



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 06:12 PM JST

PDB ID : 9X7O / pdb_00009x7o
Title : Lansoprazole derivative in complex with CRM1-Ran-RanBP1
Authors : Sun, Q.; Luo, Y.
Deposited on : 2025-10-17
Resolution : 2.00 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 : 1.8.5 (274361), 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

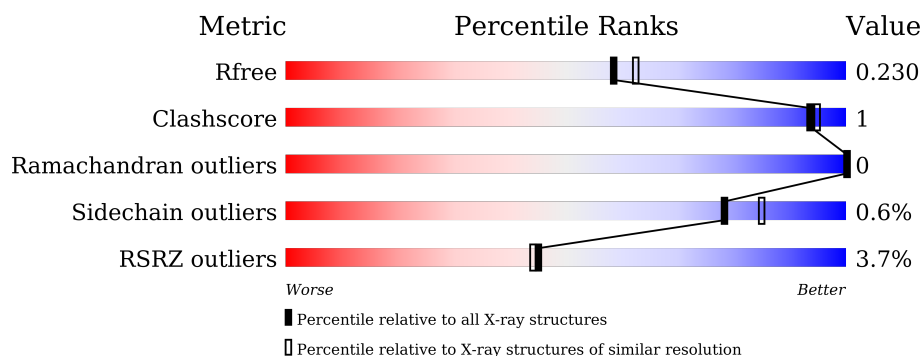
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	216	<div> <div>12%</div> <div> <div></div> <div>91%</div> <div>5% . .</div> </div> </div>
2	B	140	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>. 9%</div> </div> </div>
3	C	1003	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>. .</div> </div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12151 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	3	0
			1691	1092	288	304	7			

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	127	Total	C	N	O	S	0	0	0
			1043	663	182	194	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	12	0
			8137	5226	1341	1528	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	51	VAL	ALA	engineered mutation	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822

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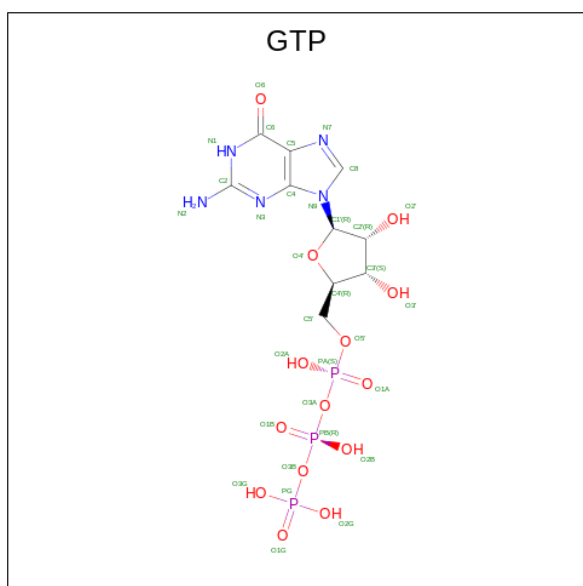
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	PRO	deletion	UNP P30822
C	?	-	ALA	deletion	UNP P30822
C	?	-	THR	deletion	UNP P30822
C	?	-	GLU	deletion	UNP P30822
C	?	-	MET	deletion	UNP P30822
C	?	-	SER	deletion	UNP P30822
C	?	-	PRO	deletion	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP P30822
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	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 GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

