:HB3	1.80	0.64
2:H:123:LEU:HD22	2:H:146:LEU:HG	1.80	0.63
1:G:176:LYS:NZ	8:G:406:HOH:O	2.33	0.61
6:C:304:GOL:O1	8:C:401:HOH:O	2.16	0.61
2:F:205:ILE:HG22	2:F:230:GLN:HB3	1.82	0.61
2:F:329:GLY:HA2	2:F:366:ILE:HD11	1.82	0.61
2:H:102:LEU:HG	2:H:146:LEU:HD12	1.83	0.61
2:F:153:ILE:O	2:F:157:ASN:ND2	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:187:THR:HG23	2:F:220:LEU:HD13	1.84	0.60
1:A:24:ASP:OD1	1:A:52:LYS:NZ	2.34	0.60
2:H:187:THR:HG23	2:H:220:LEU:HD13	1.84	0.59
1:C:232:ARG:NH2	7:C:306:SO4:O4	2.35	0.59
2:B:279:LYS:NZ	8:B:503:HOH:O	2.24	0.59
1:G:286:ARG:NH1	6:G:306:GOL:O2	2.36	0.58
1:C:167:ALA:HB1	1:C:209:LEU:HD11	1.86	0.58
2:H:158:GLN:NE2	8:H:504:HOH:O	2.35	0.57
2:F:241:ALA:HB1	2:F:283:ILE:HD13	1.85	0.57
2:H:199:LYS:NZ	8:H:505:HOH:O	2.36	0.57
1:C:218:ILE:HD11	1:C:222:ILE:HG21	1.87	0.56
2:B:306:ARG:NE	8:B:505:HOH:O	2.26	0.56
1:C:24:ASP:OD1	1:C:52:LYS:NZ	2.31	0.56
2:H:295:SER:HB3	2:H:319:LEU:HD12	1.87	0.56
2:D:319:LEU:HD21	2:D:330:ILE:HG21	1.87	0.55
1:A:249:GLY:HA2	2:B:267:MET:HE2	1.87	0.55
1:C:51:ILE:HD13	1:C:74:VAL:HG22	1.89	0.55
2:B:124:LYS:O	2:B:128:ILE:HG12	2.07	0.55
1:G:189:ARG:CD	1:G:202:MET:HE3	2.36	0.55
2:F:198:LYS:NZ	8:F:502:HOH:O	2.36	0.54
2:D:314:TYR:CE2	2:D:340:LYS:HD3	2.42	0.54
1:C:16:SER:HB2	1:C:21:LYS:HE3	1.90	0.53
6:A:306:GOL:O1	8:A:402:HOH:O	2.19	0.53
2:H:139:GLU:O	2:H:143:ILE:HG12	2.09	0.53
2:H:124:LYS:O	2:H:128:ILE:HG12	2.10	0.52
2:H:232:ILE:HG13	2:H:247:ALA:HA	1.91	0.52
1:C:176:LYS:NZ	8:C:410:HOH:O	2.42	0.52
1:C:291:ILE:O	1:C:292:LEU:HB2	2.10	0.52
2:D:241:ALA:HB1	2:D:283:ILE:HD12	1.90	0.52
1:A:54:ARG:NH1	1:A:77:GLU:OE2	2.41	0.52
1:C:286:ARG:NH2	8:C:412:HOH:O	2.43	0.52
1:A:260:VAL:HG21	1:A:267:ILE:HD11	1.91	0.51
1:E:54:ARG:HH11	1:E:73:ILE:HG23	1.75	0.51
1:A:243:ILE:HG12	1:A:269:PHE:HB2	1.92	0.51
2:F:345:MET:HE1	2:F:361:TRP:CZ3	2.45	0.51
2:D:164:GLU:O	2:D:168:SER:OG	2.22	0.51
1:C:270:ILE:HD13	6:C:304:GOL:H2	1.92	0.51
1:A:86:LYS:NZ	8:A:414:HOH:O	2.45	0.50
2:D:205:ILE:HD11	2:D:259:VAL:HG22	1.94	0.50
2:D:233:ARG:NH2	8:D:506:HOH:O	2.40	0.50
1:E:218:ILE:HD11	1:E:222:ILE:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:SER:HB3	2:D:319:LEU:HD22	1.94	0.50
2:D:345:MET:HE1	2:D:361:TRP:CZ3	2.47	0.50
1:G:243:ILE:HG12	1:G:269:PHE:HB2	1.94	0.50
1:A:22:ALA:HB1	1:A:65:GLU:HB3	1.92	0.50
2:F:235:LYS:HD2	2:F:238:ALA:HB2	1.93	0.50
2:D:150:ILE:HG23	2:D:332:LEU:HD13	1.93	0.50
2:F:205:ILE:HD11	2:F:251:ALA:HB2	1.93	0.49
1:A:215:ILE:HG12	1:A:241:SER:HB2	1.95	0.49
2:D:205:ILE:HG23	2:D:256:ILE:HG21	1.95	0.49
1:G:287:PHE:HB2	6:G:306:GOL:H11	1.94	0.49
1:A:92:PRO:HG3	1:A:181:ILE:HD11	1.95	0.49
1:C:234:HIS:HB2	1:C:263:THR:HG22	1.95	0.48
2:F:331:ALA:HB3	2:F:362:PHE:CE1	2.48	0.48
1:A:42:LYS:HB3	6:A:304:GOL:H32	1.95	0.48
2:B:88:LYS:N	2:B:132:VAL:O	2.42	0.48
2:D:92:GLU:HG2	2:D:94:ASP:HB2	1.96	0.48
1:G:82:PHE:HB2	8:G:452:HOH:O	2.13	0.48
2:F:138:VAL:O	2:F:142:VAL:HG23	2.14	0.48
1:A:234:HIS:HB2	1:A:263:THR:HG22	1.95	0.48
2:F:139:GLU:O	2:F:143:ILE:HG12	2.13	0.48
1:E:19:TYR:OH	1:E:55:LEU:O	2.23	0.47
2:F:295:SER:HB3	2:F:319:LEU:HD22	1.96	0.47
1:G:85:ASP:HA	1:G:284:ALA:HB3	1.95	0.47
1:A:189:ARG:NE	1:A:202:MET:HE3	2.30	0.47
2:F:319:LEU:HD21	2:F:330:ILE:HG21	1.96	0.47
1:C:215:ILE:HG12	1:C:241:SER:HB2	1.95	0.47
1:C:243:ILE:HG12	1:C:269:PHE:HB2	1.98	0.46
1:G:122:LYS:NZ	8:G:415:HOH:O	2.49	0.46
2:B:345:MET:HE3	2:B:345:MET:HB2	1.83	0.46
2:B:257:ASP:OD1	6:B:405:GOL:O2	2.33	0.46
1:C:174:PHE:HD1	1:C:179:MET:HE3	1.81	0.46
1:C:153[A]:GLN:NE2	8:C:407:HOH:O	2.38	0.46
1:A:189:ARG:HD2	1:A:202:MET:HE3	1.97	0.45
2:D:232:ILE:HG13	2:D:247:ALA:HA	1.98	0.45
2:F:157:ASN:O	2:F:159:LYS:NZ	2.45	0.45
1:G:16:SER:N	8:G:417:HOH:O	2.49	0.45
1:G:100:MET:HE3	1:G:211:PRO:HG3	1.98	0.45
1:G:218:ILE:HD11	1:G:222:ILE:HG21	1.98	0.45
2:F:198:LYS:HE2	2:F:198:LYS:HB3	1.84	0.45
1:A:66:ARG:HG3	1:A:69:TRP:H	1.81	0.45
2:F:206:ILE:HB	2:F:231:LEU:HD23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ALA:HB1	2:B:283:ILE:HD13	1.99	0.44
1:E:100:MET:HE1	1:E:206:TYR:HA	1.99	0.44
2:B:204[A]:THR:HG22	8:B:520:HOH:O	2.17	0.44
1:C:244:ILE:HD11	1:C:267:ILE:HD13	2.00	0.44
1:G:137:PRO:HA	5:G:303:5GP:O3'	2.17	0.44
2:B:172:LYS:HA	2:B:173:PRO:HA	1.77	0.44
1:A:22:ALA:CB	1:A:65:GLU:HB3	2.48	0.43
2:B:194:VAL:HG13	2:B:204[A]:THR:HG21	1.99	0.43
2:F:87:TYR:CE1	2:F:131:LYS:HD2	2.54	0.43
1:G:161:GLN:NE2	5:G:303:5GP:H8	2.33	0.43
2:H:102:LEU:HD21	2:H:143:ILE:HD13	2.00	0.43
2:B:195:ASN:O	2:B:199:LYS:HG2	2.19	0.43
1:C:137:PRO:HA	5:C:303:5GP:O3'	2.19	0.43
1:G:104:VAL:HA	1:G:189:ARG:O	2.19	0.43
1:G:274:GLU:OE1	8:G:402:HOH:O	2.22	0.43
2:D:127:LEU:HD21	2:D:145:THR:HG21	2.01	0.43
2:B:86:LYS:HE2	2:B:87:TYR:CZ	2.54	0.43
2:H:351:TYR:CD1	6:H:403:GOL:H32	2.54	0.43
2:F:150:ILE:HG23	2:F:332:LEU:HD13	2.01	0.42
2:B:306:ARG:HG2	2:B:338:LEU:HD21	2.02	0.42
1:A:101:LEU:HD23	1:A:215:ILE:HB	2.01	0.42
6:C:305:GOL:H31	8:D:607:HOH:O	2.19	0.42
2:F:345:MET:HE3	2:F:345:MET:HB2	1.77	0.42
2:D:209:SER:HB2	2:D:262:ASP:O	2.20	0.41
1:E:174:PHE:HB3	1:E:179:MET:HG2	2.01	0.41
2:B:98:VAL:HB	2:B:139:GLU:OE1	2.21	0.41
1:C:27:ILE:HG23	1:C:48:THR:HB	2.03	0.41
1:C:40:ASN:O	1:C:44:VAL:HG23	2.19	0.41
1:E:94:LYS:O	1:E:95:LEU:HD23	2.20	0.41
2:B:171:LYS:HA	2:B:171:LYS:HD3	1.94	0.41
1:C:19:TYR:O	1:C:23:VAL:HG23	2.21	0.41
1:E:134:VAL:HG22	8:E:443:HOH:O	2.20	0.41
2:H:124:LYS:HB2	2:H:124:LYS:HE3	1.84	0.41
1:E:234:HIS:HB2	1:E:263:THR:HG22	2.03	0.41
2:F:95:LEU:O	2:F:99:ILE:HG12	2.21	0.41
2:B:209:SER:HB2	2:B:262:ASP:O	2.21	0.41
1:C:191:GLY:HA2	1:C:195:GLU:O	2.21	0.41
1:G:82:PHE:HE1	1:G:284:ALA:HB1	1.85	0.41
1:G:189:ARG:NE	1:G:202:MET:HE3	2.36	0.41
2:H:215:ALA:HA	2:H:218:GLU:OE1	2.21	0.41
2:B:198:LYS:HG2	8:B:520:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:ASN:O	8:H:503:HOH:O	2.22	0.40
1:A:81:LEU:HG	1:A:261:VAL:HG22	2.02	0.40
1:A:189:ARG:CD	1:A:202:MET:HE3	2.51	0.40
2:F:160:THR:OG1	1:G:86:LYS:NZ	2.55	0.40
1:G:60:PRO:HB3	1:G:69:TRP:CE3	2.56	0.40
1:G:129:LEU:HD23	1:G:183:ILE:HB	2.04	0.40
2:H:138:VAL:O	2:H:142:VAL:HG23	2.21	0.40
1:E:69:TRP:O	1:E:72:SER:OG	2.33	0.40
1:E:167:ALA:HB1	1:E:209:LEU:HD11	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

