



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 12:10 PM JST

PDB ID : 7DBA
Title : RYX in complex with tubulin
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2020-10-19
Resolution : 2.46 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.23.2
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) : 2.23.2

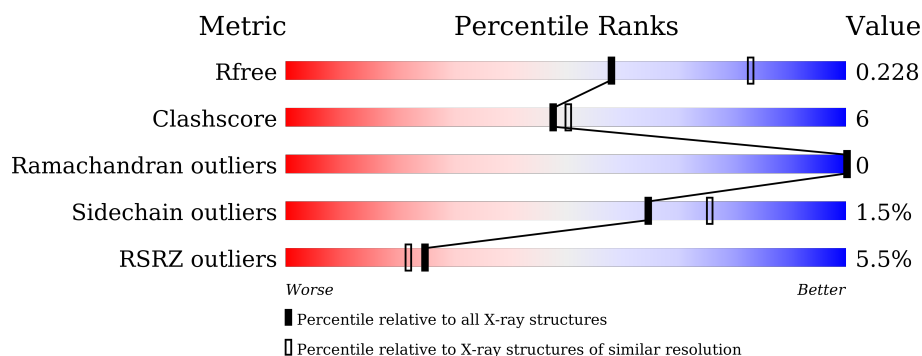
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>2%</div> <div>82% 15% .</div> </div>
1	C	451	<div> <div>87% 10% .</div> </div>
2	B	445	<div> <div>4%</div> <div>81% 13% . 5%</div> </div>
2	D	445	<div> <div>4%</div> <div>78% 16% 6%</div> </div>
3	E	143	<div> <div>8%</div> <div>73% 13% 14%</div> </div>
4	F	384	<div> <div>16%</div> <div>71% 20% . 8%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18135 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3427	2170	580	653	24			
1	C	440	Total	C	N	O	S	0	11	0
			3479	2203	586	664	26			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	5	0
			3369	2119	576	648	26			
2	D	420	Total	C	N	O	S	0	4	0
			3301	2076	557	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	3	0
			1031	637	186	202	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	5	0
			2913	1871	502	525	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- 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		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

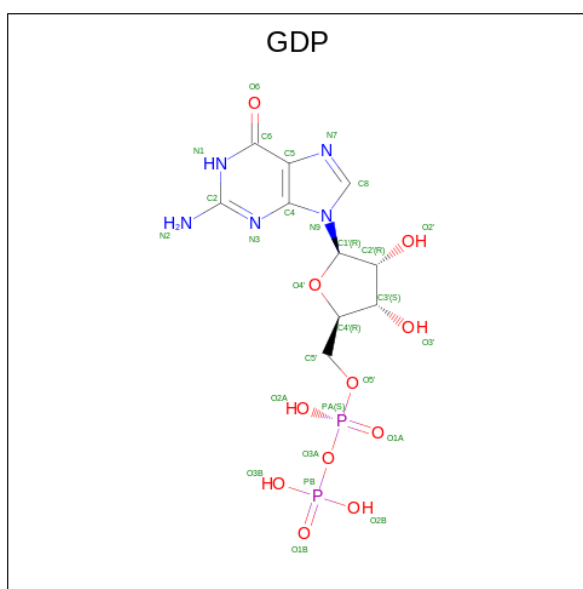
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

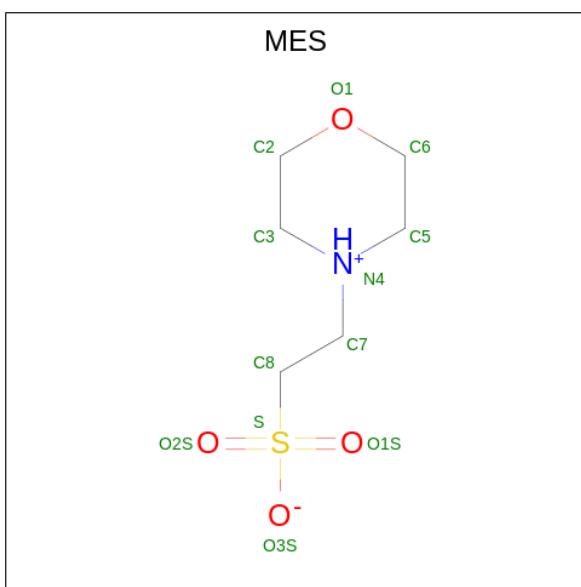
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

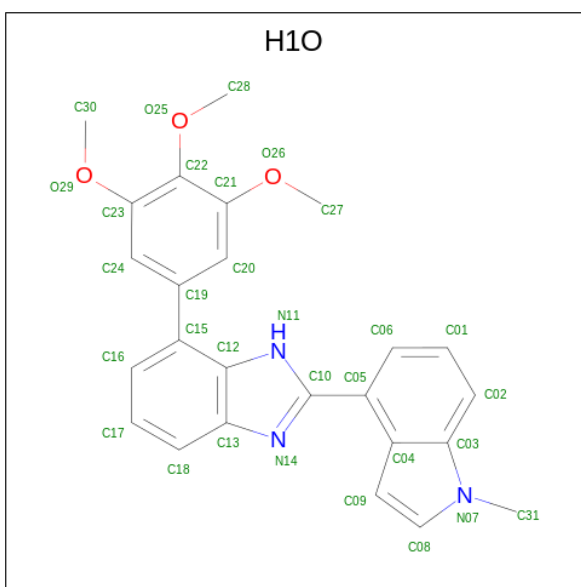
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-(1-methylindol-4-yl)-7-(3,4,5-trimethoxyphenyl)-1 {H}-benzimidazole (three-letter code: H1O) (formula: C₂₅H₂₃N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			31	25	3	3		

