



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2021 – 08:10 PM JST

PDB ID : 6M60  
Title : Plumbagin in complex with CRM1#-Ran-RanBP1  
Authors : Sun, Q.; Lei, Y.  
Deposited on : 2020-03-12  
Resolution : 2.17 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.19  
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) : 2.19

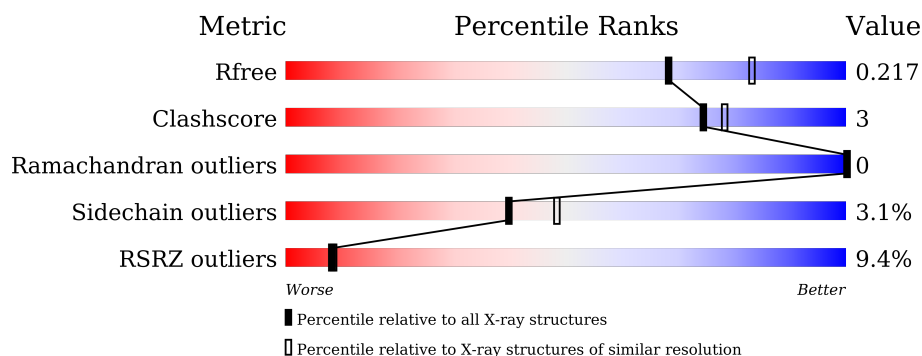
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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  $\geq 3$ , 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>16%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
2	B	140	<div> <div>13%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>
3	C	1003	<div> <div>7%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>

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	GOL	A	302	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11383 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	0	0
			1663	1074	284	299	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LEU	GLN	engineered mutation	UNP P62826
A	182	ALA	LEU	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	121	Total	C	N	O	S	0	0	0
			992	628	174	186	4			

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	995	Total	C	N	O	S	0	2	0
			8055	5178	1328	1507	42			

There are 72 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	27	GLU	SER	engineered mutation	UNP P30822
C	49	GLU	GLN	engineered mutation	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	GLY	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	ASN	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	TYR	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	LYS	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	PHE	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	ASN	deletion	UNP P30822
C	?	-	ASP	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	ILE	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	PHE	deletion	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	LYS	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	ASP	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	522	LYS	ASP	engineered mutation	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	553	ARG	SER	engineered mutation	UNP P30822
C	561	GLU	GLN	engineered mutation	UNP P30822
C	741	THR	ALA	engineered mutation	UNP P30822
C	1022	CYS	TYR	engineered mutation	UNP P30822

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

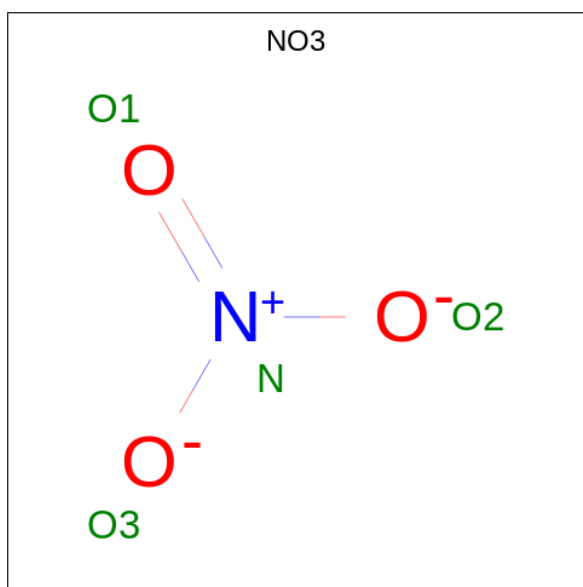
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



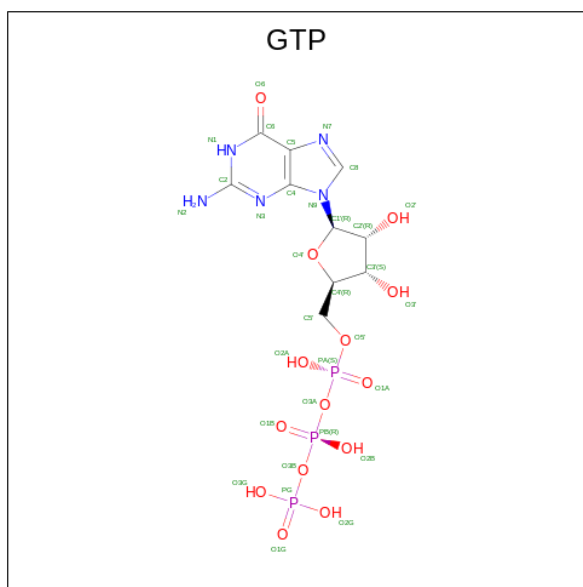
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		

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

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



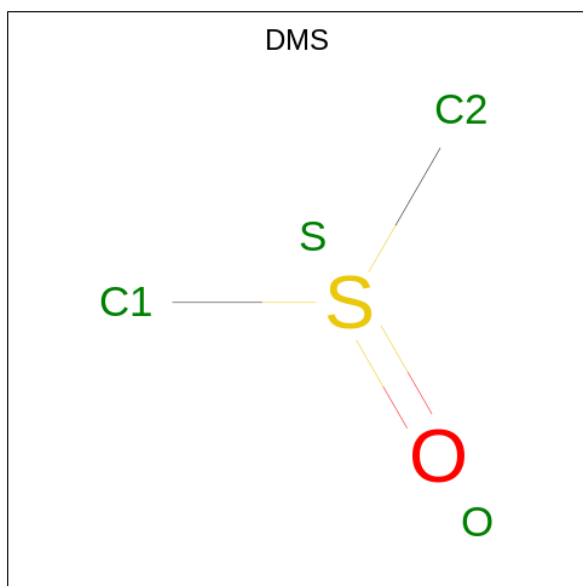
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



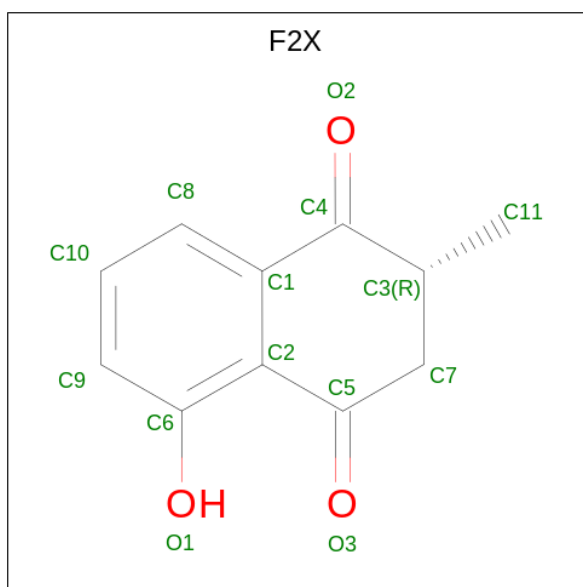
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	3	Total Cl 3 3	0	0

- Molecule 9 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O S 4 2 1 1	0	0
9	C	1	Total C O S 4 2 1 1	0	0
9	C	1	Total C O S 4 2 1 1	0	0

- Molecule 10 is (2 {R})-2-methyl-5-oxidanyl-2,3-dihydronaphthalene-1,4-dione (three-letter code: F2X) (formula:  $C_{11}H_{10}O_3$ ) (labeled as "Ligand of Interest" by depositor).