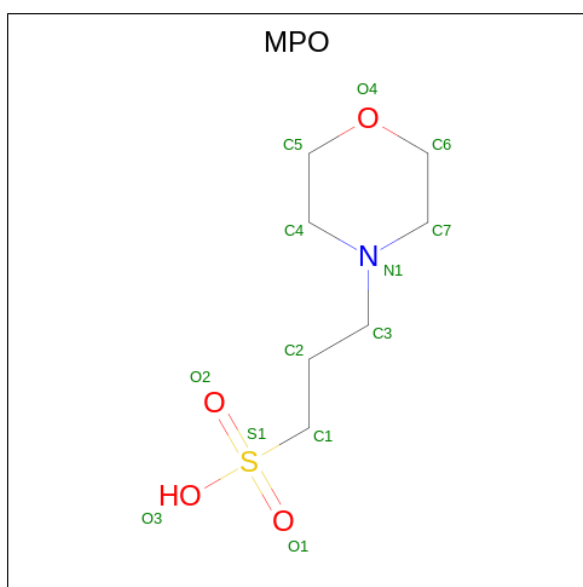


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: C₇H₁₅NO₄S).

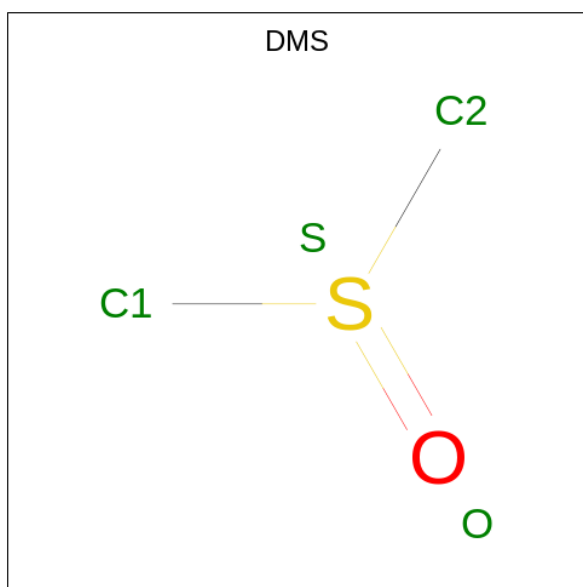


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

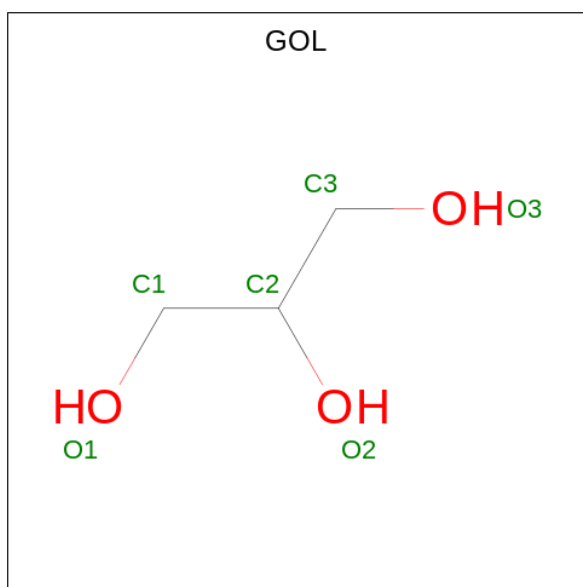
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	C	4	Total	Cl	0	0
			4	4		

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



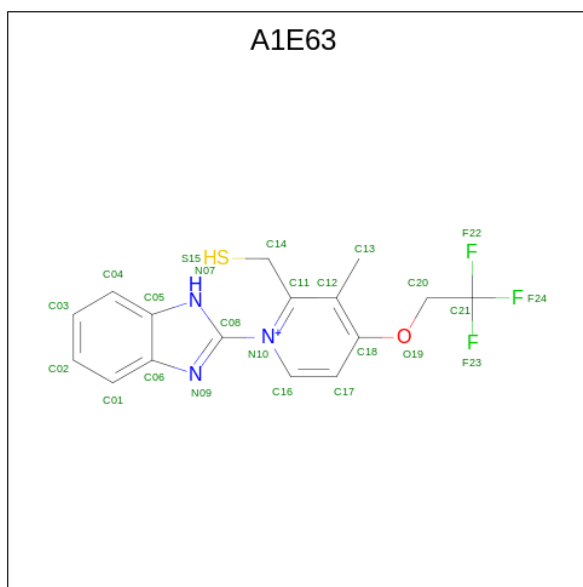
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 10 is [1-(1H-benzimidazol-2-yl)-3-methyl-4-[2,2,2-tris(fluoranyl)ethoxy]pyridin-1-ium-2-yl]methanethiol (CCD ID: A1E63) (formula: C₁₆H₁₅F₃N₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	C	1	Total	C	F	N	O	S	0	0
			24	16	3	3	1	1		

