Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 10:22 AM JST

PDB ID	:	7CND
Title	:	NCI-1 in complex with CRM1-Ran-RanBP1
Authors	:	Sun, Q.; Lei, Y.
Deposited on	:	2020-07-31
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

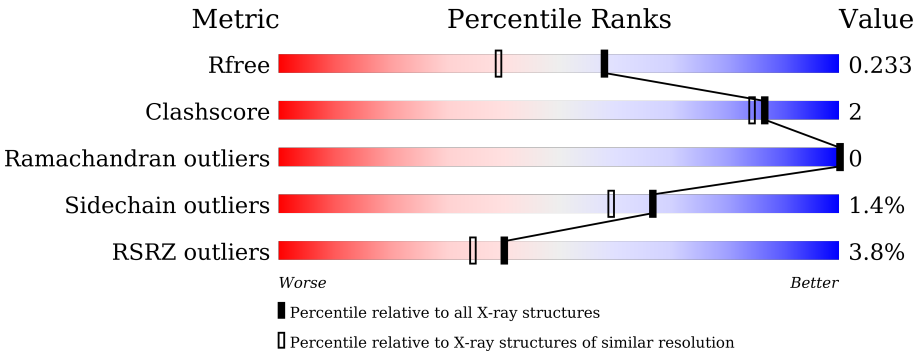
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	4% 91% 6%
2	B	140	2% 84% 14%
3	C	1003	4% 93% 6%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1664	1074	284	300	6			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called YRB1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			992	628	174	186	4			

- Molecule 3 is a protein called CRM1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	995	Total	C	N	O	S	0	4	0
			8074	5190	1328	1513	43			

There are 71 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	conflict	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	?	-	ASP	deletion	UNP A0A6A5PZI8

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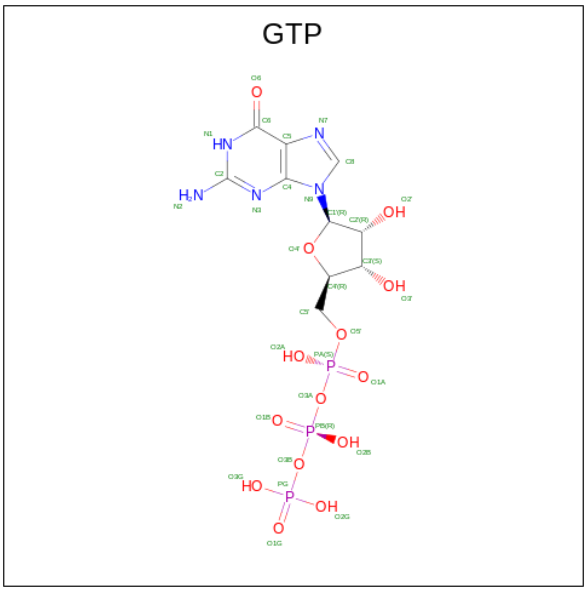
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	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	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).

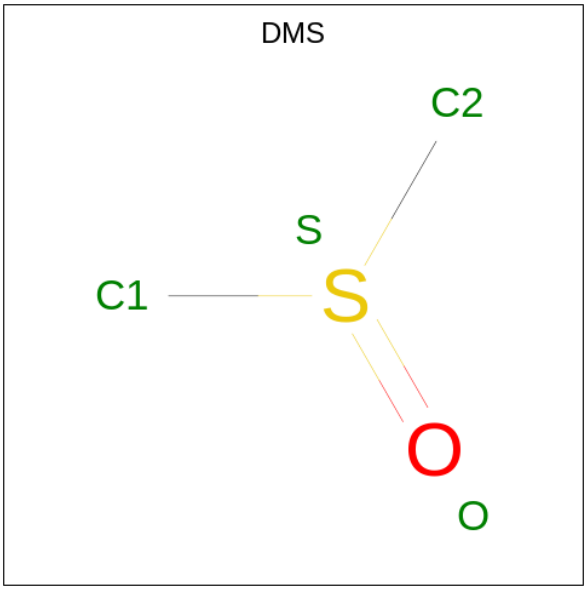
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

