



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:22 AM BST

PDB ID : 5YSU  
Title : Plumbagin in complex with CRM1-RanM189D-RanBP1  
Authors : Sun, Q.; Zhang, Y.  
Deposited on : 2017-11-15  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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 : 2.13.1  
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) : 2.13.1

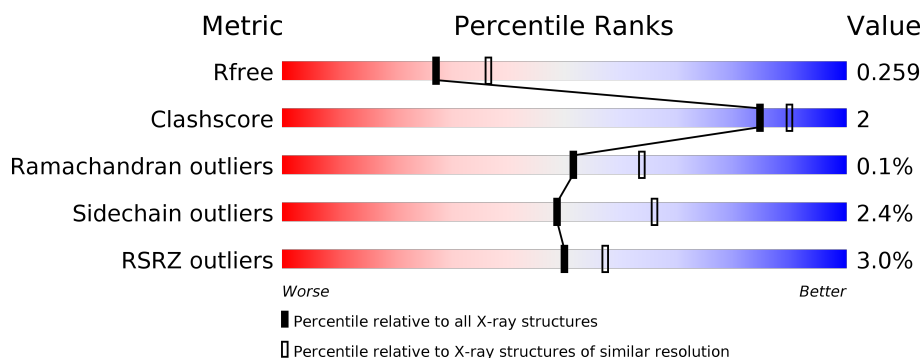
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	216	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> <div></div> </div>
2	B	140	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> <div></div> </div>
3	C	1024	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11387 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1676	1080	286	304	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	ASP	MET	engineered mutation	UNP P62826

- Molecule 2 is a protein called Ran-specific GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			1067	678	186	198	5			

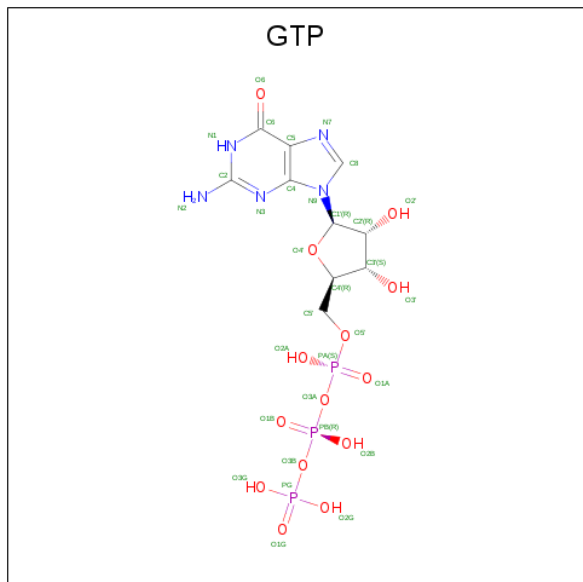
- Molecule 3 is a protein called Exportin-1,Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1017	Total	C	N	O	S	0	1	0
			8216	5277	1352	1546	41			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P30822
C	-1	GLY	-	expression tag	UNP P30822
C	0	SER	-	expression tag	UNP P30822
C	537	GLY	ASP	engineered mutation	UNP P30822
C	539	CYS	THR	engineered mutation	UNP P30822
C	540	GLU	VAL	engineered mutation	UNP P30822
C	541	GLN	LYS	engineered mutation	UNP P30822
C	1022	CYS	TYR	variant	UNP P30822

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

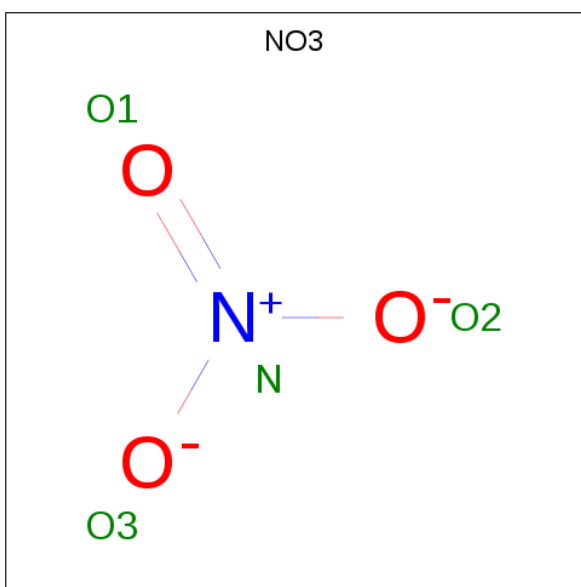
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

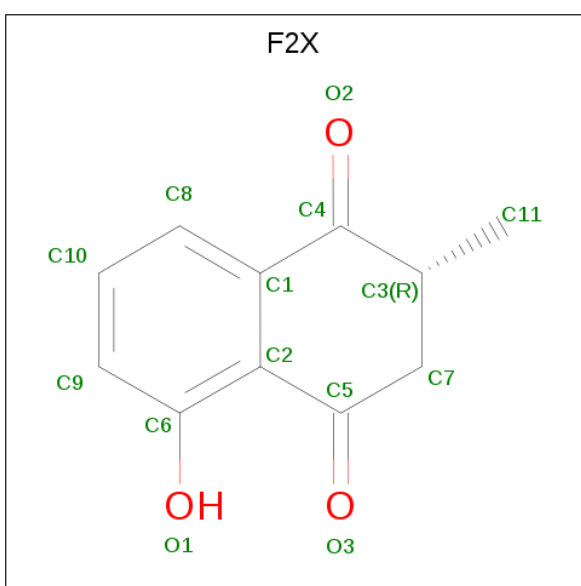
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