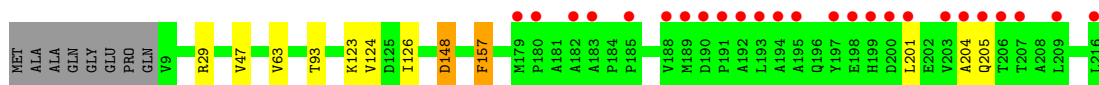
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	209	Total	O	0	0
			209	209		
11	B	63	Total	O	0	0
			63	63		
11	C	901	Total	O	0	1
			901	901		

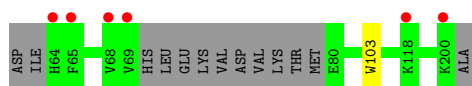
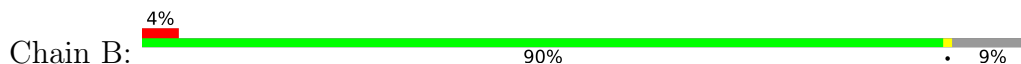
3 Residue-property plots [i](#)

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.

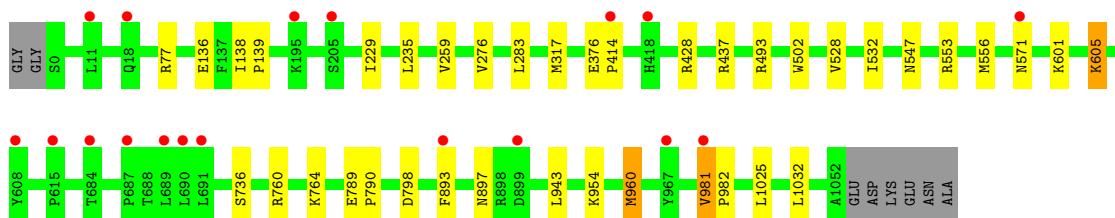
- Molecule 1: GTP-binding nuclear protein Ran



- 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, α , β , γ	105.89Å 105.89Å 305.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.35 – 2.00 32.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (32.35-2.00) 97.1 (32.35-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.187 , 0.218 0.200 , 0.230	Depositor DCC
R_{free} test set	5843 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12151	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, GTP, A1E63, DMS, MPO, CL

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	0.52	0/1733	0.86	1/2349 (0.0%)
2	B	0.47	0/1062	0.83	0/1419
3	C	0.44	0/8293	0.90	1/11238 (0.0%)
All	All	0.46	0/11088	0.88	2/15006 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ASP	CA-CB-CG	5.70	118.30	112.60
3	C	893	PHE	CA-CB-CG	5.26	119.06	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	428	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	1691	0	1687	8	0
2	B	1043	0	1038	1	0
3	C	8137	0	8213	23	0
4	A	32	0	12	1	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
6	A	13	0	15	1	0
7	A	1	0	0	0	0
7	C	4	0	0	1	0
8	A	4	0	6	0	0
8	C	8	0	12	1	0
9	A	6	0	8	1	0
9	C	12	0	16	2	0
10	C	24	0	0	0	0
11	A	209	0	0	0	0
11	B	63	0	0	0	0
11	C	901	0	0	3	0
All	All	12151	0	11007	31	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 1.

