



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 7DBG / pdb\_00007dbg  
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 wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

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

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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 : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

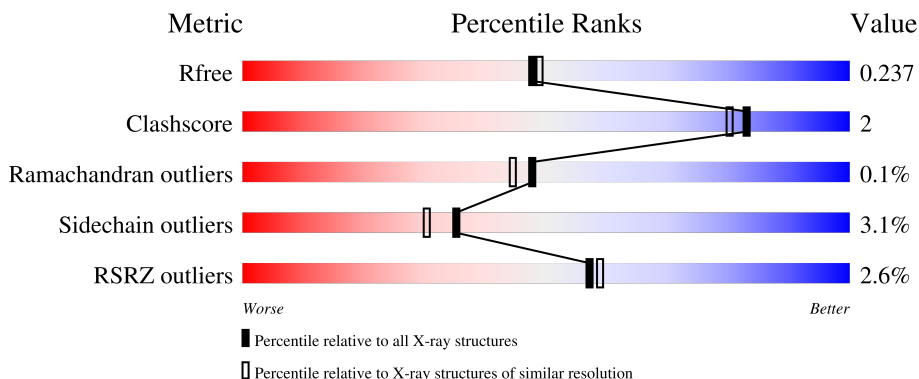
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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))
$R_{free}$	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (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	
2	B	140	
3	C	1003	

## 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
			Total	C	N	O	S			
1	A	209	1672	1079	285	302	6	0	0	0

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
			Total	C	N	O	S			
2	B	119	974	618	172	180	4	0	0	0

- Molecule 3 is a protein called CRM1 isoform 1.

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

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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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 (CCD ID: MG) (formula: Mg).

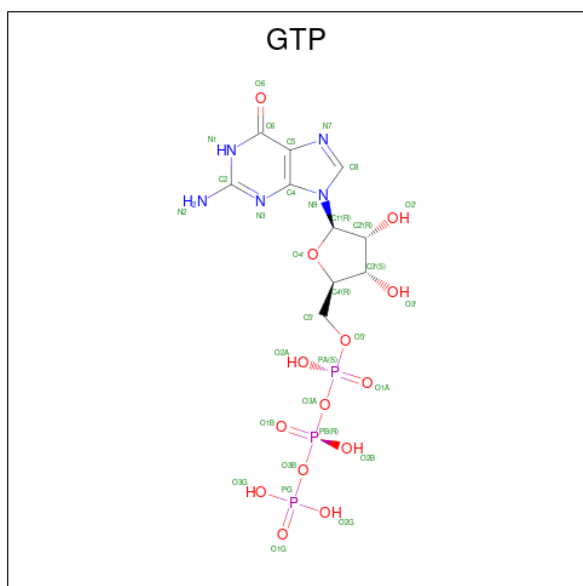
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: 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 (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