- Molecule 7 is NITRATE ION (three-letter code: NO3) (formula:  $NO_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	N	O	0	0
			4	1	3		
7	A	1	Total	N	O	0	0
			4	1	3		
7	C	1	Total	N	O	0	0
			4	1	3		
7	C	1	Total	N	O	0	0
			4	1	3		

- Molecule 8 is (2 {R})-2-methyl-5-oxidanyl-2,3-dihydronaphthalene-1,4-dione (three-letter code: F2X) (formula: C<sub>11</sub>H<sub>10</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			14	11	3		
8	C	1	Total	C	O	0	0
			14	11	3		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	60	Total	O	0	0
			60	60		
10	B	15	Total	O	0	0
			15	15		
10	C	273	Total	O	0	0
			273	273		

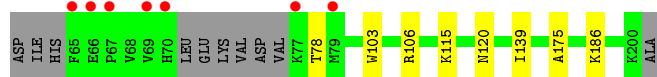
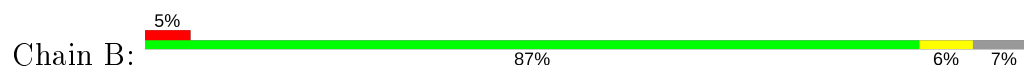
### 3 Residue-property plots [i](#)

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.

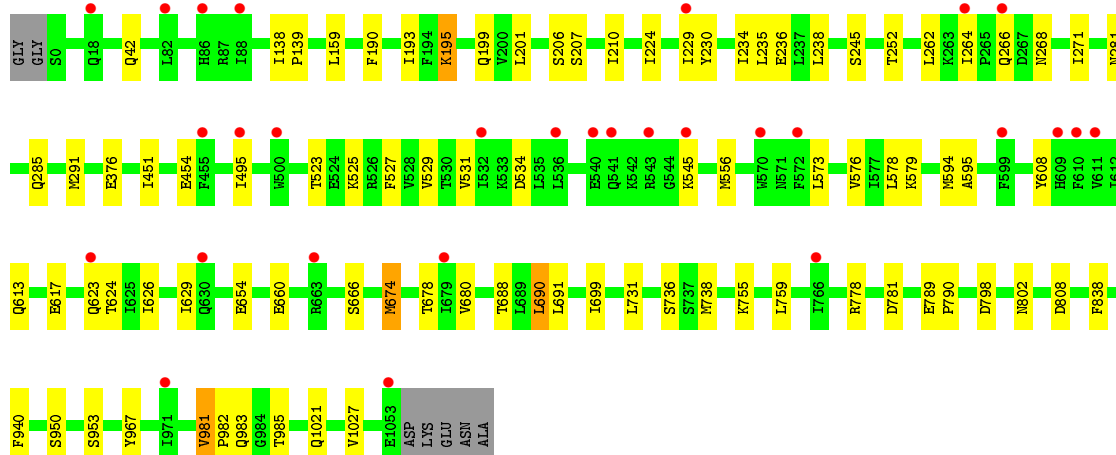
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: Ran-specific GTPase-activating protein 1



- Molecule 3: Exportin-1, Exportin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.06 Å   105.06 Å   306.53 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.74 – 2.30 49.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.74-2.30) 99.9 (49.69-2.30)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.221   ,   0.257 0.220   ,   0.259	Depositor DCC
$R_{free}$ test set	3946 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, GTP, F2X, NO3

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	0.67	0/1717	0.79	0/2328
2	B	0.67	0/1086	0.82	0/1450
3	C	0.68	1/8373 (0.0%)	0.75	0/11346
All	All	0.68	1/11176 (0.0%)	0.77	0/15124

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	376	GLU	C-N	7.03	1.47	1.34

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	1676	0	1672	5	0
2	B	1067	0	1067	4	0
3	C	8216	0	8295	44	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	8	0	0	0	0
7	C	8	0	0	0	0
8	C	28	0	0	2	0
9	C	1	0	0	0	0
10	A	60	0	0	0	0
10	B	15	0	0	0	0
10	C	273	0	0	2	0
All	All	11387	0	11046	51	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 2.