All (31) 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:437:ARG:NH1	9:C:1106:GOL:O1	2.38	0.57
1:A:124:VAL:HG11	1:A:148:ASP:HB3	1.87	0.57
3:C:943[B]:LEU:HD21	3:C:1032:LEU:HD22	1.88	0.55
6:A:303:MPO:H21	3:C:317:MET:SD	2.47	0.54
1:A:201:LEU:HG	1:A:205:GLN:HE21	1.74	0.51
3:C:502:TRP:HE1	3:C:547:ASN:HD22	1.58	0.50
1:A:204:ALA:HB1	2:B:103:TRP:CZ2	2.47	0.48
1:A:124:VAL:HG23	9:A:306:GOL:H11	1.97	0.47
3:C:229:ILE:HG22	3:C:235:LEU:HG	1.96	0.47
3:C:981:VAL:HG13	3:C:982:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:960[B]:MET:SD	3:C:1025:LEU:HA	2.56	0.46
1:A:123:LYS:HG2	4:A:301:GTP:C6	2.52	0.45
3:C:571:ASN:HB2	7:C:1103:CL:CL	2.53	0.45
3:C:77:ARG:HB3	8:C:1107:DMS:C1	2.47	0.44
3:C:553:ARG:HA	3:C:556:MET:HE3	1.98	0.44
3:C:235:LEU:HD21	3:C:259:VAL:HG11	1.99	0.44
1:A:29:ARG:HG2	1:A:157[B]:PHE:CE1	2.53	0.44
3:C:789:GLU:HB3	3:C:790:PRO:HD3	1.99	0.44
3:C:601:LYS:O	3:C:605:LYS:HD3	2.17	0.43
3:C:276:VAL:HG21	9:C:1105:GOL:H2	1.99	0.43
1:A:93:THR:HG21	1:A:126:ILE:HD12	2.00	0.43
3:C:760:ARG:HD3	11:C:1318:HOH:O	2.18	0.43
3:C:897[B]:ASN:OD1	3:C:897[B]:ASN:N	2.49	0.43
3:C:376:GLU:HA	3:C:414:PRO:HD3	1.87	0.42
3:C:493:ARG:NH2	11:C:1226:HOH:O	2.51	0.42
3:C:138:ILE:HB	3:C:139:PRO:HD3	2.01	0.42
3:C:528:VAL:O	3:C:532:ILE:HG12	2.21	0.41
1:A:47:VAL:HA	1:A:63:VAL:O	2.21	0.41
3:C:502:TRP:HE1	3:C:547:ASN:ND2	2.19	0.41
3:C:736:SER:HB3	3:C:798[A]:ASP:OD1	2.21	0.41
3:C:764:LYS:NZ	11:C:1240:HOH:O	2.54	0.41

There are no symmetry-related clashes.

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	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
2	B	123/140 (88%)	116 (94%)	7 (6%)	0	100	100
3	C	1005/1003 (100%)	989 (98%)	16 (2%)	0	100	100
All	All	1337/1359 (98%)	1309 (98%)	28 (2%)	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	182/184 (99%)	180 (99%)	2 (1%)	65	73
2	B	109/121 (90%)	109 (100%)	0	100	100
3	C	922/915 (101%)	915 (99%)	7 (1%)	73	80
All	All	1213/1220 (99%)	1204 (99%)	9 (1%)	78	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157[A]	PHE
1	A	157[B]	PHE
3	C	136	GLU
3	C	283	LEU
3	C	605	LYS
3	C	954	LYS
3	C	960[A]	MET
3	C	960[B]	MET
3	C	981	VAL

