



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2021 – 12:12 PM JST

PDB ID : 6LQ9  
Title : S109 in complex with CRM1-Ran-RanBP1  
Authors : Sun, Q.; Lei, Y.  
Deposited on : 2020-01-13  
Resolution : 2.50 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 : 2.20  
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) : 2.20

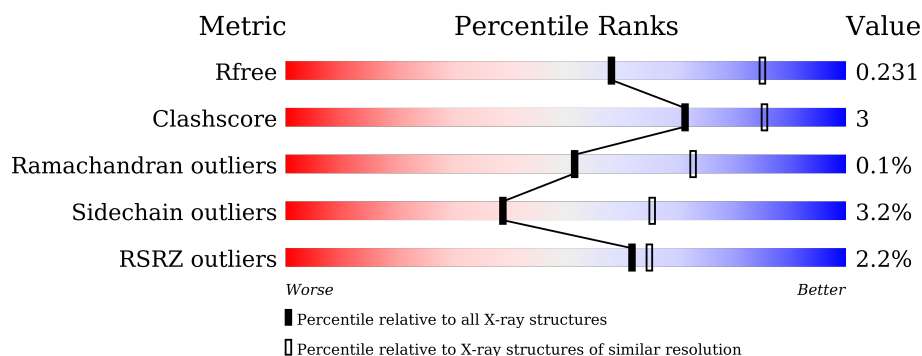
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	235	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>•</div> <div>11%</div> </div> </div>
2	B	143	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>•</div> <div>10%</div> </div> </div>
3	C	1024	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11483 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1676	1081	286	302	7			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP P62826
A	-17	SER	-	expression tag	UNP P62826
A	-16	SER	-	expression tag	UNP P62826
A	-15	HIS	-	expression tag	UNP P62826
A	-14	HIS	-	expression tag	UNP P62826
A	-13	HIS	-	expression tag	UNP P62826
A	-12	HIS	-	expression tag	UNP P62826
A	-11	HIS	-	expression tag	UNP P62826
A	-10	HIS	-	expression tag	UNP P62826
A	-9	SER	-	expression tag	UNP P62826
A	-8	SER	-	expression tag	UNP P62826
A	-7	GLY	-	expression tag	UNP P62826
A	-6	LEU	-	expression tag	UNP P62826
A	-5	VAL	-	expression tag	UNP P62826
A	-4	PRO	-	expression tag	UNP P62826
A	-3	ARG	-	expression tag	UNP P62826
A	-2	GLY	-	expression tag	UNP P62826
A	-1	SER	-	expression tag	UNP P62826
A	0	HIS	-	expression tag	UNP P62826

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			1048	666	181	196	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	59	GLY	-	expression tag	UNP P41920
B	60	GLY	-	expression tag	UNP P41920
B	61	SER	-	expression tag	UNP P41920

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1017	Total	C	N	O	S	0	3	0
			8238	5292	1356	1549	41			

There are 45 discrepancies between the modelled and reference sequences:

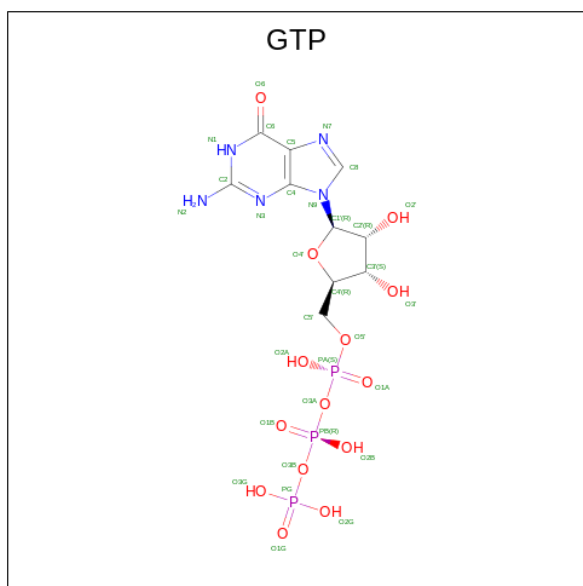
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P30822
C	-1	GLY	-	expression tag	UNP P30822
C	0	SER	-	expression tag	UNP P30822
C	?	-	VAL	deletion	UNP P30822
C	?	-	GLN	deletion	UNP P30822
C	?	-	ARG	deletion	UNP P30822
C	?	-	LEU	deletion	UNP P30822
C	?	-	PRO	deletion	UNP 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	537	GLY	ASP	engineered mutation	UNP P30822
C	539	CYS	THR	engineered mutation	UNP P30822
C	540	GLU	VAL	engineered mutation	UNP P30822
C	541	GLN	LYS	engineered mutation	UNP P30822
C	1022	CYS	TYR	engineered mutation	UNP P30822