All (51) 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)
3:C:190:PHE:CZ	3:C:224:ILE:HG21	2.25	0.71
3:C:967:TYR:HB2	8:C:1101:F2X:C5	2.23	0.69
3:C:556:MET:HE1	3:C:594:MET:C	2.14	0.68
3:C:556:MET:HE1	3:C:594:MET:HB3	1.79	0.62
3:C:982:PRO:O	3:C:985:THR:HG22	2.01	0.61
3:C:495:ILE:HD11	3:C:534:ASP:HB3	1.82	0.60
1:A:178:ALA:HB3	2:B:78:THR:HG22	1.84	0.59
3:C:613:GLN:NE2	3:C:617:GLU:O	2.35	0.59
3:C:556:MET:HE1	3:C:595:ALA:N	2.19	0.57
2:B:115:LYS:HE2	2:B:120:ASN:HD22	1.70	0.56
3:C:699:ILE:HG21	3:C:731:LEU:HD21	1.89	0.54
3:C:738:MET:HE1	3:C:759:LEU:HD21	1.90	0.54
1:A:186:GLU:HA	2:B:139:ILE:HG13	1.91	0.54
3:C:691:LEU:HD22	3:C:755:LYS:NZ	2.23	0.53
3:C:573:LEU:O	3:C:576:VAL:HG22	2.10	0.50
1:A:77:ASP:HA	1:A:80:TYR:CE2	2.47	0.50
1:A:199:HIS:O	1:A:203:VAL:HG23	2.10	0.49
3:C:229:ILE:HG13	3:C:262:LEU:HD11	1.94	0.49
3:C:556:MET:CE	3:C:594:MET:C	2.81	0.48
3:C:268:ASN:CG	3:C:271:ILE:HD12	2.33	0.48
3:C:688:THR:O	3:C:691:LEU:HG	2.13	0.48
3:C:967:TYR:CB	8:C:1101:F2X:C5	2.93	0.47
2:B:103:TRP:CH2	2:B:175:ALA:HB2	2.50	0.47
3:C:268:ASN:OD1	3:C:271:ILE:HD12	2.16	0.46
3:C:808:ASP:HA	10:C:1377:HOH:O	2.16	0.46
3:C:138:ILE:HB	3:C:139:PRO:HD3	1.98	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:981:VAL:CG1	3:C:985:THR:CG2	2.94	0.46
3:C:236:GLU:OE1	10:C:1201:HOH:O	2.21	0.45
3:C:981:VAL:HG13	3:C:985:THR:HG21	1.97	0.45
3:C:527:PHE:O	3:C:531:VAL:HG23	2.16	0.45
3:C:525:LYS:O	3:C:529:VAL:HG23	2.17	0.45
3:C:690:LEU:HB3	3:C:738:MET:HE3	1.99	0.45
3:C:206:SER:O	3:C:210:ILE:HG12	2.17	0.44
3:C:281:ASN:O	3:C:285:GLN:HG2	2.17	0.44
3:C:556:MET:HE1	3:C:594:MET:CB	2.45	0.44
3:C:264:ILE:HG22	3:C:266:GLN:OE1	2.18	0.43
3:C:608:TYR:HA	3:C:654:GLU:HG2	2.00	0.43
3:C:674:MET:O	3:C:678:THR:HG23	2.18	0.43
3:C:1021:GLN:CD	3:C:1027:VAL:HG12	2.38	0.43
3:C:736:SER:HB3	3:C:798:ASP:OD1	2.18	0.43
3:C:201:LEU:CD1	3:C:234:ILE:HD11	2.49	0.42
3:C:626:ILE:O	3:C:629:ILE:HG22	2.20	0.42
3:C:230:TYR:CE1	3:C:264:ILE:HD11	2.55	0.41
3:C:238:LEU:O	3:C:252:THR:HG21	2.20	0.41
3:C:691:LEU:HD22	3:C:755:LYS:HZ1	1.85	0.41
3:C:578:LEU:HA	3:C:578:LEU:HD23	1.95	0.41
3:C:159:LEU:HD13	3:C:193:ILE:HG23	2.01	0.41
1:A:39:TYR:OH	1:A:69:GLN:NE2	2.42	0.41
3:C:235:LEU:HA	3:C:235:LEU:HD23	1.84	0.40
3:C:789:GLU:HB2	3:C:790:PRO:HD3	2.03	0.40
3:C:195:LYS:O	3:C:199:GLN:HG3	2.21	0.40

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	207/216 (96%)	200 (97%)	7 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	126/140 (90%)	118 (94%)	8 (6%)	0	100	100
3	C	1016/1024 (99%)	984 (97%)	31 (3%)	1 (0%)	51	64
All	All	1349/1380 (98%)	1302 (96%)	46 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	838	PHE

### 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	181/185 (98%)	179 (99%)	2 (1%)	73	86
2	B	112/121 (93%)	110 (98%)	2 (2%)	59	75
3	C	930/933 (100%)	905 (97%)	25 (3%)	44	61
All	All	1223/1239 (99%)	1194 (98%)	29 (2%)	49	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	202	GLU
2	B	106	ARG
2	B	186	LYS
3	C	42	GLN
3	C	195	LYS
3	C	207	SER
3	C	245	SER
3	C	291	MET
3	C	451	ILE
3	C	454	GLU
3	C	523	THR
3	C	545	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	579	LYS
3	C	623	GLN
3	C	624	THR
3	C	660	GLU
3	C	666	SER
3	C	674	MET
3	C	680	VAL
3	C	690	LEU
3	C	778	ARG
3	C	781	ASP
3	C	802	ASN
3	C	940	PHE
3	C	950	SER
3	C	953	SER
3	C	981	VAL
3	C	983	GLN