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	154	ASN
1	A	205	GLN
3	C	30	GLN
3	C	31	GLN
3	C	274	GLN
3	C	477	HIS
3	C	494	GLN
3	C	547	ASN
3	C	730	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	A	301	5	30,34,34	0.56	0	46,54,54	0.55	0
8	DMS	A	305	-	3,3,3	0.21	0	3,3,3	0.20	0
10	A1E63	C	1111	-	23,26,26	1.58	4 (17%)	28,38,38	1.53	3 (10%)
9	GOL	C	1105	-	5,5,5	0.11	0	5,5,5	0.30	0
9	GOL	A	306	-	5,5,5	0.09	0	5,5,5	0.33	0
6	MPO	A	303	-	13,13,13	0.71	1 (7%)	17,17,17	0.97	1 (5%)
8	DMS	C	1107	-	3,3,3	0.23	0	3,3,3	0.08	0
9	GOL	C	1106	-	5,5,5	0.10	0	5,5,5	0.31	0
8	DMS	C	1108	-	3,3,3	0.24	0	3,3,3	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	301	5	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	C	1105	-	-	2/4/4/4	-
9	GOL	A	306	-	-	0/4/4/4	-
6	MPO	A	303	-	-	6/7/15/15	0/1/1/1
9	GOL	C	1106	-	-	0/4/4/4	-
10	A1E63	C	1111	-	-	5/6/12/12	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1111	A1E63	C14-C11	4.28	1.55	1.50
10	C	1111	A1E63	C06-N09	-2.93	1.33	1.39
10	C	1111	A1E63	C05-N07	-2.36	1.34	1.38
6	A	303	MPO	O3-S1	2.33	1.55	1.47
10	C	1111	A1E63	C16-N10	-2.18	1.33	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1111	A1E63	O19-C18-C12	4.80	120.28	115.33
10	C	1111	A1E63	C20-O19-C18	-2.69	111.11	117.67
6	A	303	MPO	C3-N1-C7	2.59	117.85	111.23
10	C	1111	A1E63	C06-N09-C08	2.12	108.29	104.30

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	303	MPO	C2-C1-S1-O1
6	A	303	MPO	C1-C2-C3-N1
9	C	1105	GOL	O1-C1-C2-C3
10	C	1111	A1E63	O19-C20-C21-F22
10	C	1111	A1E63	O19-C20-C21-F24
10	C	1111	A1E63	O19-C20-C21-F23
6	A	303	MPO	C2-C3-N1-C7
6	A	303	MPO	C2-C1-S1-O3
6	A	303	MPO	C2-C3-N1-C4
9	C	1105	GOL	O1-C1-C2-O2
6	A	303	MPO	C2-C1-S1-O2
10	C	1111	A1E63	C12-C18-O19-C20
10	C	1111	A1E63	C17-C18-O19-C20