5.3.1 Protein backbone ⓘ

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	70	73
1	C	228/252 (90%)	226 (99%)	2 (1%)	70	73
1	E	228/252 (90%)	226 (99%)	2 (1%)	70	73
1	G	233/252 (92%)	230 (99%)	3 (1%)	61	61
2	B	247/259 (95%)	244 (99%)	3 (1%)	63	63
2	D	235/259 (91%)	231 (98%)	4 (2%)	53	52
2	F	246/259 (95%)	237 (96%)	9 (4%)	30	22
2	H	243/259 (94%)	235 (97%)	8 (3%)	33	26
All	All	1892/2044 (93%)	1859 (98%)	33 (2%)	51	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	94	LYS
2	B	283	ILE
2	B	358	SER
2	B	366	ILE
1	C	141	ASP
1	C	179	MET
2	D	128	ILE
2	D	239	ASP
2	D	279	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	366	ILE
1	E	94	LYS
1	E	275	LYS
2	F	102	LEU
2	F	137	GLU
2	F	197	LEU
2	F	198	LYS
2	F	231	LEU
2	F	235	LYS
2	F	283	ILE
2	F	338	LEU
2	F	366	ILE
1	G	66	ARG
1	G	242	VAL
1	G	276	ILE
2	H	102	LEU
2	H	146	LEU
2	H	197	LEU
2	H	220	LEU
2	H	231	LEU
2	H	279	LYS
2	H	319	LEU
2	H	366	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	177	ASN
2	B	195	ASN
2	B	200	ASN
2	B	304	GLN
2	D	304	GLN
2	D	349	GLN
1	E	177	ASN
2	F	255	ASN
2	F	304	GLN
1	G	56	ASN
2	H	230	GLN
2	H	311	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	GNP	B	401	4	33,34,34	1.46	3 (9%)	46,54,54	0.75	1 (2%)
6	GOL	A	305	-	5,5,5	0.36	0	5,5,5	0.50	0
6	GOL	E	304	-	5,5,5	0.34	0	5,5,5	0.30	0
6	GOL	G	305	-	5,5,5	0.40	0	5,5,5	0.51	0
5	5GP	E	303	-	26,26,26	0.53	0	40,40,40	0.57	0
3	GNP	C	301	4	33,34,34	1.46	5 (15%)	46,54,54	1.29	5 (10%)
7	SO4	A	307	-	4,4,4	0.14	0	6,6,6	0.05	0
5	5GP	G	303	-	26,26,26	0.60	1 (3%)	40,40,40	0.67	1 (2%)
6	GOL	C	305	-	5,5,5	0.34	0	5,5,5	0.39	0
7	SO4	B	407	-	4,4,4	0.16	0	6,6,6	0.13	0
3	GNP	D	401	4	33,34,34	1.36	3 (9%)	46,54,54	0.89	2 (4%)
6	GOL	B	405	-	5,5,5	0.43	0	5,5,5	0.29	0
5	5GP	C	303	-	26,26,26	0.57	0	40,40,40	0.70	0
7	SO4	G	307	-	4,4,4	0.14	0	6,6,6	0.07	0
7	SO4	A	309	-	4,4,4	0.15	0	6,6,6	0.13	0
7	SO4	C	306	-	4,4,4	0.15	0	6,6,6	0.05	0
5	5GP	A	303	-	26,26,26	0.55	0	40,40,40	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	G	304	-	5,5,5	0.35	0	5,5,5	0.97	0
7	SO4	E	306	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GNP	E	301	4	33,34,34	1.35	6 (18%)	46,54,54	1.26	6 (13%)
6	GOL	H	404	-	5,5,5	0.37	0	5,5,5	0.16	0
7	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	H	403	-	5,5,5	0.51	0	5,5,5	0.54	0
6	GOL	B	403	-	5,5,5	0.40	0	5,5,5	0.47	0
6	GOL	A	306	-	5,5,5	0.35	0	5,5,5	0.32	0
3	GNP	H	401	4	33,34,34	1.31	4 (12%)	46,54,54	0.76	1 (2%)
3	GNP	F	401	4	33,34,34	1.44	4 (12%)	46,54,54	1.06	3 (6%)
6	GOL	A	304	-	5,5,5	0.34	0	5,5,5	0.28	0
6	GOL	F	403	-	5,5,5	0.40	0	5,5,5	0.34	0
6	GOL	G	306	-	5,5,5	0.35	0	5,5,5	0.32	0
7	SO4	A	308	-	4,4,4	0.13	0	6,6,6	0.13	0
6	GOL	D	403	-	5,5,5	0.43	0	5,5,5	0.48	0
7	SO4	H	405	-	4,4,4	0.16	0	6,6,6	0.14	0
3	GNP	A	301	4	33,34,34	1.36	4 (12%)	46,54,54	1.44	6 (13%)
6	GOL	E	305	-	5,5,5	0.35	0	5,5,5	0.55	0
6	GOL	B	404	-	5,5,5	0.30	0	5,5,5	0.37	0
6	GOL	C	304	-	5,5,5	0.31	0	5,5,5	0.30	0
3	GNP	G	301	4	33,34,34	1.33	5 (15%)	46,54,54	1.29	5 (10%)

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	B	401	4	-	3/18/38/38	0/3/3/3
6	GOL	A	305	-	-	0/4/4/4	-
6	GOL	E	304	-	-	4/4/4/4	-
6	GOL	G	305	-	-	0/4/4/4	-
5	5GP	E	303	-	-	2/10/26/26	0/3/3/3
3	GNP	C	301	4	-	2/18/38/38	0/3/3/3
5	5GP	G	303	-	-	2/10/26/26	0/3/3/3
6	GOL	C	305	-	-	0/4/4/4	-
3	GNP	D	401	4	-	3/18/38/38	0/3/3/3
6	GOL	B	405	-	-	0/4/4/4	-
5	5GP	C	303	-	-	2/10/26/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5GP	A	303	-	-	1/10/26/26	0/3/3/3
6	GOL	B	406	-	-	2/4/4/4	-
6	GOL	G	304	-	-	2/4/4/4	-
3	GNP	E	301	4	-	2/18/38/38	0/3/3/3
6	GOL	H	404	-	-	2/4/4/4	-
6	GOL	H	403	-	-	3/4/4/4	-
6	GOL	B	403	-	-	2/4/4/4	-
6	GOL	A	306	-	-	2/4/4/4	-
3	GNP	H	401	4	-	3/18/38/38	0/3/3/3
3	GNP	F	401	4	-	3/18/38/38	0/3/3/3
6	GOL	A	304	-	-	4/4/4/4	-
6	GOL	F	403	-	-	2/4/4/4	-
6	GOL	G	306	-	-	4/4/4/4	-
6	GOL	D	403	-	-	2/4/4/4	-
3	GNP	A	301	4	-	2/18/38/38	0/3/3/3
6	GOL	E	305	-	-	2/4/4/4	-
6	GOL	B	404	-	-	0/4/4/4	-
6	GOL	C	304	-	-	2/4/4/4	-
3	GNP	G	301	4	-	2/18/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	GNP	PB-O3A	-5.75	1.51	1.59
3	F	401	GNP	PB-O3A	-5.69	1.51	1.59
3	D	401	GNP	PB-O3A	-5.06	1.52	1.59
3	A	301	GNP	PG-O1G	4.99	1.54	1.46
3	C	301	GNP	PG-O1G	4.53	1.53	1.46
3	E	301	GNP	PG-O1G	4.34	1.53	1.46
3	H	401	GNP	PB-O3A	-4.20	1.53	1.59
3	G	301	GNP	PB-O3A	-4.09	1.53	1.59
3	C	301	GNP	PB-O2B	-3.89	1.46	1.56
3	E	301	GNP	PB-O3A	-3.67	1.54	1.59
3	D	401	GNP	PB-O2B	-3.60	1.47	1.56
3	C	301	GNP	PB-O3A	-3.57	1.54	1.59
3	G	301	GNP	PB-O2B	-3.48	1.47	1.56
3	B	401	GNP	PB-O2B	-3.43	1.47	1.56
3	B	401	GNP	PG-O1G	3.40	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	401	GNP	PB-O2B	-3.36	1.47	1.56
3	F	401	GNP	PG-O1G	3.23	1.51	1.46
3	G	301	GNP	PG-O1G	3.23	1.51	1.46
3	A	301	GNP	PB-O3A	-3.20	1.55	1.59
3	H	401	GNP	PG-O1G	3.16	1.51	1.46
3	A	301	GNP	PB-O2B	-3.08	1.48	1.56
3	D	401	GNP	PG-O1G	3.03	1.51	1.46
3	F	401	GNP	PB-O2B	-2.94	1.48	1.56
3	E	301	GNP	PB-O2B	-2.60	1.49	1.56
3	C	301	GNP	PG-O2G	-2.56	1.49	1.56
3	E	301	GNP	PB-O1B	2.48	1.50	1.46
3	G	301	GNP	PG-O2G	-2.34	1.50	1.56
3	G	301	GNP	PB-O1B	2.31	1.49	1.46
3	E	301	GNP	PG-O2G	-2.30	1.50	1.56
3	F	401	GNP	PG-O3G	-2.29	1.50	1.56
3	A	301	GNP	PG-O2G	-2.23	1.50	1.56
3	H	401	GNP	PB-O1B	2.22	1.49	1.46
3	C	301	GNP	PB-O1B	2.15	1.49	1.46
3	E	301	GNP	PG-O3G	-2.11	1.51	1.56
5	G	303	5GP	P-OP2	-2.04	1.47	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	GNP	O2B-PB-O1B	5.03	120.46	109.92
3	A	301	GNP	O1B-PB-N3B	-4.64	104.94	111.77
3	G	301	GNP	O1G-PG-N3B	-4.55	105.06	111.77
3	A	301	GNP	O2B-PB-O1B	4.30	118.93	109.92
3	F	401	GNP	O2B-PB-O1B	4.15	118.63	109.92
3	F	401	GNP	O1B-PB-N3B	-4.02	105.86	111.77
3	D	401	GNP	O2B-PB-O1B	3.84	117.97	109.92
3	C	301	GNP	O2B-PB-O1B	3.81	117.91	109.92
3	C	301	GNP	O3G-PG-O1G	-3.71	104.13	113.45
3	G	301	GNP	O2B-PB-O1B	3.65	117.57	109.92
3	A	301	GNP	O1G-PG-N3B	-3.41	106.75	111.77
3	A	301	GNP	O3G-PG-O1G	-3.24	105.30	113.45
3	E	301	GNP	O3G-PG-O1G	-3.19	105.44	113.45
3	C	301	GNP	O2G-PG-O3G	3.11	115.92	107.64
3	C	301	GNP	O1G-PG-N3B	-3.08	107.23	111.77
3	G	301	GNP	O2G-PG-O3G	2.80	115.09	107.64
3	A	301	GNP	O2G-PG-O3G	2.69	114.81	107.64
3	E	301	GNP	O1B-PB-N3B	-2.65	107.88	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	GNP	O3G-PG-O1G	-2.61	106.89	113.45
3	E	301	GNP	O1G-PG-N3B	-2.51	108.08	111.77
3	G	301	GNP	O1B-PB-N3B	-2.45	108.16	111.77
3	E	301	GNP	O2G-PG-O3G	2.41	114.07	107.64
3	D	401	GNP	O1G-PG-N3B	-2.36	108.30	111.77
5	G	303	5GP	OP3-P-OP1	2.26	119.52	110.68
3	B	401	GNP	O1G-PG-N3B	-2.21	108.52	111.77
3	E	301	GNP	C2'-C1'-N9	2.16	119.34	113.22
3	F	401	GNP	O1G-PG-N3B	-2.14	108.62	111.77
3	H	401	GNP	O2B-PB-O1B	2.13	114.39	109.92
3	C	301	GNP	O1B-PB-N3B	-2.05	108.75	111.77
3	A	301	GNP	C2'-C1'-N9	2.00	118.89	113.22