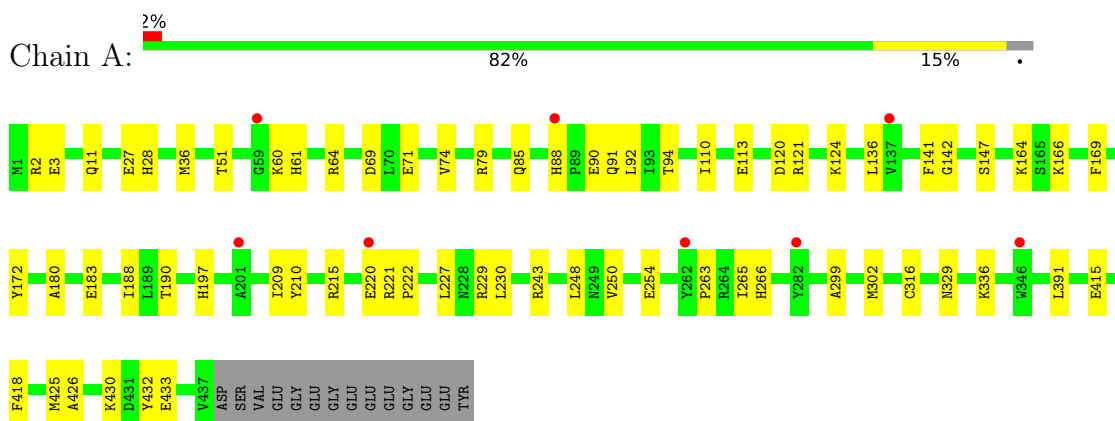
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	89	Total 89	O 89	0	0
12	B	83	Total 83	O 83	0	0
12	C	174	Total 174	O 174	0	0
12	D	41	Total 41	O 41	0	0
12	E	18	Total 18	O 18	0	0
12	F	28	Total 28	O 28	0	0

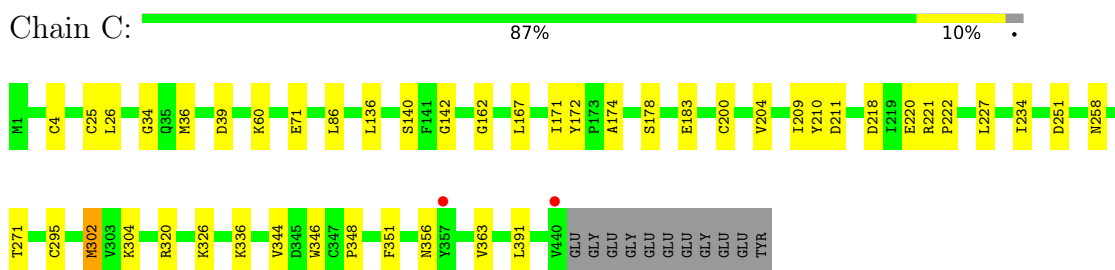
3 Residue-property plots [i](#)

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.

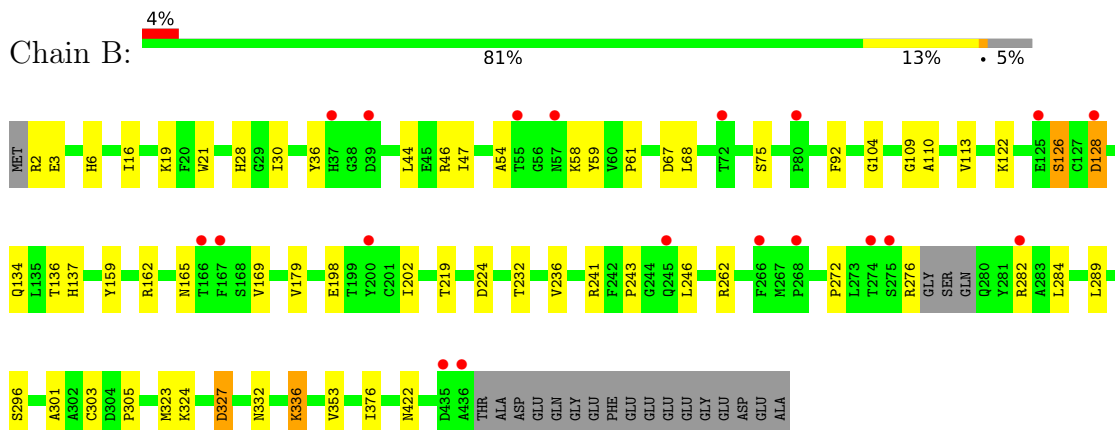
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain



Protein	Residue	Score	Category	
MET	R2	0.00	Low	
	H6	0.00	Low	
	I7	0.00	Low	
	W21	0.00	Low	
	I30	0.00	Low	
	H37	0.00	Low	
	T55	0.00	Low	
	Y59	0.00	Low	
	E69	0.00	Low	
	S75	0.00	Low	
G79	S78	0.00	Low	
	P80	0.00	Low	
	F81	0.00	Low	
	T84	0.00	Low	
	W101	0.00	Low	
	G104	0.00	Low	
	H105	0.00	Low	
	Y106	0.00	Low	
	G109	0.00	Low	
	L117	0.00	Low	
D118	D118	0.00	Low	
	R121	0.00	Low	
	Q134	0.00	Low	
	L135	0.00	Low	
	T136	0.00	Low	
	H137	0.00	Low	
	S138	0.00	Low	
	L139	0.00	Low	
	G140	0.00	Low	
	G141	0.00	Low	
M165	M165	0.00	Low	
	S168	0.00	Low	
	V169	0.00	Low	
	K174	0.00	Low	
	D177	0.00	Low	
	T178	0.00	Low	
	V179	0.00	Low	
	V180	0.00	Low	
	I202	I202	0.00	Low
		E205	0.00	Low
C211		0.00	Low	
F212		0.00	Low	
R213		0.00	Low	
T214		0.00	Low	
L215		0.00	Low	
K216		0.00	Low	
L217		0.00	Low	
T218		0.00	Low	
T219	0.00	Low		
P220	0.00	Low		
T221	0.00	Low		
T238	T238	0.00	Low	
	C239	0.00	Low	
	F242	0.00	Low	
	L246	0.00	Low	
	L273	0.00	Low	
	T284	0.00	Low	
	SER	0.00	Low	
	ARG	0.00	Low	
	GLY	0.00	Low	
	SER	0.00	Low	
GLN	0.00	Low		
TTR	0.00	Low		
ALA	0.00	Low		
L284	L284	0.00	Low	
	T285	0.00	Low	
	V286	0.00	Low	
	P287	0.00	Low	
	E288	0.00	Low	
	L289	0.00	Low	
	T290	0.00	Low	
	M293	0.00	Low	
	S296	0.00	Low	
	P305	0.00	Low	
R318	0.00	Low		
K324	K324	0.00	Low	
	E328	0.00	Low	
	Q329	0.00	Low	
	V333	0.00	Low	
	A352	0.00	Low	

