



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 21, 2021 – 12:19 PM EDT

PDB ID : 5S59
Title : Tubulin-Z1324080698-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.60 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 : 2.20
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

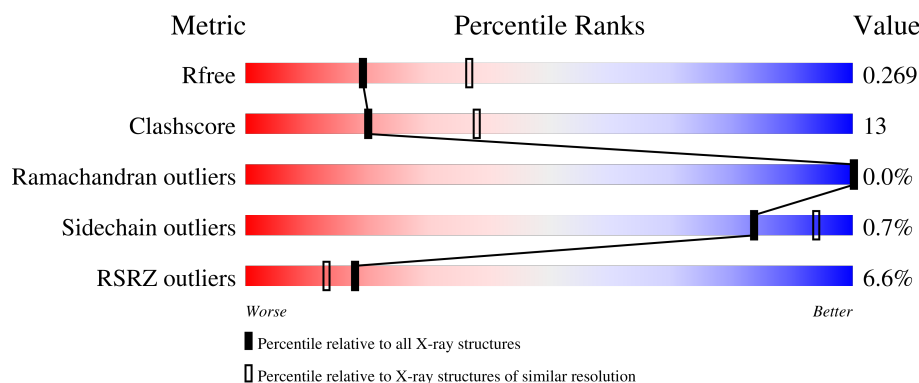
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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>4%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	C	451	<div> <div>72%</div> <div>25%</div> <div>.</div> </div>
2	B	445	<div> <div>2%</div> <div>72%</div> <div>23%</div> <div>.</div> </div>
2	D	445	<div> <div>5%</div> <div>64%</div> <div>31%</div> <div>.</div> </div>
3	E	143	<div> <div>10%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (21%), green (63%), yellow (27%), and grey (9%). The percentages are labeled above or below the corresponding segments.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17828 atoms, of which 24 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	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	1	1	0
			3359	2109	577	646	27			
2	D	426	Total	C	N	O	S	5	0	0
			3343	2098	570	648	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	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	0	0
			2864	1836	492	522	14			

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		

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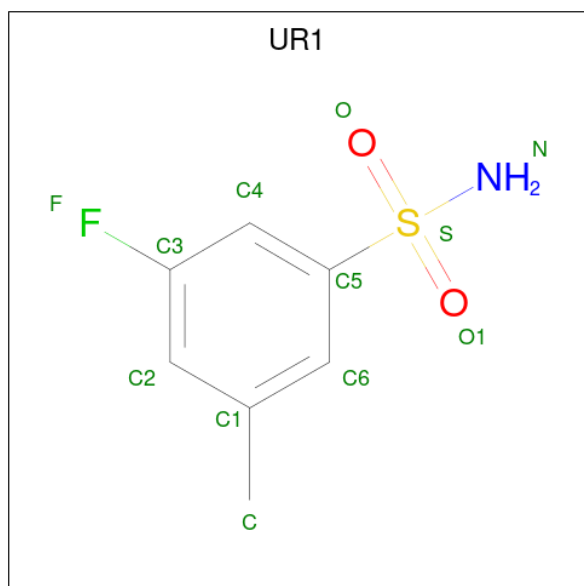
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- 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	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 3-fluoro-5-methylbenzene-1-sulfonamide (three-letter code: UR1) (formula: C₇H₈FNO₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	A	1	Total	C	F	H	N	O	S	0	0
			20	7	1	8	1	2	1		
8	C	1	Total	C	F	H	N	O	S	0	0
			20	7	1	8	1	2	1		
8	D	1	Total	C	F	H	N	O	S	0	0
			20	7	1	8	1	2	1		