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GNP	PG-N3B-PB-O1B
3	A	301	GNP	PG-N3B-PB-O3A
3	B	401	GNP	PB-N3B-PG-O1G
3	B	401	GNP	PG-N3B-PB-O1B
3	B	401	GNP	PG-N3B-PB-O3A
3	C	301	GNP	PG-N3B-PB-O1B
3	C	301	GNP	PG-N3B-PB-O3A
3	D	401	GNP	PB-N3B-PG-O1G
3	D	401	GNP	PG-N3B-PB-O1B
3	E	301	GNP	PG-N3B-PB-O1B
3	E	301	GNP	PG-N3B-PB-O3A
3	F	401	GNP	PB-N3B-PG-O1G
3	F	401	GNP	PG-N3B-PB-O1B
3	F	401	GNP	PG-N3B-PB-O3A
3	G	301	GNP	PG-N3B-PB-O1B
3	G	301	GNP	PG-N3B-PB-O3A
3	H	401	GNP	PB-N3B-PG-O1G
3	H	401	GNP	PG-N3B-PB-O1B
3	H	401	GNP	PG-N3B-PB-O3A
5	C	303	5GP	C4'-C5'-O5'-P
5	G	303	5GP	C4'-C5'-O5'-P
6	A	304	GOL	O1-C1-C2-C3
6	A	304	GOL	C1-C2-C3-O3
6	A	306	GOL	O1-C1-C2-C3
6	B	403	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	406	GOL	O1-C1-C2-C3
6	D	403	GOL	O1-C1-C2-C3
6	E	305	GOL	O1-C1-C2-C3
6	F	403	GOL	O1-C1-C2-C3
6	G	304	GOL	C1-C2-C3-O3
6	G	306	GOL	O1-C1-C2-C3
6	G	306	GOL	C1-C2-C3-O3
6	H	403	GOL	O1-C1-C2-C3
6	H	404	GOL	O1-C1-C2-C3
6	A	304	GOL	O1-C1-C2-O2
6	D	403	GOL	O1-C1-C2-O2
5	E	303	5GP	C4'-C5'-O5'-P
6	E	304	GOL	C1-C2-C3-O3
6	B	403	GOL	O1-C1-C2-O2
6	B	406	GOL	O1-C1-C2-O2
6	E	304	GOL	O2-C2-C3-O3
6	F	403	GOL	O1-C1-C2-O2
5	A	303	5GP	C4'-C5'-O5'-P
6	A	306	GOL	O1-C1-C2-O2
6	E	305	GOL	O1-C1-C2-O2
6	G	306	GOL	O1-C1-C2-O2
6	G	306	GOL	O2-C2-C3-O3
6	H	403	GOL	O1-C1-C2-O2
6	H	404	GOL	O1-C1-C2-O2
6	A	304	GOL	O2-C2-C3-O3
6	E	304	GOL	O1-C1-C2-O2
6	C	304	GOL	C1-C2-C3-O3
3	D	401	GNP	PG-N3B-PB-O3A
6	G	304	GOL	O2-C2-C3-O3
6	C	304	GOL	O2-C2-C3-O3
5	E	303	5GP	O4'-C4'-C5'-O5'
5	G	303	5GP	O4'-C4'-C5'-O5'
6	E	304	GOL	O1-C1-C2-C3
5	C	303	5GP	O4'-C4'-C5'-O5'
6	H	403	GOL	O2-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 14 short contacts:

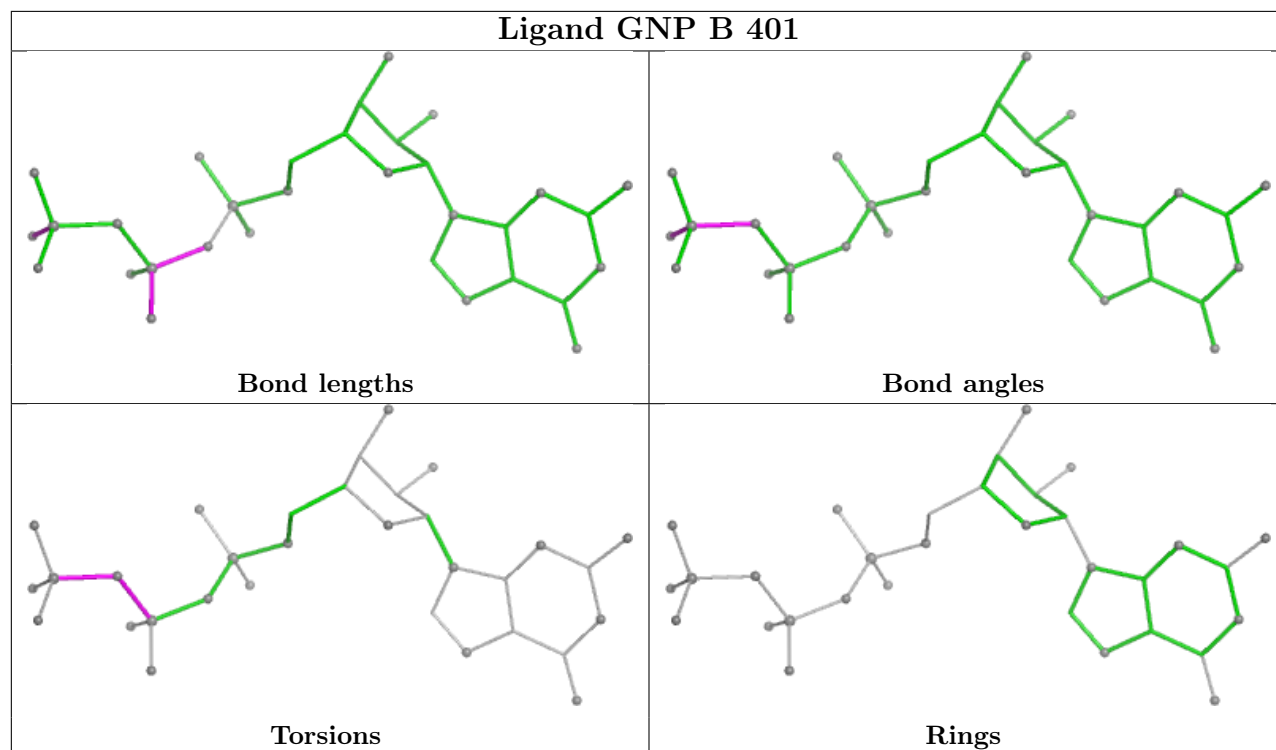
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	305	GOL	1	0
5	G	303	5GP	2	0

Continued on next page...

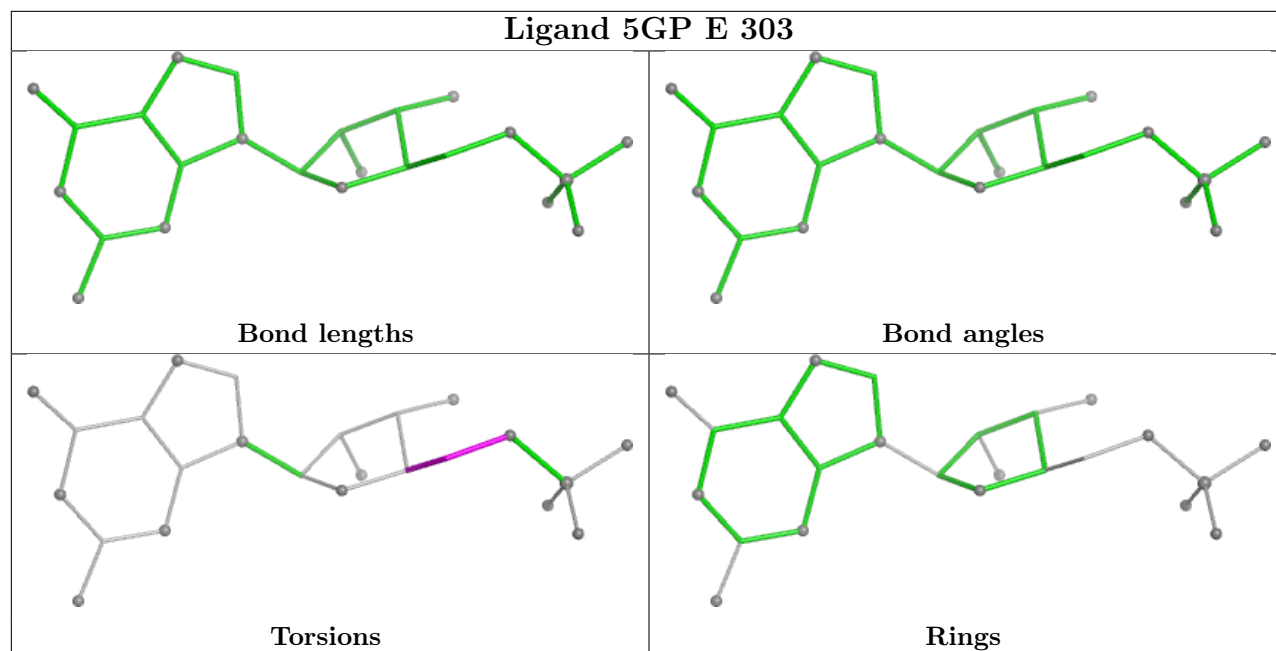
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	305	GOL	1	0
6	B	405	GOL	1	0
5	C	303	5GP	1	0
7	C	306	SO4	1	0
6	H	403	GOL	1	0
6	A	306	GOL	1	0
6	A	304	GOL	1	0
6	G	306	GOL	2	0
6	C	304	GOL	2	0

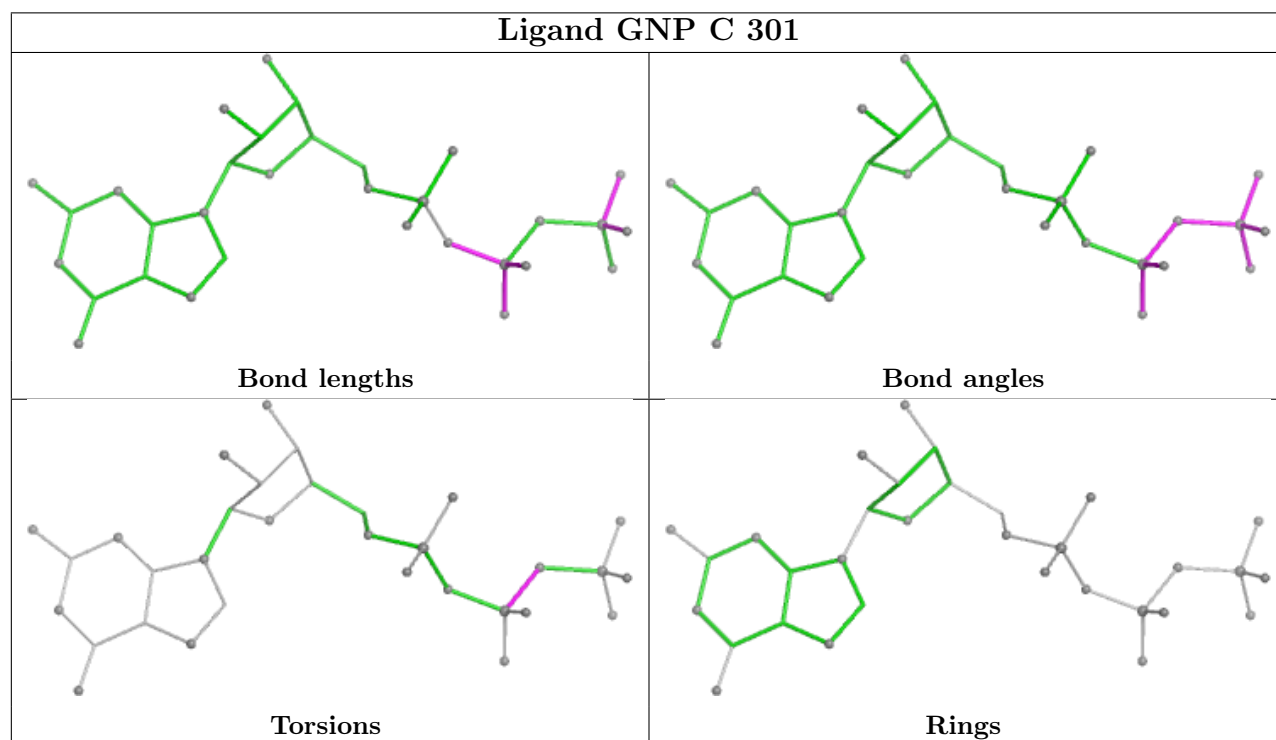
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