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



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

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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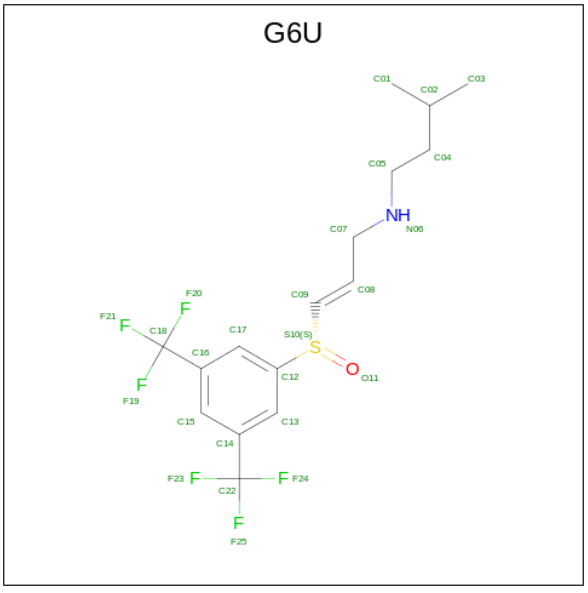
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O S 4 2 1 1	0	0
6	C	1	Total C O S 4 2 1 1	0	0
6	C	1	Total C O S 4 2 1 1	0	0

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

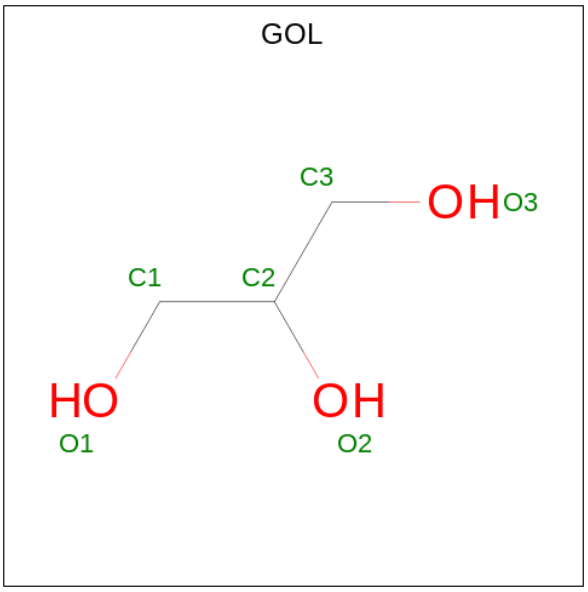
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	B	1	Total Cl 1 1	0	0
7	C	7	Total Cl 7 7	0	0

- Molecule 8 is {N}-[({E})-3-[3,5-bis(trifluoromethyl)phenyl]sulfinylprop-2-enyl]-3-methyl-butan-1-amine (three-letter code: G6U) (formula: $C_{16}H_{19}F_6NOS$) (labeled as "Ligand of Interest" by depositor).



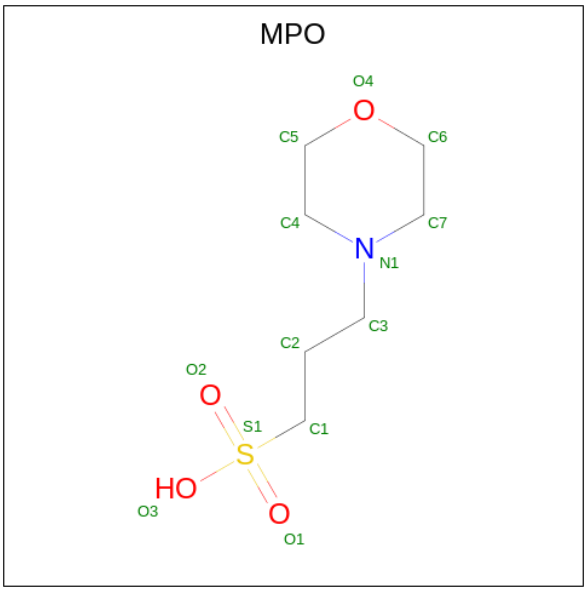
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C F N O S 25 16 6 1 1 1	0	0

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



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

- Molecule 10 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



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

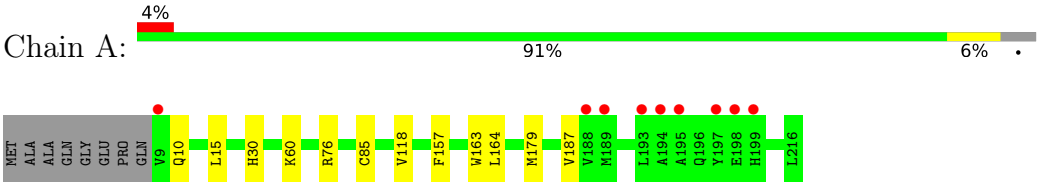
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	138	Total O 138 138	0	0
11	B	46	Total O 46 46	0	0
11	C	589	Total O 590 590	0	1

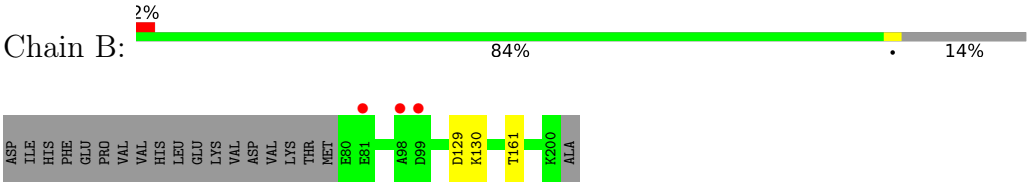
3 Residue-property plots (i)

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.