[illegible]

I330	R197	THR	M1
Q340	D200	ARG	F4
Y343	L206	T125	V5
A354	Y211	D126	
L361	R217	E127	R10
A362	E218	R128	
ASP	G219	E129	Y14
THR	V220	F131	A15
GLY	L221	L132	E16
GLN	R222	A133	V17
LYS	S225	A134	S13
THR		Y135	R19
SER		M136	
GLN	A231	R137	T24
PRO	N232	R138	G25
T372	R233	R139	
H379	Q234	E140	R29
H380	D235	G141	L30
H381	K236	R142	R31
H384	T237	E143	K32
		G144	
		M145	M45
		N146	R46
		W147	
	L240		I81
	H243	K150	E86
	C244	S151	L87
	I245	ALA	S83
	Q246	GLY	E89
	K247	ALA	
	E248	LYS	P95
	Y249	GLY	E96
	S250	E158	S97
	K251	G159	Y93
	N252	I160	V99
	Y253	L161	I100
	G254	I162	Y101
	R255	S163	P102
	Y256	S164	T103
	E257	E165	N104
		A166	
		S167	K106
	F263	E168	THR
	Q269	L169	PRO
	T277	I173	ALA
	T278	D174	PRO
	S282	E175	ALA
		Q176	GLN
	Q286	G177	ASN
		Q178	GLY
			ILE
	I290		ARG
	D318	Q183	HIS
		L191	LEU
	L325	H196	ILE
			ASN
			ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.45Å 158.88Å 181.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.30 – 2.46 31.30 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.1 (31.30-2.46) 99.1 (31.30-2.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.188 , 0.228 0.189 , 0.228	Depositor DCC
R_{free} test set	1997 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18135	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, H1O, GTP, CA, GDP, MG, 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	0.29	0/3517	0.48	0/4776
1	C	0.31	0/3587	0.50	0/4870
2	B	0.32	0/3455	0.49	1/4678 (0.0%)
2	D	0.31	0/3383	0.49	0/4586
3	E	0.34	0/1049	0.45	0/1392
4	F	0.32	0/2996	0.55	2/4048 (0.0%)
All	All	0.31	0/17987	0.50	3/24350 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	282	ARG	NE-CZ-NH1	-5.85	117.37	120.30
4	F	159	GLY	N-CA-C	5.60	127.09	113.10
4	F	225	SER	C-N-CA	5.31	134.98	121.70

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	3427	0	3340	44	0
1	C	3479	0	3405	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3369	0	3257	41	0
2	D	3301	0	3172	44	0
3	E	1031	0	1051	14	0
4	F	2913	0	2889	53	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	24	0	24	0	0
11	B	31	0	0	1	0
12	A	89	0	0	1	0
12	B	83	0	0	2	0
12	C	174	0	0	1	0
12	D	41	0	0	2	0
12	E	18	0	0	3	0
12	F	28	0	0	0	0
All	All	18135	0	17186	212	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 6.

The worst 5 of 212 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)
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.19	0.83
2:D:399:ARG:HD2	2:D:401:ALA:HB2	1.66	0.77
2:D:105:HIS:HD2	2:D:106:TYR:CE2	2.03	0.76
4:F:86:GLU:O	4:F:87:LEU:HD23	1.86	0.75
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.25	0.69

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	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
1	C	448/451 (99%)	437 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	D	419/445 (94%)	406 (97%)	13 (3%)	0	100	100
3	E	122/143 (85%)	122 (100%)	0	0	100	100
4	F	349/384 (91%)	333 (95%)	16 (5%)	0	100	100
All	All	2202/2319 (95%)	2135 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/379 (98%)	367 (99%)	4 (1%)	73	82
1	C	381/379 (100%)	375 (98%)	6 (2%)	62	74
2	B	371/383 (97%)	365 (98%)	6 (2%)	62	74
2	D	364/383 (95%)	358 (98%)	6 (2%)	62	74
3	E	113/127 (89%)	111 (98%)	2 (2%)	59	71
4	F	321/342 (94%)	313 (98%)	8 (2%)	47	60
All	All	1921/1993 (96%)	1889 (98%)	32 (2%)	65	73

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	222	ARG
4	F	255[A]	ARG
1	C	221	ARG
1	C	218	ASP
4	F	255[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	48	ASN
2	D	57	ASN
2	D	105	HIS
1	A	285	GLN
1	A	266	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 [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	GDP	D	501	6	24,30,30	1.21	2 (8%)	31,47,47	1.81	6 (19%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.67	6 (18%)
9	GDP	B	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.95	9 (29%)
10	MES	B	504	-	12,12,12	4.48	7 (58%)	14,16,16	2.27	4 (28%)
11	H1O	B	505	-	31,35,35	1.27	6 (19%)	38,51,51	1.34	8 (21%)
10	MES	B	503	-	12,12,12	4.83	7 (58%)	14,16,16	2.77	6 (42%)
5	GTP	A	501	6	26,34,34	1.03	1 (3%)	33,54,54	1.72	6 (18%)