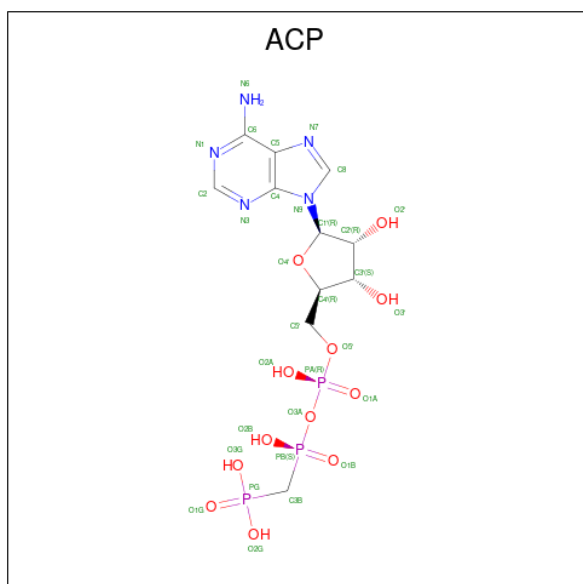
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- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group having a hydroxyl group and a carboxylate group. The structure is labeled with various atoms and bonds, including the 5' and 3' positions of the ribose sugar and the phosphate groups.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- MES
-
- The chemical structure of MES (3-(Trimethylsilyl)urea) is shown. It consists of a central urea group (C=O, N-H) where the nitrogen atom is substituted with a trimethylsilyl group (Si(CH₃)₃). The structure is labeled with atom names: O1 (oxygen), C2, C3, C4, C5, C6, C7, C8, S (sulfur), O2S, O1S, and O3S (oxygen). The nitrogen atom is labeled N4.

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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

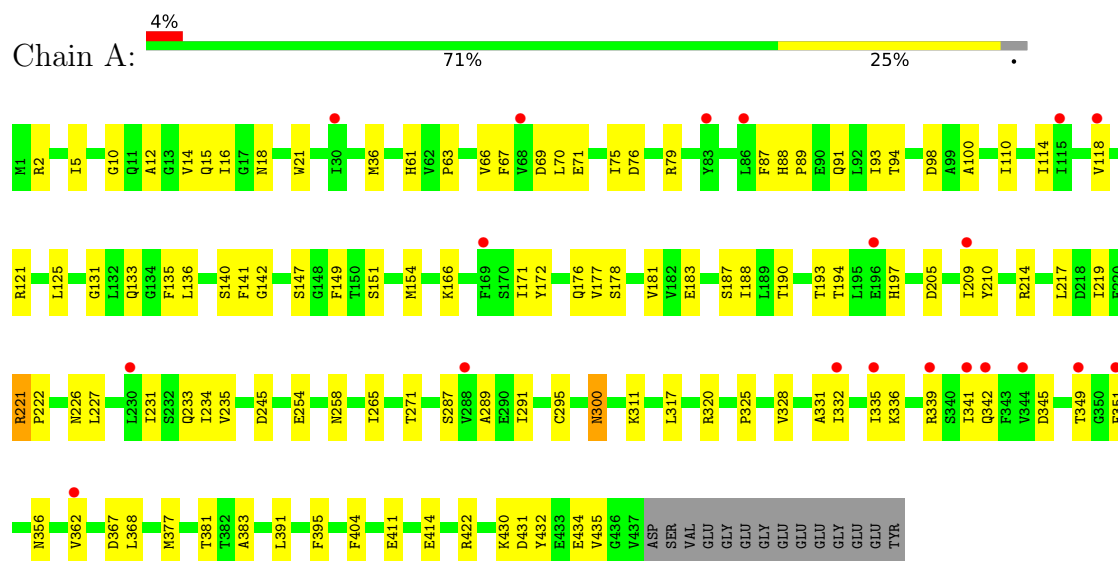
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	28	Total O 28 28	0	0
12	B	38	Total O 38 38	0	0
12	C	77	Total O 77 77	0	0
12	D	9	Total O 9 9	0	0
12	E	2	Total O 2 2	0	0
12	F	3	Total O 3 3	0	0

