



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2021 – 10:12 AM JST

PDB ID : 7DBG  
Title : Yeast CRM1e (apo) in complex with Ran-RanBP1  
Authors : Sun, Q.; Lei, Y.  
Deposited on : 2020-10-20  
Resolution : 2.06 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 : 2.23.1  
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) : 2.23.1

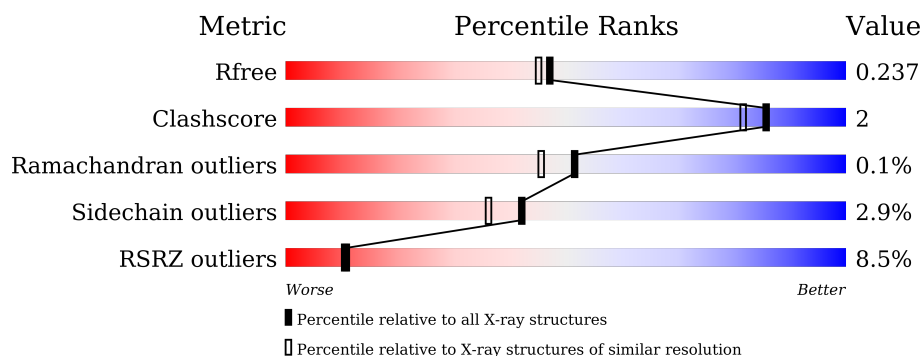
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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>18%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
2	B	140	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div></div> </div> <div>15%</div> </div>
3	C	1003	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div></div> </div> <div>8%</div> </div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11398 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	209	Total	C	N	O	S	0	0	0
			1672	1079	285	302	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLU	GLN	conflict	UNP P62826
A	69	LEU	GLN	engineered mutation	UNP P62826
A	182	ALA	LEU	engineered mutation	UNP P62826

- Molecule 2 is a protein called YRB1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	S	0	0	0
			974	618	172	180	4			

- Molecule 3 is a protein called CRM1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	996	Total	C	N	O	S	0	3	0
			8073	5189	1328	1512	44			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A6A5PZI8
C	-1	GLY	-	expression tag	UNP A0A6A5PZI8
C	0	SER	-	expression tag	UNP A0A6A5PZI8
C	27	GLU	SER	engineered mutation	UNP A0A6A5PZI8
C	49	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	51	VAL	ALA	engineered mutation	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	TYR	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8

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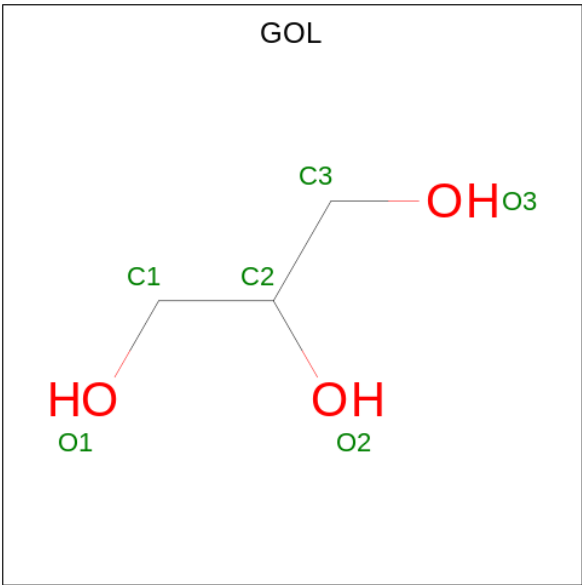
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	ASP	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	537	GLY	ASP	engineered mutation	UNP A0A6A5PZI8
C	539	CYS	THR	engineered mutation	UNP A0A6A5PZI8
C	540	GLU	VAL	engineered mutation	UNP A0A6A5PZI8
C	541	GLN	LYS	engineered mutation	UNP A0A6A5PZI8
C	553	ARG	SER	engineered mutation	UNP A0A6A5PZI8
C	561	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	741	THR	ALA	engineered mutation	UNP A0A6A5PZI8
C	1022	CYS	TYR	engineered mutation	UNP A0A6A5PZI8