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	GDP	D	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
11	H1O	B	505	-	-	3/14/14/14	0/5/5/5
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C7-N4	-8.46	1.28	1.47
10	B	503	MES	O1S-S	8.23	1.69	1.45
10	B	503	MES	C7-N4	-7.77	1.29	1.47
10	B	503	MES	O2S-S	7.63	1.67	1.45
10	B	504	MES	O1S-S	7.27	1.66	1.45

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	C6-C5-N4	5.79	118.88	110.10
5	A	501	GTP	N3-C2-N1	-5.33	120.12	127.22
5	C	501	GTP	N3-C2-N1	-5.23	120.25	127.22
10	B	504	MES	C2-C3-N4	4.92	117.57	110.10
10	B	504	MES	C5-N4-C3	4.68	119.37	108.83

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

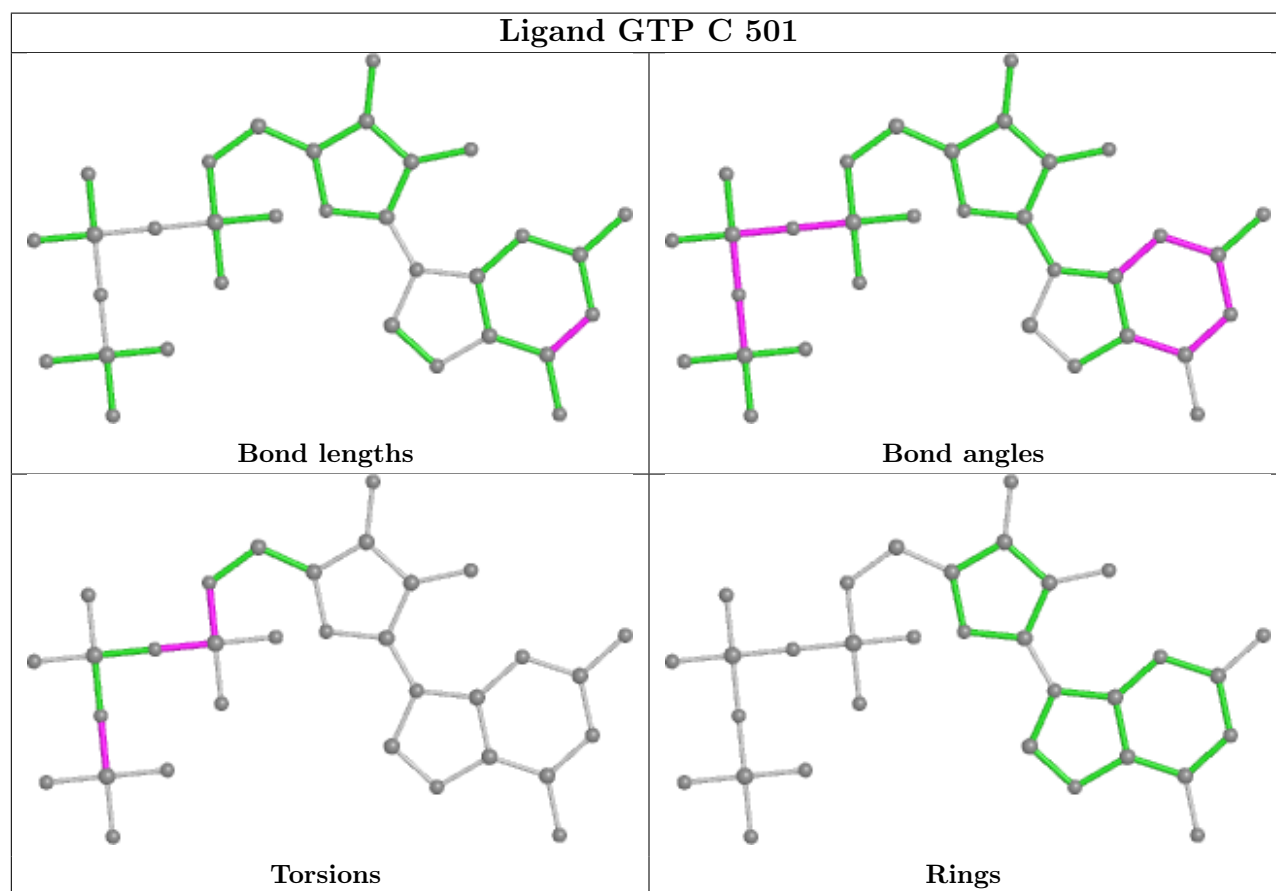
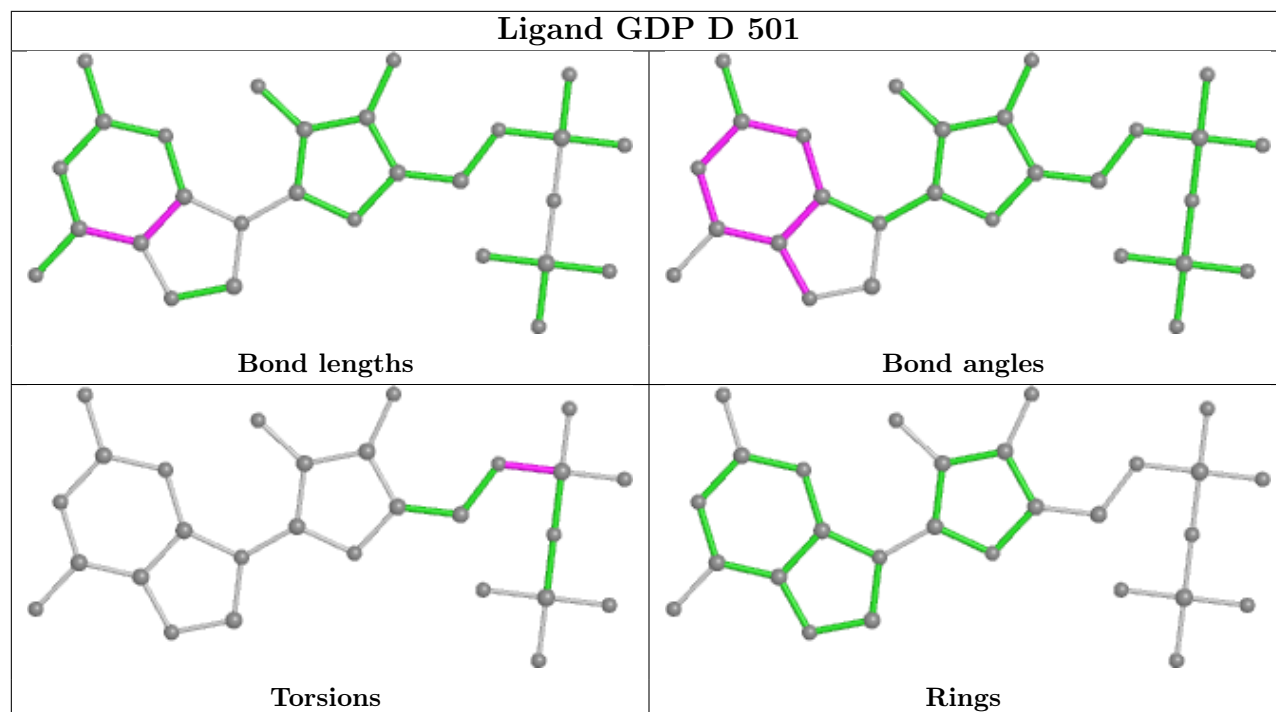
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A