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

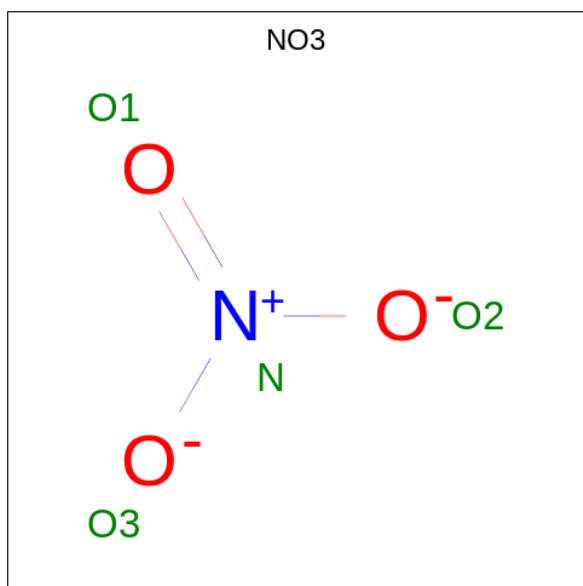


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	10	5	14		

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

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

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

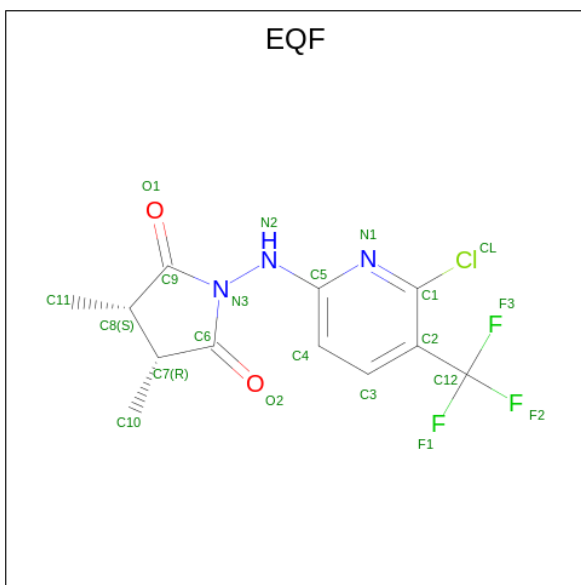


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		

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

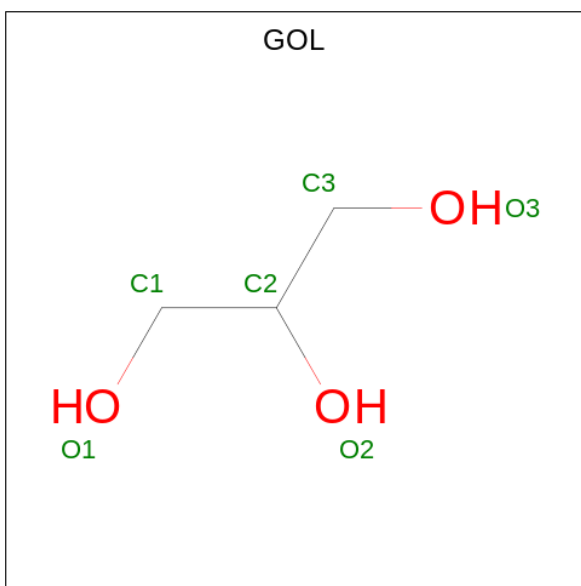
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is (3 {R},4 {S})-1-[[6-chloranyl-5-(trifluoromethyl)pyridin-2-yl]amino]-3,4-dimethyl-pyrrolidine-2,5-dione (three-letter code: EQF) (formula: C<sub>12</sub>H<sub>11</sub>ClF<sub>3</sub>N<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	Cl	F	N	O	0	0
			21	12	1	3	3	2		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

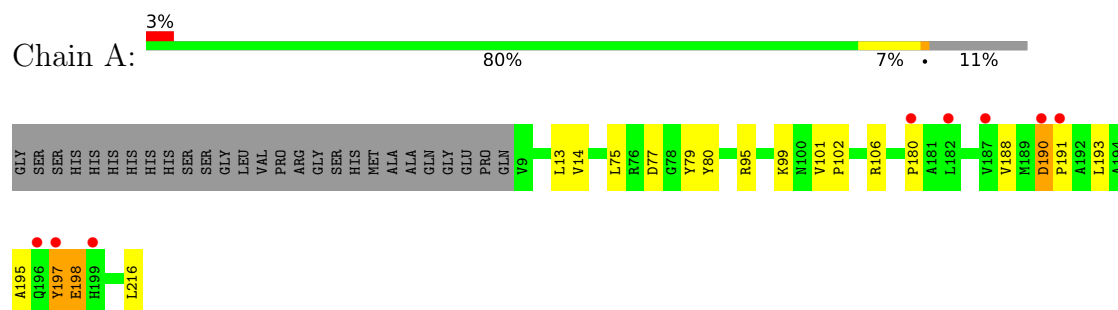
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	87	Total 87	O 87	0	0
10	B	20	Total 20	O 20	0	0
10	C	333	Total 333	O 333	0	0