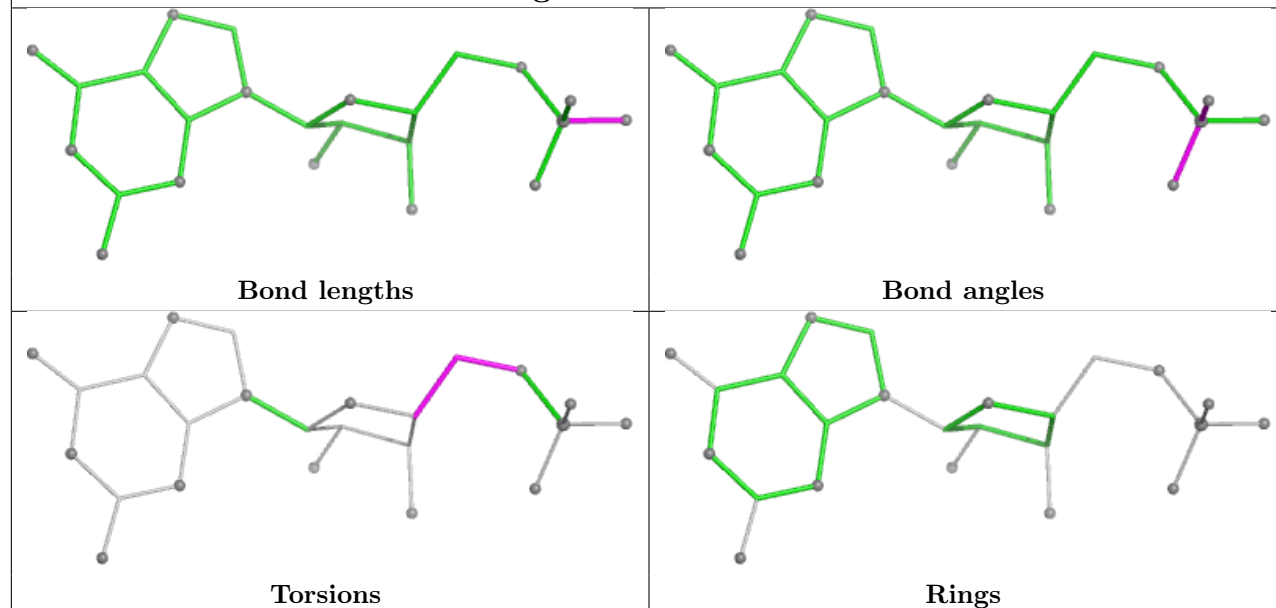
Ligand 5GP E 303



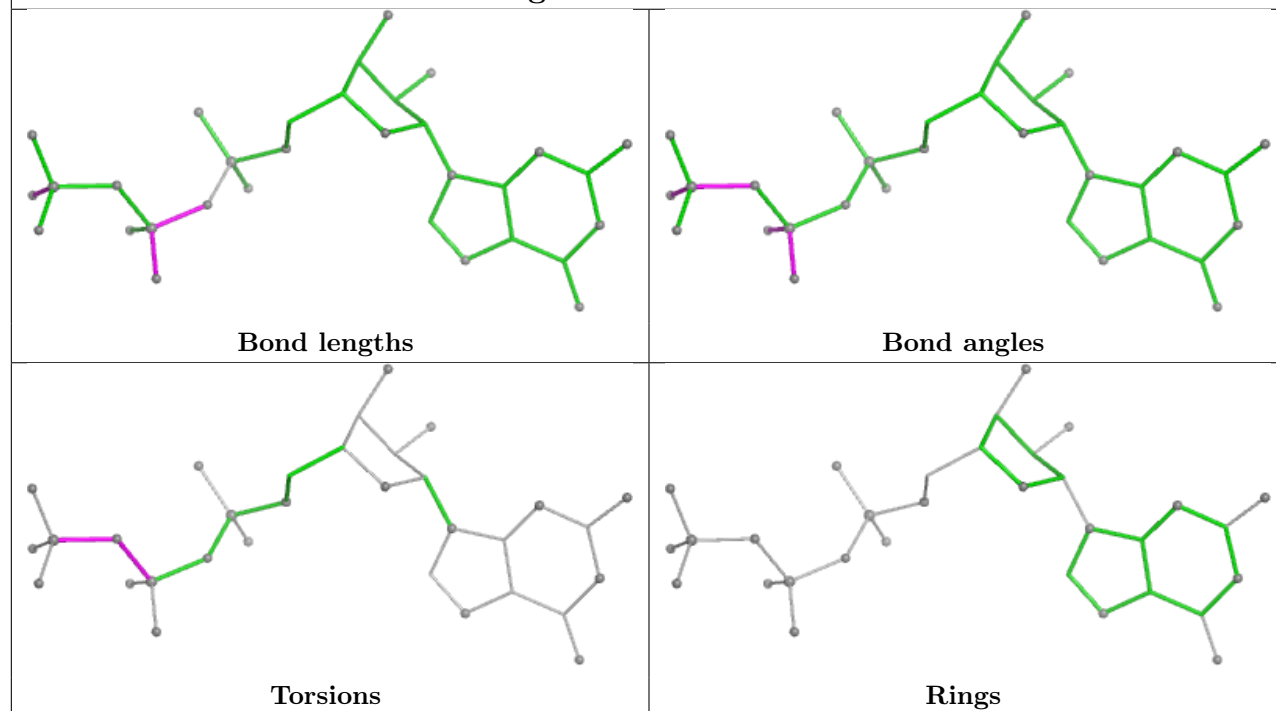
Ligand GNP C 301



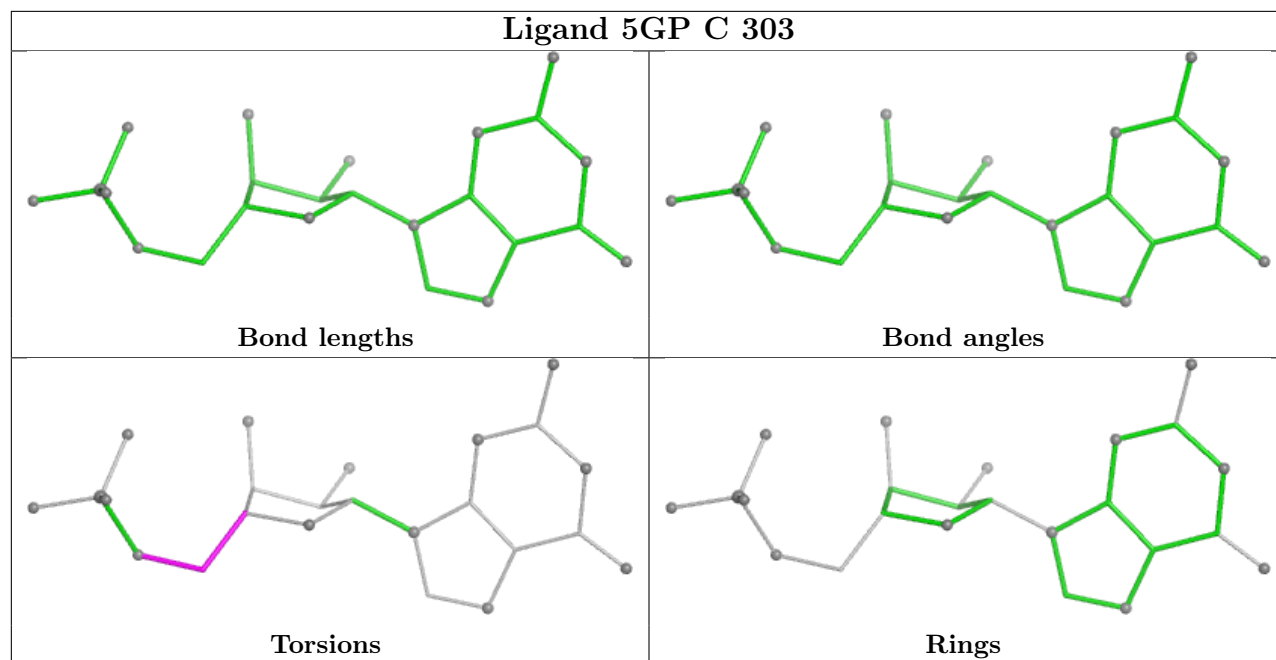