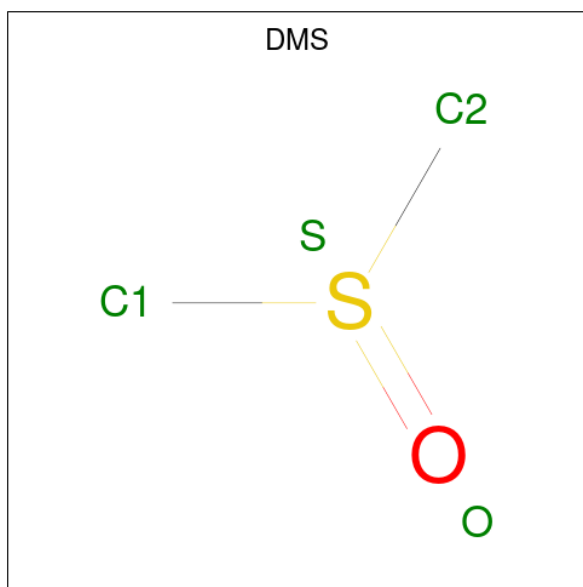


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

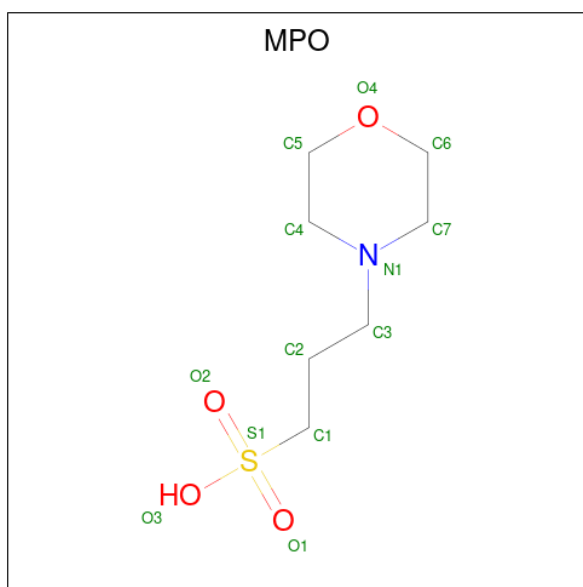
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	C	11	Total Cl 11 11	0	0

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



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

- Molecule 9 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



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

- 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.

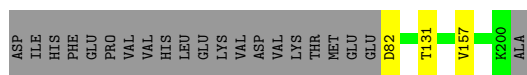
- Molecule 1: GTP-binding nuclear protein Ran

Chain A: 



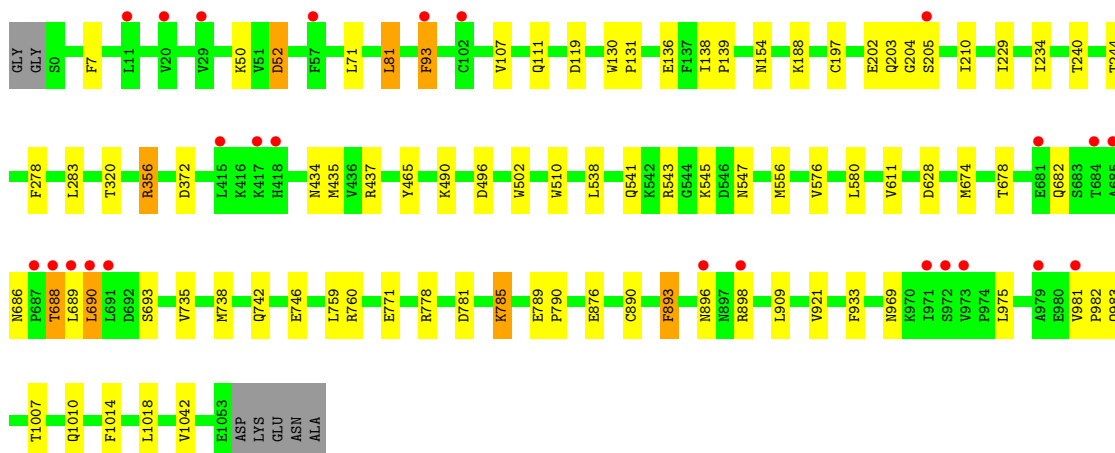
- Molecule 2: YRB1 isoform 1

Chain B: 



- Molecule 3: CRM1 isoform 1

Chain C: 



## 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) 99.9 (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)	Xtrriage
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 (5.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage'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: GOL, MPO, MG, GTP, DMS, 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	0.94	0/1713	1.28	0/2322
2	B	0.95	0/991	1.29	0/1323
3	C	0.97	0/8229	1.45	5/11149 (0.0%)
All	All	0.97	0/10933	1.41	5/14794 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	93	PHE	CA-CB-CG	5.75	119.56	113.80
3	C	52	ASP	CB-CA-C	5.61	120.39	110.85
3	C	893	PHE	CB-CA-C	-5.54	101.27	110.68
3	C	496	ASP	CA-CB-CG	5.37	117.97	112.60
3	C	278	PHE	CA-CB-CG	5.24	119.04	113.80

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	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	0
All	All	11398	0	10867	52	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.