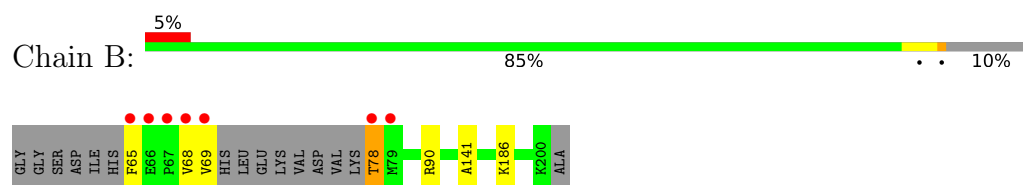
### 3 Residue-property plots [i](#)

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.

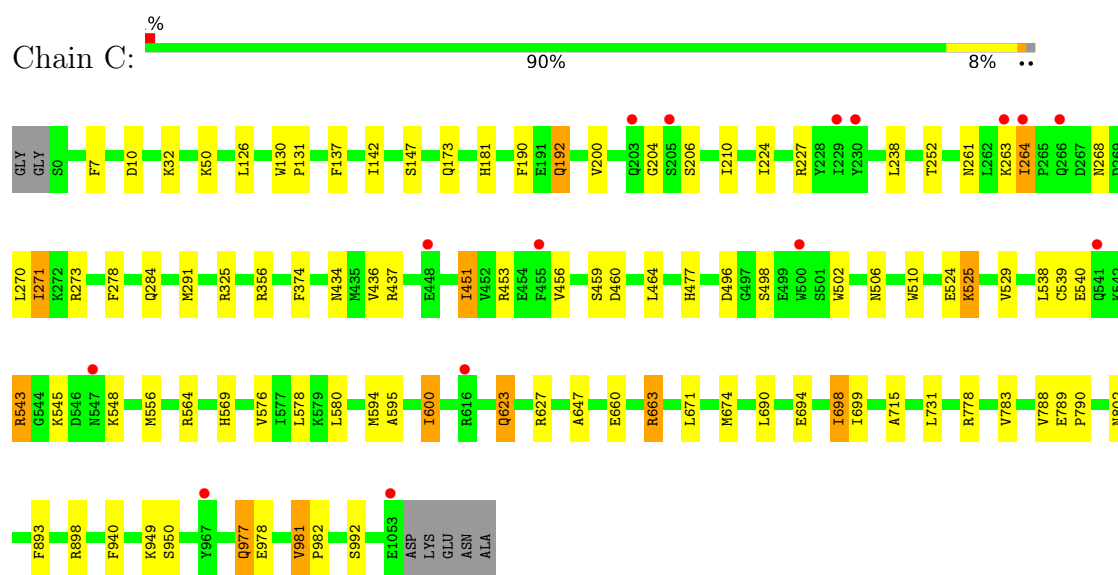
- Molecule 1: GTP-binding nuclear protein Ran



- 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, $\alpha$ , $\beta$ , $\gamma$	105.11Å 105.11Å 303.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.50 49.66 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.71-2.50) 99.5 (49.66-2.49)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.190 , 0.228 0.193 , 0.231	Depositor DCC
$R_{free}$ test set	3030 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11483	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 3.60% 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: EQF, CL, NO3, GTP, GOL, MG