Ligand 5GP G 303



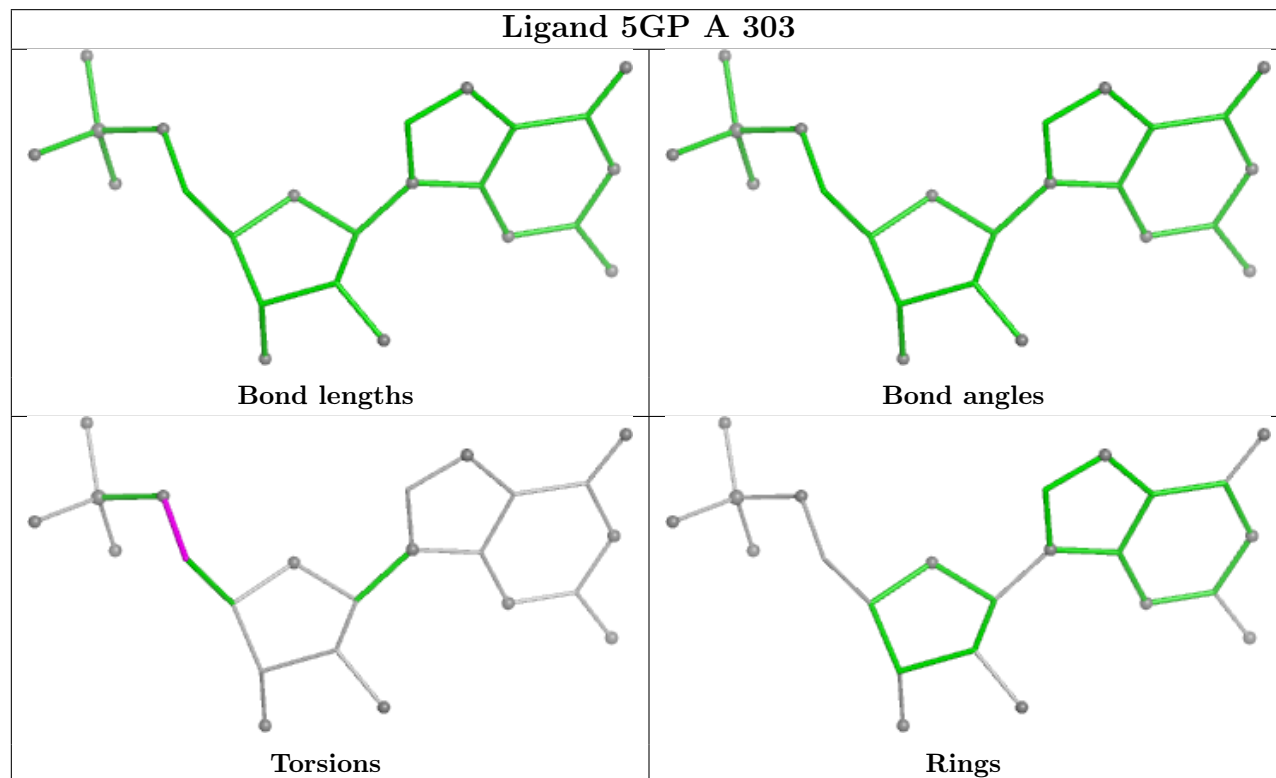
Ligand GNP D 401

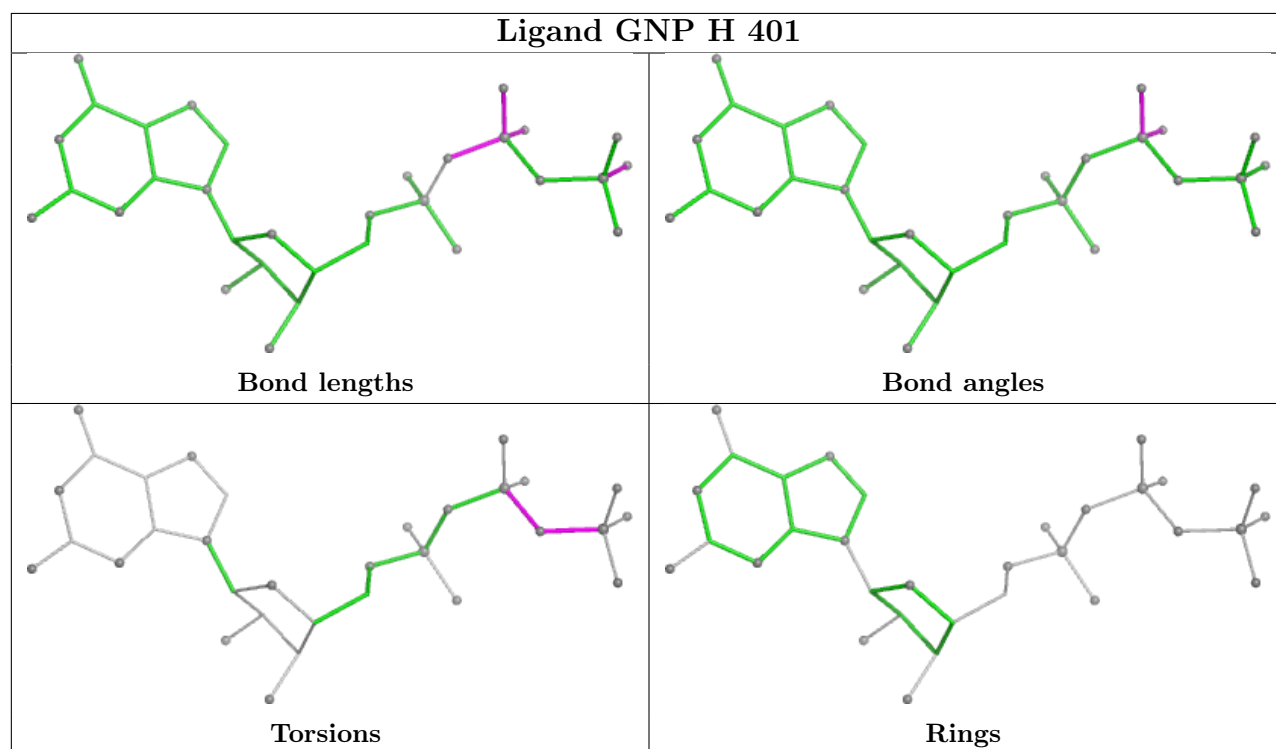
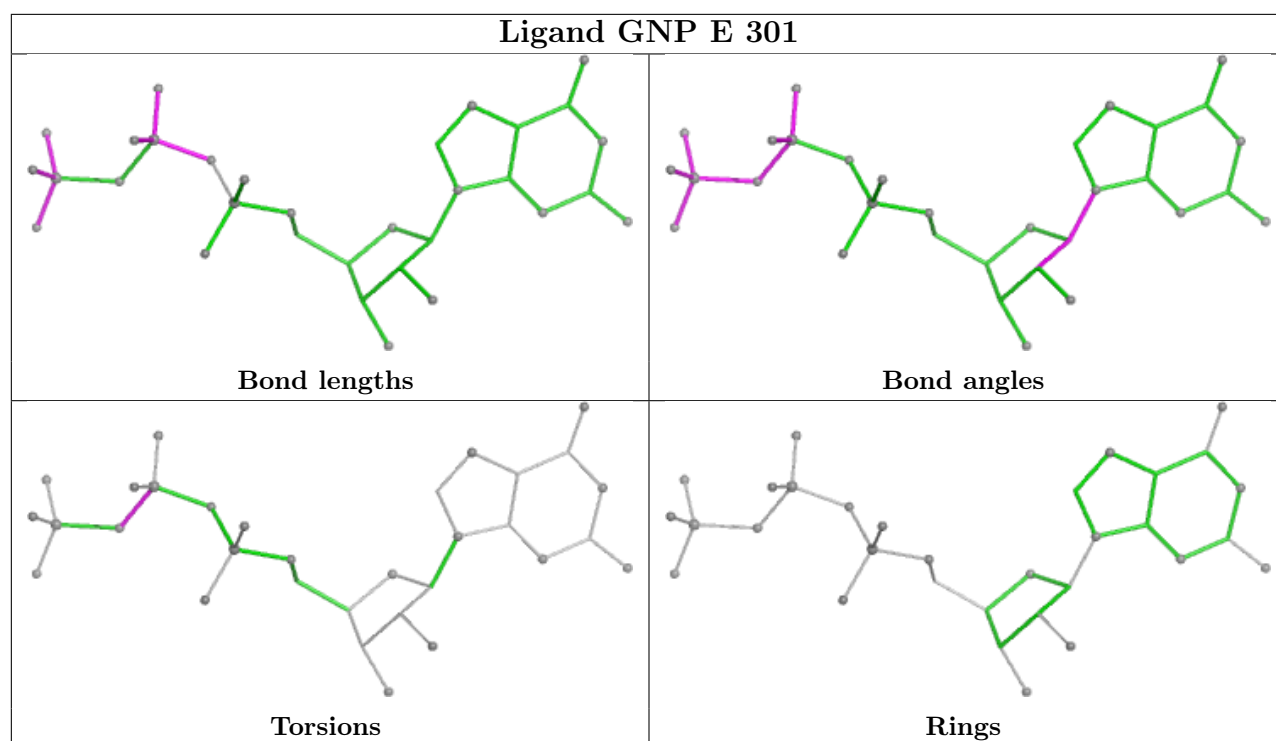