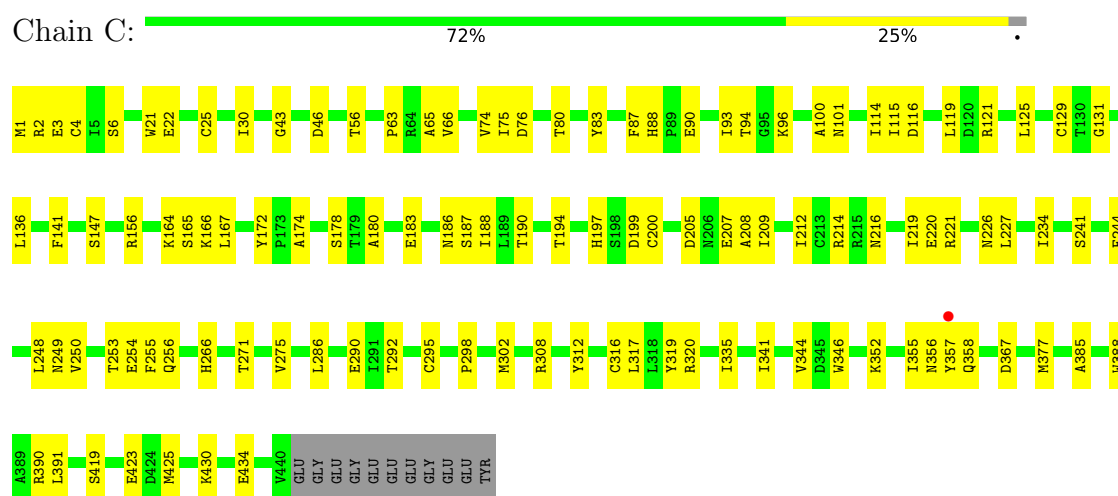
3 Residue-property plots

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

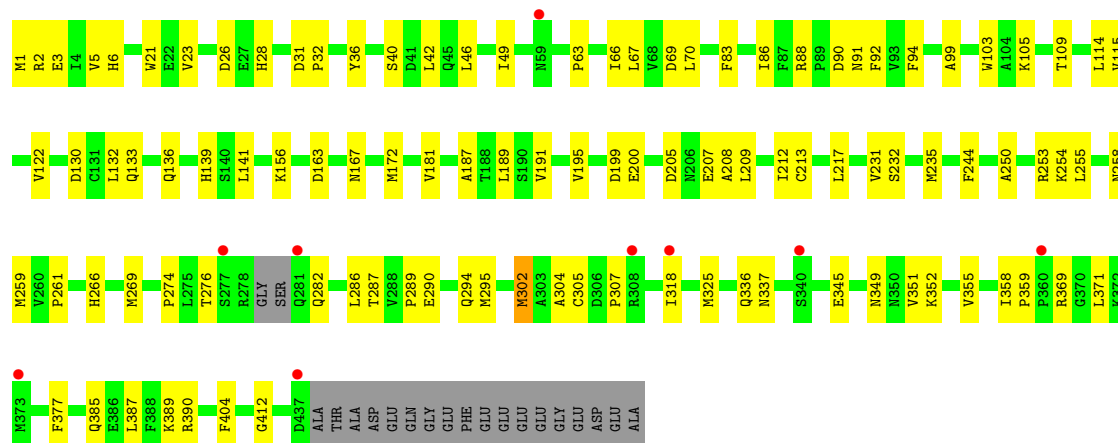


• Molecule 1: Tubulin alpha-1B chain

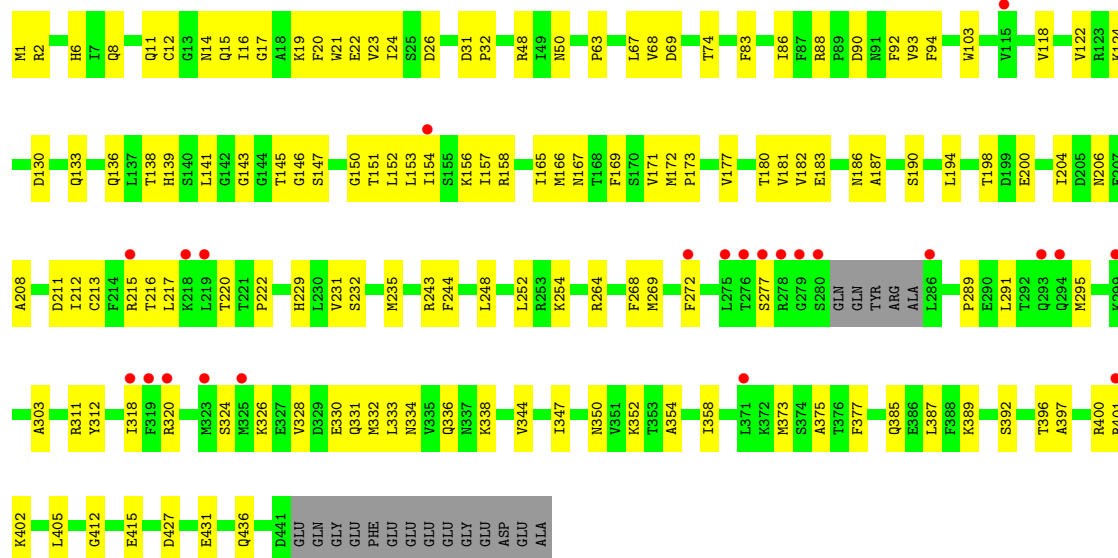


• Molecule 2: Tubulin beta-2B chain

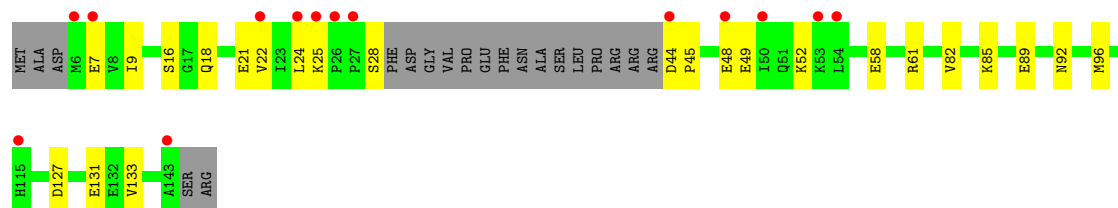




• Molecule 2: Tubulin beta-2B chain

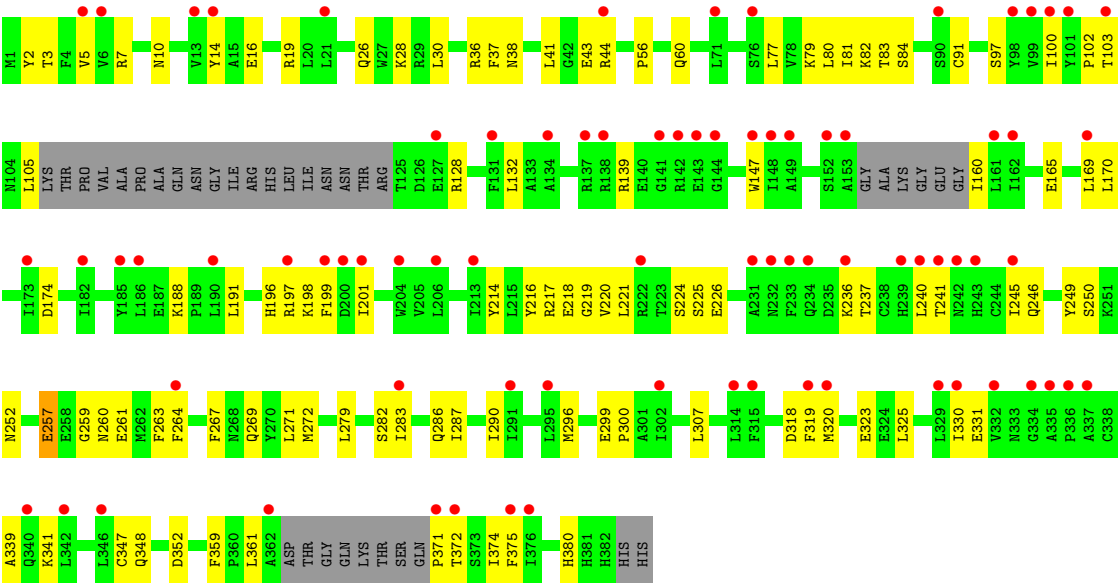


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 158.90Å 179.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.84 – 2.60 89.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (59.84-2.60) 99.3 (89.67-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.220 , 0.268 0.220 , 0.269	Depositor DCC
R_{free} test set	4548 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17828	wwPDB-VP
Average B, all atoms (Å ²)	96.0	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: MG, GDP, ACP, UR1, CA, GTP, MES

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	0.25	0/3494	0.42	0/4743
1	C	0.27	0/3521	0.42	0/4780
2	B	0.26	0/3433	0.41	0/4647
2	D	0.25	0/3416	0.41	0/4626
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2931	0.39	0/3961
All	All	0.25	0/17817	0.41	0/24113