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	0.46	0/1717	0.63	0/2327
2	B	0.41	0/1066	0.61	0/1424
3	C	0.44	0/8397	0.57	1/11379 (0.0%)
All	All	0.44	0/11180	0.58	1/15130 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	893	PHE	CB-CA-C	-5.02	100.37	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1676	0	1677	16	0
2	B	1048	0	1047	4	0
3	C	8238	0	8311	61	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0
6	A	12	0	0	1	0
6	C	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	C	21	0	0	0	0
9	C	6	0	8	0	0
10	A	87	0	0	1	0
10	B	20	0	0	0	0
10	C	333	0	0	5	0
All	All	11483	0	11055	77	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 (77) 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:268:ASN:ND2	3:C:271:ILE:HD12	1.54	1.20
3:C:356:ARG:HD2	3:C:464:LEU:HD22	1.43	0.96
3:C:268:ASN:ND2	3:C:271:ILE:CD1	2.33	0.89
3:C:268:ASN:HD22	3:C:271:ILE:CD1	1.87	0.87
3:C:268:ASN:HD22	3:C:271:ILE:HD12	1.40	0.86
3:C:981:VAL:HG22	3:C:982:PRO:HD2	1.57	0.86
3:C:325:ARG:HH21	3:C:325:ARG:HG3	1.41	0.83
3:C:556:MET:HE1	3:C:594:MET:C	2.06	0.76
3:C:356:ARG:HD2	3:C:464:LEU:CD2	2.18	0.72
3:C:981:VAL:HG22	3:C:982:PRO:CD	2.19	0.72
3:C:270:LEU:HD23	3:C:273:ARG:HH12	1.58	0.68
3:C:623:GLN:O	3:C:627:ARG:HG3	1.93	0.68
3:C:268:ASN:HD21	3:C:271:ILE:HD12	1.51	0.68
3:C:325:ARG:HH21	3:C:325:ARG:CG	2.08	0.66
3:C:181:HIS:ND1	10:C:1201:HOH:O	2.28	0.65
3:C:556:MET:HE1	3:C:595:ALA:N	2.13	0.63
1:A:193:LEU:HD12	1:A:195:ALA:H	1.64	0.63
1:A:106:ARG:HH12	3:C:173:GLN:HE22	1.48	0.62
3:C:978:GLU:H	3:C:978:GLU:CD	2.03	0.61
3:C:270:LEU:HD23	3:C:273:ARG:NH1	2.17	0.60
1:A:188:VAL:HG11	2:B:141:ALA:HB2	1.87	0.56
3:C:460:ASP:OD1	3:C:460:ASP:N	2.39	0.56
1:A:190:ASP:HB2	1:A:191:PRO:HD3	1.85	0.56
1:A:190:ASP:HB2	1:A:191:PRO:CD	2.36	0.55
3:C:600:ILE:HG12	3:C:647:ALA:HB2	1.89	0.54
3:C:264:ILE:H	3:C:264:ILE:HD13	1.72	0.54
3:C:227:ARG:NH1	10:C:1207:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:268:ASN:HD22	3:C:271:ILE:HD13	1.71	0.53
3:C:789:GLU:HB2	3:C:790:PRO:HD3	1.90	0.52
1:A:216:LEU:HD11	2:B:90:ARG:HG2	1.92	0.51
3:C:434:ASN:HB2	10:C:1495:HOH:O	2.10	0.51
3:C:525:LYS:HE2	3:C:569:HIS:HE1	1.75	0.51
3:C:436:VAL:HG11	3:C:464:LEU:HD23	1.91	0.51
3:C:525:LYS:HE2	3:C:569:HIS:CE1	2.46	0.51
1:A:77:ASP:HA	1:A:80:TYR:CE2	2.47	0.50
1:A:180:PRO:HA	2:B:78:THR:HA	1.94	0.49
3:C:325:ARG:CG	3:C:325:ARG:NH2	2.72	0.49
3:C:506:ASN:HB3	3:C:510:TRP:CZ2	2.49	0.48
3:C:200:VAL:O	3:C:204:GLY:HA3	2.13	0.48
3:C:576:VAL:O	3:C:580:LEU:HG	2.14	0.47
3:C:699:ILE:HG21	3:C:731:LEU:HD21	1.97	0.47
3:C:694:GLU:O	3:C:698:ILE:HD13	2.15	0.47
3:C:437:ARG:HH11	3:C:437:ARG:HG2	1.79	0.46
1:A:14:VAL:HG11	1:A:80:TYR:HA	1.97	0.46
3:C:715:ALA:CB	3:C:778:ARG:HG3	2.46	0.46
3:C:524:GLU:CD	3:C:564:ARG:HH21	2.18	0.46
1:A:197:TYR:CD1	1:A:198:GLU:N	2.84	0.45
3:C:238:LEU:O	3:C:252:THR:HG21	2.16	0.45
3:C:715:ALA:HB2	3:C:778:ARG:HG3	1.98	0.45
3:C:663:ARG:HA	3:C:663:ARG:HD3	1.84	0.45
3:C:192:GLN:HG3	10:C:1378:HOH:O	2.16	0.45
2:B:68:VAL:O	2:B:69:VAL:C	2.56	0.44
3:C:206:SER:O	3:C:210:ILE:HG12	2.17	0.44
3:C:543:ARG:HA	3:C:543:ARG:HE	1.82	0.44
3:C:949:LYS:N	10:C:1220:HOH:O	2.51	0.44
3:C:263:LYS:HA	3:C:325:ARG:HD3	2.00	0.44
1:A:95:ARG:HG3	6:A:304:NO3:O1	2.18	0.43
10:A:402:HOH:O	3:C:460:ASP:HA	2.18	0.43
3:C:374:PHE:HE1	3:C:477[A]:HIS:CG	2.36	0.43
3:C:525:LYS:O	3:C:529:VAL:HG23	2.18	0.43
1:A:13:LEU:C	1:A:13:LEU:HD23	2.38	0.43
3:C:977:GLN:H	3:C:977:GLN:HG2	1.54	0.43
3:C:374:PHE:CE1	3:C:477[A]:HIS:CD2	3.07	0.43
3:C:898:ARG:HD3	3:C:950:SER:HB2	2.00	0.43
3:C:142:ILE:HD13	3:C:192:GLN:HB3	2.01	0.42
3:C:190:PHE:CZ	3:C:224:ILE:HG21	2.53	0.42
3:C:451:ILE:HD11	3:C:502:TRP:CE3	2.55	0.42
3:C:539:CYS:O	3:C:548:LYS:NZ	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:496:ASP:OD1	3:C:498:SER:OG	2.29	0.41
3:C:126:LEU:HD11	3:C:137:PHE:CZ	2.56	0.41
1:A:75:LEU:HB2	1:A:79:TYR:CZ	2.56	0.41
1:A:190:ASP:CB	1:A:191:PRO:CD	2.98	0.41
1:A:190:ASP:CB	1:A:191:PRO:HD3	2.50	0.41
3:C:7:PHE:CE2	3:C:50:LYS:HE3	2.56	0.41
1:A:101:VAL:N	1:A:102:PRO:CD	2.83	0.40
3:C:783:VAL:O	3:C:788:VAL:HG23	2.21	0.40
3:C:130:TRP:HA	3:C:131:PRO:HA	1.77	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/235 (88%)	199 (96%)	7 (3%)	1 (0%)	29	48
2	B	124/143 (87%)	117 (94%)	7 (6%)	0	100	100
3	C	1018/1024 (99%)	1001 (98%)	17 (2%)	0	100	100
All	All	1349/1402 (96%)	1317 (98%)	31 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASP

### 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	181/201 (90%)	178 (98%)	3 (2%)	60	82
2	B	110/122 (90%)	107 (97%)	3 (3%)	44	71
3	C	932/933 (100%)	899 (96%)	33 (4%)	36	62
All	All	1223/1256 (97%)	1184 (97%)	39 (3%)	39	65

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	A	197	TYR
1	A	198	GLU
2	B	65	PHE
2	B	78	THR
2	B	186	LYS
3	C	10	ASP
3	C	32	LYS
3	C	147	SER
3	C	192	GLN
3	C	261	ASN
3	C	264	ILE
3	C	271	ILE
3	C	278	PHE
3	C	284	GLN
3	C	291	MET
3	C	451	ILE
3	C	453	ARG
3	C	456	VAL
3	C	459	SER
3	C	525	LYS
3	C	538	LEU
3	C	540	GLU
3	C	543	ARG
3	C	545	LYS
3	C	578	LEU
3	C	600	ILE
3	C	623	GLN
3	C	660	GLU
3	C	663	ARG
3	C	671	LEU

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Mol	Chain	Res	Type
3	C	674	MET
3	C	690	LEU
3	C	698	ILE
3	C	802	ASN
3	C	940	PHE
3	C	977	GLN
3	C	981	VAL
3	C	992	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	120	ASN
3	C	33	GLN
3	C	35	GLN
3	C	173	GLN
3	C	261	ASN
3	C	266	GLN
3	C	284	GLN
3	C	342	ASN
3	C	494	GLN
3	C	609	HIS
3	C	614	GLN
3	C	802	ASN
3	C	955	GLN
3	C	1005	HIS

### 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

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	NO3	C	1102	-	1,3,3	0.11	0	0,3,3	0.00	-
6	NO3	A	304	-	1,3,3	0.47	0	0,3,3	0.00	-
4	GTP	A	301	5	26,34,34	1.14	2 (7%)	33,54,54	1.73	10 (30%)
9	GOL	C	1104	-	5,5,5	0.40	0	5,5,5	0.36	0
6	NO3	A	303	-	1,3,3	0.05	0	0,3,3	0.00	-
8	EQF	C	1101	3	21,22,22	1.69	4 (19%)	29,34,34	2.70	8 (27%)
6	NO3	C	1103	-	1,3,3	0.14	0	0,3,3	0.00	-
6	NO3	A	305	-	1,3,3	0.09	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
9	GOL	C	1104	-	-	0/4/4/4	-
4	GTP	A	301	5	-	4/18/38/38	0/3/3/3
8	EQF	C	1101	3	-	0/10/30/30	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1101	EQF	C6-N3	-4.27	1.32	1.39
8	C	1101	EQF	C9-N3	-3.81	1.33	1.39
8	C	1101	EQF	C1-CL	3.77	1.80	1.74
4	A	301	GTP	C6-C5	3.72	1.47	1.41
4	A	301	GTP	C5-C4	2.77	1.48	1.40
8	C	1101	EQF	C5-N2	-2.08	1.35	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1101	EQF	C2-C1-N1	-9.05	118.75	126.13
8	C	1101	EQF	F2-C12-C2	-5.02	103.96	112.70
8	C	1101	EQF	C2-C1-CL	4.83	124.00	119.14
8	C	1101	EQF	C7-C6-N3	4.55	111.10	107.50
4	A	301	GTP	C6-C5-C4	-4.06	116.92	120.80
8	C	1101	EQF	C8-C9-N3	3.88	110.57	107.50
4	A	301	GTP	C5-C6-N1	-3.53	118.61	123.43
4	A	301	GTP	C6-N1-C2	3.07	120.81	115.93
4	A	301	GTP	C1'-N9-C4	-2.88	121.58	126.64
8	C	1101	EQF	C1-N1-C5	2.55	122.00	116.08
4	A	301	GTP	PA-O3A-PB	-2.40	124.59	132.83
8	C	1101	EQF	F1-C12-F3	2.33	114.26	105.72
8	C	1101	EQF	C12-C2-C1	-2.31	118.56	122.82
4	A	301	GTP	O4'-C4'-C5'	-2.28	101.87	109.37
4	A	301	GTP	C2-N3-C4	2.28	117.96	115.36
4	A	301	GTP	PB-O3B-PG	-2.27	125.03	132.83
4	A	301	GTP	O2A-PA-O1A	2.22	123.19	112.24
4	A	301	GTP	O3G-PG-O2G	2.17	115.95	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