Ligand 5GP C 303

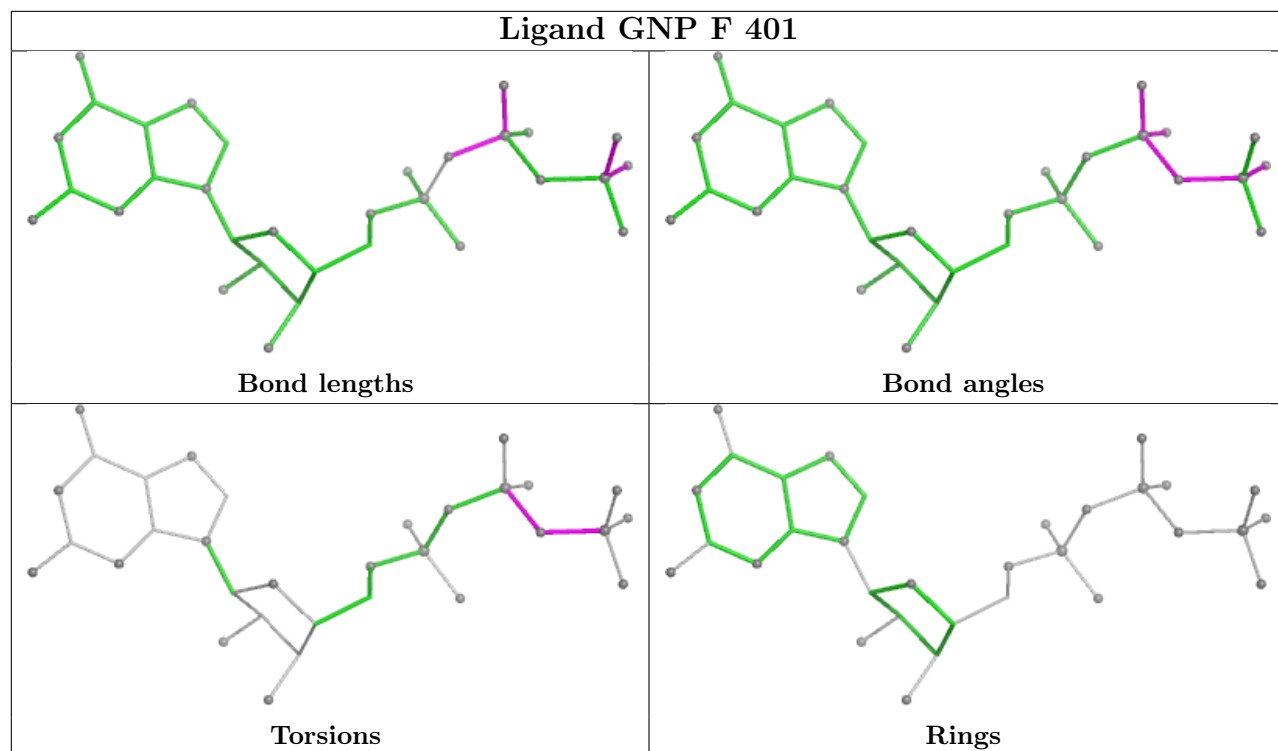


Ligand 5GP A 303

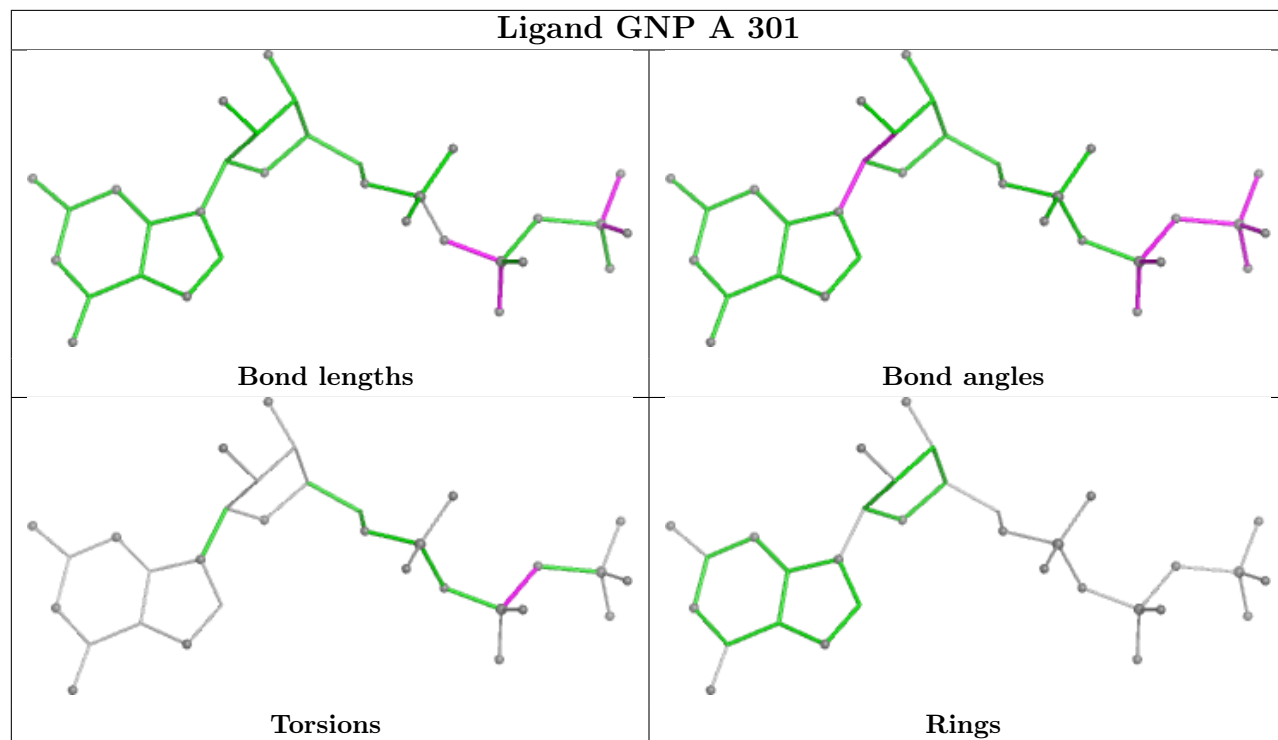


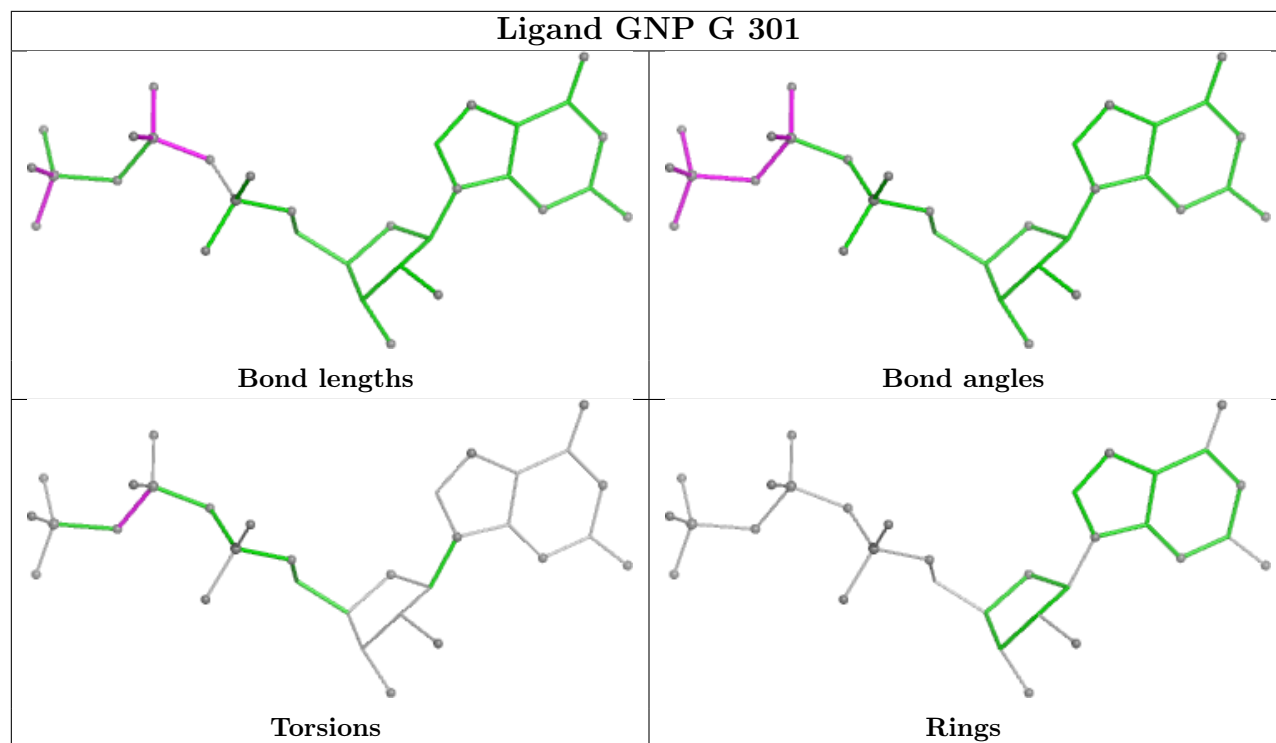


Ligand GNP F 401



Ligand GNP A 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.17	13 (4%)	36	39	16, 34, 73, 113	2 (0%)
1	C	270/298 (90%)	0.56	28 (10%)	11	12	19, 44, 106, 135	2 (0%)
1	E	271/298 (90%)	0.39	23 (8%)	16	17	17, 39, 97, 126	1 (0%)
1	G	277/298 (92%)	0.23	9 (3%)	50	54	18, 38, 70, 112	0
2	B	283/296 (95%)	0.08	10 (3%)	47	50	19, 33, 64, 107	1 (0%)
2	D	271/296 (91%)	0.58	26 (9%)	13	14	22, 44, 100, 120	1 (0%)
2	F	283/296 (95%)	0.67	22 (7%)	19	20	23, 46, 79, 123	0
2	H	278/296 (93%)	0.29	18 (6%)	25	26	19, 35, 90, 117	2 (0%)
All	All	2207/2376 (92%)	0.37	149 (6%)	23	24	16, 39, 89, 135	9 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	85	LEU	6.7
1	G	63	VAL	6.0
2	F	236	TYR	5.5
1	A	63	VAL	5.3
2	D	130	LYS	4.9
1	A	64	LEU	4.7
2	H	368	SER	4.5
2	F	132	VAL	4.4
1	A	83	GLY	4.4
1	E	23	VAL	4.4
1	A	82	PHE	4.3
2	D	236	TYR	4.2
2	F	87	TYR	4.1
1	E	292	LEU	4.0
2	D	104	PHE	4.0
2	F	362	PHE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	292	LEU	3.9
1	C	17	THR	3.8
2	F	133	SER	3.8
1	A	86	LYS	3.7
1	C	23	VAL	3.7
1	E	59	LYS	3.7
1	G	292	LEU	3.6
1	C	19	TYR	3.6
1	C	59	LYS	3.6
2	B	132	VAL	3.6
2	D	368	SER	3.5
2	H	132	VAL	3.5
1	E	70	PHE	3.5
2	D	138	VAL	3.4
1	G	64	LEU	3.4
2	F	86	LYS	3.4
2	H	128	ILE	3.4
2	H	137	GLU	3.3
1	E	22	ALA	3.3
2	D	237	GLY	3.3
2	B	86	LYS	3.2
2	H	366	ILE	3.2
1	A	93	THR	3.2
2	B	87	TYR	3.1
1	C	18	PRO	3.1
2	D	170	GLY	3.1
1	A	65	GLU	3.1
2	D	128	ILE	3.1
1	E	27	ILE	3.0
2	F	168	SER	2.9
2	D	235	LYS	2.9
1	C	55	LEU	2.9
1	E	85	ASP	2.9
1	E	69	TRP	2.9
2	F	131	LYS	2.9
2	D	119	ILE	2.9
1	C	56	ASN	2.9
1	C	82	PHE	2.9
2	H	131	LYS	2.8
2	H	126	ASN	2.8
1	A	196	THR	2.8
1	C	291	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	90	ILE	2.8
1	A	59	LYS	2.7
1	E	17	THR	2.7
2	D	143	ILE	2.7
2	F	366	ILE	2.7
1	C	69	TRP	2.7
2	B	133	SER	2.7
2	D	112	SER	2.6
1	G	82	PHE	2.6
1	A	81	LEU	2.6
1	E	47	LEU	2.6
1	E	18	PRO	2.6
1	E	54	ARG	2.6
2	D	106	LEU	2.6
2	F	235	LYS	2.6
1	C	135[A]	TYR	2.5
1	C	22	ALA	2.5
1	C	194	GLU	2.5
1	E	67	LYS	2.5
2	H	95	LEU	2.5
1	C	58	GLU	2.5
1	E	58	GLU	2.5
1	E	196	THR	2.5
1	E	19	TYR	2.4
2	F	368	SER	2.4
2	D	141	ILE	2.4
1	E	66	ARG	2.4
2	D	122	ASP	2.4
2	F	135	ARG	2.4
2	D	95	LEU	2.4
2	D	127	LEU	2.4
1	E	82	PHE	2.4
2	F	357	PHE	2.4
1	C	71	ILE	2.4
2	B	366	ILE	2.4
2	B	135	ARG	2.3
1	E	73	ILE	2.3
1	G	86	LYS	2.3
1	C	75	TYR	2.3
2	F	255	ASN	2.3
1	C	86	LYS	2.3
1	E	21	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	57	LYS	2.3
2	B	168	SER	2.3
2	D	361	TRP	2.3
2	D	126	ASN	2.3
1	C	45	PHE	2.3
2	B	236	TYR	2.3
1	G	61	PRO	2.3
2	D	92	GLU	2.3
2	F	88	LYS	2.2
1	C	30	LEU	2.2
1	E	16	SER	2.2
1	C	73	ILE	2.2
2	F	363	VAL	2.2
1	C	292	LEU	2.2
1	A	16	SER	2.2
1	G	62	SER	2.2
1	C	28	LYS	2.2
2	H	138	VAL	2.2
2	D	123	LEU	2.2
1	G	60	PRO	2.2
1	C	126	LYS	2.2
2	D	113	TYR	2.1
2	F	114	GLU	2.1
2	F	367	PHE	2.1
2	H	117	GLU	2.1
2	H	236[A]	TYR	2.1
2	F	163	ILE	2.1
2	H	97	ASP	2.1
2	H	98	VAL	2.1
1	E	55	LEU	2.1
2	D	97	ASP	2.1
1	C	228	ASP	2.1
2	B	368	SER	2.1
2	F	164	GLU	2.1
2	H	130	LYS	2.1
2	H	102	LEU	2.1
2	H	127	LEU	2.1
2	D	161	ASP	2.1
1	C	16	SER	2.0
1	C	196	THR	2.0
1	C	177	ASN	2.0
2	D	98	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	138	VAL	2.0
1	A	69	TRP	2.0
1	C	57	LYS	2.0
1	G	291	ILE	2.0
2	H	141	ILE	2.0
2	B	126	ASN	2.0
2	D	96	ASN	2.0

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 oligosaccharides 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	0.51	0.18	74,84,86,87	0
7	SO4	C	306	5/5	0.68	0.12	108,109,110,111	0
6	GOL	C	305	6/6	0.71	0.22	67,76,78,79	0
6	GOL	A	304	6/6	0.73	0.21	54,63,71,73	0
5	5GP	A	303	24/24	0.74	0.22	84,97,107,109	24
7	SO4	B	408	5/5	0.79	0.11	119,121,122,122	0
7	SO4	E	306	5/5	0.79	0.14	134,135,136,137	0
7	SO4	G	307	5/5	0.79	0.14	103,104,104,107	0
5	5GP	E	303	24/24	0.80	0.19	58,83,95,99	24
6	GOL	A	306	6/6	0.85	0.17	56,59,63,64	0
6	GOL	E	304	6/6	0.86	0.14	45,46,55,63	0
5	5GP	C	303	24/24	0.86	0.19	53,83,110,112	0
5	5GP	G	303	24/24	0.87	0.18	35,80,100,105	24
6	GOL	B	404	6/6	0.87	0.14	46,58,60,61	0
6	GOL	C	304	6/6	0.87	0.12	46,51,56,59	0
7	SO4	A	307	5/5	0.87	0.10	59,67,71,72	0

Continued on next page...