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

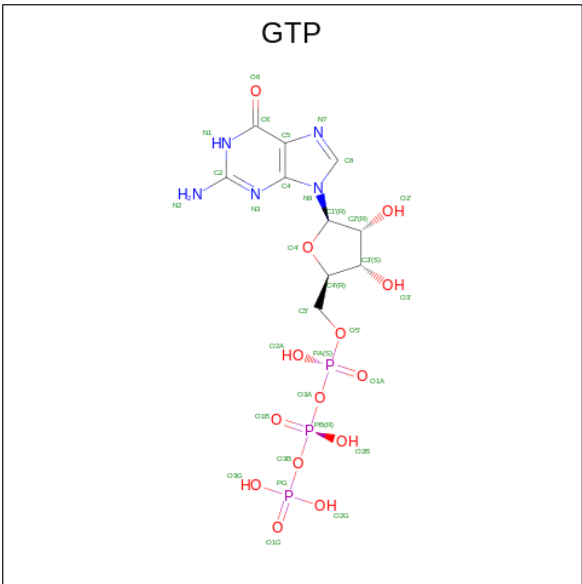
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- 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		

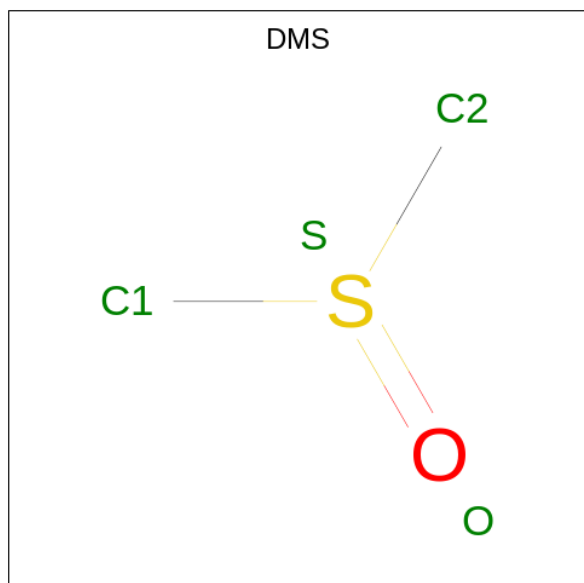
- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

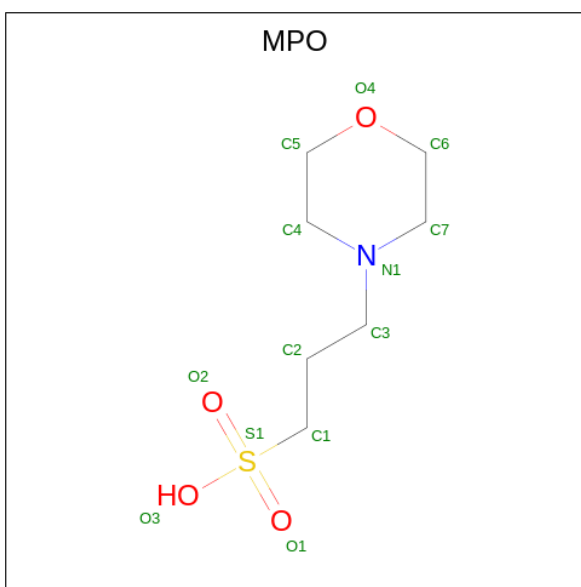
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	C	11	Total	Cl	0	0
			11	11		

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



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

- Molecule 10 is water.

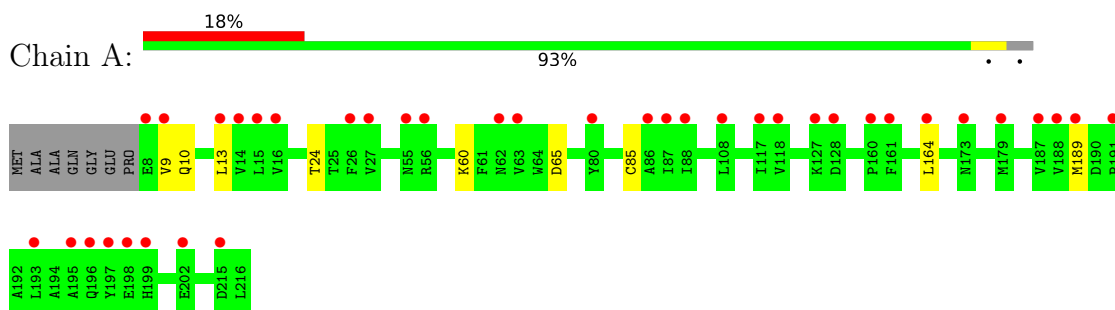
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	123	Total	O	0	1
			124	124		
10	B	28	Total	O	0	0
			28	28		
10	C	449	Total	O	0	0
			449	449		