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

Mol	Chain	Res	Type
1	A	173	ASN
2	B	120	ASN
3	C	33	GLN
3	C	35	GLN
3	C	49	GLN
3	C	199	GLN
3	C	261	ASN
3	C	342	ASN
3	C	494	GLN
3	C	623	GLN
3	C	730	GLN
3	C	955	GLN
3	C	1005	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	NO3	A	305	-	1,3,3	0.32	0	0,3,3	0.00	-
4	GTP	A	301	5	26,34,34	1.05	1 (3%)	33,54,54	2.17	5 (15%)
8	F2X	C	1102	3	14,15,15	1.41	1 (7%)	17,22,22	1.70	3 (17%)
7	NO3	A	304	-	1,3,3	0.15	0	0,3,3	0.00	-
8	F2X	C	1101	3	14,15,15	1.23	2 (14%)	17,22,22	1.77	5 (29%)
7	NO3	C	1105	-	1,3,3	0.12	0	0,3,3	0.00	-
7	NO3	C	1106	-	1,3,3	0.36	0	0,3,3	0.00	-

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	GTP	A	301	5	-	7/18/38/38	0/3/3/3
8	F2X	C	1101	3	-	-	0/2/2/2
8	F2X	C	1102	3	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GTP	C6-N1	3.94	1.39	1.33
8	C	1101	F2X	C1-C2	-3.07	1.36	1.41
8	C	1102	F2X	C1-C2	-2.90	1.36	1.41
8	C	1101	F2X	C2-C6	-2.34	1.37	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	GTP	C5-C6-N1	-9.02	111.10	123.43
4	A	301	GTP	C6-N1-C2	6.01	125.48	115.93
8	C	1102	F2X	C11-C3-C7	-4.63	96.57	112.52
8	C	1101	F2X	C7-C5-C2	3.94	124.01	117.12
8	C	1101	F2X	C1-C2-C6	3.43	121.60	118.41
4	A	301	GTP	C2-N3-C4	-2.95	111.99	115.36
8	C	1102	F2X	C1-C2-C6	2.83	121.05	118.41
8	C	1102	F2X	C7-C5-C2	2.79	122.00	117.12
8	C	1101	F2X	O3-C5-C7	-2.75	116.92	120.79
4	A	301	GTP	N3-C2-N1	-2.75	123.56	127.22
8	C	1101	F2X	C1-C4-C3	2.25	121.94	117.53
4	A	301	GTP	PA-O3A-PB	-2.15	125.44	132.83
8	C	1101	F2X	O3-C5-C2	-2.09	119.06	122.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GTP	C5'-O5'-PA-O3A
4	A	301	GTP	O4'-C4'-C5'-O5'
4	A	301	GTP	C3'-C4'-C5'-O5'
4	A	301	GTP	PA-O3A-PB-O2B
4	A	301	GTP	C5'-O5'-PA-O1A
4	A	301	GTP	C5'-O5'-PA-O2A
4	A	301	GTP	PA-O3A-PB-O1B

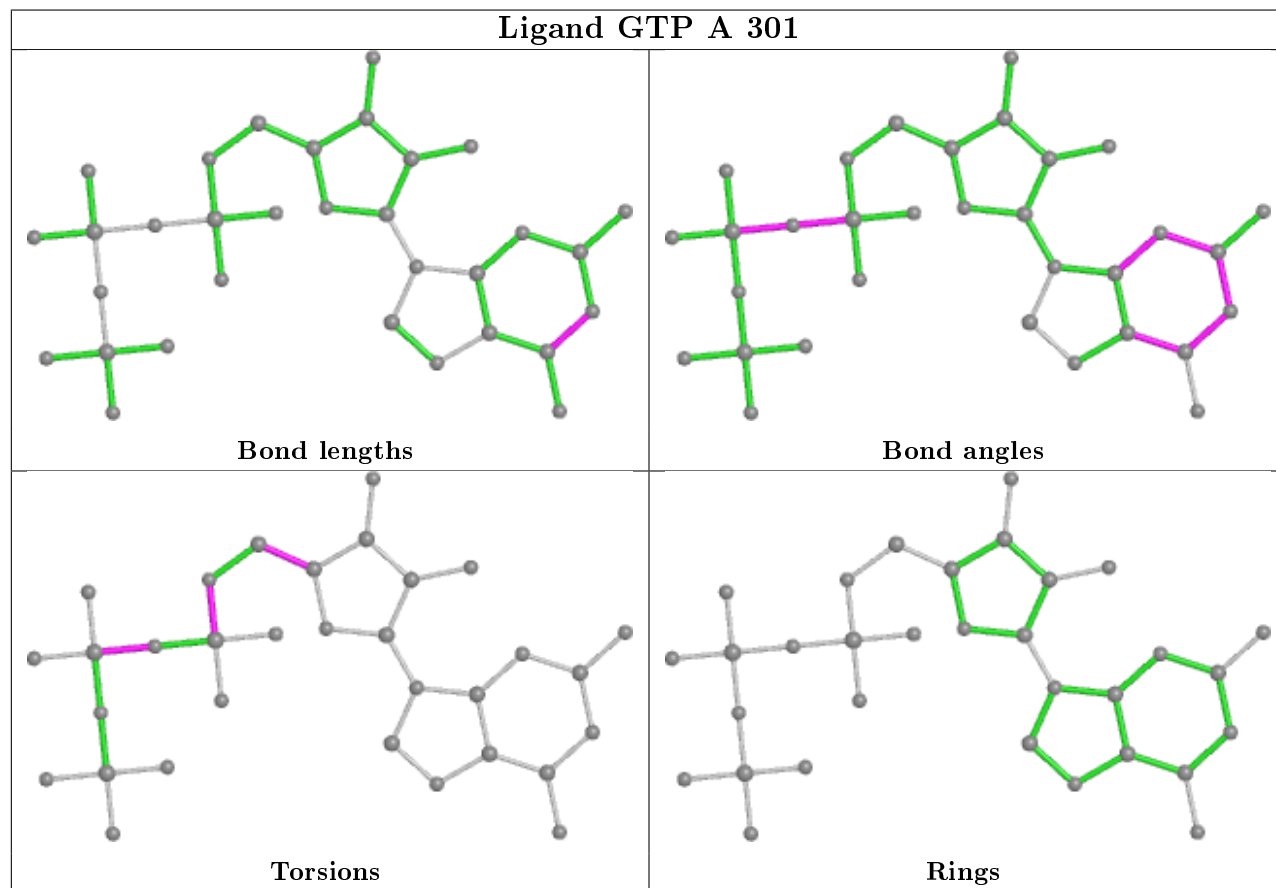
There are no ring outliers.