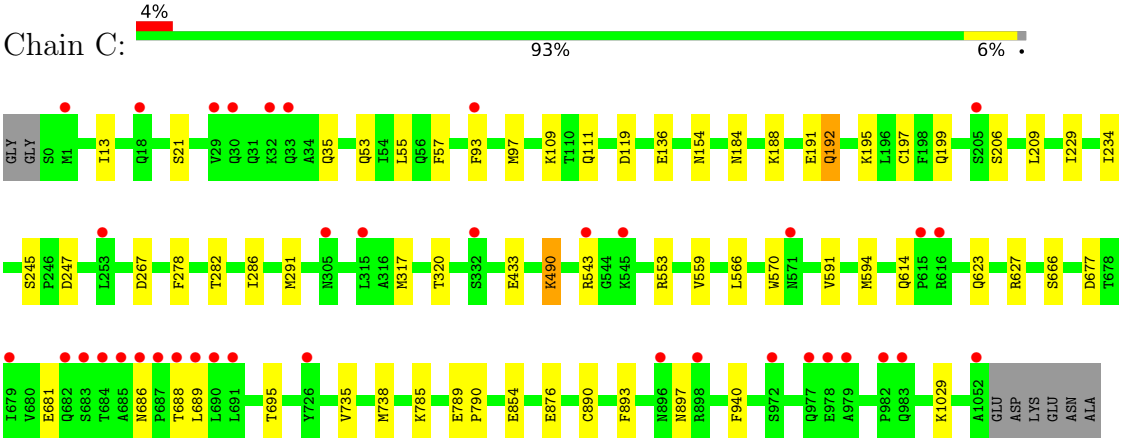
• Molecule 1: GTP-binding nuclear protein Ran



• Molecule 2: YRB1 isoform 1



• Molecule 3: CRM1 isoform 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.33Å 105.33Å 304.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.56 – 1.80 37.54 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.56-1.80) 100.0 (37.54-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.202 , 0.232 0.207 , 0.233	Depositor DCC
R_{free} test set	7985 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11614	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DMS, GTP, MG, G6U, CL, MPO, GOL

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	0.62	0/1705	0.74	0/2312
2	B	0.63	0/1009	0.74	0/1347
3	C	0.65	0/8230	0.68	0/11151
All	All	0.64	0/10944	0.70	0/14810