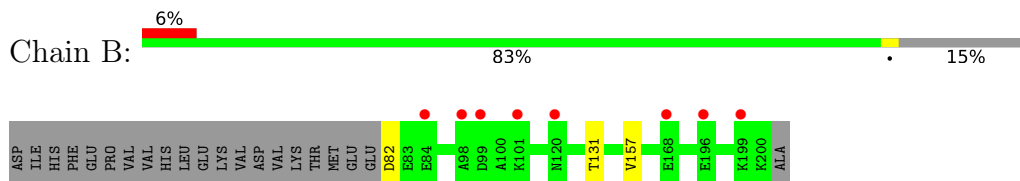
### 3 Residue-property plots [i](#)

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.

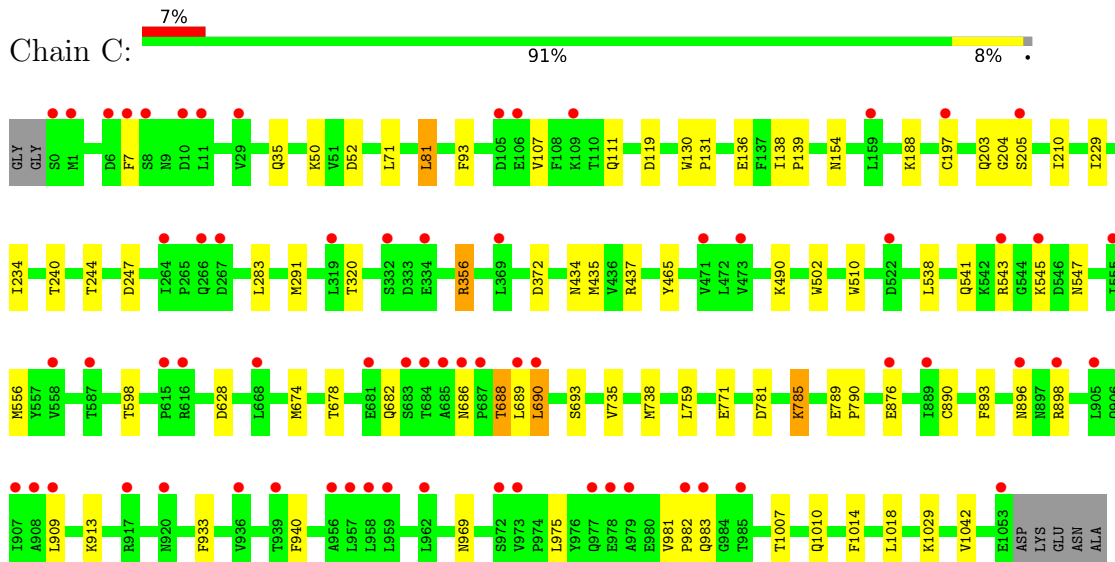
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: YRB1 isoform 1



- Molecule 3: CRM1 isoform 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.90Å 105.90Å 304.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.12 – 2.06 30.12 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.12-2.06) 100.0 (30.12-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.201 , 0.228 0.210 , 0.237	Depositor DCC
$R_{free}$ test set	5615 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, MPO, MG, CL, GOL, GTP

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	0.61	0/1713	0.74	0/2322
2	B	0.63	0/991	0.75	0/1323
3	C	0.64	0/8229	0.70	0/11149
All	All	0.63	0/10933	0.71	0/14794