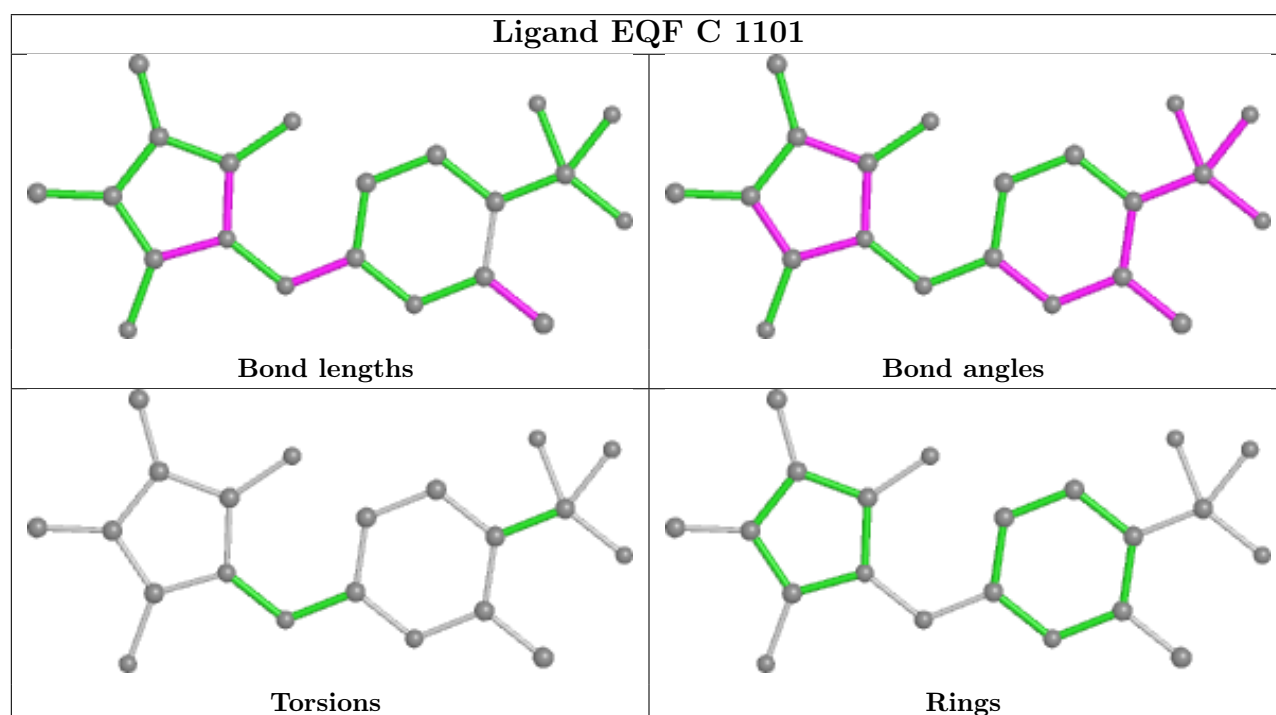
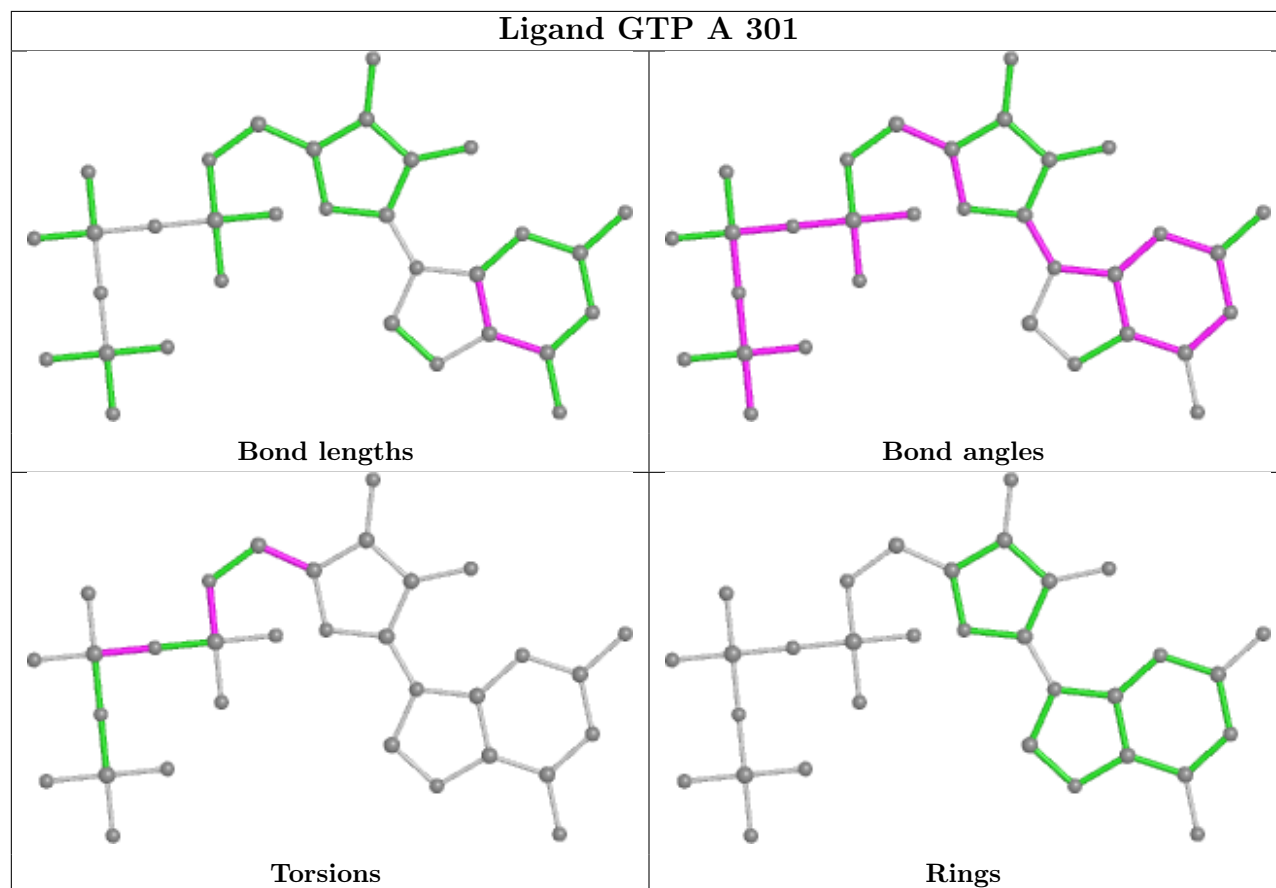
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	304	NO3	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	208/235 (88%)	-0.04	8 (3%)	40 43	40, 56, 136, 185	0
2	B	128/143 (89%)	-0.17	7 (5%)	25 26	54, 68, 125, 279	0
3	C	1017/1024 (99%)	-0.26	15 (1%)	73 75	42, 61, 97, 135	0
All	All	1353/1402 (96%)	-0.22	30 (2%)	62 65	40, 62, 101, 279	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ASP	8.3
2	B	68	VAL	6.2
2	B	67	PRO	5.9
2	B	79	MET	5.6
1	A	187	VAL	5.2
1	A	196	GLN	4.7
1	A	197	TYR	4.6
2	B	65	PHE	4.1
3	C	205	SER	3.9
1	A	182	LEU	3.6
2	B	66	GLU	3.1
3	C	264	ILE	2.9
3	C	500	TRP	2.9
2	B	69	VAL	2.7
3	C	541	GLN	2.6
3	C	616	ARG	2.6
2	B	78	THR	2.6
1	A	199	HIS	2.5
3	C	455	PHE	2.4
1	A	191	PRO	2.4
1	A	180	PRO	2.3
3	C	266	GLN	2.3
3	C	1053	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	547	ASN	2.3
3	C	203	GLN	2.2
3	C	230	TYR	2.2
3	C	967	TYR	2.1
3	C	229	ILE	2.0
3	C	263	LYS	2.0
3	C	448	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