1 monomer is involved in 2 short contacts:

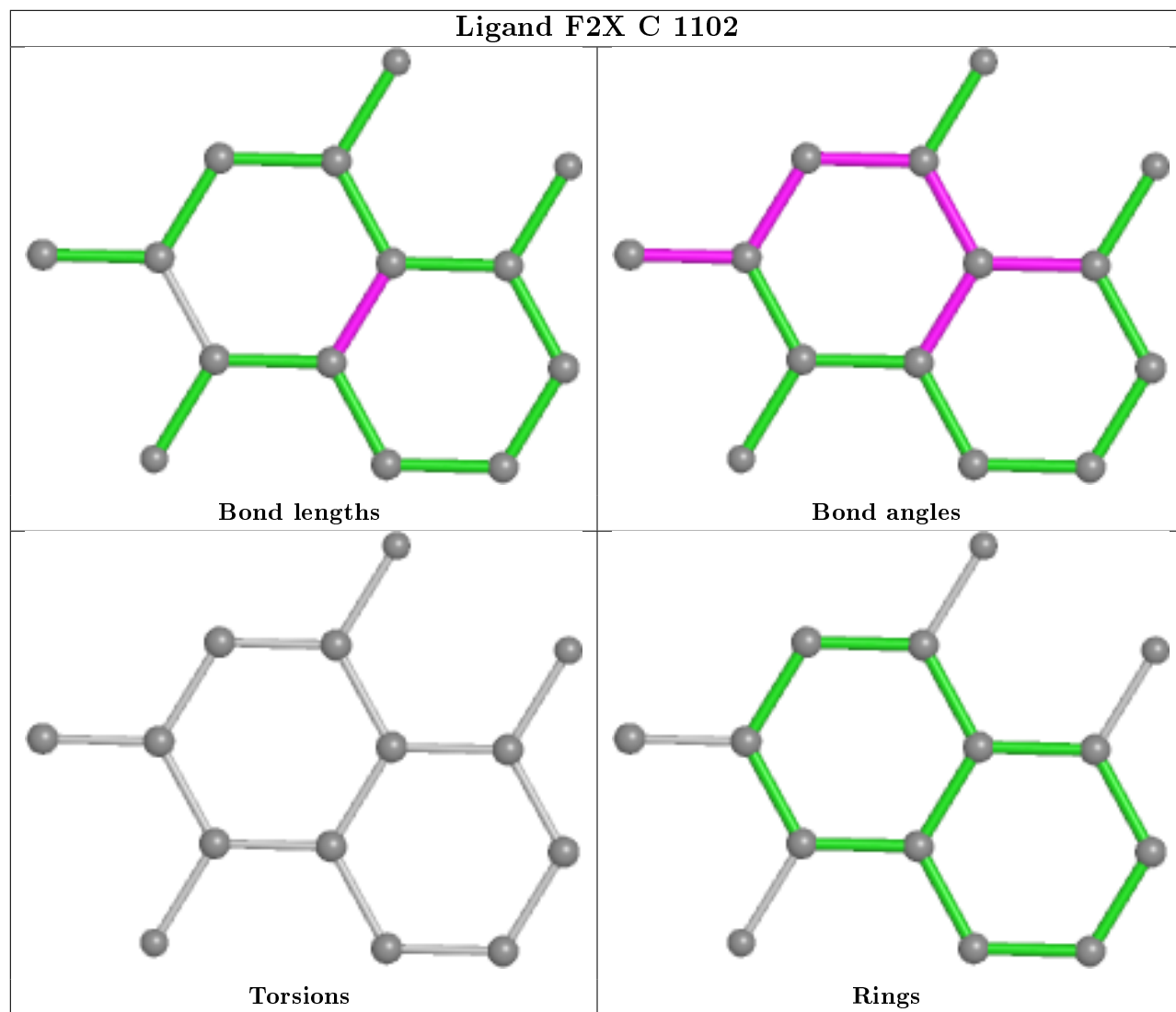
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1101	F2X	2	0