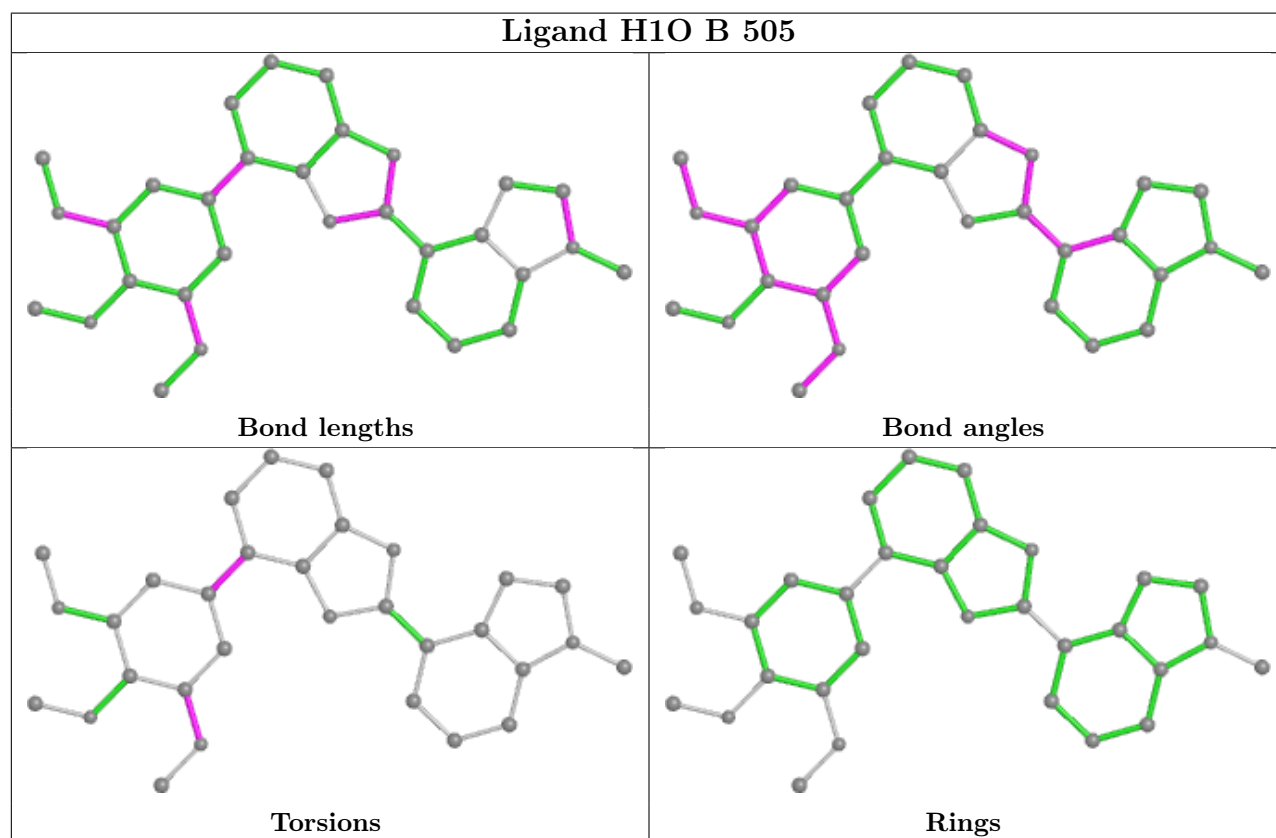
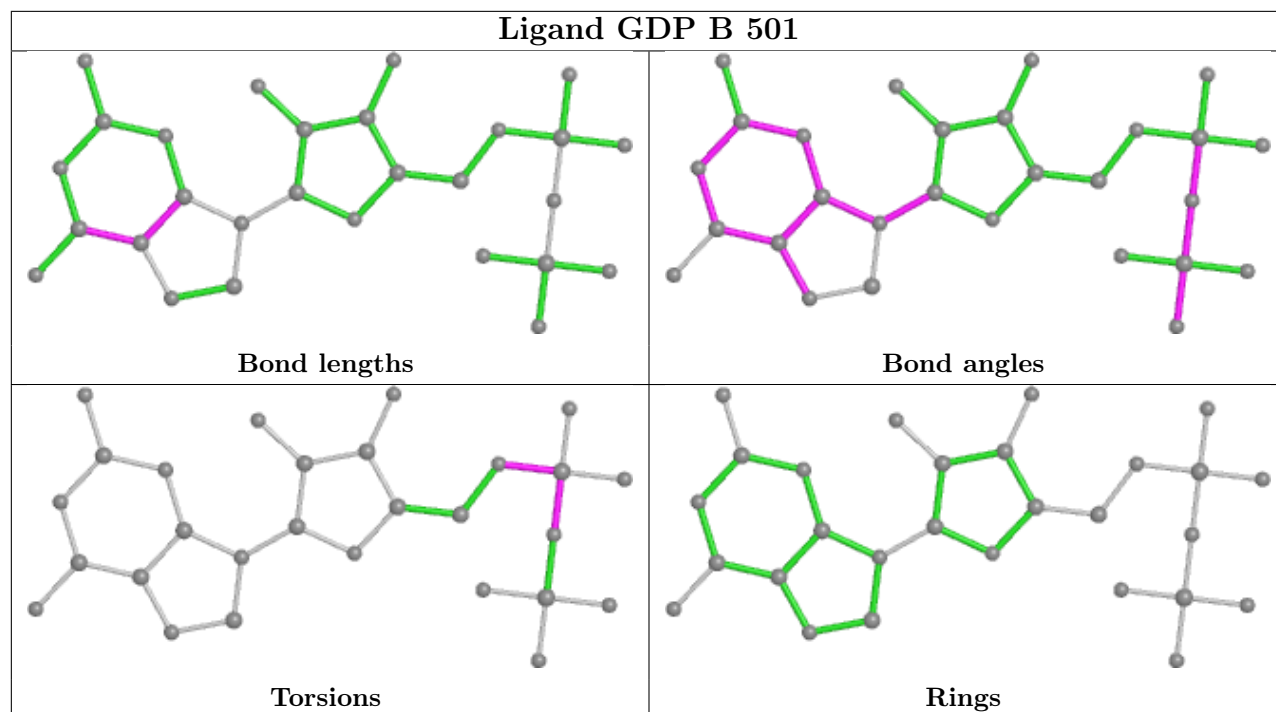
There are no ring outliers.