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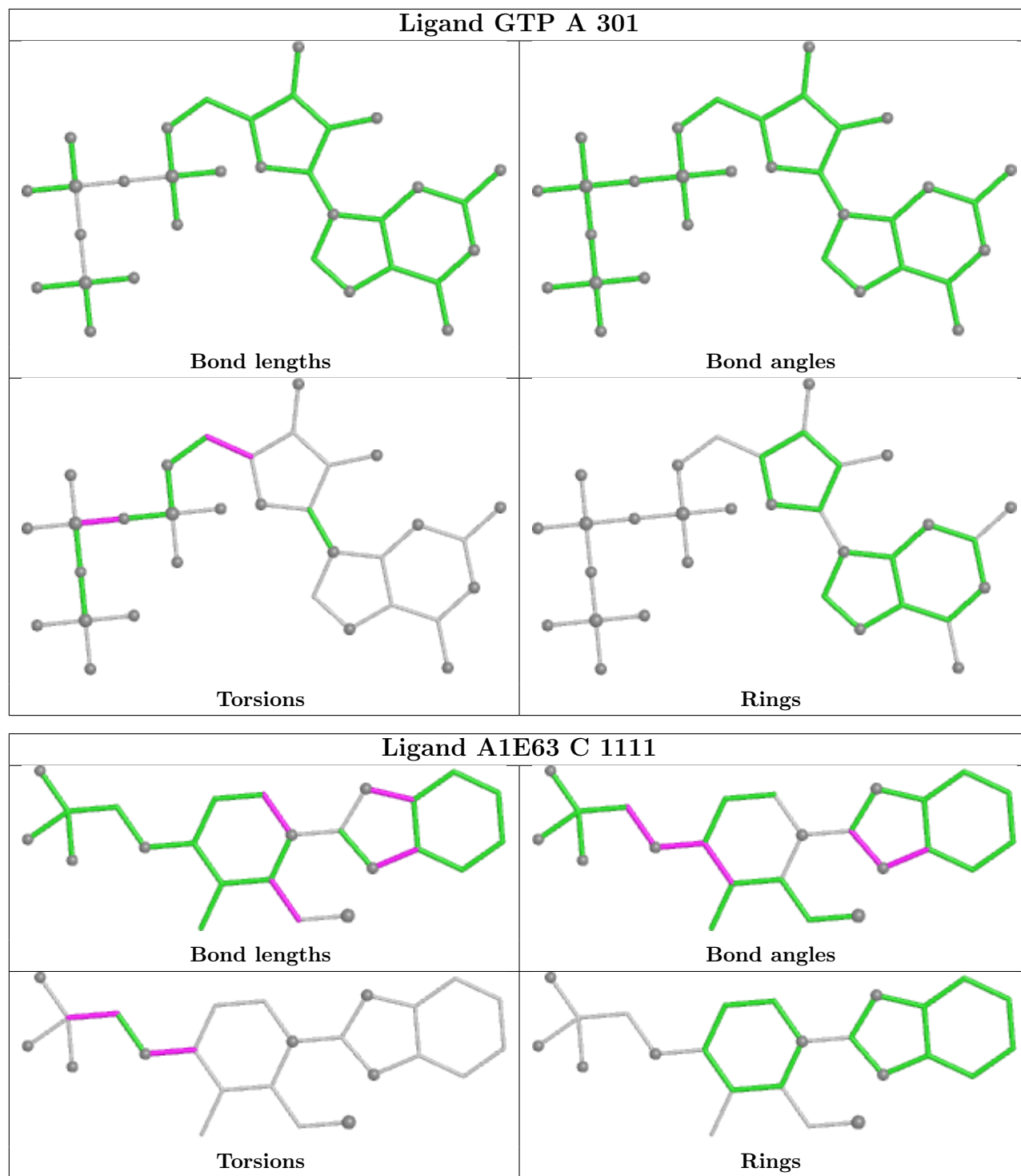
Mol	Chain	Res	Type	Atoms
4	A	301	GTP	PA-O3A-PB-O2B
4	A	301	GTP	O4'-C4'-C5'-O5'
4	A	301	GTP	PA-O3A-PB-O1B

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GTP	1	0
9	C	1105	GOL	1	0
9	A	306	GOL	1	0
6	A	303	MPO	1	0
8	C	1107	DMS	1	0
9	C	1106	GOL	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	208/216 (96%)	0.35	25 (12%) 9 8	14, 45, 109, 136	3 (1%)
2	B	127/140 (90%)	0.64	6 (4%) 36 35	47, 66, 99, 116	0
3	C	995/1003 (99%)	0.25	18 (1%) 67 67	19, 49, 81, 113	12 (1%)
All	All	1330/1359 (97%)	0.30	49 (3%) 45 44	14, 50, 90, 136	15 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	HIS	5.4
1	A	197	TYR	5.4
3	C	571	ASN	5.0
1	A	206	THR	4.9
1	A	195	ALA	4.5
3	C	689	LEU	3.9
2	B	64	HIS	3.9
1	A	194	ALA	3.8
2	B	65	PHE	3.8
1	A	193	LEU	3.7
3	C	690	LEU	3.6
1	A	191	PRO	3.5
1	A	188	VAL	3.5
1	A	198	GLU	3.2
3	C	195[A]	LYS	3.2
1	A	192	ALA	3.1
3	C	893	PHE	3.1
3	C	205	SER	3.1
1	A	216	LEU	3.1
3	C	414	PRO	3.0
1	A	183	ALA	2.9
2	B	68	VAL	2.8
1	A	180	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	967	TYR	2.7
1	A	201	LEU	2.7
3	C	11	LEU	2.7
1	A	179	MET	2.7
2	B	69	VAL	2.6
3	C	981	VAL	2.6
1	A	203	VAL	2.6
3	C	608	TYR	2.5
1	A	182	ALA	2.5
1	A	205	GLN	2.4
3	C	684	THR	2.4
3	C	687	PRO	2.4
3	C	691	LEU	2.3
1	A	185	PRO	2.3
3	C	18	GLN	2.3
3	C	418	HIS	2.3
3	C	899	ASP	2.3
3	C	615	PRO	2.2
2	B	118	LYS	2.2
2	B	200	LYS	2.2
1	A	204	ALA	2.2
1	A	209	LEU	2.2
1	A	189	MET	2.0
1	A	190	ASP	2.0
1	A	200	ASP	2.0
1	A	207	THR	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](#)