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	1672	0	1672	4	0
2	B	974	0	980	1	0
3	C	8073	0	8161	43	0
4	A	1	0	0	0	0
5	A	6	0	8	0	0
5	C	6	0	8	3	0
6	A	32	0	12	0	0
7	A	1	0	0	0	0
7	C	11	0	0	0	0
8	C	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	13	0	14	1	0
10	A	124	0	0	0	0
10	B	28	0	0	1	0
10	C	449	0	0	2	0
All	All	11398	0	10867	48	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 (48) 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:356:ARG:HH21	3:C:356:ARG:HB2	1.44	0.83
3:C:502:TRP:HE1	3:C:547:ASN:HD22	1.37	0.73
3:C:556[B]:MET:HA	3:C:556[B]:MET:CE	2.18	0.71
3:C:320:THR:HB	9:C:1115:MPO:H52	1.71	0.71
3:C:981:VAL:HG22	3:C:982:PRO:HD2	1.73	0.71
3:C:556[B]:MET:HA	3:C:556[B]:MET:HE2	1.74	0.68
3:C:197[A]:CYS:SG	10:C:1290:HOH:O	2.52	0.67
3:C:502:TRP:HE1	3:C:547:ASN:ND2	1.93	0.66
3:C:204:GLY:HA2	3:C:210:ILE:HD11	1.76	0.66
3:C:556[B]:MET:HE2	3:C:556[B]:MET:CA	2.31	0.58
3:C:686:ASN:HD21	3:C:688:THR:HG22	1.69	0.56
3:C:435:MET:HE1	3:C:465:TYR:CE1	2.42	0.55
3:C:435:MET:HE1	3:C:465:TYR:CD1	2.41	0.55
3:C:356:ARG:NH2	5:C:1109:GOL:O2	2.40	0.54
1:A:10:GLN:HA	1:A:60:LYS:O	2.11	0.51
3:C:682:GLN:HB3	3:C:689:LEU:HD13	1.91	0.51
3:C:356:ARG:HH21	3:C:356:ARG:CB	2.20	0.51
3:C:1029:LYS:NZ	10:C:1207:HOH:O	2.39	0.50
3:C:674:MET:O	3:C:678:THR:HG23	2.13	0.49
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.44	0.48
1:A:85:CYS:HB2	1:A:164:LEU:HD22	1.96	0.48
3:C:240:THR:O	3:C:244:THR:HG23	2.15	0.47
3:C:81:LEU:HD13	3:C:1042:VAL:HG11	1.98	0.46
3:C:7:PHE:CE2	3:C:50:LYS:HE3	2.51	0.46
3:C:434:ASN:OD1	5:C:1109:GOL:H31	2.15	0.46
3:C:356:ARG:HA	5:C:1109:GOL:C1	2.46	0.45
2:B:131:THR:HA	10:B:321:HOH:O	2.16	0.45
3:C:556[B]:MET:HE2	3:C:598:THR:HG21	1.99	0.45
3:C:690:LEU:HB3	3:C:738:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:ILE:HB	3:C:139:PRO:HD3	1.98	0.44
3:C:229:ILE:HA	3:C:234:ILE:CG2	2.48	0.44
3:C:130:TRP:CD1	3:C:131:PRO:HA	2.53	0.43
3:C:107:VAL:HG13	3:C:111:GLN:HG3	1.99	0.43
3:C:686:ASN:ND2	3:C:688:THR:HG22	2.33	0.43
3:C:890:CYS:O	3:C:893:PHE:HB2	2.19	0.43
1:A:13:LEU:C	1:A:13:LEU:HD23	2.39	0.42
1:A:24:THR:OG1	1:A:65:ASP:OD2	2.37	0.42
3:C:437:ARG:HB3	3:C:510:TRP:CZ2	2.54	0.42
3:C:789:GLU:HB3	3:C:790:PRO:HD3	2.00	0.42
3:C:81:LEU:HD12	3:C:81:LEU:HA	1.90	0.42
3:C:556[B]:MET:HE2	3:C:556[B]:MET:HB3	1.94	0.42
3:C:682:GLN:HB3	3:C:689:LEU:CD1	2.50	0.42
3:C:247:ASP:N	3:C:247:ASP:OD1	2.53	0.42
3:C:933:PHE:HE2	3:C:975:LEU:HB3	1.85	0.42
3:C:781:ASP:O	3:C:785:LYS:HB2	2.19	0.41
3:C:1007:THR:H	3:C:1010:GLN:HE21	1.69	0.41
3:C:735:VAL:HG13	3:C:759:LEU:HB3	2.03	0.41
3:C:1014:PHE:CZ	3:C:1018:LEU:HD22	2.56	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	207/216 (96%)	202 (98%)	5 (2%)	0	100	100
2	B	117/140 (84%)	112 (96%)	5 (4%)	0	100	100
3	C	997/1003 (99%)	984 (99%)	12 (1%)	1 (0%)	51	45
All	All	1321/1359 (97%)	1298 (98%)	22 (2%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	205	SER