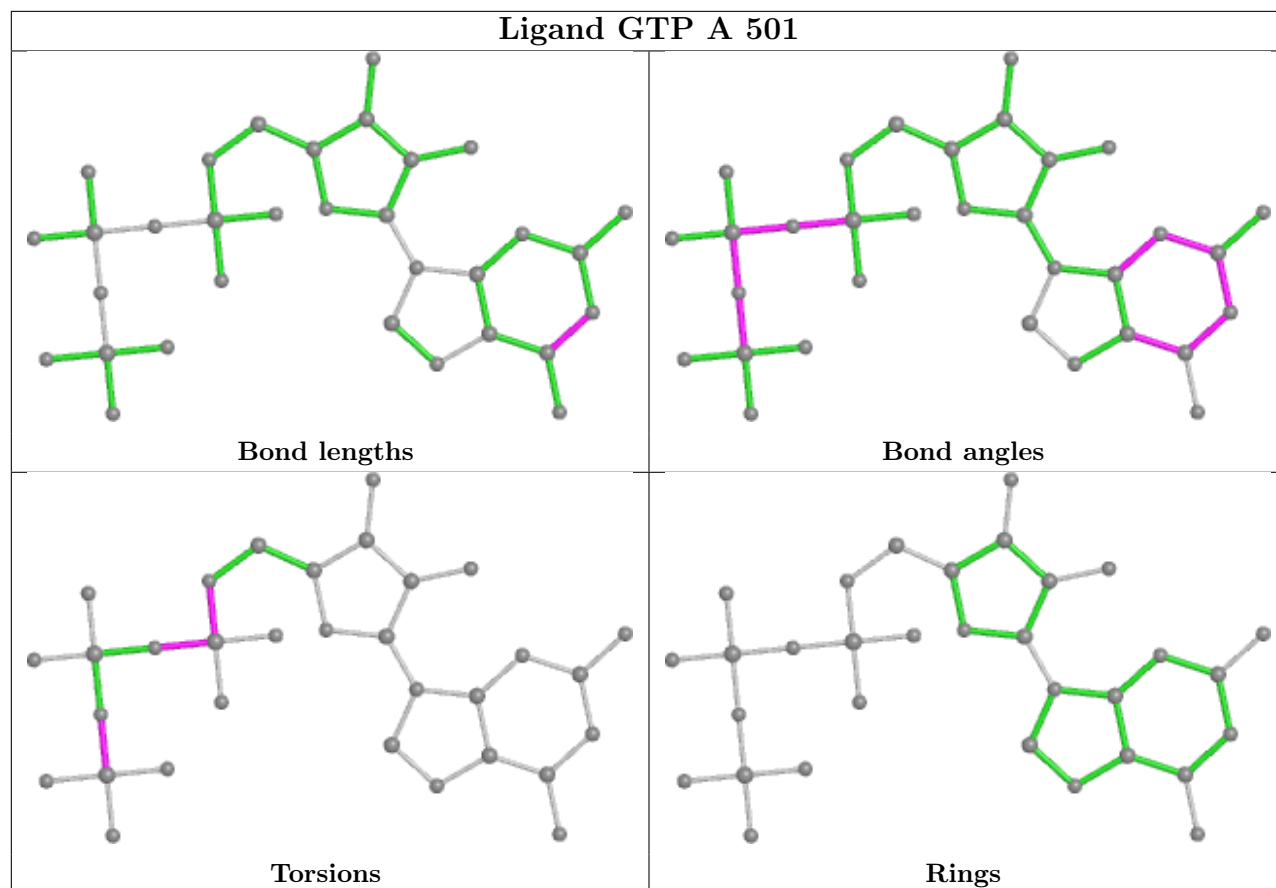
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
11	B	505	H1O	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	0.01	8 (1%) 68 65	30, 45, 71, 88	0
1	C	440/451 (97%)	-0.26	2 (0%) 91 92	22, 35, 58, 94	0
2	B	424/445 (95%)	0.11	19 (4%) 33 30	23, 44, 74, 117	2 (0%)
2	D	420/445 (94%)	0.20	20 (4%) 30 28	30, 54, 84, 126	3 (0%)
3	E	123/143 (86%)	0.45	11 (8%) 9 6	32, 57, 92, 125	0
4	F	352/384 (91%)	0.73	61 (17%) 1 1	35, 69, 141, 163	0
All	All	2196/2319 (94%)	0.15	121 (5%) 25 22	22, 48, 96, 163	5 (0%)