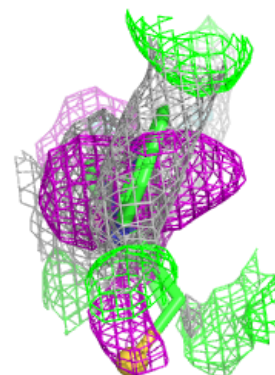
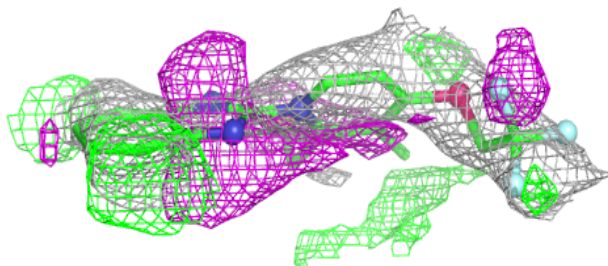
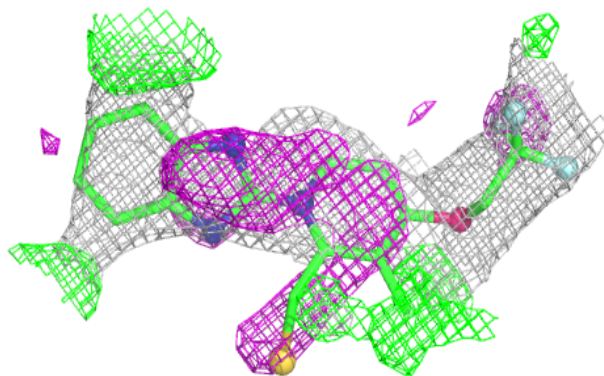
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