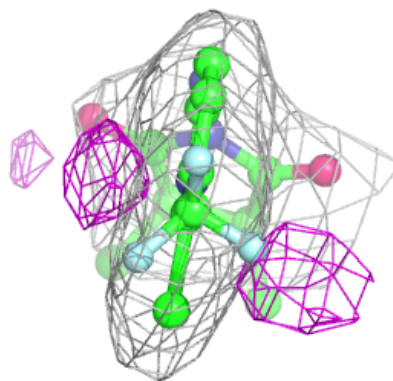
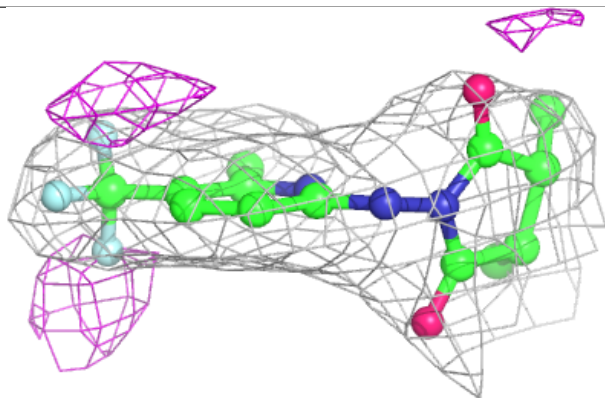
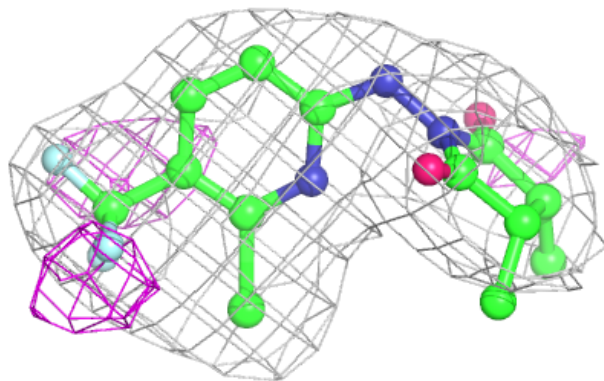
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NO3	C	1102	4/4	0.56	0.34	82,90,92,94	0
6	NO3	A	305	4/4	0.86	0.25	91,91,94,98	0
9	GOL	C	1104	6/6	0.86	0.24	78,89,93,95	0
6	NO3	C	1103	4/4	0.91	0.27	66,68,70,71	0
6	NO3	A	303	4/4	0.91	0.28	81,82,85,86	0
7	CL	A	306	1/1	0.95	0.26	100,100,100,100	0
8	EQF	C	1101	21/21	0.95	0.18	77,80,85,88	0
6	NO3	A	304	4/4	0.95	0.17	78,84,86,91	0
4	GTP	A	301	32/32	0.98	0.12	41,44,48,49	0
5	MG	A	302	1/1	0.99	0.08	48,48,48,48	0