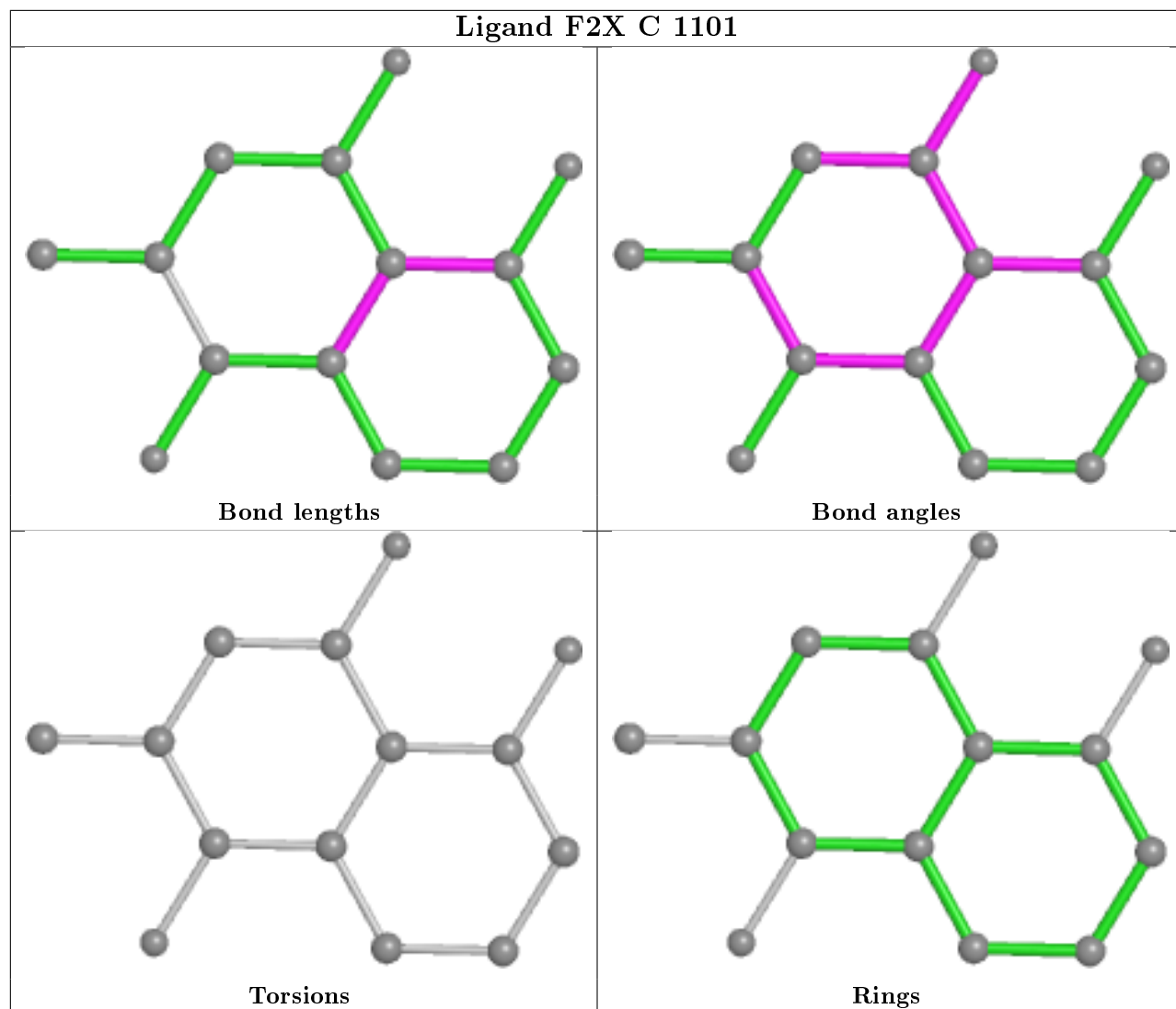
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	208/216 (96%)	0.03	4 (1%) 66 73	44, 58, 101, 122	0
2	B	130/140 (92%)	0.02	7 (5%) 25 32	53, 72, 110, 169	0
3	C	1017/1024 (99%)	0.09	29 (2%) 51 58	47, 69, 106, 145	0
All	All	1355/1380 (98%)	0.08	40 (2%) 50 57	44, 68, 106, 169	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	70	HIS	6.3
2	B	65	PHE	6.1
2	B	69	VAL	5.6
3	C	572	PHE	5.1
1	A	180	PRO	5.0
1	A	179	MET	4.5
3	C	543	ARG	4.1
2	B	67	PRO	3.8
3	C	610	PHE	3.6
2	B	79	MET	3.4
3	C	545	LYS	3.3
3	C	611	VAL	3.2
3	C	623	GLN	3.1
2	B	66	GLU	3.0
3	C	541	GLN	2.9
3	C	536	LEU	2.9
2	B	77	LYS	2.9
3	C	532	ILE	2.9
3	C	455	PHE	2.8
3	C	766	ILE	2.6
3	C	266	GLN	2.6
3	C	1053	GLU	2.6
3	C	495	ILE	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	599	PHE	2.5
3	C	609	HIS	2.5
3	C	264	ILE	2.4
3	C	679	ILE	2.4
3	C	500	TRP	2.4
3	C	630	GLN	2.3
3	C	88	ILE	2.3
1	A	76	ARG	2.2
3	C	971	ILE	2.2
3	C	663	ARG	2.2
3	C	18	GLN	2.2
3	C	86	HIS	2.2
3	C	570	TRP	2.2
3	C	82	LEU	2.1
3	C	229	ILE	2.1
1	A	187	VAL	2.1
3	C	540	GLU	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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NO3	C	1105	4/4	0.76	0.36	94,101,104,107	0
6	CL	A	303	1/1	0.78	0.14	101,101,101,101	0
8	F2X	C	1102	14/14	0.89	0.14	107,114,120,122	0
8	F2X	C	1101	14/14	0.89	0.39	94,103,108,114	0
9	NA	C	1104	1/1	0.92	0.98	79,79,79,79	0
7	NO3	C	1106	4/4	0.93	0.31	84,91,92,96	0