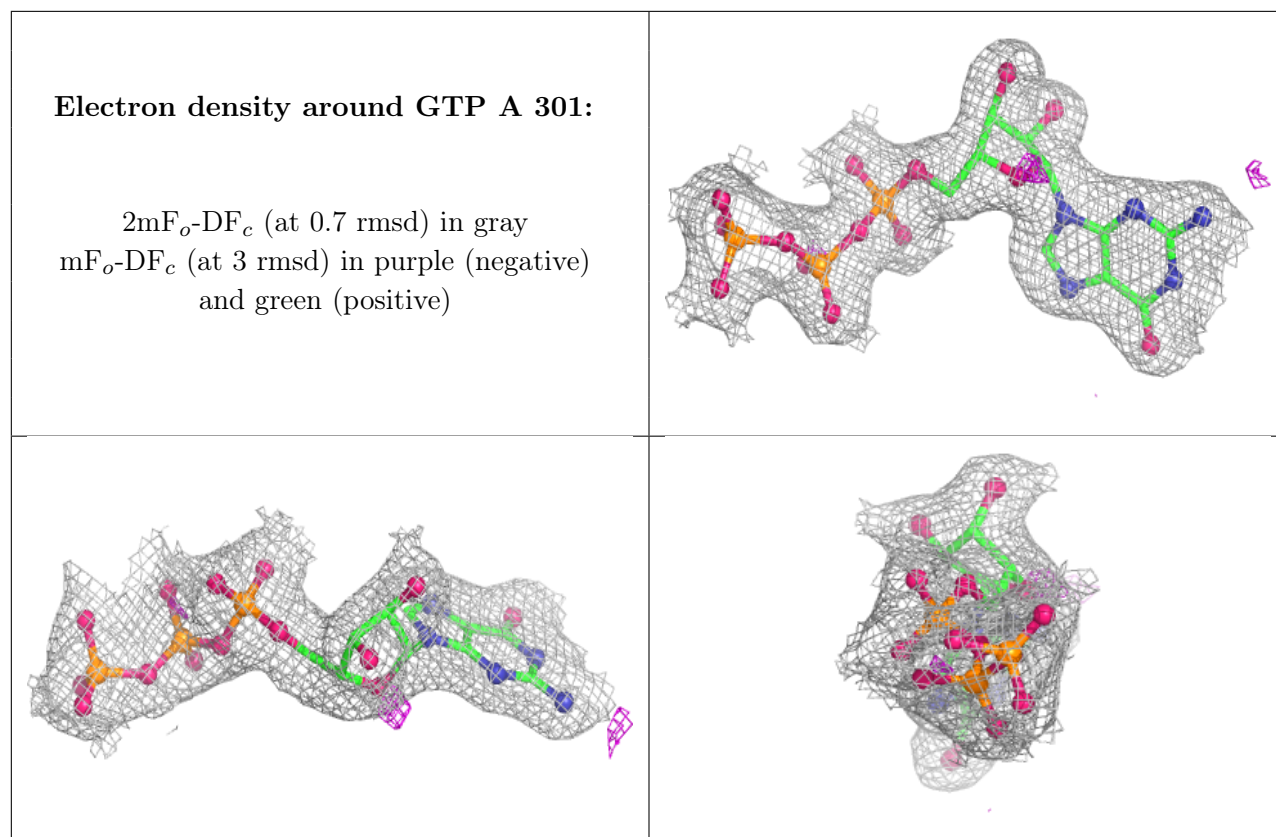
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	A1E63	C	1111	24/24	0.43	0.26	89,100,108,111	0
9	GOL	A	306	6/6	0.54	0.35	20,20,20,20	0
8	DMS	C	1108	4/4	0.68	0.28	90,92,94,95	0
9	GOL	C	1105	6/6	0.82	0.14	66,70,71,71	0
8	DMS	A	305	4/4	0.85	0.20	62,66,68,69	0
8	DMS	C	1107	4/4	0.85	0.19	83,83,87,87	0
6	MPO	A	303	13/13	0.86	0.17	55,66,70,70	0
9	GOL	C	1106	6/6	0.87	0.13	66,67,68,69	0
5	MG	C	1110	1/1	0.87	0.18	30,30,30,30	0
7	CL	C	1102	1/1	0.88	0.13	90,90,90,90	0
7	CL	C	1104	1/1	0.88	0.17	80,80,80,80	0
7	CL	A	304	1/1	0.88	0.14	87,87,87,87	0
5	MG	C	1101	1/1	0.89	0.13	70,70,70,70	1
7	CL	C	1103	1/1	0.90	0.09	93,93,93,93	0
7	CL	C	1109	1/1	0.91	0.12	74,74,74,74	0
4	GTP	A	301	32/32	0.98	0.05	30,35,38,40	0
5	MG	A	302	1/1	0.99	0.02	36,36,36,36	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 A1E63 C 1111:

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.