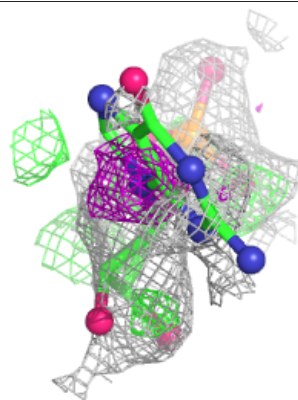
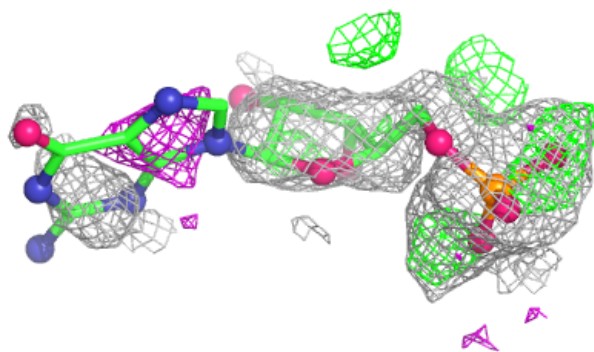
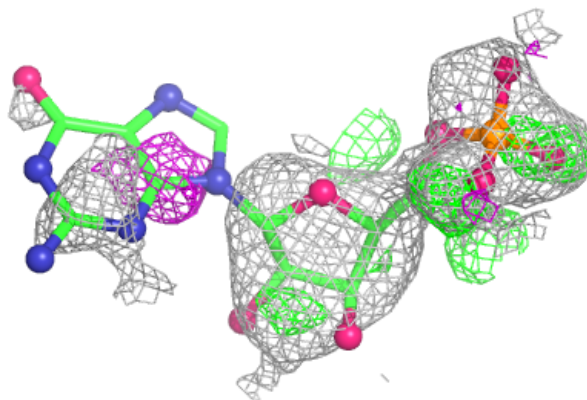
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	A	309	5/5	0.88	0.10	52,66,81,84	0
6	GOL	B	406	6/6	0.88	0.12	65,72,74,77	0
6	GOL	G	305	6/6	0.88	0.13	45,54,60,60	0
6	GOL	B	403	6/6	0.88	0.14	45,47,52,52	0
6	GOL	B	405	6/6	0.88	0.12	40,45,52,54	0
6	GOL	E	305	6/6	0.89	0.14	41,55,59,63	0
6	GOL	F	403	6/6	0.89	0.12	50,55,58,58	0
6	GOL	G	306	6/6	0.90	0.12	39,52,53,56	0
7	SO4	A	308	5/5	0.90	0.09	56,58,62,71	0
6	GOL	G	304	6/6	0.90	0.11	30,37,51,61	0
7	SO4	B	407	5/5	0.90	0.09	38,44,60,65	0
7	SO4	H	405	5/5	0.92	0.09	58,60,68,70	0
6	GOL	A	305	6/6	0.93	0.11	29,35,43,45	0
6	GOL	H	403	6/6	0.93	0.09	35,40,43,45	0
6	GOL	D	403	6/6	0.94	0.08	40,43,47,48	0
3	GNP	E	301	32/32	0.98	0.05	16,23,30,31	0
3	GNP	F	401	32/32	0.98	0.05	18,22,27,30	0
4	MG	B	402	1/1	0.98	0.03	19,19,19,19	0
4	MG	H	402	1/1	0.98	0.04	21,21,21,21	0
3	GNP	C	301	32/32	0.98	0.05	17,24,28,28	0
4	MG	C	302	1/1	0.99	0.03	25,25,25,25	0
4	MG	D	402	1/1	0.99	0.04	22,22,22,22	0
4	MG	E	302	1/1	0.99	0.05	25,25,25,25	0
4	MG	G	302	1/1	0.99	0.02	22,22,22,22	0
3	GNP	B	401	32/32	0.99	0.04	12,18,23,24	0
3	GNP	A	301	32/32	0.99	0.04	13,20,23,24	0
3	GNP	G	301	32/32	0.99	0.04	14,20,24,27	0
3	GNP	H	401	32/32	0.99	0.04	16,22,25,26	0
3	GNP	D	401	32/32	0.99	0.05	17,23,29,31	0
4	MG	F	402	1/1	1.00	0.01	24,24,24,24	0
4	MG	A	302	1/1	1.00	0.01	20,20,20,20	0

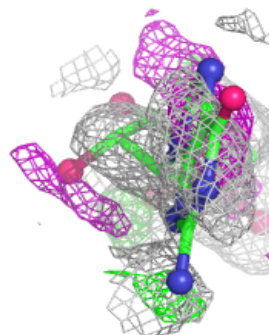
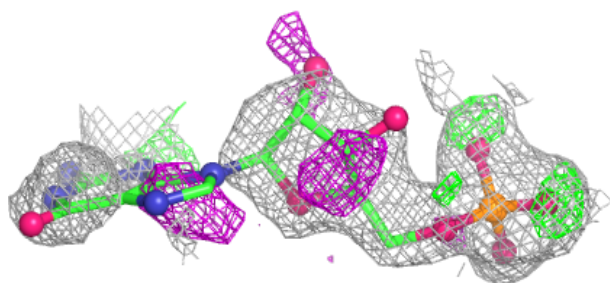
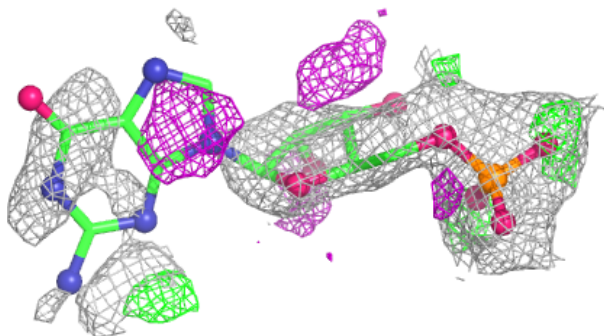
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5GP A 303:

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

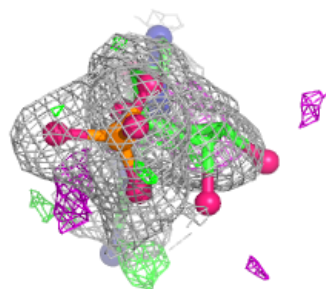
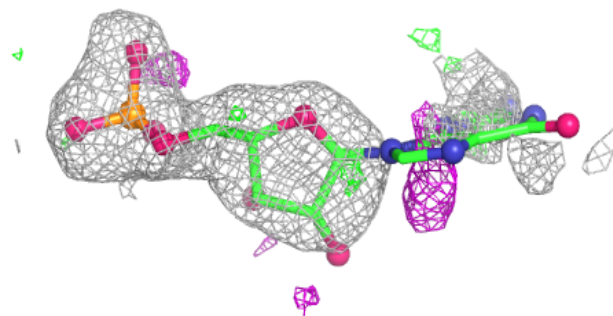
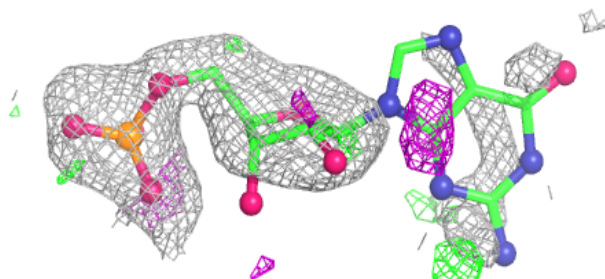
**Electron density around 5GP E 303:**

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

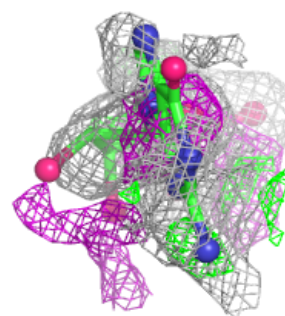
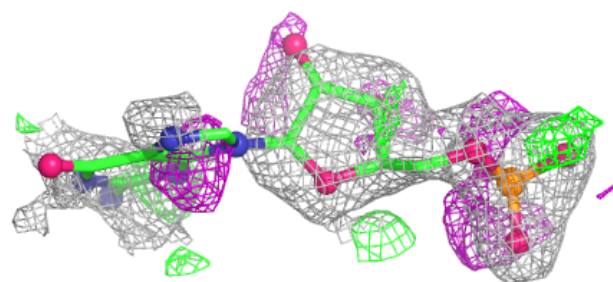
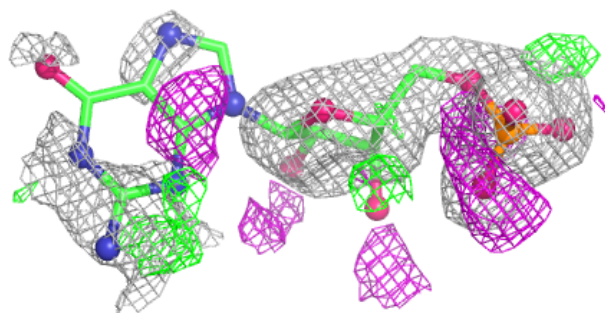


Electron density around 5GP C 303:

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

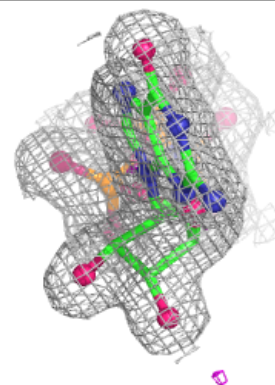
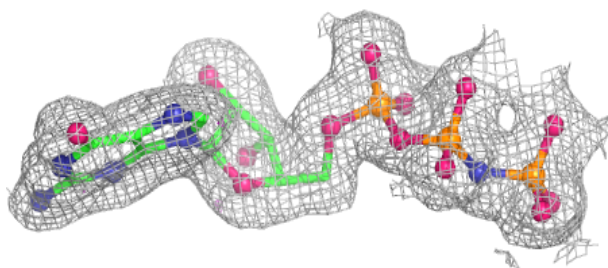
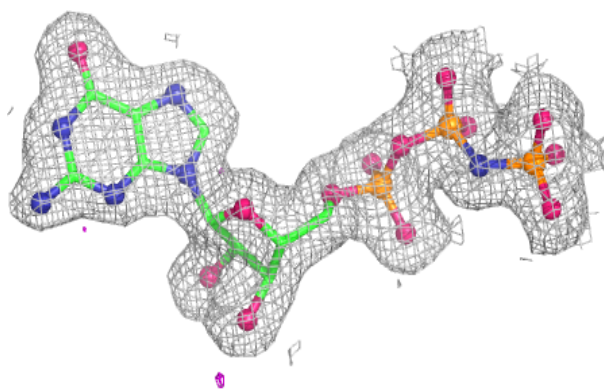
**Electron density around 5GP G 303:**