### 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	180/184 (98%)	178 (99%)	2 (1%)	73	72
2	B	101/121 (84%)	99 (98%)	2 (2%)	55	51
3	C	914/915 (100%)	883 (97%)	31 (3%)	37	30
All	All	1195/1220 (98%)	1160 (97%)	35 (3%)	42	36

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	189	MET
2	B	82	ASP
2	B	157	VAL
3	C	35	GLN
3	C	52	ASP
3	C	71	LEU
3	C	81	LEU
3	C	93	PHE
3	C	136	GLU
3	C	188	LYS
3	C	203	GLN
3	C	283	LEU
3	C	291	MET
3	C	356	ARG
3	C	372	ASP
3	C	490	LYS
3	C	538	LEU
3	C	541	GLN
3	C	543	ARG
3	C	545	LYS
3	C	628	ASP

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Mol	Chain	Res	Type
3	C	688	THR
3	C	690	LEU
3	C	693	SER
3	C	771	GLU
3	C	785	LYS
3	C	876	GLU
3	C	896	ASN
3	C	898	ARG
3	C	909	LEU
3	C	913	LYS
3	C	940	PHE
3	C	969	ASN
3	C	983	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
3	C	541	GLN
3	C	547	ASN
3	C	742	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 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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	$\# Z  > 2$
6	GTP	A	303	4	26,34,34	1.16	1 (3%)	33,54,54	2.00	4 (12%)
5	GOL	C	1109	-	5,5,5	0.13	0	5,5,5	0.44	0
8	DMS	C	1105	-	3,3,3	0.25	0	3,3,3	0.10	0
5	GOL	A	302	-	5,5,5	0.10	0	5,5,5	0.27	0
8	DMS	C	1106	-	3,3,3	0.23	0	3,3,3	0.08	0
9	MPO	C	1115	-	13,13,13	0.90	1 (7%)	17,17,17	1.02	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTP	A	303	4	-	3/18/38/38	0/3/3/3
9	MPO	C	1115	-	-	2/7/15/15	0/1/1/1
5	GOL	A	302	-	-	3/4/4/4	-
5	GOL	C	1109	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	303	GTP	C6-N1	3.88	1.39	1.33
9	C	1115	MPO	O2-S1	2.93	1.53	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	303	GTP	C5-C6-N1	-8.53	111.77	123.43
6	A	303	GTP	C6-N1-C2	5.44	124.58	115.93
9	C	1115	MPO	O3-S1-O1	3.07	118.78	111.27
6	A	303	GTP	C2-N3-C4	-2.57	112.42	115.36
6	A	303	GTP	N3-C2-N1	-2.44	123.96	127.22
9	C	1115	MPO	O2-S1-C1	-2.22	104.25	106.92



There are no chirality outliers.

All (8) torsion outliers are listed below:

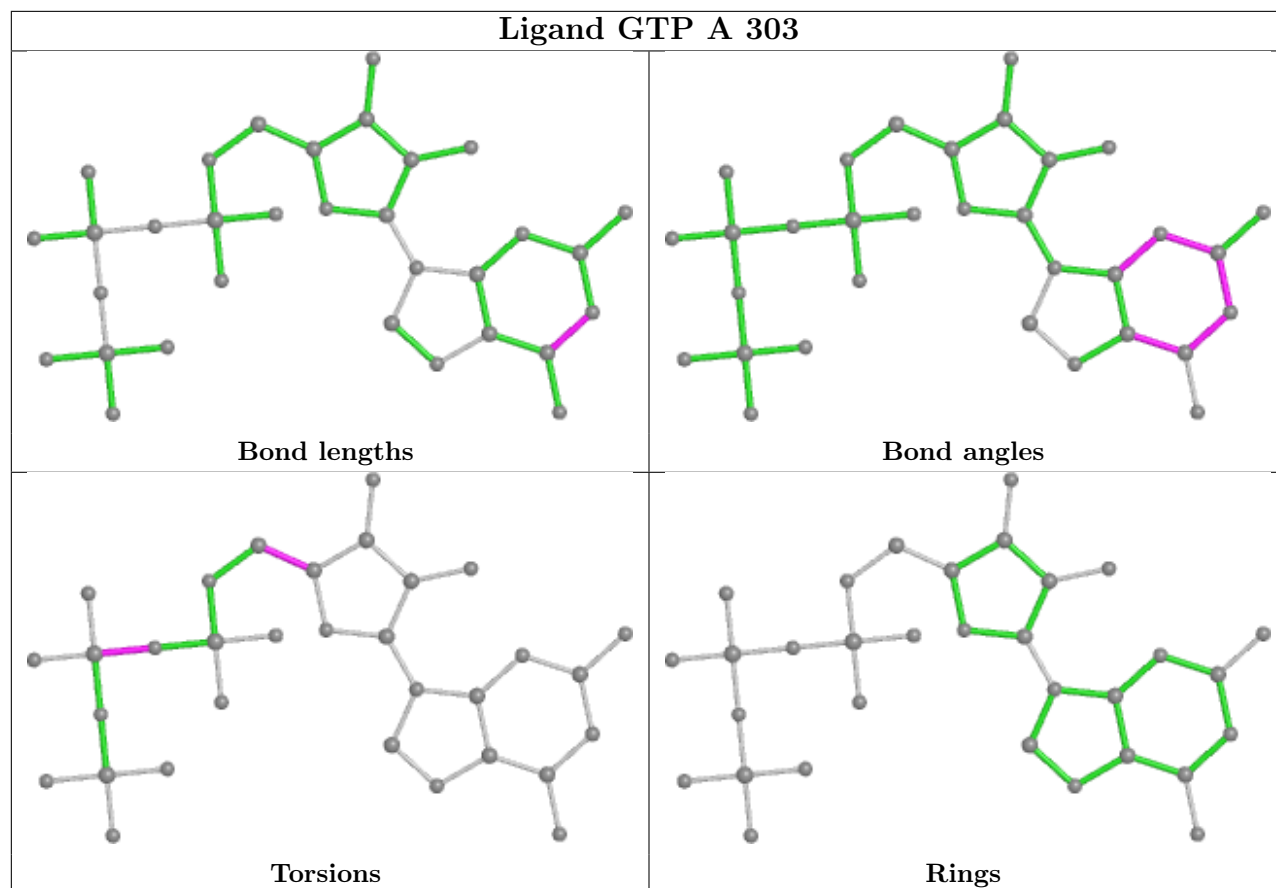
Mol	Chain	Res	Type	Atoms
5	A	302	GOL	C1-C2-C3-O3
5	A	302	GOL	O2-C2-C3-O3
9	C	1115	MPO	C2-C3-N1-C7
6	A	303	GTP	PA-O3A-PB-O1B
5	A	302	GOL	O1-C1-C2-O2
9	C	1115	MPO	C2-C1-S1-O2
6	A	303	GTP	PA-O3A-PB-O2B
6	A	303	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1109	GOL	3	0
9	C	1115	MPO	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	209/216 (96%)	0.97	38 (18%) <b>1</b> <b>1</b>	33, 46, 86, 110	0
2	B	119/140 (85%)	0.56	8 (6%) <b>17</b> <b>18</b>	44, 57, 78, 89	0
3	C	996/1003 (99%)	0.44	66 (6%) <b>18</b> <b>18</b>	29, 48, 75, 126	0
All	All	1324/1359 (97%)	0.53	112 (8%) <b>10</b> <b>11</b>	29, 49, 78, 126	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	684	THR	7.5
1	A	9	VAL	7.0
3	C	689	LEU	6.7
3	C	979	ALA	6.2
1	A	13	LEU	5.4
1	A	188	VAL	5.3
1	A	87	ILE	5.2
3	C	690	LEU	5.1
1	A	14	VAL	5.1
1	A	15	LEU	5.0
3	C	616	ARG	4.5
3	C	685	ALA	4.4
1	A	8	GLU	4.3
3	C	898	ARG	4.2
1	A	86	ALA	4.0
3	C	958	LEU	3.9
1	A	118	VAL	3.8
1	A	189	MET	3.8
3	C	972	SER	3.8
1	A	16	VAL	3.8
1	A	197	TYR	3.6
3	C	205	SER	3.6
1	A	27	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	959	LEU	3.6
3	C	106	GLU	3.6
1	A	127	LYS	3.6
3	C	7	PHE	3.5
3	C	978	GLU	3.5
3	C	332	SER	3.4
1	A	198	GLU	3.4
3	C	543	ARG	3.4
3	C	983	GLN	3.4
1	A	88	ILE	3.4
1	A	215	ASP	3.4
3	C	1053	GLU	3.3
3	C	29	VAL	3.3
3	C	267	ASP	3.3