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

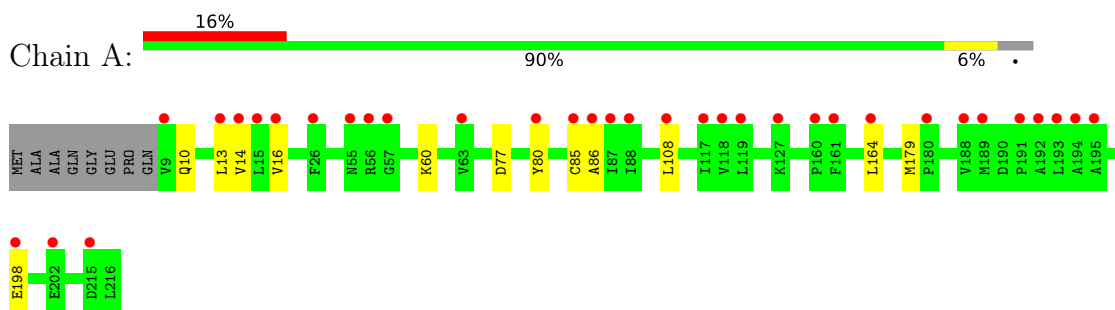
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	104	Total	O	0	0
			104	104		
11	B	25	Total	O	0	0
			25	25		
11	C	400	Total	O	0	0
			400	400		

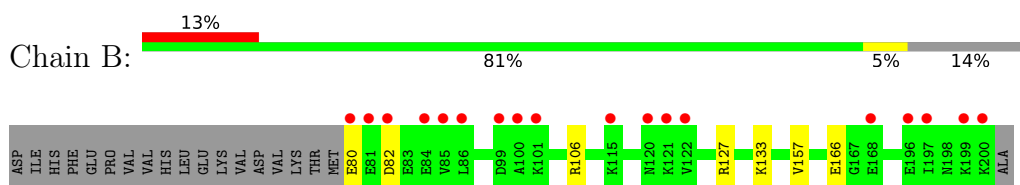
### 3 Residue-property plots [i](#)

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.

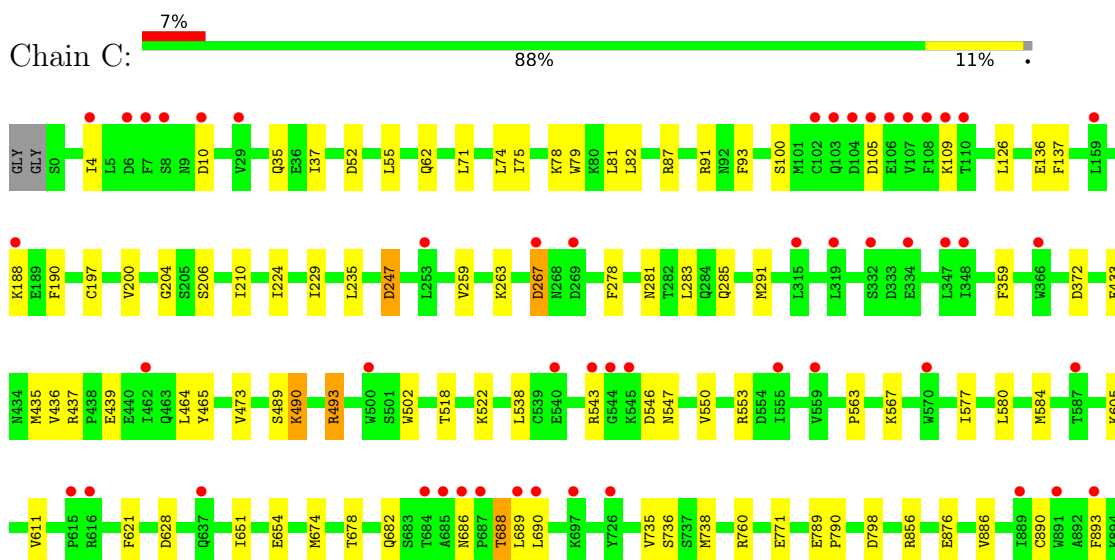
- Molecule 1: GTP-binding nuclear protein Ran

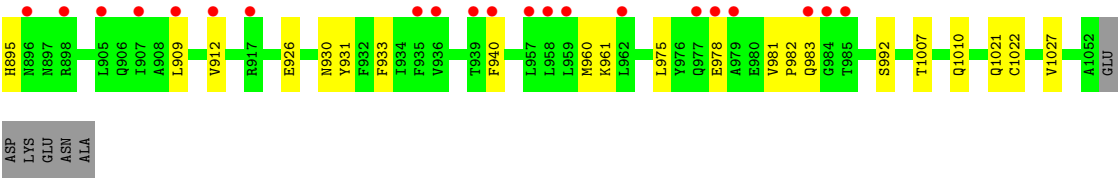


- Molecule 2: Ran-specific GTPase-activating protein 1



- Molecule 3: Exportin-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.59Å 105.59Å 305.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.72 – 2.17 31.72 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.72-2.17) 100.0 (31.72-2.17)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.181 , 0.213 0.188 , 0.217	Depositor DCC
$R_{free}$ test set	4620 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: DMS, CL, MG, GTP, GOL, 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	0.66	0/1704	0.82	0/2310
2	B	0.64	0/1009	0.81	0/1347
3	C	0.66	0/8211	0.75	0/11125
All	All	0.66	0/10924	0.76	0/14782

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	1663	0	1666	8	0
2	B	992	0	992	4	0
3	C	8055	0	8146	57	0
4	A	1	0	0	0	0
5	A	6	0	8	0	0
5	C	12	0	16	1	0
6	A	12	0	0	0	0
6	C	24	0	0	0	0
7	A	32	0	12	0	0
8	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	12	0	18	0	0
10	C	42	0	0	2	0
11	A	104	0	0	0	0
11	B	25	0	0	0	0
11	C	400	0	0	3	0
All	All	11383	0	10858	70	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 3.