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	8.3
4	F	104	ASN	6.2
4	F	177	GLY	5.6
4	F	102	PRO	5.3
4	F	106	LYS	5.3

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

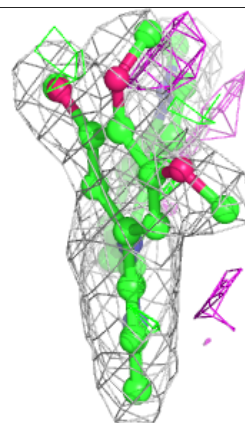
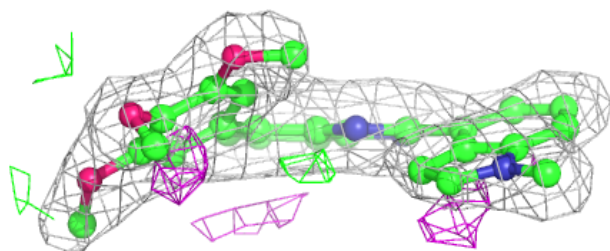
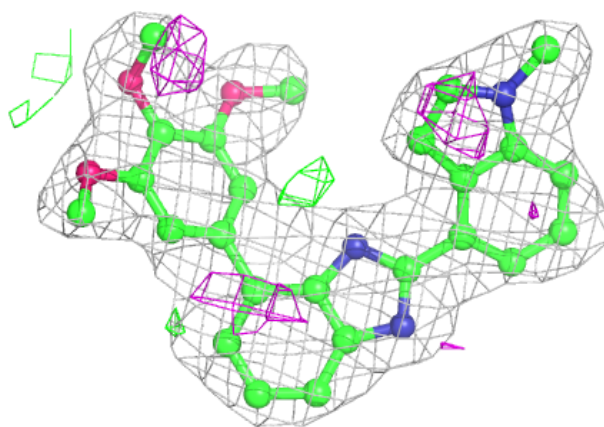
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.89	0.11	57,57,57,57	0
8	CL	A	504	1/1	0.90	0.09	79,79,79,79	0
11	H1O	B	505	31/31	0.90	0.15	30,48,55,58	0
6	MG	C	502	1/1	0.91	0.14	31,31,31,31	0
10	MES	B	504	12/12	0.94	0.24	65,73,82,92	0
7	CA	A	503	1/1	0.95	0.06	66,66,66,66	0
10	MES	B	503	12/12	0.96	0.14	38,54,60,61	0
7	CA	C	503	1/1	0.96	0.04	49,49,49,49	0
9	GDP	D	501	28/28	0.96	0.12	43,50,68,80	0
6	MG	A	502	1/1	0.97	0.09	32,32,32,32	0
5	GTP	C	501	32/32	0.98	0.14	22,29,34,40	0
5	GTP	A	501	32/32	0.98	0.11	24,37,42,48	0
6	MG	B	502	1/1	0.98	0.13	23,23,23,23	0
9	GDP	B	501	28/28	0.99	0.13	20,31,40,41	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.

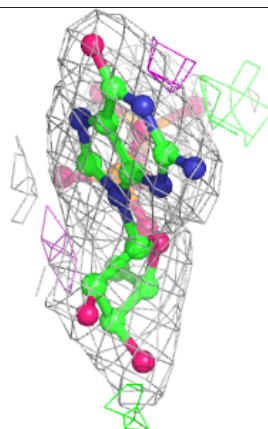
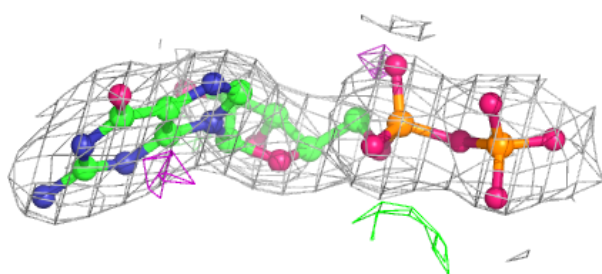
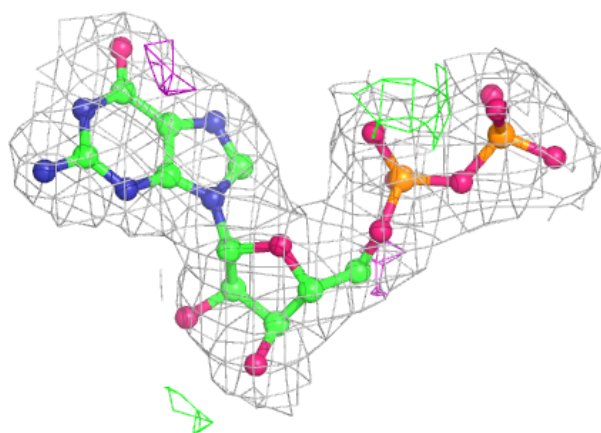
Electron density around H1O B 505:

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

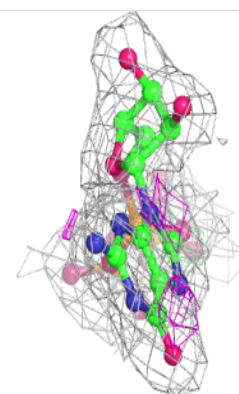
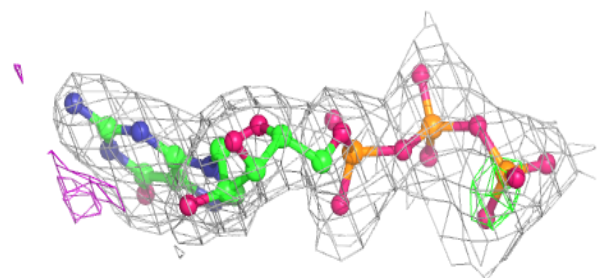
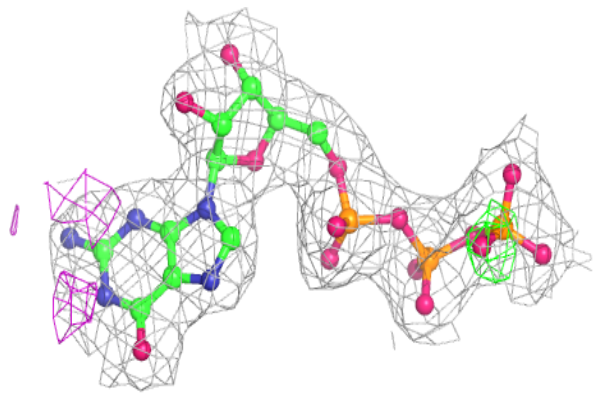


Electron density around GDP D 501:

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

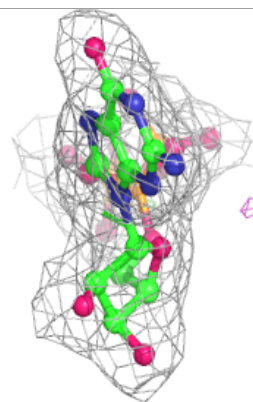
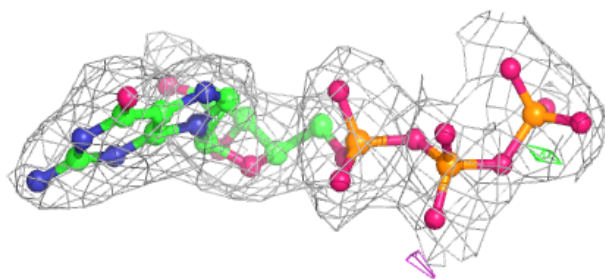
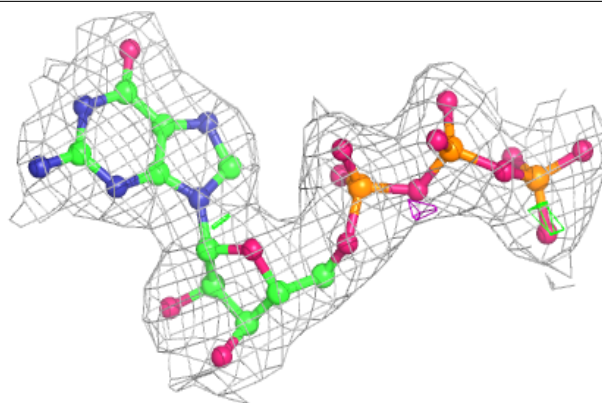
**Electron density around GTP C 501:**

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

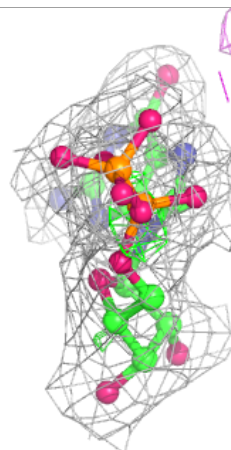
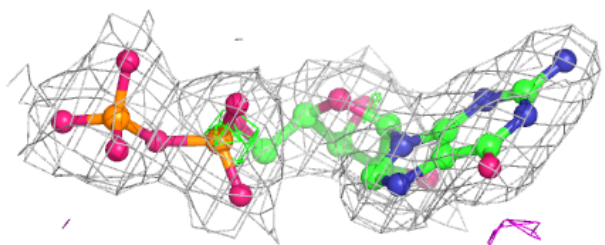
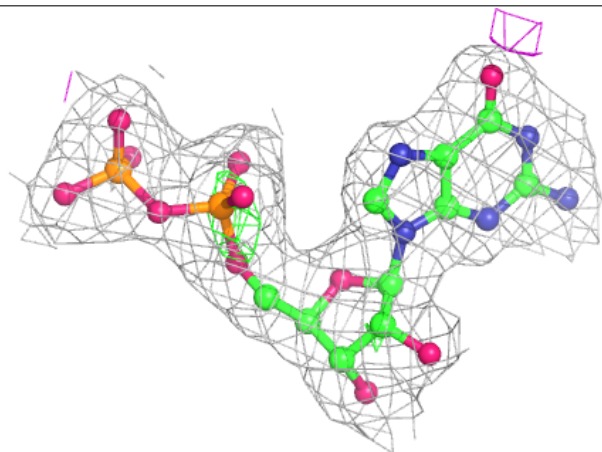


Electron density around GTP A 501:

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

**Electron density around GDP B 501:**

$2mF_o-DF_c$ (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.