*Continued on next page...*

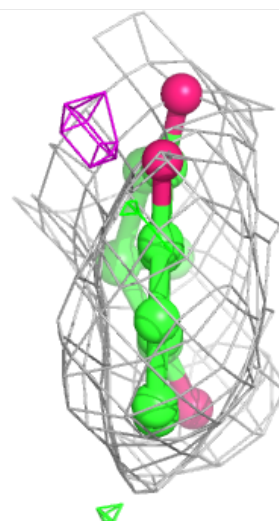
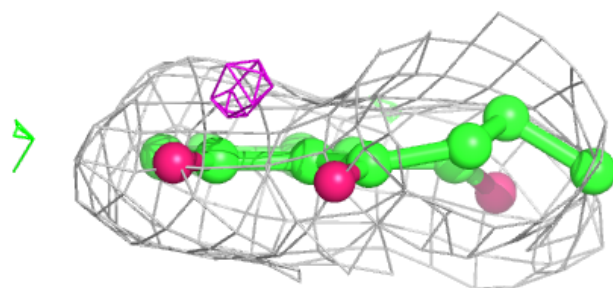
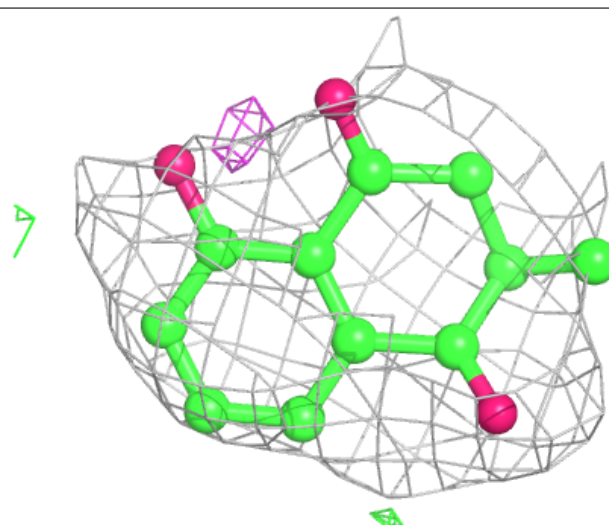
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NO3	A	304	4/4	0.94	0.15	74,84,87,87	0
6	CL	C	1103	1/1	0.95	0.36	92,92,92,92	0
7	NO3	A	305	4/4	0.96	0.09	80,82,83,88	0
5	MG	A	302	1/1	0.98	0.17	50,50,50,50	0
4	GTP	A	301	32/32	0.98	0.14	46,49,52,56	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.