1	A	63	VAL	3.3
3	C	681	GLU	3.2
2	B	98	ALA	3.2
3	C	109	LYS	3.1
3	C	962	LEU	3.1
3	C	896	ASN	3.0
1	A	195	ALA	3.0
3	C	266	GLN	3.0
1	A	187	VAL	3.0
3	C	683	SER	2.9
3	C	587	THR	2.9
3	C	159	LEU	2.9
1	A	179	MET	2.9
2	B	84	GLU	2.9
3	C	105	ASP	2.8
1	A	56	ARG	2.8
2	B	168	GLU	2.8
2	B	99	ASP	2.7
1	A	193	LEU	2.7
3	C	917	ARG	2.7
1	A	196	GLN	2.7
3	C	686	ASN	2.7
1	A	191	PRO	2.7
1	A	161	PHE	2.6
3	C	471	VAL	2.6
3	C	939	THR	2.6
1	A	108	LEU	2.6
3	C	973	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	1	MET	2.5
3	C	197[A]	CYS	2.5
3	C	957	LEU	2.4
3	C	889	ILE	2.4
3	C	909	LEU	2.4
1	A	173	ASN	2.4
3	C	545	LYS	2.4
3	C	982	PRO	2.4
1	A	26	PHE	2.4
3	C	0	SER	2.4
3	C	977	GLN	2.4
3	C	908	ALA	2.4
3	C	615	PRO	2.4
3	C	8	SER	2.4
3	C	369	LEU	2.4
3	C	936	VAL	2.4
3	C	905	LEU	2.3
1	A	55	ASN	2.3
1	A	164	LEU	2.3
3	C	920	ASN	2.3
3	C	985	THR	2.3
3	C	522	ASP	2.3
3	C	555	ILE	2.3
2	B	199	LYS	2.3
1	A	202	GLU	2.3
2	B	196	GLU	2.3
1	A	199	HIS	2.2
3	C	956	ALA	2.2
3	C	687	PRO	2.2
3	C	6	ASP	2.2
3	C	334	GLU	2.2
3	C	558	VAL	2.2
1	A	160	PRO	2.2
3	C	10	ASP	2.2
3	C	876	GLU	2.2
3	C	11	LEU	2.1
1	A	128	ASP	2.1
3	C	907	ILE	2.1
1	A	117	ILE	2.1
2	B	120	ASN	2.1
2	B	101	LYS	2.1
3	C	319	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	473	VAL	2.1
1	A	80	TYR	2.0
3	C	264	ILE	2.0
1	A	62	ASN	2.0
3	C	668	LEU	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.