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

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	1664	0	1666	8	0
2	B	992	0	992	4	0
3	C	8074	0	8162	34	0
4	A	1	0	0	0	0
5	A	32	0	12	0	0
6	A	8	0	12	0	0
6	C	16	0	24	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	25	0	0	0	0
9	C	6	0	8	0	0
10	C	13	0	14	4	0
11	A	138	0	0	1	0
11	B	46	0	0	0	0
11	C	590	0	0	5	0
All	All	11614	0	10890	45	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 (45) 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:320:THR:HB	10:C:1109:MPO:H61	1.77	0.65
3:C:623:GLN:O	3:C:627:ARG:HG3	2.01	0.60
3:C:195:LYS:O	3:C:199:GLN:HG3	2.02	0.59
3:C:206:SER:HB3	3:C:209:LEU:HB3	1.83	0.59
3:C:55:LEU:HD22	3:C:97:MET:HE1	1.84	0.59
1:A:187:VAL:HG11	2:B:161:THR:OG1	2.03	0.58
3:C:317:MET:SD	10:C:1109:MPO:H21	2.45	0.56
3:C:553:ARG:HG2	3:C:594[B]:MET:HG2	1.89	0.55
3:C:686:ASN:ND2	3:C:688:THR:HG22	2.21	0.54
3:C:735:VAL:HA	3:C:738:MET:HE2	1.88	0.54
1:A:76:ARG:HD2	11:A:415:HOH:O	2.10	0.52
3:C:543:ARG:HA	3:C:543:ARG:NE	2.24	0.52
1:A:187:VAL:HG21	2:B:161:THR:OG1	2.10	0.51
3:C:433:GLU:HG2	3:C:490:LYS:HE3	1.92	0.51
3:C:184:ASN:O	3:C:188:LYS:HD3	2.11	0.50
3:C:13:ILE:HD11	3:C:53:GLN:HG2	1.94	0.50
3:C:247:ASP:N	3:C:247:ASP:OD1	2.44	0.50
3:C:111:GLN:HE21	3:C:111:GLN:HA	1.77	0.49
3:C:191:GLU:HB3	3:C:192:GLN:HE21	1.78	0.49
3:C:890:CYS:O	3:C:893:PHE:HB2	2.14	0.48
3:C:433:GLU:CG	3:C:490:LYS:HE3	2.43	0.47
2:B:129:ASP:C	2:B:130:LYS:HG2	2.35	0.47
3:C:789:GLU:HB3	3:C:790:PRO:HD3	1.96	0.47
10:C:1109:MPO:H71	11:C:1648:HOH:O	2.14	0.46
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.44	0.46
3:C:591:VAL:O	3:C:594[B]:MET:HG3	2.16	0.45
1:A:10:GLN:HA	1:A:60:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:897:ASN:ND2	11:C:1219:HOH:O	2.49	0.45
3:C:109:LYS:HD3	3:C:109:LYS:HA	1.78	0.44
3:C:197[A]:CYS:SG	11:C:1251:HOH:O	2.62	0.43
1:A:85:CYS:HB2	1:A:164:LEU:HD22	2.01	0.43
1:A:187:VAL:HG11	2:B:161:THR:HG1	1.80	0.43
3:C:13:ILE:HD12	3:C:57:PHE:HB2	2.00	0.43
3:C:559:VAL:HG13	3:C:566:LEU:HD21	1.99	0.43
1:A:30:HIS:CD2	1:A:157:PHE:CE2	3.07	0.43
3:C:677:ASP:O	3:C:681:GLU:HG2	2.19	0.42
3:C:686:ASN:HD21	3:C:688:THR:HG22	1.84	0.42
3:C:282:THR:O	3:C:286:ILE:HG12	2.19	0.42
3:C:229:ILE:HA	3:C:234:ILE:CG2	2.50	0.42
10:C:1109:MPO:H42	11:C:1709:HOH:O	2.21	0.41
1:A:118:VAL:HG22	1:A:163:TRP:CE3	2.56	0.41
3:C:689:LEU:HD23	3:C:695:THR:HG21	2.02	0.41
3:C:735:VAL:HA	3:C:738:MET:CE	2.50	0.41
3:C:570:TRP:CE2	3:C:614:GLN:HG3	2.56	0.40
3:C:1029:LYS:NZ	11:C:1215:HOH:O	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/216 (95%)	200 (97%)	6 (3%)	0	100	100
2	B	119/140 (85%)	113 (95%)	6 (5%)	0	100	100
3	C	997/1003 (99%)	979 (98%)	18 (2%)	0	100	100
All	All	1322/1359 (97%)	1292 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	179/184 (97%)	177 (99%)	2 (1%)	73 68
2	B	103/121 (85%)	103 (100%)	0	100 100
3	C	914/915 (100%)	898 (98%)	16 (2%)	59 48
All	All	1196/1220 (98%)	1178 (98%)	18 (2%)	67 56

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	179	MET
3	C	21	SER
3	C	35	GLN
3	C	93	PHE
3	C	136[A]	GLU
3	C	136[B]	GLU
3	C	192	GLN
3	C	245	SER
3	C	267	ASP
3	C	278	PHE
3	C	291	MET
3	C	490	LYS
3	C	666	SER
3	C	785	LYS
3	C	854	GLU
3	C	876	GLU
3	C	940	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	9	ASN
3	C	33	GLN
3	C	111	GLN