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3330	94	0
1	C	3443	0	3352	78	0
2	B	3359	0	3235	78	0
2	D	3343	0	3222	101	0
3	E	1014	0	1029	22	0
4	F	2864	0	2828	87	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	12	8	0	0	0
8	C	12	8	0	0	0
8	D	12	8	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	2	0
10	B	12	0	12	1	0
11	F	31	0	14	3	0
12	A	28	0	0	4	0
12	B	38	0	0	1	0
12	C	77	0	0	2	0
12	D	9	0	0	2	0
12	E	2	0	0	0	0
12	F	3	0	0	0	0
All	All	17804	24	17070	435	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 13.

The worst 5 of 435 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)
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.28	0.99
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.49	0.95
4:F:269:GLN:HA	4:F:272:MET:HE2	1.49	0.92
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.57	0.85
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.59	0.83

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	435/451 (96%)	422 (97%)	13 (3%)	0	100	100
1	C	439/451 (97%)	428 (98%)	11 (2%)	0	100	100
2	B	422/445 (95%)	402 (95%)	19 (4%)	1 (0%)	47	71
2	D	422/445 (95%)	408 (97%)	14 (3%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	341/384 (89%)	328 (96%)	13 (4%)	0	100	100
All	All	2178/2319 (94%)	2105 (97%)	72 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	ALA

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	368/379 (97%)	364 (99%)	4 (1%)	73	88
1	C	372/379 (98%)	370 (100%)	2 (0%)	88	96
2	B	368/383 (96%)	366 (100%)	2 (0%)	88	96
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	92
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	313 (99%)	2 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1901/1993 (95%)	1888 (99%)	13 (1%)	84 94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	266	HIS
2	D	26	ASP
4	F	257	GLU
2	D	229	HIS
4	F	91	CYS

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	133	GLN
2	B	258	ASN
3	E	18	GLN
4	F	180	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.77	6 (18%)
9	GDP	D	501	6	24,30,30	1.16	2 (8%)	31,47,47	1.88	7 (22%)
5	GTP	C	501	6	26,34,34	1.01	2 (7%)	33,54,54	1.68	6 (18%)
11	ACP	F	401	6	27,33,33	1.40	5 (18%)	32,52,52	1.52	4 (12%)
10	MES	B	504	-	12,12,12	2.26	1 (8%)	14,16,16	1.99	6 (42%)
8	UR1	A	504	-	12,12,12	0.53	0	18,18,18	1.19	2 (11%)
8	UR1	C	504	-	12,12,12	0.46	0	18,18,18	1.08	1 (5%)
9	GDP	B	501	6	24,30,30	1.17	2 (8%)	31,47,47	2.00	8 (25%)
8	UR1	D	503	-	12,12,12	0.52	0	18,18,18	1.30	3 (16%)