The worst 5 of 52 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:556[B]:MET:HE3	3:C:556[B]:MET:HA	1.37	1.06
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

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%)	202 (98%)	5 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	117/140 (84%)	112 (96%)	5 (4%)	0	100	100
3	C	997/1003 (99%)	984 (99%)	12 (1%)	1 (0%)	48	44
All	All	1321/1359 (97%)	1298 (98%)	22 (2%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	205	SER

### 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	180/184 (98%)	177 (98%)	3 (2%)	53	53
2	B	101/121 (84%)	99 (98%)	2 (2%)	48	47
3	C	914/915 (100%)	882 (96%)	32 (4%)	32	26
All	All	1195/1220 (98%)	1158 (97%)	37 (3%)	35	30

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	778	ARG
3	C	969	ASN
3	C	785	LYS
3	C	898	ARG
3	C	203	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	742	GLN
3	C	896	ASN
3	C	1010	GLN

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Mol	Chain	Res	Type
3	C	418	HIS
3	C	494	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 oligosaccharides 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
9	MPO	C	1115	-	13,13,13	0.91	1 (7%)	17,17,17	0.93	1 (5%)
8	DMS	C	1106	-	3,3,3	0.22	0	3,3,3	0.08	0
5	GOL	A	302	-	5,5,5	0.09	0	5,5,5	0.26	0
6	GTP	A	303	4	33,34,34	0.68	0	50,54,54	0.53	0
8	DMS	C	1105	-	3,3,3	0.24	0	3,3,3	0.10	0
5	GOL	C	1109	-	5,5,5	0.12	0	5,5,5	0.44	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
5	GOL	A	302	-	-	3/4/4/4	-
9	MPO	C	1115	-	-	2/7/15/15	0/1/1/1
5	GOL	C	1109	-	-	0/4/4/4	-
6	GTP	A	303	4	-	2/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1115	MPO	O2-S1	3.03	1.53	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1115	MPO	O3-S1-O1	2.95	118.78	111.40

There are no chirality outliers.