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

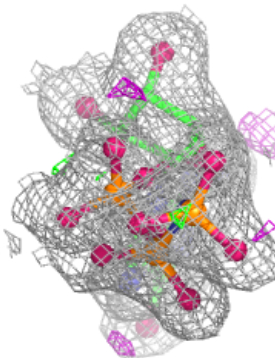
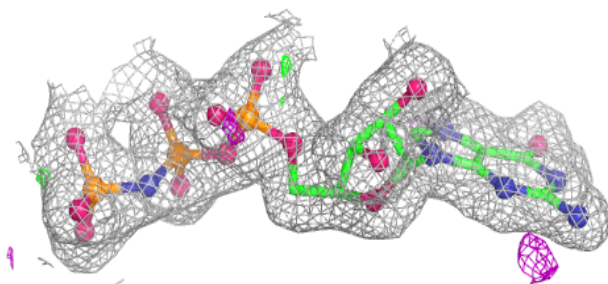
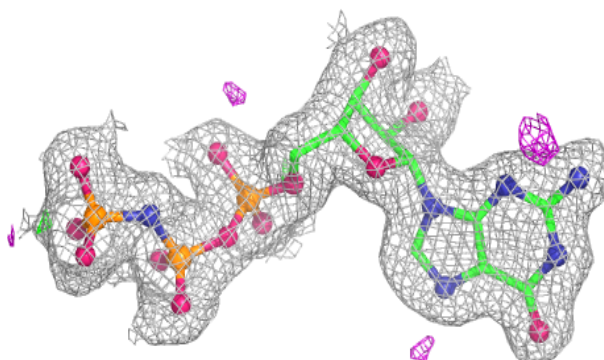


Electron density around GNP E 301:

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

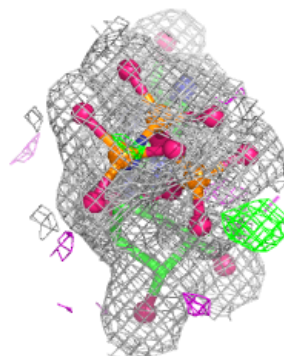
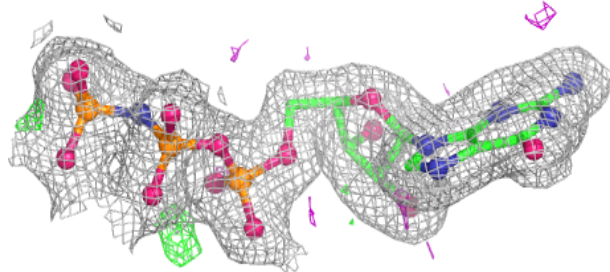
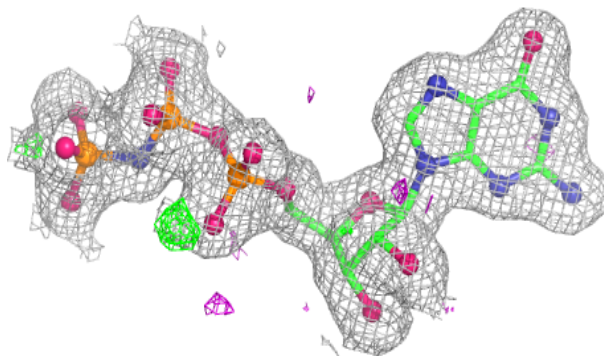
**Electron density around GNP F 401:**

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

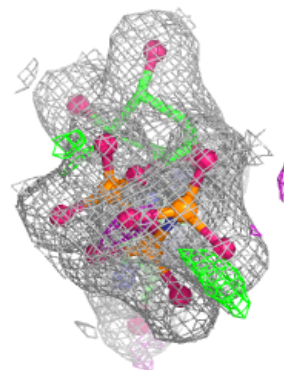
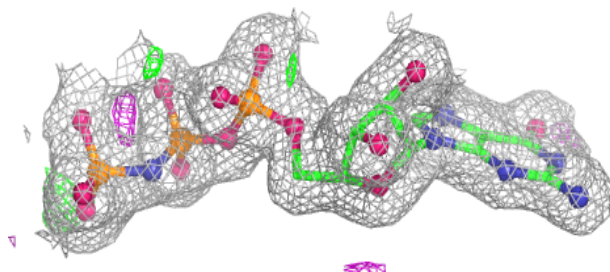
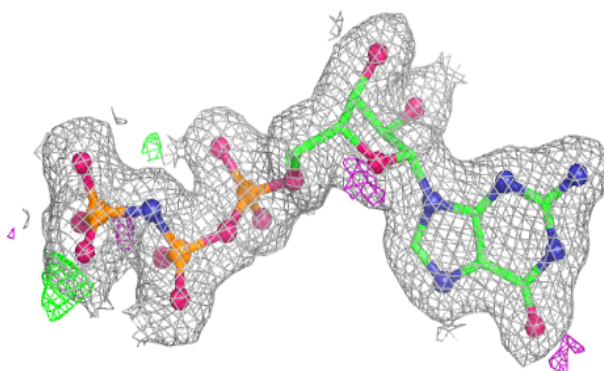


Electron density around GNP C 301:

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

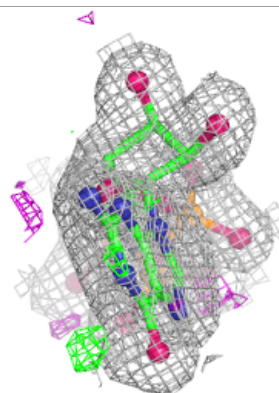
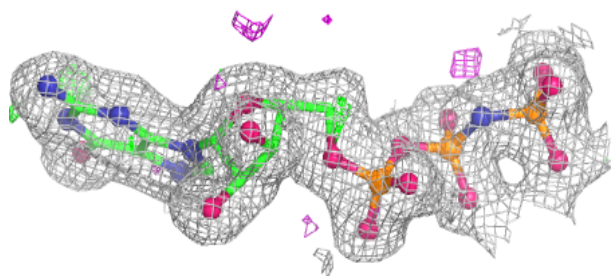
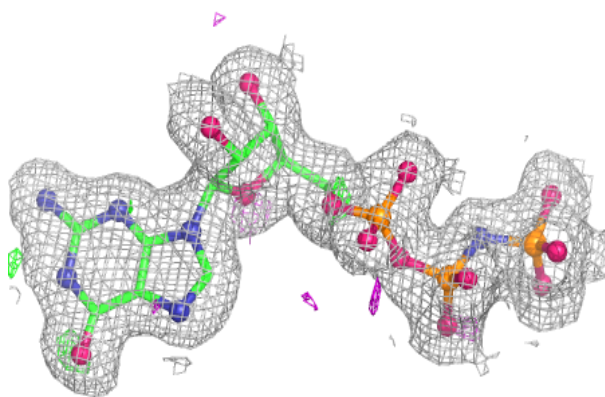
**Electron density around GNP B 401:**

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

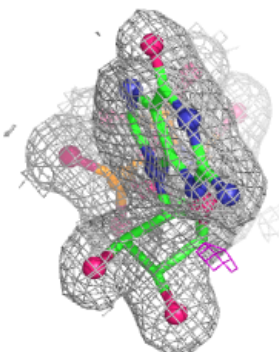
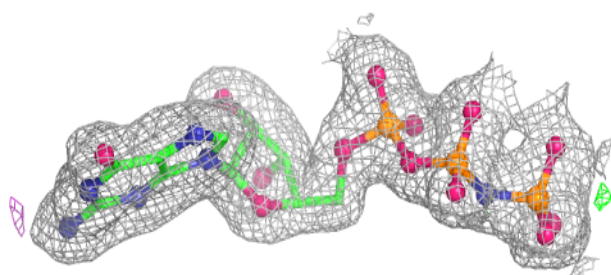
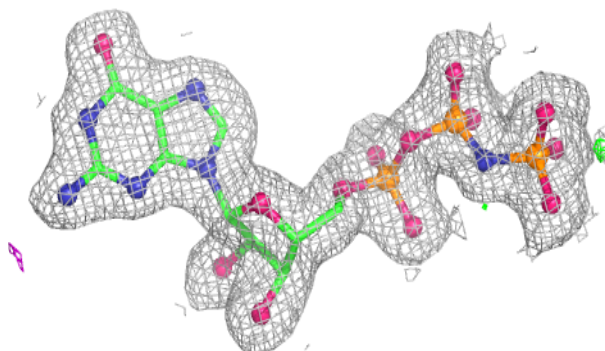


Electron density around GNP A 301:

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

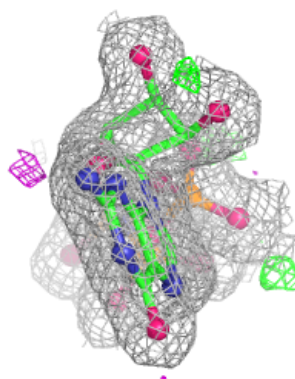
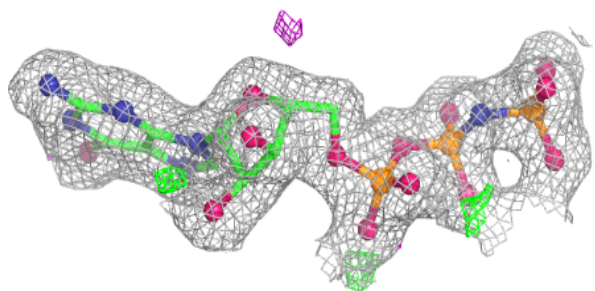
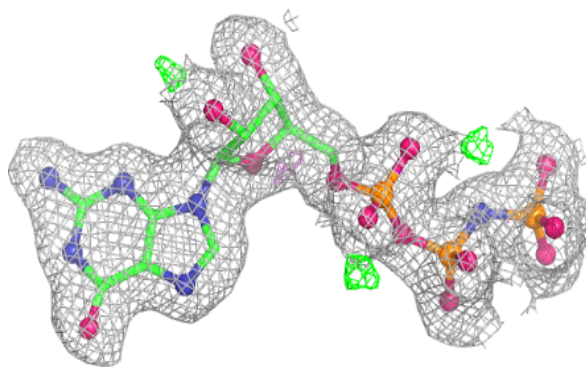
**Electron density around GNP G 301:**

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

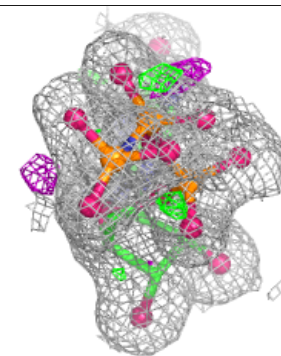
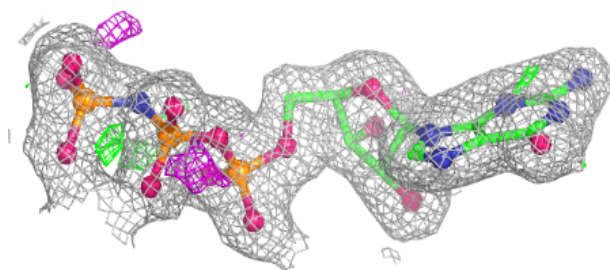
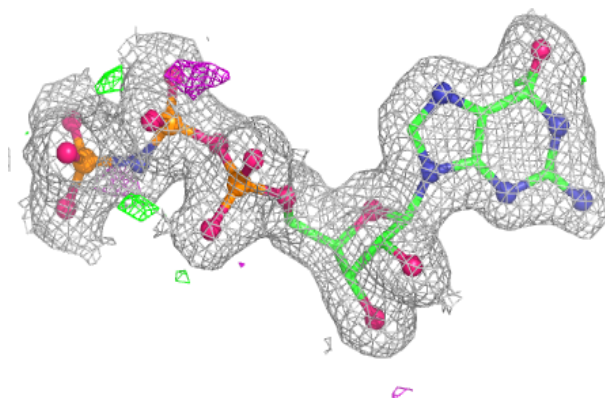


Electron density around GNP H 401:

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

**Electron density around GNP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.