All (70) 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:981:VAL:HG22	3:C:982:PRO:HD2	1.58	0.86
3:C:197[A]:CYS:SG	11:C:1224:HOH:O	2.44	0.74
3:C:674:MET:O	3:C:678:THR:HG23	1.89	0.73
3:C:502:TRP:HE1	3:C:547:ASN:HD22	1.38	0.71
3:C:502:TRP:HE1	3:C:547:ASN:ND2	1.92	0.68
3:C:435:MET:HE1	3:C:465:TYR:CE1	2.35	0.61
3:C:981:VAL:HG22	3:C:982:PRO:CD	2.29	0.60
3:C:735:VAL:HA	3:C:738:MET:HE3	1.82	0.60
3:C:204:GLY:HA3	3:C:210:ILE:HD11	1.84	0.60
3:C:686:ASN:HD21	3:C:688:THR:HG22	1.67	0.59
3:C:856:ARG:HD3	3:C:895:HIS:NE2	2.22	0.55
3:C:200:VAL:O	3:C:204:GLY:N	2.39	0.54
3:C:960:MET:HG2	3:C:1022:CYS:O	2.10	0.52
3:C:789:GLU:HB3	3:C:790:PRO:HD3	1.91	0.52
3:C:433:GLU:CG	3:C:490:LYS:HE3	2.40	0.51
10:C:1117:F2X:O1	10:C:1117:F2X:O3	2.26	0.51
10:C:1115:F2X:O1	10:C:1115:F2X:O3	2.25	0.51
3:C:437:ARG:HD2	3:C:439:GLU:HB2	1.92	0.51
3:C:489:SER:O	3:C:493:ARG:HD2	2.11	0.50
1:A:179:MET:HE1	2:B:133:LYS:HG2	1.93	0.50
3:C:229:ILE:HG22	3:C:235:LEU:HG	1.93	0.50
3:C:978:GLU:HA	3:C:978:GLU:OE1	2.12	0.50
3:C:247:ASP:N	3:C:247:ASP:OD1	2.45	0.49
3:C:690:LEU:HB3	3:C:738:MET:CE	2.43	0.49
1:A:10:GLN:HA	1:A:60:LYS:O	2.12	0.48
2:B:80:GLU:OE1	2:B:127:ARG:NH2	2.42	0.48
3:C:736:SER:HB3	3:C:798:ASP:OD1	2.13	0.48
3:C:235:LEU:HD21	3:C:259:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1007:THR:H	3:C:1010:GLN:HE21	1.61	0.48
2:B:106:ARG:NH2	2:B:166:GLU:HG2	2.30	0.47
3:C:686:ASN:ND2	3:C:689:LEU:HG	2.30	0.47
1:A:86:ALA:CB	1:A:108:LEU:HD21	2.45	0.46
3:C:580:LEU:O	3:C:584:MET:HG3	2.15	0.46
1:A:85:CYS:HB2	1:A:164:LEU:HD22	1.98	0.46
3:C:78:LYS:NZ	11:C:1217:HOH:O	2.45	0.46
3:C:682:GLN:HB3	3:C:689:LEU:HD13	1.98	0.46
3:C:473:VAL:HG13	3:C:518:THR:HG22	1.98	0.45
2:B:166:GLU:OE2	2:B:166:GLU:HA	2.16	0.45
3:C:267:ASP:OD1	3:C:267:ASP:N	2.50	0.45
3:C:563:PRO:HG3	3:C:605:LYS:HD3	1.98	0.44
3:C:890:CYS:O	3:C:893:PHE:HB2	2.17	0.44
3:C:281:ASN:O	3:C:285:GLN:HG2	2.17	0.44
1:A:14:VAL:HG12	1:A:16:VAL:HG13	2.01	0.43
3:C:200:VAL:O	3:C:204:GLY:HA3	2.18	0.43
3:C:91:ARG:NE	11:C:1208:HOH:O	2.38	0.43
1:A:13:LEU:C	1:A:13:LEU:HD23	2.40	0.42
3:C:206:SER:O	3:C:210:ILE:HG12	2.18	0.42
3:C:55:LEU:HD12	3:C:93:PHE:HE2	1.84	0.42
3:C:200:VAL:O	3:C:204:GLY:CA	2.68	0.42
3:C:79:TRP:NE1	3:C:87:ARG:HD2	2.35	0.42
3:C:235:LEU:HD23	3:C:235:LEU:HA	1.88	0.42
3:C:912:VAL:HG11	3:C:961:LYS:HG3	2.01	0.42
3:C:359:PHE:CB	5:C:1107:GOL:H12	2.50	0.41
3:C:926:GLU:O	3:C:930:ASN:ND2	2.53	0.41
3:C:74:LEU:HD21	3:C:82:LEU:HD11	2.02	0.41
3:C:126:LEU:HD11	3:C:137:PHE:CZ	2.55	0.41
3:C:567:LYS:CE	3:C:605:LYS:O	2.68	0.41
3:C:1021:GLN:CD	3:C:1027:VAL:HG12	2.40	0.41
3:C:190:PHE:CZ	3:C:224:ILE:HG21	2.56	0.41
3:C:651:ILE:O	3:C:654:GLU:HB2	2.20	0.41
3:C:1007:THR:H	3:C:1010:GLN:NE2	2.19	0.41
1:A:77:ASP:HA	1:A:80:TYR:CD2	2.56	0.41
3:C:436:VAL:HG11	3:C:464:LEU:HD23	2.01	0.41
3:C:933:PHE:HE2	3:C:975:LEU:HB3	1.86	0.41
1:A:10:GLN:OE1	1:A:60:LYS:HE2	2.21	0.41
3:C:546:ASP:O	3:C:550:VAL:HG23	2.21	0.41
3:C:577:ILE:HG21	3:C:621:PHE:HE2	1.86	0.41
3:C:4:ILE:HD11	3:C:37:ILE:HG22	2.02	0.40
3:C:886:VAL:HG11	3:C:931:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:ILE:O	3:C:79:TRP:HB2	2.22	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	206/216 (95%)	202 (98%)	4 (2%)	0	100	100
2	B	119/140 (85%)	115 (97%)	4 (3%)	0	100	100
3	C	995/1003 (99%)	976 (98%)	19 (2%)	0	100	100
All	All	1320/1359 (97%)	1293 (98%)	27 (2%)	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	179/184 (97%)	178 (99%)	1 (1%)	86	92
2	B	103/121 (85%)	101 (98%)	2 (2%)	57	68
3	C	911/914 (100%)	877 (96%)	34 (4%)	34	40
All	All	1193/1219 (98%)	1156 (97%)	37 (3%)	40	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLU
2	B	82	ASP
2	B	157	VAL
3	C	10	ASP
3	C	35	GLN
3	C	52	ASP
3	C	62	GLN
3	C	71	LEU
3	C	81	LEU
3	C	100	SER
3	C	105	ASP
3	C	109	LYS
3	C	136	GLU
3	C	188	LYS
3	C	247	ASP
3	C	263	LYS
3	C	267	ASP
3	C	278	PHE
3	C	283	LEU
3	C	291	MET
3	C	372	ASP
3	C	490	LYS
3	C	493	ARG
3	C	522	LYS
3	C	538	LEU
3	C	543	ARG
3	C	553	ARG
3	C	611	VAL
3	C	628	ASP
3	C	688	THR
3	C	760	ARG
3	C	771	GLU
3	C	876	GLU
3	C	909	LEU
3	C	940	PHE
3	C	983	GLN
3	C	992	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	205	GLN
3	C	30	GLN
3	C	56	GLN
3	C	541	GLN
3	C	547	ASN
3	C	930	ASN
3	C	988	GLN
3	C	1010	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	$\# Z  > 2$
5	GOL	C	1107	-	5,5,5	0.15	0	5,5,5	0.42	0
9	DMS	C	1114	-	3,3,3	0.29	0	3,3,3	0.10	0
6	NO3	C	1101	-	1,3,3	0.56	0	0,3,3	0.00	-
7	GTP	A	305	4	26,34,34	1.05	1 (3%)	33,54,54	2.14	4 (12%)
6	NO3	C	1106	-	1,3,3	0.11	0	0,3,3	0.00	-
9	DMS	C	1112	-	3,3,3	0.27	0	3,3,3	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	F2X	C	1115	3	14,15,15	1.55	2 (14%)	17,22,22	2.05	6 (35%)
9	DMS	C	1105	-	3,3,3	0.24	0	3,3,3	0.12	0
6	NO3	A	304	-	1,3,3	0.50	0	0,3,3	0.00	-
5	GOL	A	302	-	5,5,5	0.16	0	5,5,5	0.36	0
6	NO3	A	303	-	1,3,3	0.76	0	0,3,3	0.00	-
6	NO3	C	1113	-	1,3,3	0.14	0	0,3,3	0.00	-
6	NO3	C	1110	-	1,3,3	0.27	0	0,3,3	0.00	-
5	GOL	C	1108	-	5,5,5	0.13	0	5,5,5	0.40	0
10	F2X	C	1116	3	14,15,15	1.31	2 (14%)	17,22,22	1.67	5 (29%)
6	NO3	C	1111	-	1,3,3	0.20	0	0,3,3	0.00	-
6	NO3	C	1109	-	1,3,3	0.10	0	0,3,3	0.00	-
10	F2X	C	1117	3	14,15,15	1.13	2 (14%)	17,22,22	1.58	5 (29%)
6	NO3	A	306	-	1,3,3	0.23	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
5	GOL	A	302	-	-	1/4/4/4	-
5	GOL	C	1107	-	-	2/4/4/4	-
10	F2X	C	1117	3	-	-	0/2/2/2
10	F2X	C	1115	3	-	-	0/2/2/2
5	GOL	C	1108	-	-	0/4/4/4	-
10	F2X	C	1116	3	-	-	0/2/2/2
7	GTP	A	305	4	-	2/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1115	F2X	C1-C2	-3.94	1.35	1.41
7	A	305	GTP	C6-N1	3.74	1.39	1.33
10	C	1115	F2X	C2-C6	-3.56	1.35	1.41
10	C	1117	F2X	C2-C6	-3.24	1.36	1.41
10	C	1116	F2X	C1-C2	-2.97	1.36	1.41
10	C	1116	F2X	C7-C5	2.32	1.54	1.50
10	C	1117	F2X	C1-C2	-2.22	1.38	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	305	GTP	C5-C6-N1	-8.86	111.31	123.43
7	A	305	GTP	C6-N1-C2	6.03	125.51	115.93
10	C	1115	F2X	C1-C2-C6	4.12	122.24	118.41
10	C	1115	F2X	C7-C5-C2	3.60	123.42	117.12
10	C	1115	F2X	O3-C5-C2	-3.56	116.74	122.38
10	C	1116	F2X	C7-C5-C2	3.41	123.09	117.12
10	C	1117	F2X	C1-C2-C6	3.19	121.38	118.41
10	C	1115	F2X	O2-C4-C1	-3.19	116.87	121.98
7	A	305	GTP	C2-N3-C4	-3.05	111.87	115.36
10	C	1117	F2X	C6-C2-C5	-2.95	116.67	120.81
7	A	305	GTP	N3-C2-N1	-2.81	123.48	127.22
10	C	1117	F2X	C7-C5-C2	2.65	121.75	117.12
10	C	1116	F2X	C6-C2-C5	2.56	124.40	120.81
10	C	1115	F2X	C6-C2-C5	-2.49	117.31	120.81
10	C	1116	F2X	O3-C5-C2	-2.47	118.47	122.38
10	C	1116	F2X	C1-C4-C3	-2.44	112.73	117.53
10	C	1117	F2X	O3-C5-C2	-2.30	118.74	122.38
10	C	1115	F2X	C1-C4-C3	2.21	121.88	117.53
10	C	1116	F2X	C2-C1-C4	-2.05	115.68	120.53
10	C	1117	F2X	O1-C6-C2	-2.01	117.38	121.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1107	GOL	O1-C1-C2-C3
5	C	1107	GOL	O1-C1-C2-O2
7	A	305	GTP	O4'-C4'-C5'-O5'
5	A	302	GOL	C1-C2-C3-O3
7	A	305	GTP	PA-O3A-PB-O2B