5 of 7 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

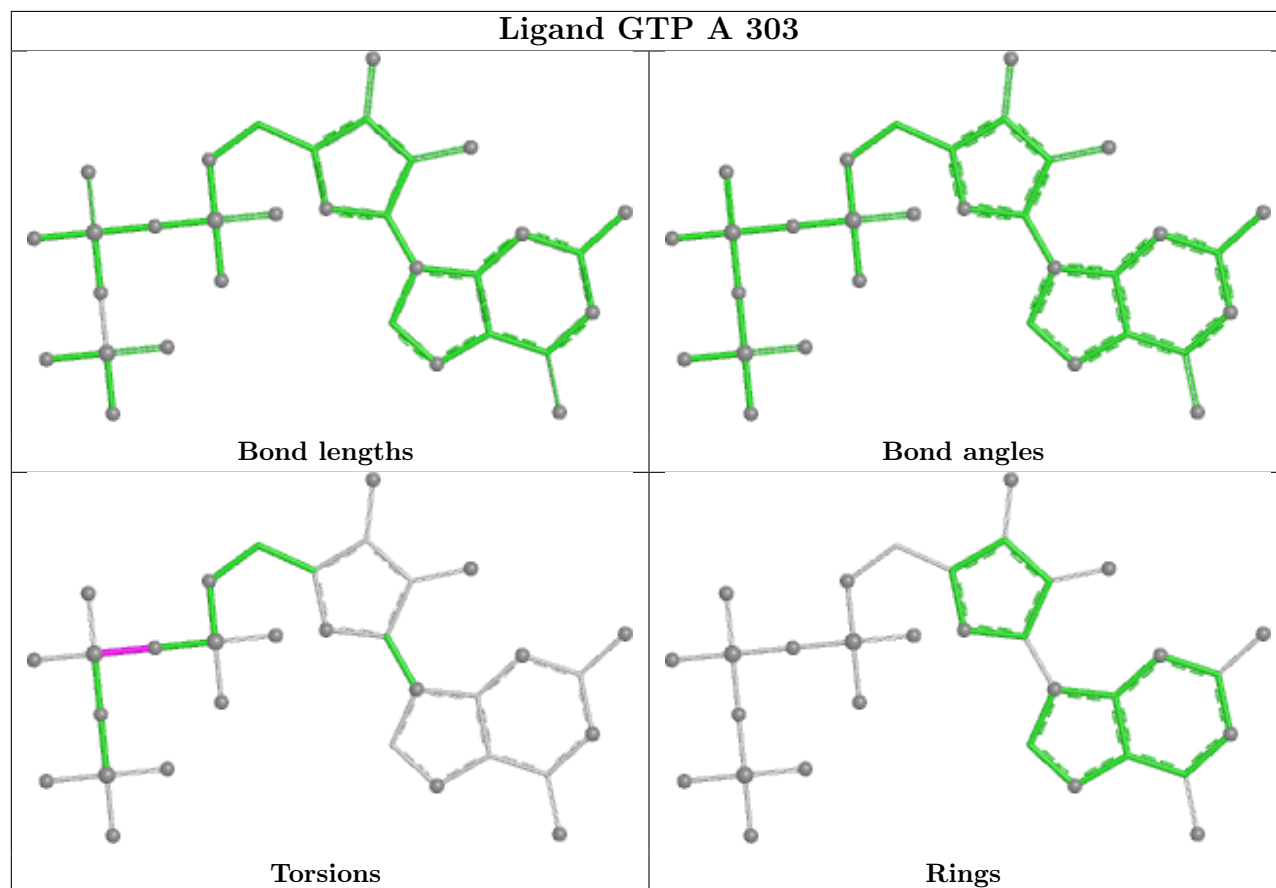
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1115	MPO	1	0
5	C	1109	GOL	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.41	10 (4%) 35 35	33, 46, 86, 110	0
2	B	119/140 (85%)	0.45	0 100 100	44, 57, 78, 89	0
3	C	996/1003 (99%)	0.30	25 (2%) 58 60	22, 48, 75, 126	3 (0%)
All	All	1324/1359 (97%)	0.33	35 (2%) 57 59	22, 49, 78, 126	3 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	690	LEU	4.4
3	C	691	LEU	4.1
1	A	188	VAL	3.8
3	C	687	PRO	3.6
1	A	9	VAL	3.6