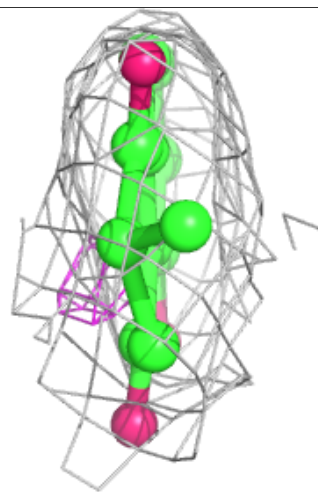
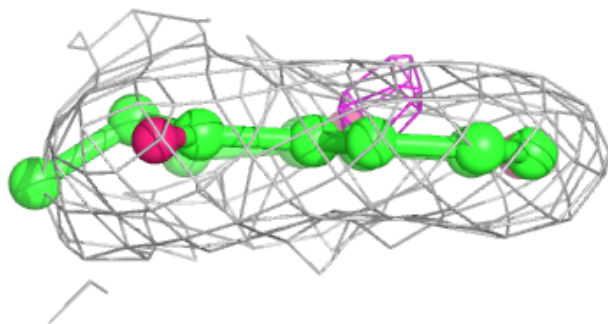
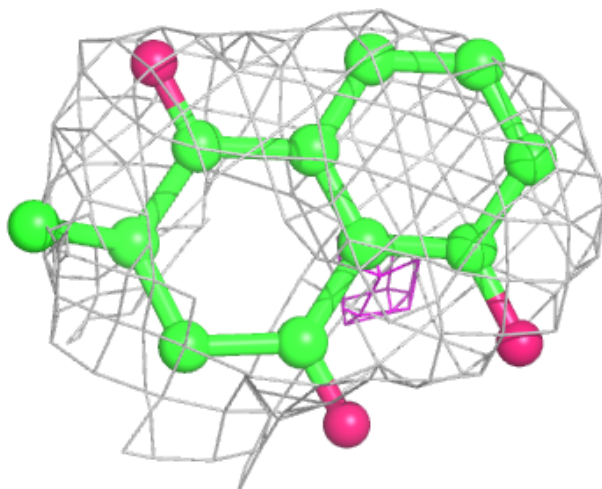
**Electron density around F2X C 1102:**

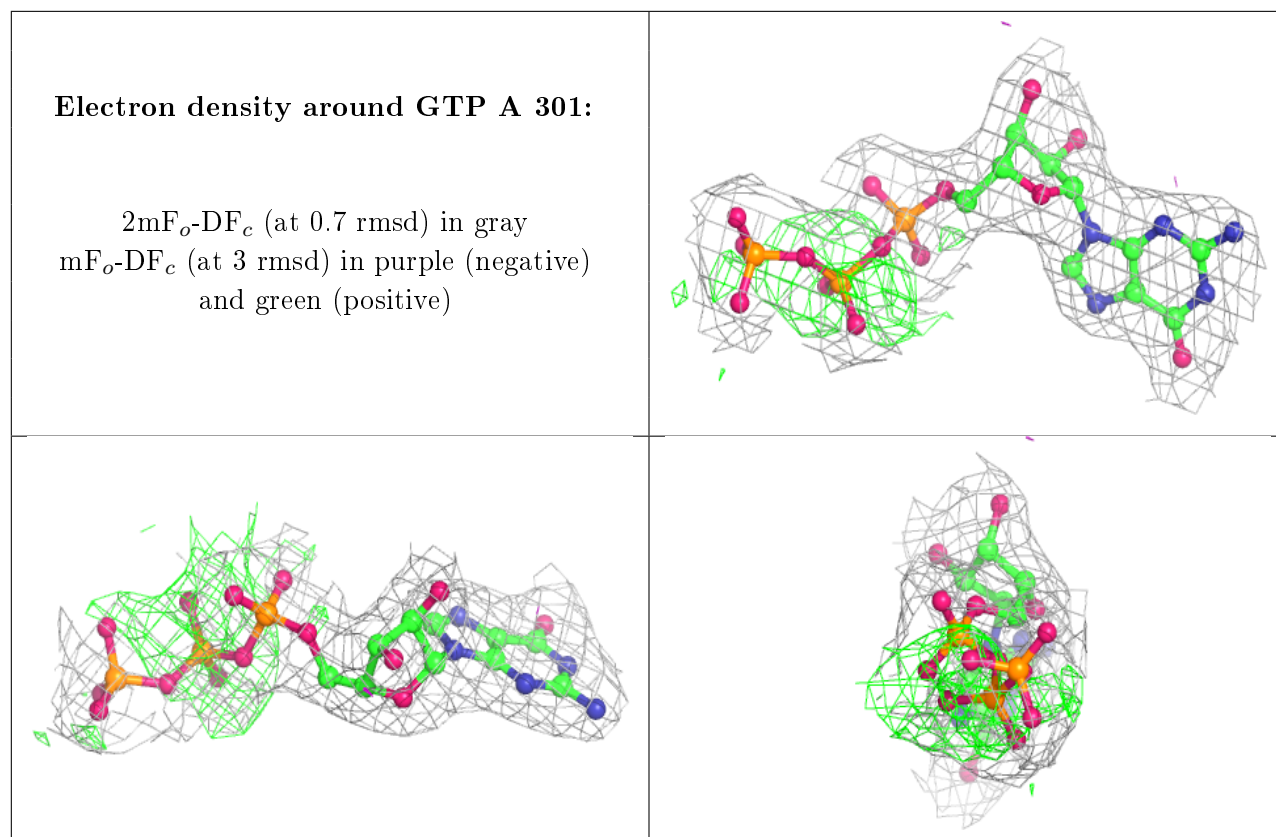
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around F2X C 1101:**

$2mF_o-DF_c$  (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.