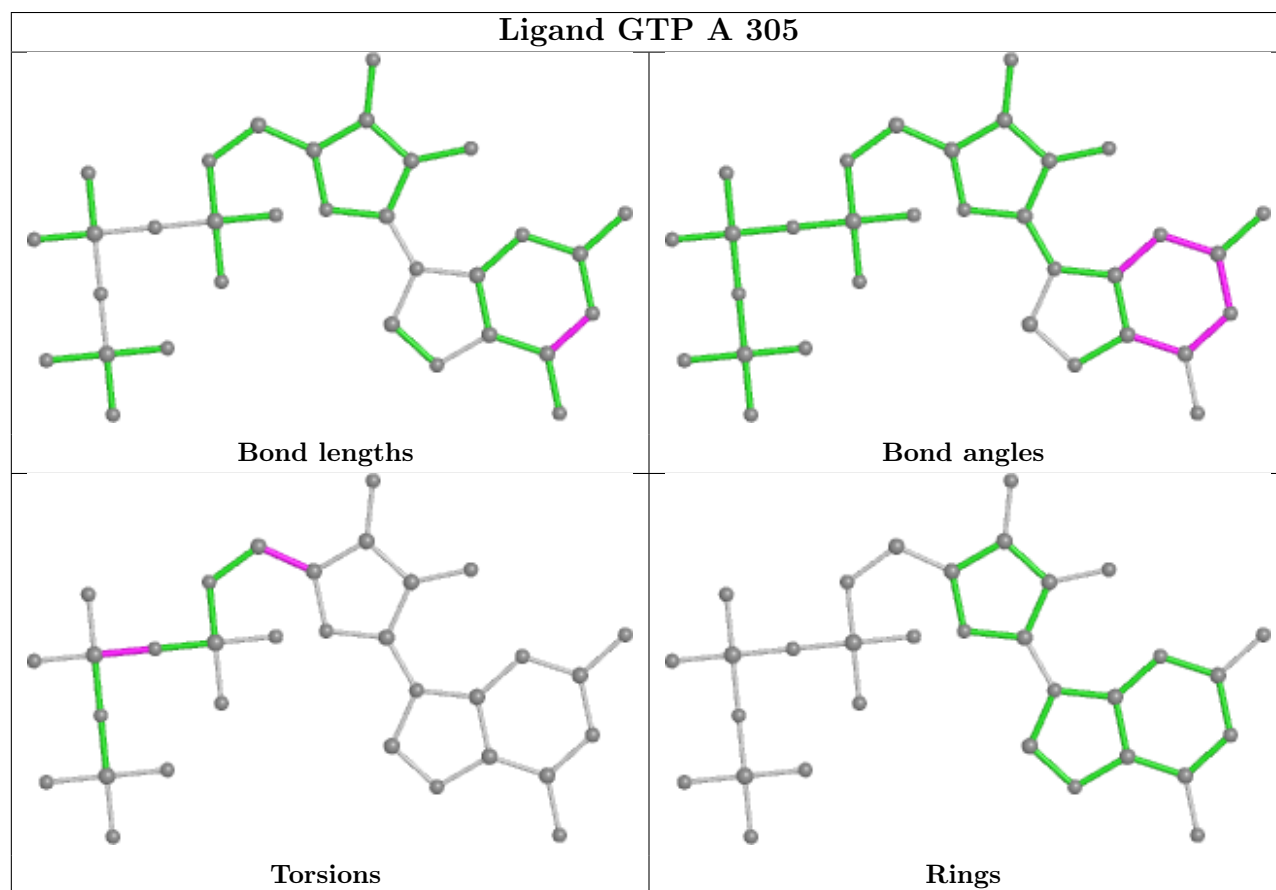
There are no ring outliers.