### 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](#)

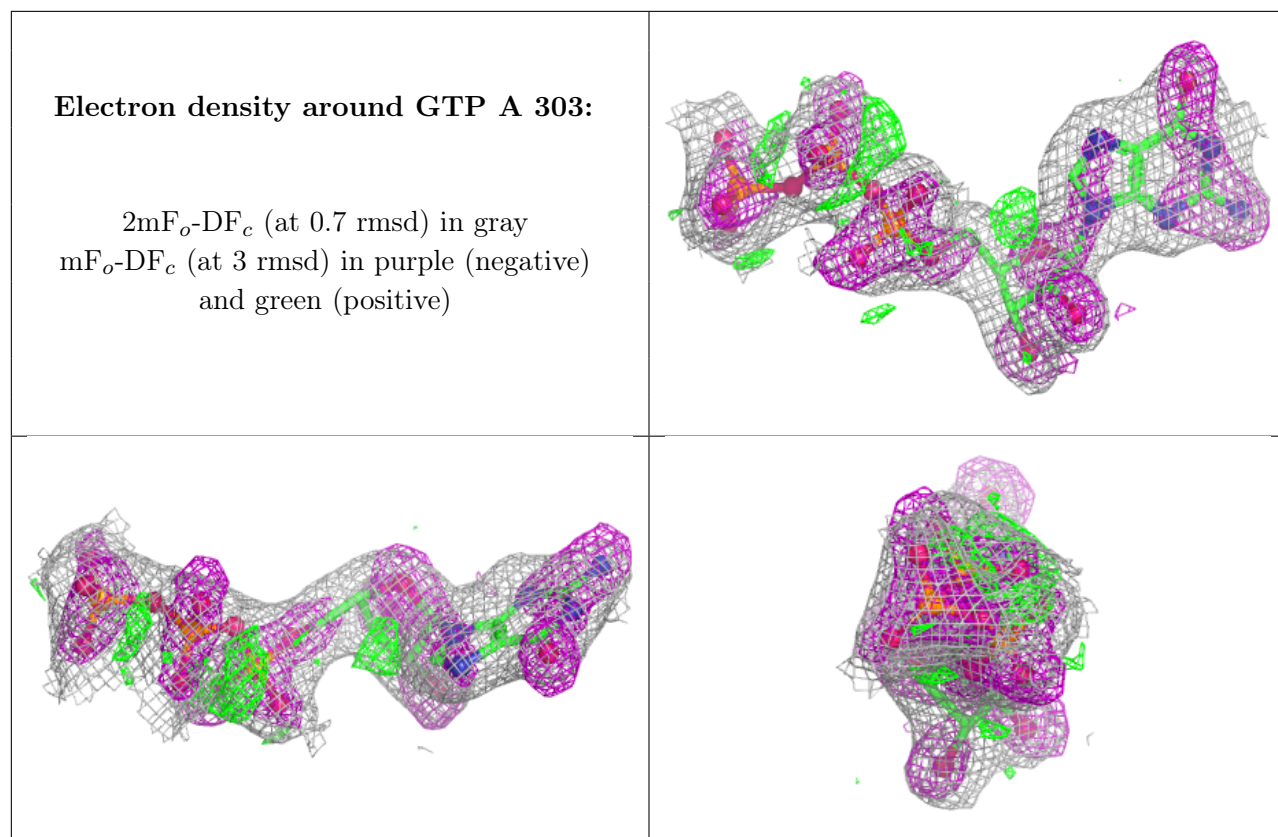
There are no oligosaccharides in this entry.

### 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, 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
8	DMS	C	1105	4/4	0.79	0.25	90,91,93,95	0
7	CL	C	1113	1/1	0.80	0.16	90,90,90,90	0
8	DMS	C	1106	4/4	0.81	0.23	87,88,89,90	0
9	MPO	C	1115	13/13	0.82	0.22	71,79,89,96	0
5	GOL	A	302	6/6	0.87	0.13	68,74,76,77	0
5	GOL	C	1109	6/6	0.87	0.12	55,63,66,68	0
7	CL	C	1114	1/1	0.88	0.14	76,76,76,76	0
7	CL	C	1102	1/1	0.88	0.13	76,76,76,76	0
7	CL	C	1108	1/1	0.89	0.13	80,80,80,80	0
7	CL	C	1104	1/1	0.90	0.13	81,81,81,81	0
7	CL	C	1110	1/1	0.91	0.07	81,81,81,81	1
7	CL	A	304	1/1	0.92	0.10	72,72,72,72	0
7	CL	C	1107	1/1	0.92	0.11	76,76,76,76	0
7	CL	C	1103	1/1	0.92	0.19	81,81,81,81	0
7	CL	C	1111	1/1	0.93	0.14	83,83,83,83	0
7	CL	C	1101	1/1	0.95	0.11	74,74,74,74	0
6	GTP	A	303	32/32	0.95	0.08	20,20,20,20	0
7	CL	C	1112	1/1	0.95	0.15	66,66,66,66	0
4	MG	A	301	1/1	0.95	0.05	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.