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Mol	Chain	Res	Type
3	C	192	GLN
3	C	233	ASN
3	C	682	GLN
3	C	686	ASN
3	C	742	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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	A	302	4	26,34,34	0.96	2 (7%)	32,54,54	0.83	1 (3%)
6	DMS	C	1103	-	3,3,3	0.28	0	3,3,3	0.14	0
6	DMS	C	1102	-	3,3,3	0.29	0	3,3,3	0.17	0
6	DMS	C	1112	-	3,3,3	0.29	0	3,3,3	0.14	0
9	GOL	C	1104	-	5,5,5	0.12	0	5,5,5	0.31	0
10	MPO	C	1109	-	13,13,13	1.10	1 (7%)	17,17,17	1.24	2 (11%)
6	DMS	C	1105	-	3,3,3	0.25	0	3,3,3	0.16	0
8	G6U	C	1101	-	22,25,25	2.97	1 (4%)	32,36,36	1.76	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	DMS	A	303	-	3,3,3	0.34	0	3,3,3	0.18	0
6	DMS	A	304	-	3,3,3	0.33	0	3,3,3	0.12	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
9	GOL	C	1104	-	-	2/4/4/4	-
10	MPO	C	1109	-	-	5/7/15/15	0/1/1/1
5	GTP	A	302	4	-	6/18/38/38	0/3/3/3
8	G6U	C	1101	-	-	4/24/25/25	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1101	G6U	C12-S10	-13.64	1.67	1.79
10	C	1109	MPO	O2-S1	3.66	1.55	1.45
5	A	302	GTP	C5-C6	-2.74	1.41	1.47
5	A	302	GTP	C8-N7	-2.18	1.31	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1101	G6U	O11-S10-C09	6.23	118.86	105.27
8	C	1101	G6U	O11-S10-C12	-3.81	101.78	106.14
8	C	1101	G6U	C13-C12-S10	2.89	123.14	119.10
10	C	1109	MPO	O3-S1-O1	2.68	117.83	111.27
10	C	1109	MPO	C6-C7-N1	2.63	114.09	110.10
8	C	1101	G6U	F20-C18-C16	-2.33	107.81	112.93
5	A	302	GTP	O6-C6-C5	2.21	128.70	124.37
8	C	1101	G6U	C17-C16-C18	2.06	122.37	119.58

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	GTP	C5'-O5'-PA-O3A
5	A	302	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	C	1101	G6U	C13-C12-S10-C09
8	C	1101	G6U	C17-C12-S10-C09
10	C	1109	MPO	C2-C1-S1-O2
5	A	302	GTP	C3'-C4'-C5'-O5'
10	C	1109	MPO	C2-C1-S1-O3
10	C	1109	MPO	C2-C3-N1-C4
10	C	1109	MPO	C2-C3-N1-C7
9	C	1104	GOL	O1-C1-C2-C3
9	C	1104	GOL	O1-C1-C2-O2
8	C	1101	G6U	C08-C07-N06-C05
10	C	1109	MPO	C2-C1-S1-O1
8	C	1101	G6U	C02-C04-C05-N06
5	A	302	GTP	C5'-O5'-PA-O1A
5	A	302	GTP	C5'-O5'-PA-O2A
5	A	302	GTP	PA-O3A-PB-O2B

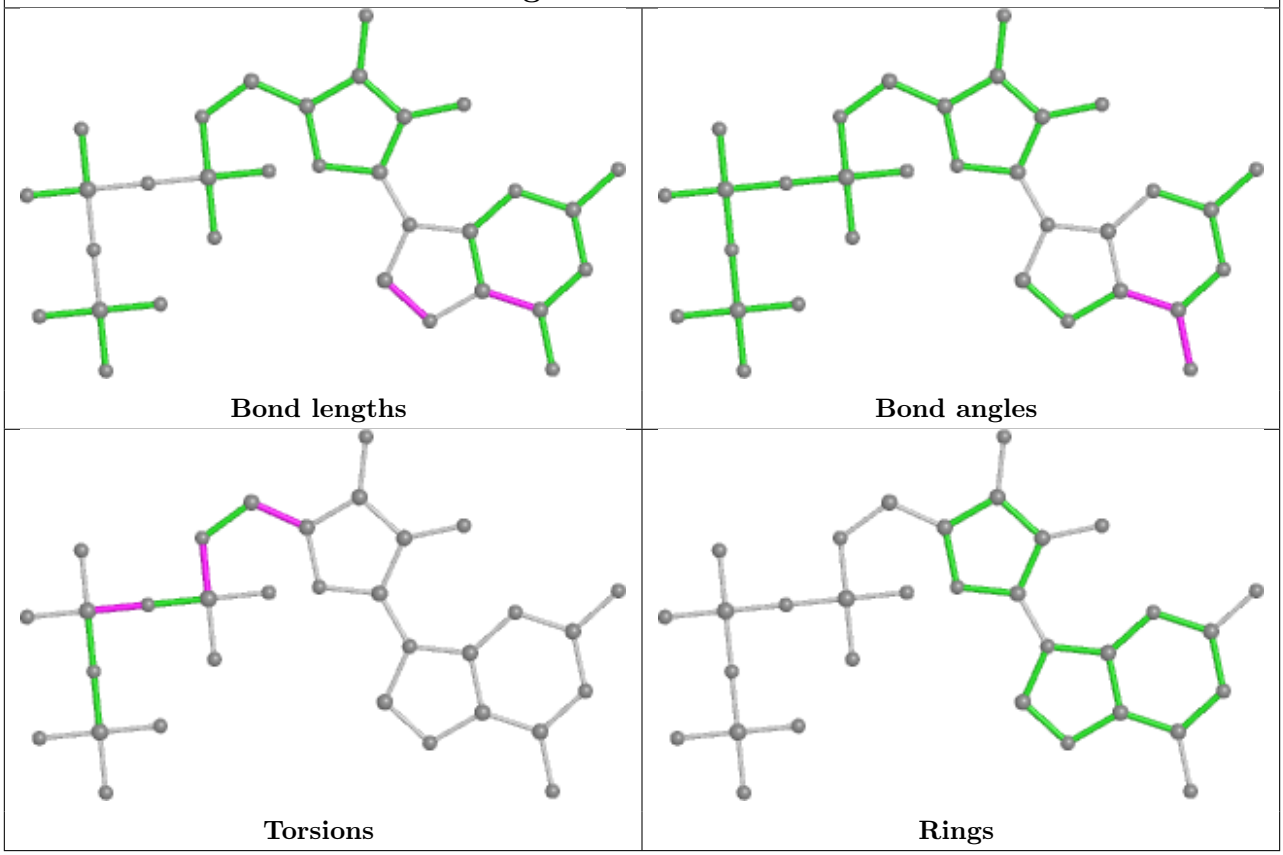
There are no ring outliers.