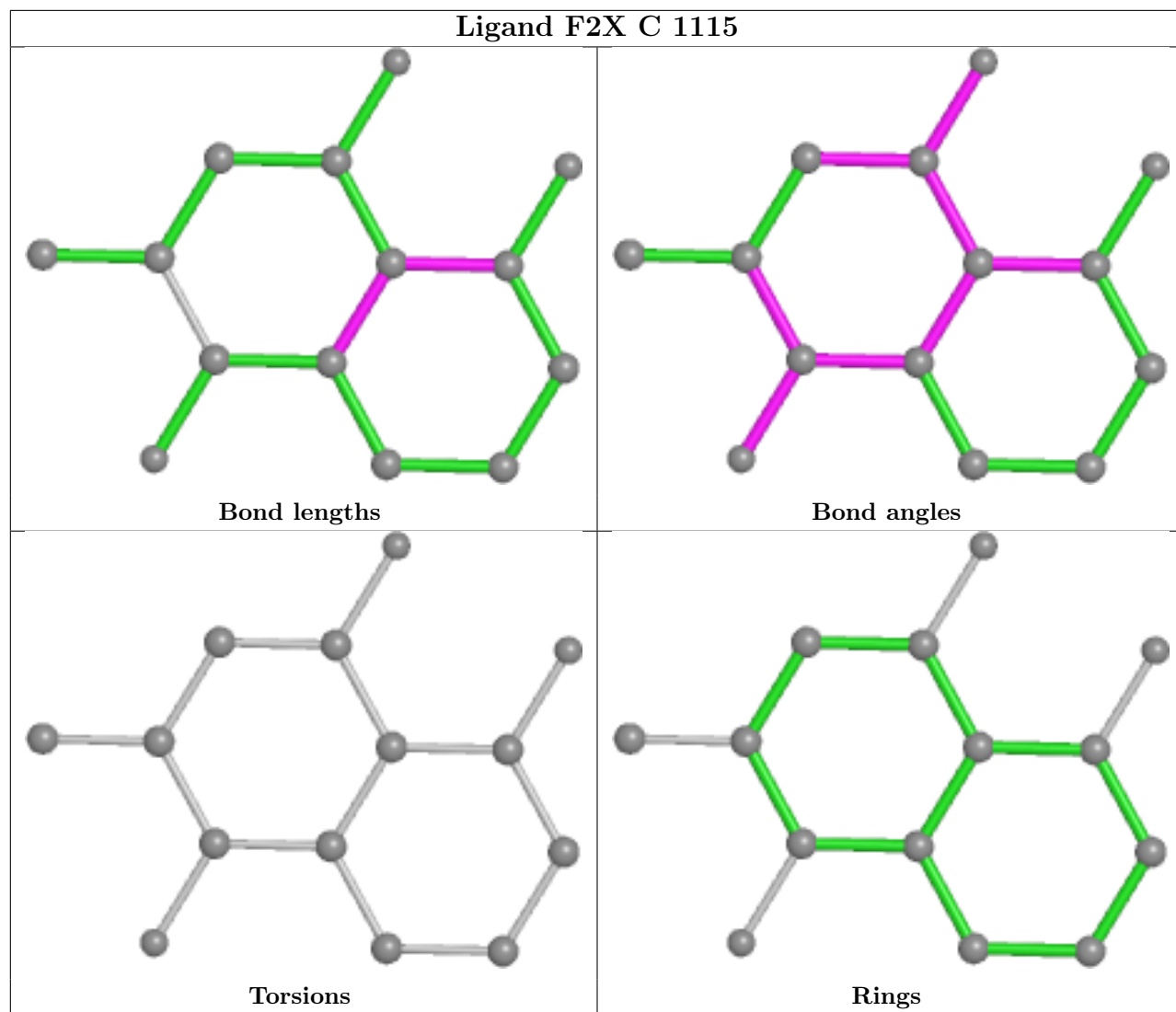
3 monomers are involved in 3 short contacts:

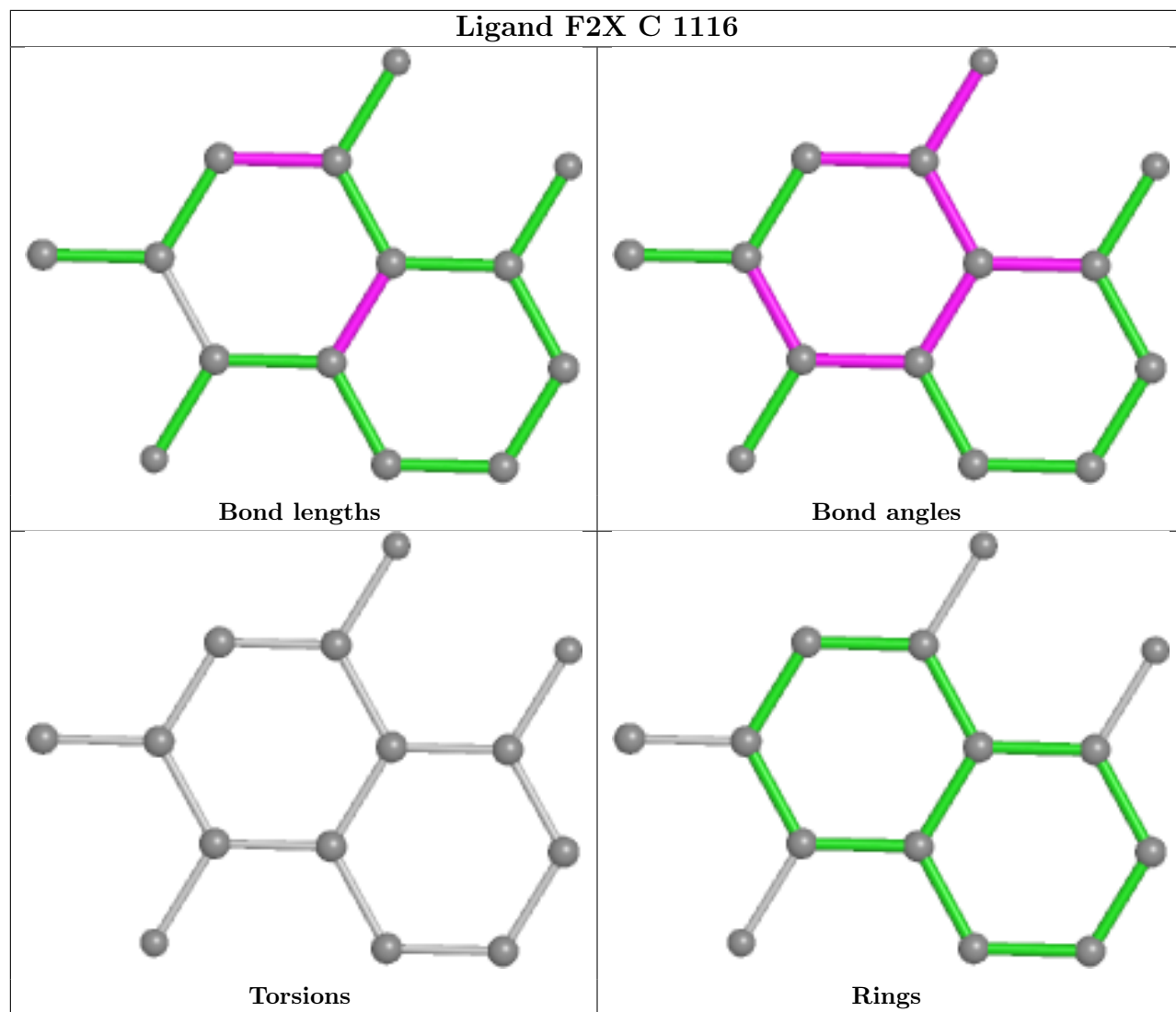
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1107	GOL	1	0
10	C	1115	F2X	1	0
10	C	1117	F2X	1	0