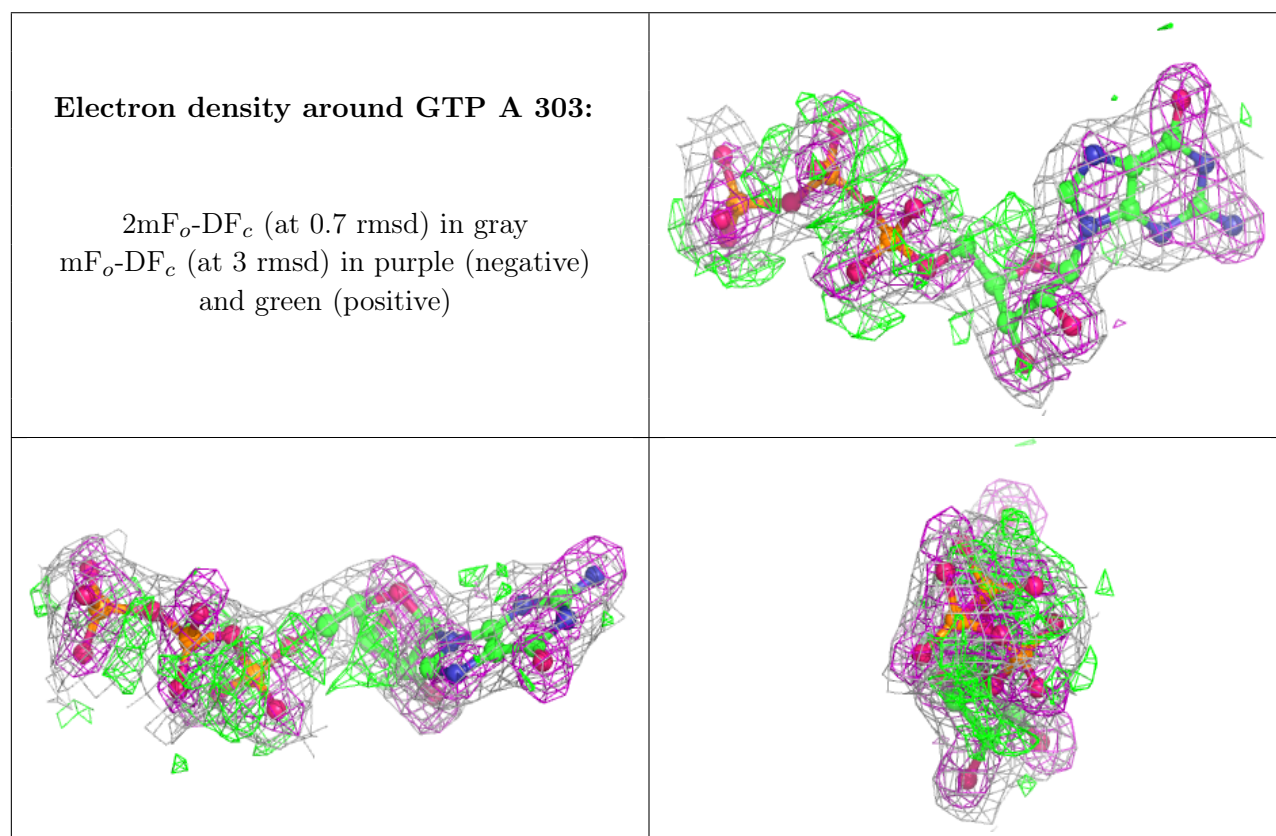
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	C	1104	1/1	0.59	0.16	81,81,81,81	0
7	CL	C	1111	1/1	0.73	0.14	83,83,83,83	0
7	CL	C	1108	1/1	0.74	0.38	80,80,80,80	0
7	CL	A	304	1/1	0.74	0.12	72,72,72,72	0
7	CL	C	1113	1/1	0.76	0.14	90,90,90,90	0
5	GOL	C	1109	6/6	0.78	0.28	55,63,66,68	0
5	GOL	A	302	6/6	0.80	0.33	68,74,76,77	0
7	CL	C	1101	1/1	0.81	0.12	74,74,74,74	0
7	CL	C	1107	1/1	0.83	0.11	76,76,76,76	0
7	CL	C	1114	1/1	0.83	0.14	76,76,76,76	0
7	CL	C	1103	1/1	0.84	0.20	81,81,81,81	0
9	MPO	C	1115	13/13	0.84	0.25	71,79,89,96	0
7	CL	C	1102	1/1	0.86	0.14	76,76,76,76	0
8	DMS	C	1105	4/4	0.86	0.27	90,91,93,95	0
7	CL	C	1110	1/1	0.86	0.11	81,81,81,81	1
8	DMS	C	1106	4/4	0.87	0.22	87,88,89,90	0
7	CL	C	1112	1/1	0.91	0.17	66,66,66,66	0
6	GTP	A	303	32/32	0.95	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	301	1/1	0.97	0.15	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.