1 monomer is involved in 4 short contacts:

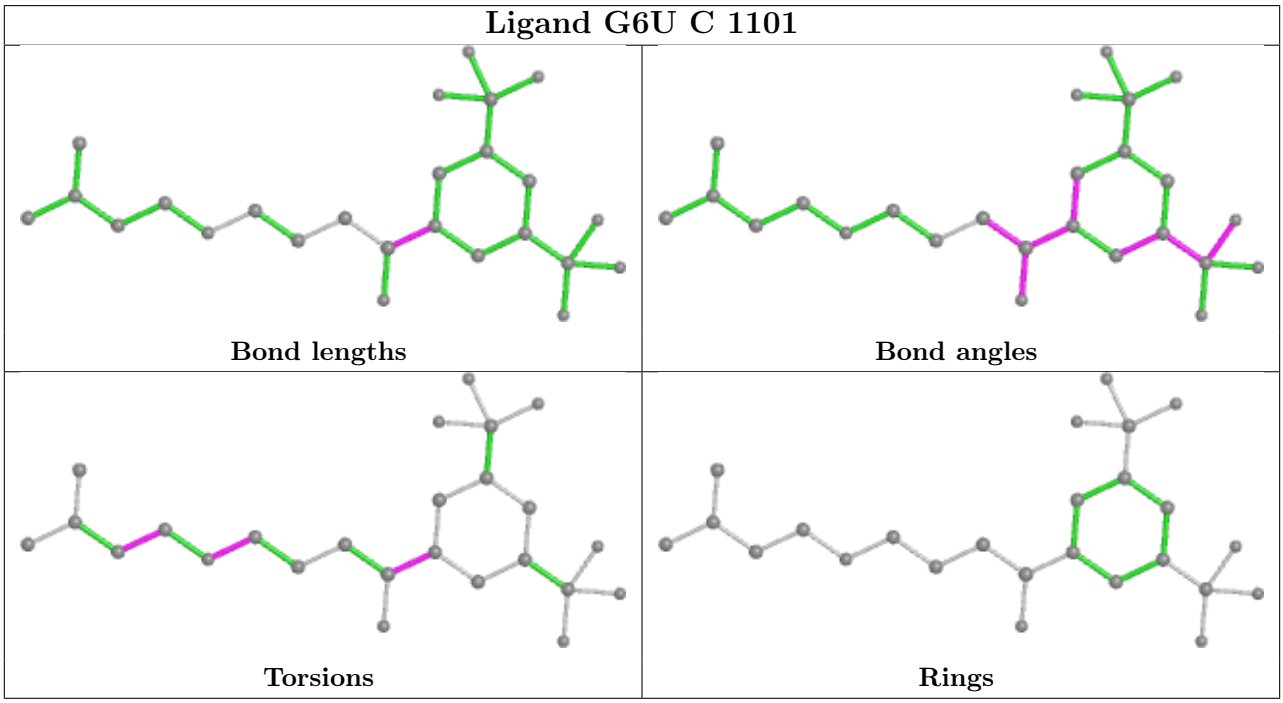
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1109	MPO	4	0

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 then 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.