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

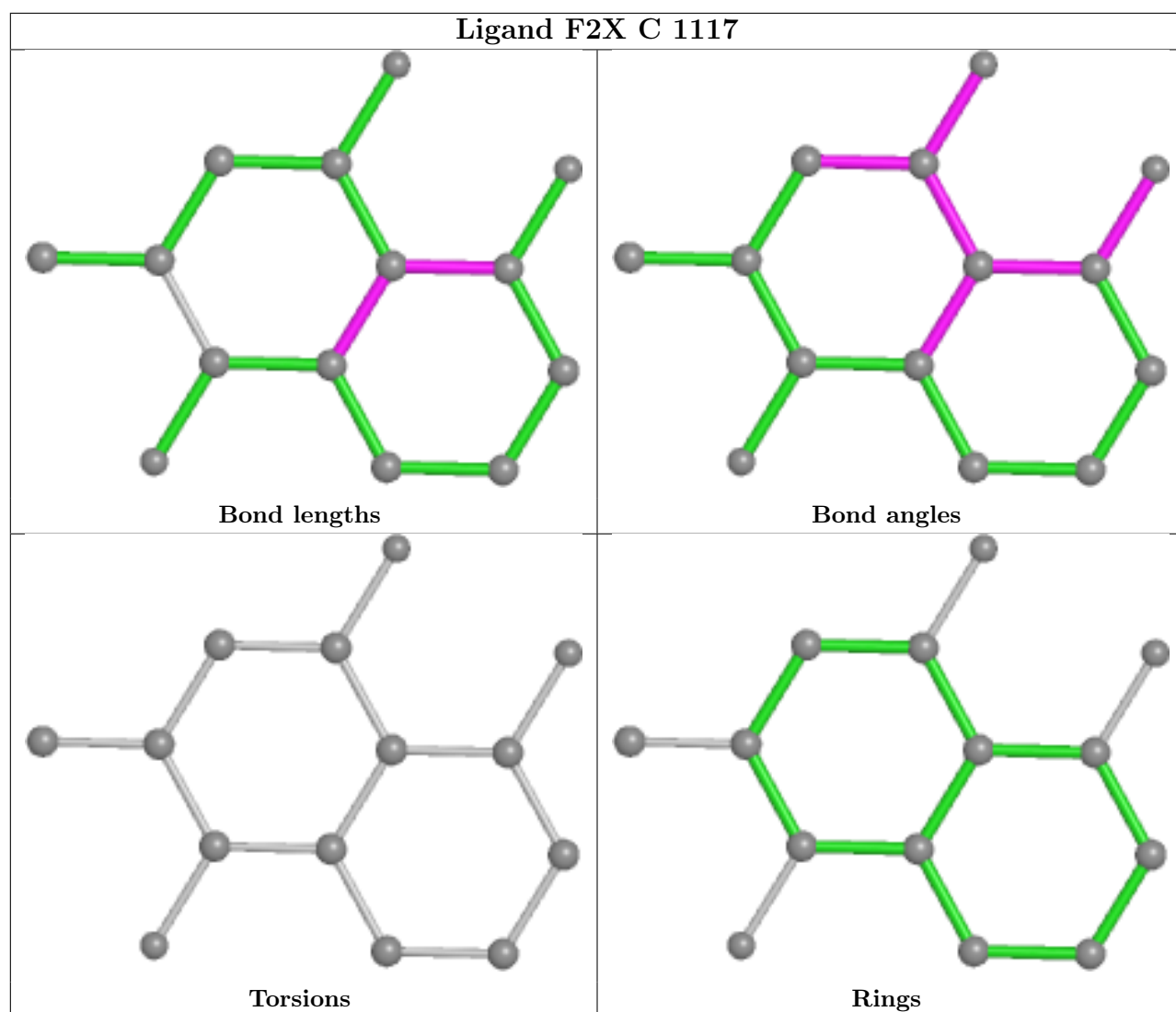
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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