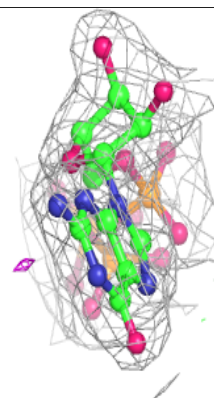
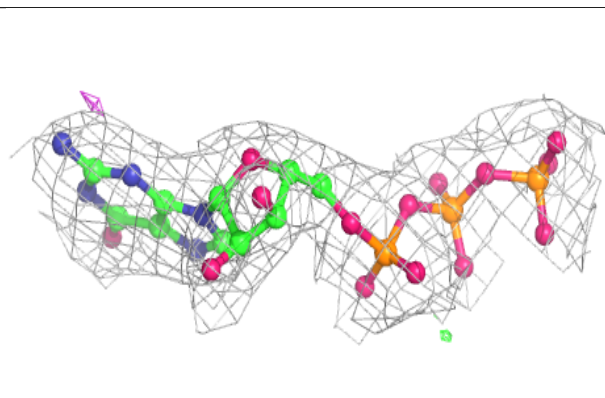
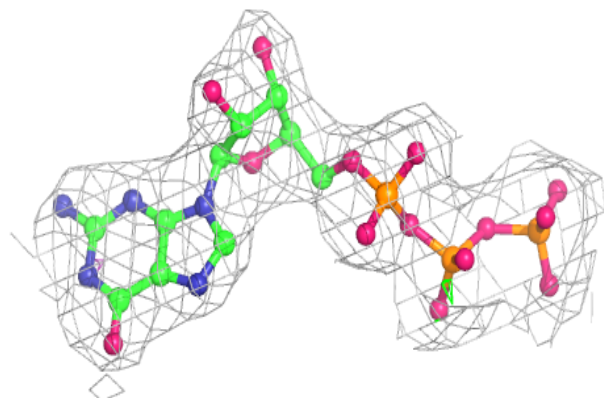
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around EQF C 1101:**

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

**Electron density around GTP A 301:**

$2mF_o-DF_c$  (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.