Ligand GTP A 302



Ligand G6U C 1101



5.7 Other polymers

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^{th} 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%)	0.03	9 (4%) 35 29	25, 37, 89, 101	0
2	B	121/140 (86%)	0.12	3 (2%) 57 52	38, 49, 75, 88	0
3	C	995/1003 (99%)	0.08	38 (3%) 40 35	25, 40, 68, 110	0
All	All	1324/1359 (97%)	0.07	50 (3%) 40 35	25, 41, 71, 110	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	689	LEU	8.8
3	C	691	LEU	8.2
3	C	684	THR	6.0
1	A	199	HIS	5.4
3	C	616	ARG	5.4
3	C	690	LEU	5.2
1	A	188	VAL	4.9
3	C	686	ASN	4.9
3	C	688	THR	4.3
3	C	979	ALA	4.1
3	C	978	GLU	3.9
3	C	687	PRO	3.9
3	C	685	ALA	3.5
1	A	197	TYR	3.5
3	C	543	ARG	3.4
3	C	898	ARG	3.4
3	C	332	SER	3.3
1	A	9	VAL	3.3
3	C	977	GLN	3.2
3	C	30	GLN	3.2
3	C	683	SER	3.2
3	C	982	PRO	3.1
3	C	545	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	18	GLN	2.9
3	C	29	VAL	2.9
2	B	99	ASP	2.7
3	C	205	SER	2.7
2	B	81	GLU	2.7
3	C	32	LYS	2.7
1	A	189	MET	2.6
3	C	972	SER	2.6
3	C	33	GLN	2.6
3	C	983	GLN	2.6
3	C	305	ASN	2.5
1	A	194	ALA	2.4
1	A	195	ALA	2.4
2	B	98	ALA	2.4
1	A	198	GLU	2.3
3	C	896	ASN	2.3
3	C	682	GLN	2.3
3	C	615	PRO	2.2
3	C	1052	ALA	2.2
3	C	1	MET	2.2
3	C	571	ASN	2.2
3	C	253	LEU	2.1
3	C	726	TYR	2.1
3	C	93	PHE	2.1
1	A	193	LEU	2.1
3	C	679	ILE	2.0
3	C	315	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,

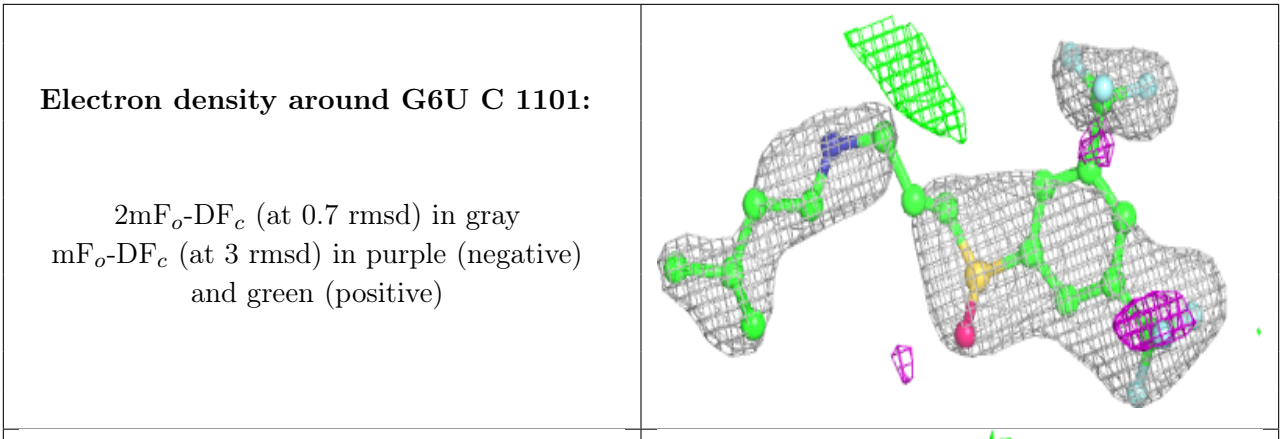
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DMS	C	1112	4/4	0.72	0.24	85,87,87,87	0
9	GOL	C	1104	6/6	0.73	0.13	78,79,80,81	0
8	G6U	C	1101	25/25	0.79	0.23	72,79,84,85	25
7	CL	C	1108	1/1	0.80	0.18	80,80,80,80	1
7	CL	A	305	1/1	0.82	0.09	73,73,73,73	0
7	CL	C	1113	1/1	0.84	0.35	77,77,77,77	0
7	CL	C	1106	1/1	0.86	0.18	70,70,70,70	0
6	DMS	C	1105	4/4	0.89	0.21	81,84,84,84	0
6	DMS	A	304	4/4	0.89	0.14	57,60,64,65	0
6	DMS	C	1103	4/4	0.90	0.20	79,81,82,82	0
7	CL	C	1114	1/1	0.92	0.10	86,86,86,86	0
6	DMS	A	303	4/4	0.92	0.11	67,68,69,69	0
7	CL	C	1107	1/1	0.92	0.09	71,71,71,71	0
10	MPO	C	1109	13/13	0.92	0.15	45,48,51,51	0
6	DMS	C	1102	4/4	0.93	0.17	66,70,70,72	0
7	CL	C	1111	1/1	0.95	0.16	61,61,61,61	0
7	CL	C	1110	1/1	0.95	0.09	73,73,73,73	0
7	CL	B	301	1/1	0.97	0.42	30,30,30,30	0
4	MG	A	301	1/1	0.99	0.03	29,29,29,29	0
5	GTP	A	302	32/32	0.99	0.07	26,30,32,32	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.