### 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%)	0.84	34 (16%) <b>1</b> <b>1</b>	39, 56, 122, 151	0
2	B	121/140 (86%)	0.62	18 (14%) <b>2</b> <b>2</b>	55, 70, 102, 131	0
3	C	995/1003 (99%)	0.42	72 (7%) <b>15</b> <b>16</b>	39, 63, 91, 142	0
All	All	1324/1359 (97%)	0.51	124 (9%) <b>8</b> <b>8</b>	39, 64, 96, 151	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	81	GLU	7.7
3	C	689	LEU	6.9
3	C	616	ARG	5.6
3	C	684	THR	5.5
3	C	543	ARG	5.5
2	B	80	GLU	5.3
1	A	15	LEU	5.1
1	A	195	ALA	5.1
1	A	86	ALA	5.0
1	A	87	ILE	4.9
1	A	13	LEU	4.7
3	C	896	ASN	4.5
1	A	194	ALA	4.4
1	A	14	VAL	4.3
3	C	958	LEU	4.2
3	C	615	PRO	4.2
3	C	685	ALA	4.1
3	C	979	ALA	4.0
3	C	962	LEU	3.9
1	A	192	ALA	3.8
3	C	105	ASP	3.8
1	A	189	MET	3.8
1	A	88	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	898	ARG	3.7
1	A	118	VAL	3.7
1	A	63	VAL	3.7
2	B	85	VAL	3.7
3	C	983	GLN	3.6
1	A	108	LEU	3.6
2	B	120	ASN	3.5
1	A	16	VAL	3.5
3	C	726	TYR	3.5
3	C	104	ASP	3.5
3	C	687	PRO	3.4
1	A	9	VAL	3.4
3	C	957	LEU	3.4
2	B	168	GLU	3.3
3	C	8	SER	3.2
3	C	978	GLU	3.2
2	B	84	GLU	3.1
1	A	215	ASP	3.1
3	C	959	LEU	3.1
3	C	893	PHE	3.0
3	C	267	ASP	3.0
1	A	117	ILE	3.0
1	A	127	LYS	3.0
3	C	315	LEU	2.9
3	C	106	GLU	2.9
3	C	587	THR	2.9
3	C	905	LEU	2.8
2	B	196	GLU	2.8
1	A	202	GLU	2.8
1	A	164	LEU	2.7
3	C	10	ASP	2.7
1	A	180	PRO	2.7
3	C	917	ARG	2.7
3	C	939	THR	2.7
1	A	56	ARG	2.7
3	C	6	ASP	2.6
3	C	319	LEU	2.6
2	B	82	ASP	2.6
1	A	85	CYS	2.6
1	A	57	GLY	2.6
3	C	500	TRP	2.6
3	C	7	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	110	THR	2.5
3	C	936	VAL	2.5
3	C	334	GLU	2.5
3	C	935	PHE	2.5
2	B	197	ILE	2.5
3	C	891	TRP	2.5
3	C	889	ILE	2.5
2	B	101	LYS	2.5
1	A	55	ASN	2.4
3	C	4	ILE	2.4
3	C	347	LEU	2.4
1	A	188	VAL	2.4
2	B	200	LYS	2.4
2	B	199	LYS	2.4
3	C	690	LEU	2.4
3	C	109	LYS	2.4
1	A	80	TYR	2.4
3	C	108	PHE	2.4
3	C	269	ASP	2.4
3	C	555	ILE	2.3
1	A	193	LEU	2.3
2	B	86	LEU	2.3
3	C	637	GLN	2.3
3	C	462	ILE	2.3
1	A	191	PRO	2.3
2	B	99	ASP	2.3
3	C	909	LEU	2.3
3	C	697	LYS	2.3
3	C	907	ILE	2.3
3	C	686	ASN	2.3
3	C	570	TRP	2.3
1	A	161	PHE	2.2
3	C	985	THR	2.2
3	C	540	GLU	2.2
3	C	29	VAL	2.2
3	C	544	GLY	2.2
3	C	984	GLY	2.2
2	B	122	VAL	2.1
2	B	100	ALA	2.1
2	B	121	LYS	2.1
1	A	26	PHE	2.1
3	C	332	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	366	TRP	2.1
3	C	107	VAL	2.1
3	C	912	VAL	2.1
1	A	160	PRO	2.1
1	A	119	LEU	2.1
3	C	159	LEU	2.1
3	C	253	LEU	2.1
1	A	198	GLU	2.1
3	C	103	GLN	2.1
3	C	940	PHE	2.1
3	C	545	LYS	2.0
2	B	115	LYS	2.0
3	C	348	ILE	2.0
3	C	188	LYS	2.0
3	C	102	CYS	2.0
3	C	559	VAL	2.0
3	C	977	GLN	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
6	NO3	C	1110	4/4	0.65	0.27	99,100,105,107	0
5	GOL	A	302	6/6	0.67	0.41	73,89,95,98	0
8	CL	C	1103	1/1	0.76	0.15	91,91,91,91	0
9	DMS	C	1114	4/4	0.77	0.32	129,139,141,142	0
8	CL	C	1102	1/1	0.80	0.17	92,92,92,92	0
6	NO3	C	1106	4/4	0.81	0.21	106,106,111,115	0

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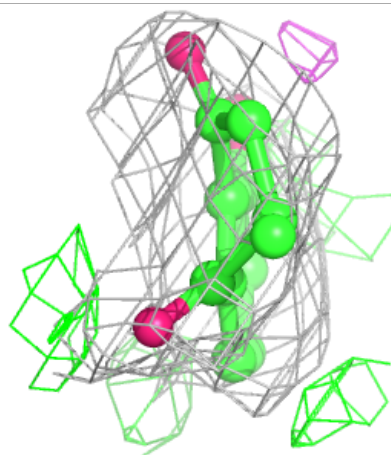
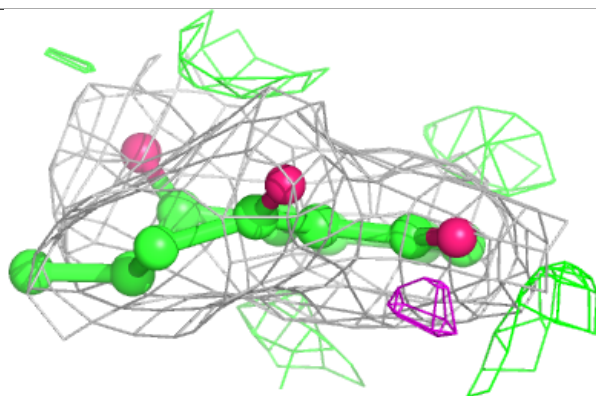
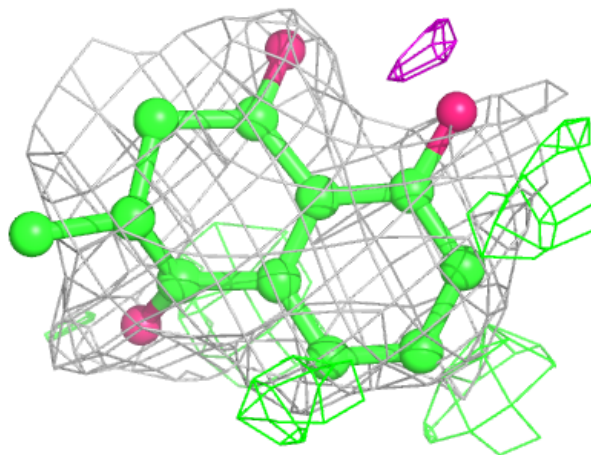
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NO3	C	1109	4/4	0.82	0.51	81,85,89,93	0
5	GOL	C	1108	6/6	0.83	0.25	72,80,84,85	0
6	NO3	C	1101	4/4	0.84	0.48	74,76,81,85	0
5	GOL	C	1107	6/6	0.84	0.35	77,86,87,88	0
6	NO3	C	1113	4/4	0.84	0.28	83,89,92,95	0
6	NO3	C	1111	4/4	0.85	0.17	92,93,97,100	0
10	F2X	C	1116	14/14	0.85	0.20	96,108,110,112	0
6	NO3	A	304	4/4	0.87	0.20	82,86,92,93	0
9	DMS	C	1112	4/4	0.87	0.30	139,139,140,140	0
9	DMS	C	1105	4/4	0.88	0.28	110,111,113,114	0
10	F2X	C	1117	14/14	0.88	0.12	86,99,103,103	0
6	NO3	A	306	4/4	0.91	0.17	82,83,85,95	0
6	NO3	A	303	4/4	0.91	0.19	62,64,66,74	0
8	CL	C	1104	1/1	0.93	0.17	97,97,97,97	0
10	F2X	C	1115	14/14	0.94	0.13	69,71,74,76	0
7	GTP	A	305	32/32	0.98	0.10	40,46,49,52	0
4	MG	A	301	1/1	0.99	0.06	44,44,44,44	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.