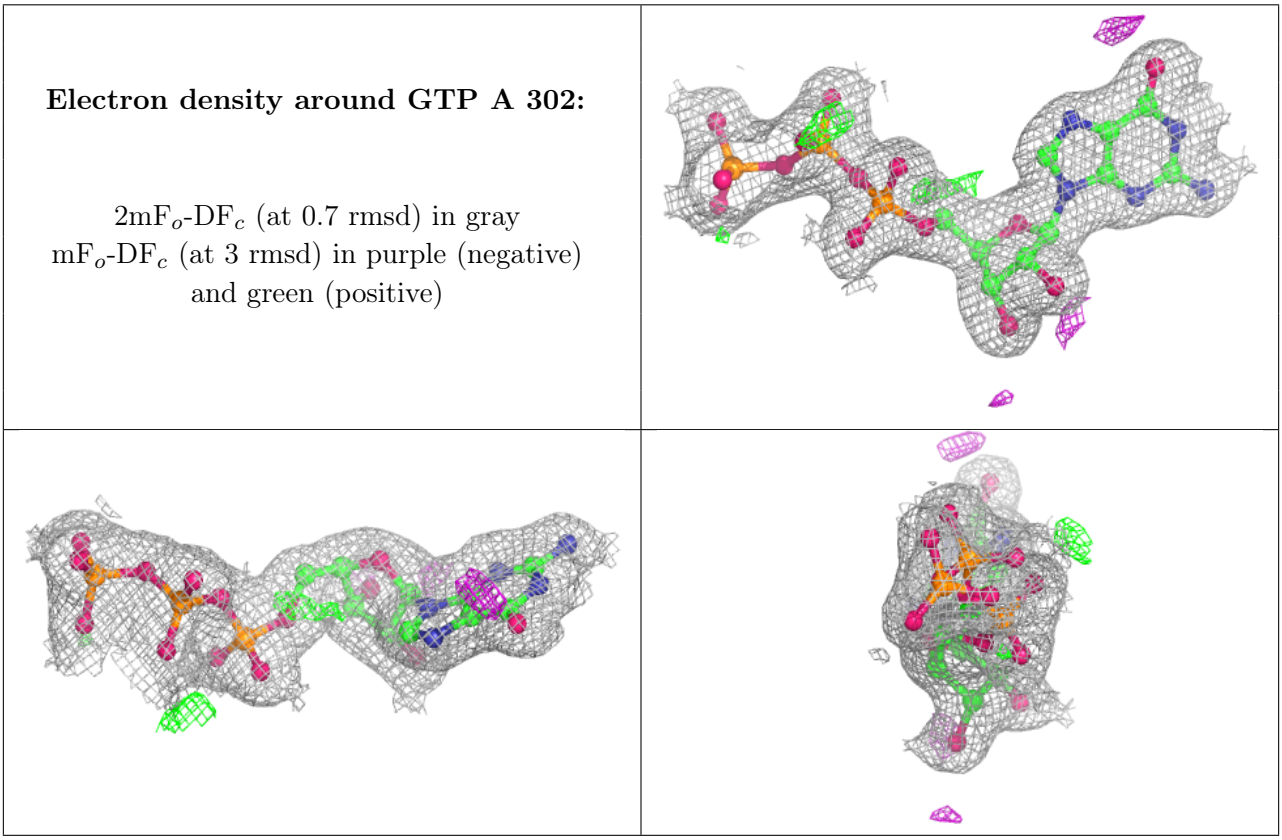
Electron density around G6U C 1101:

$2mF_o$-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 302:

$2mF_o$-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.