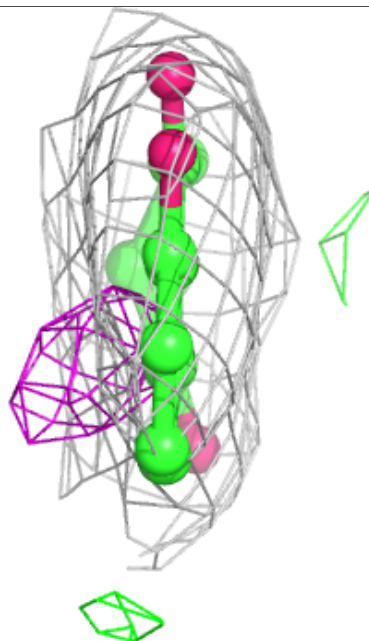
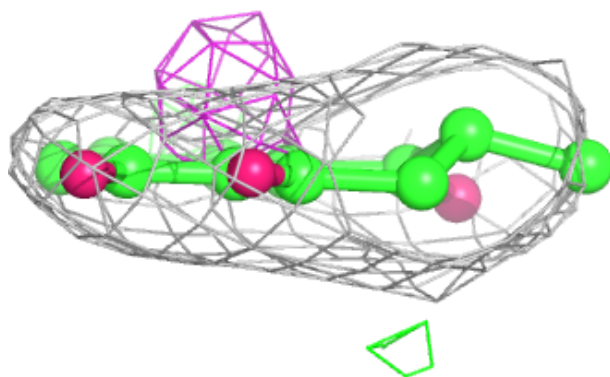
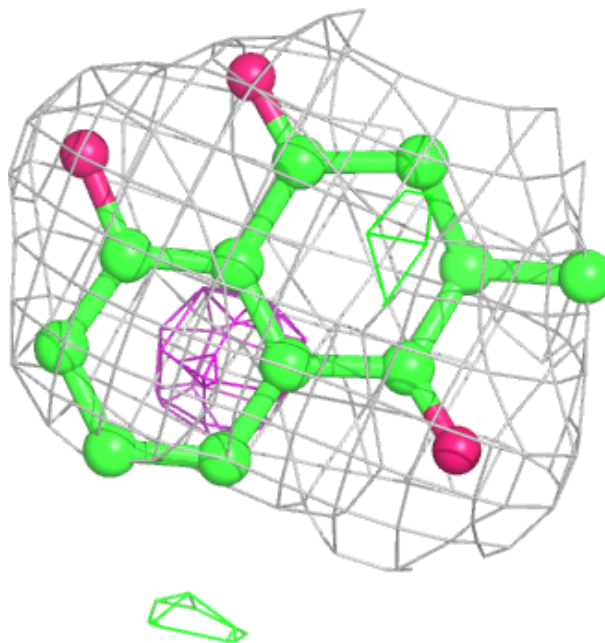
**Electron density around F2X C 1116:**

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



**Electron density around F2X C 1117:**

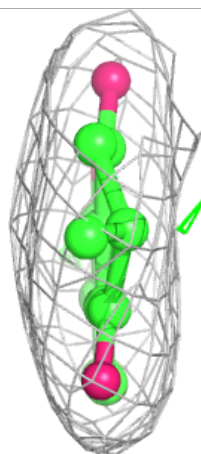
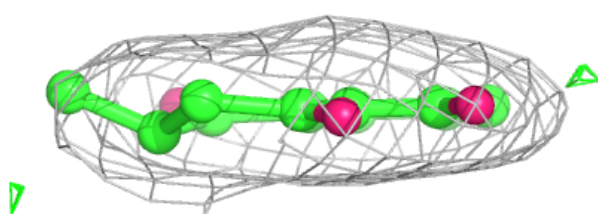
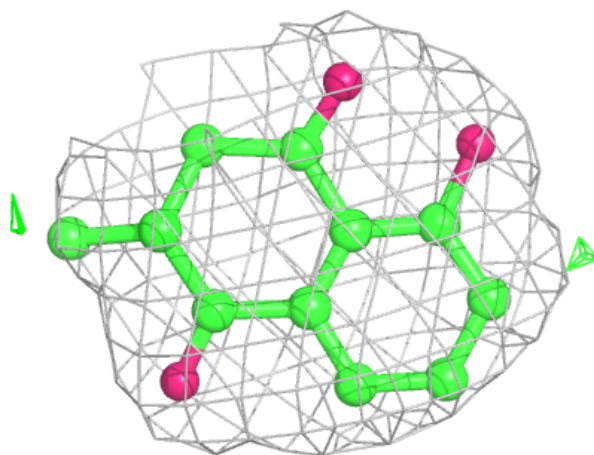
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

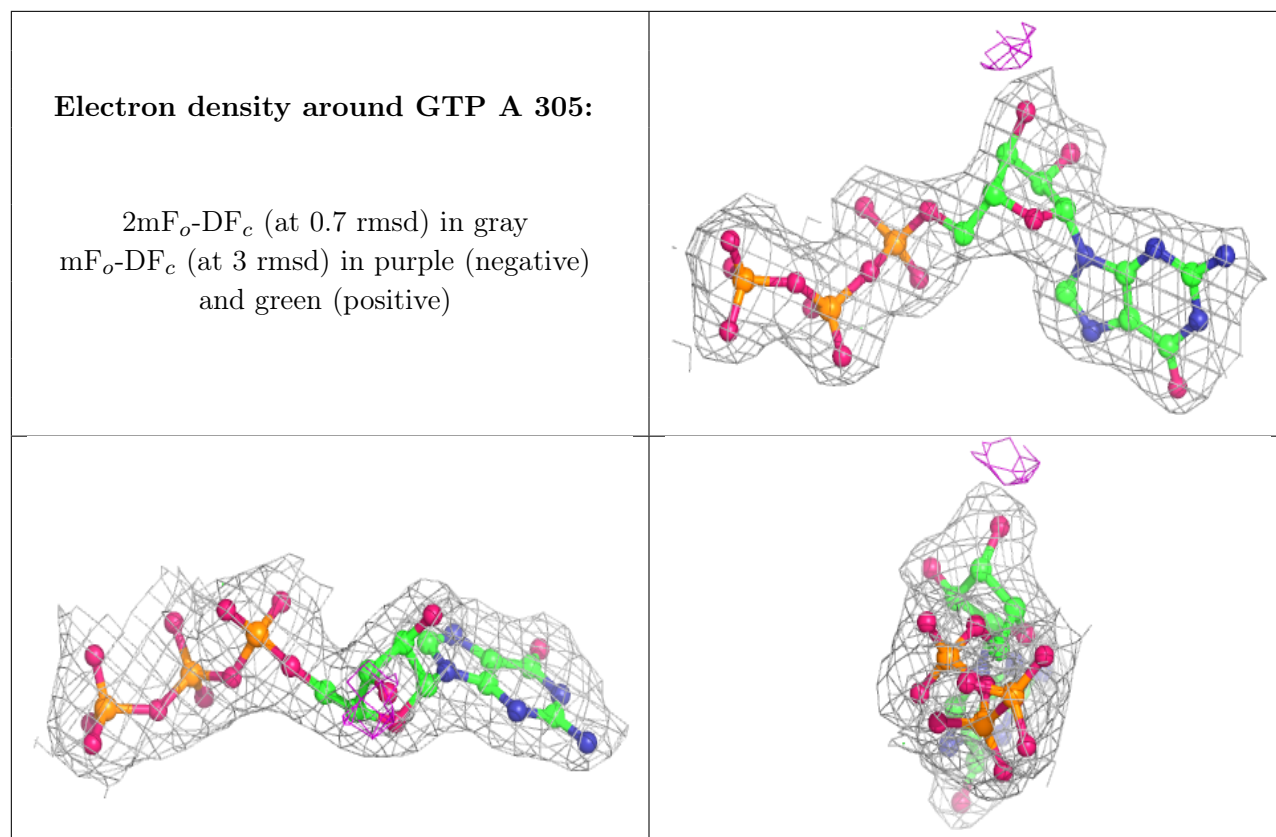




**Electron density around F2X C 1115:**

$2mF_o-DF_c$  (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.