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	GTP	A	501	6	-	6/18/38/38	0/3/3/3
9	GDP	D	501	6	-	2/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	UR1	A	504	-	-	4/6/6/6	0/1/1/1
8	UR1	C	504	-	-	4/6/6/6	0/1/1/1
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	UR1	D	503	-	-	4/6/6/6	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.54	1.66	1.77
9	B	501	GDP	C6-C5	4.12	1.48	1.41
9	D	501	GDP	C6-C5	4.03	1.48	1.41
5	C	501	GTP	C6-N1	3.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PG-O3G	2.94	1.61	1.54

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.25	120.22	127.22
5	C	501	GTP	N3-C2-N1	-5.03	120.51	127.22
9	B	501	GDP	C2-N3-C4	4.97	121.03	115.36
9	D	501	GDP	C2-N3-C4	4.75	120.79	115.36
11	F	401	ACP	PA-O3A-PB	-4.30	118.93	132.56

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

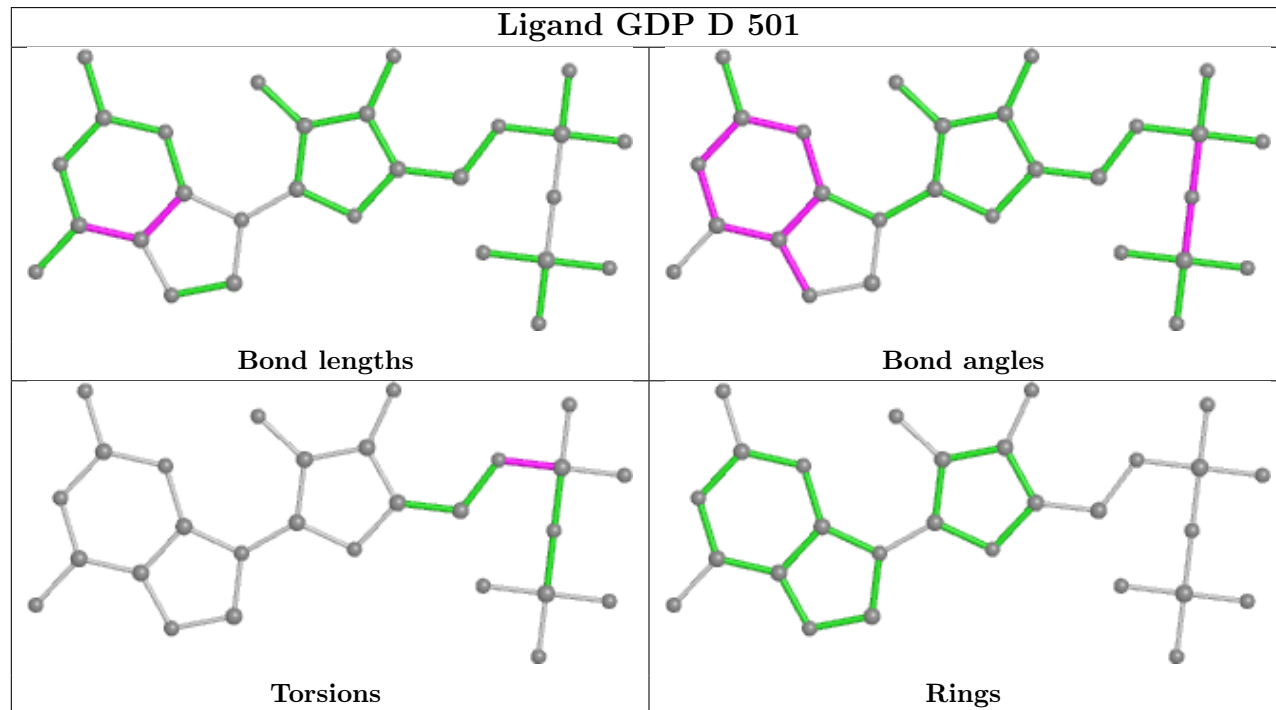
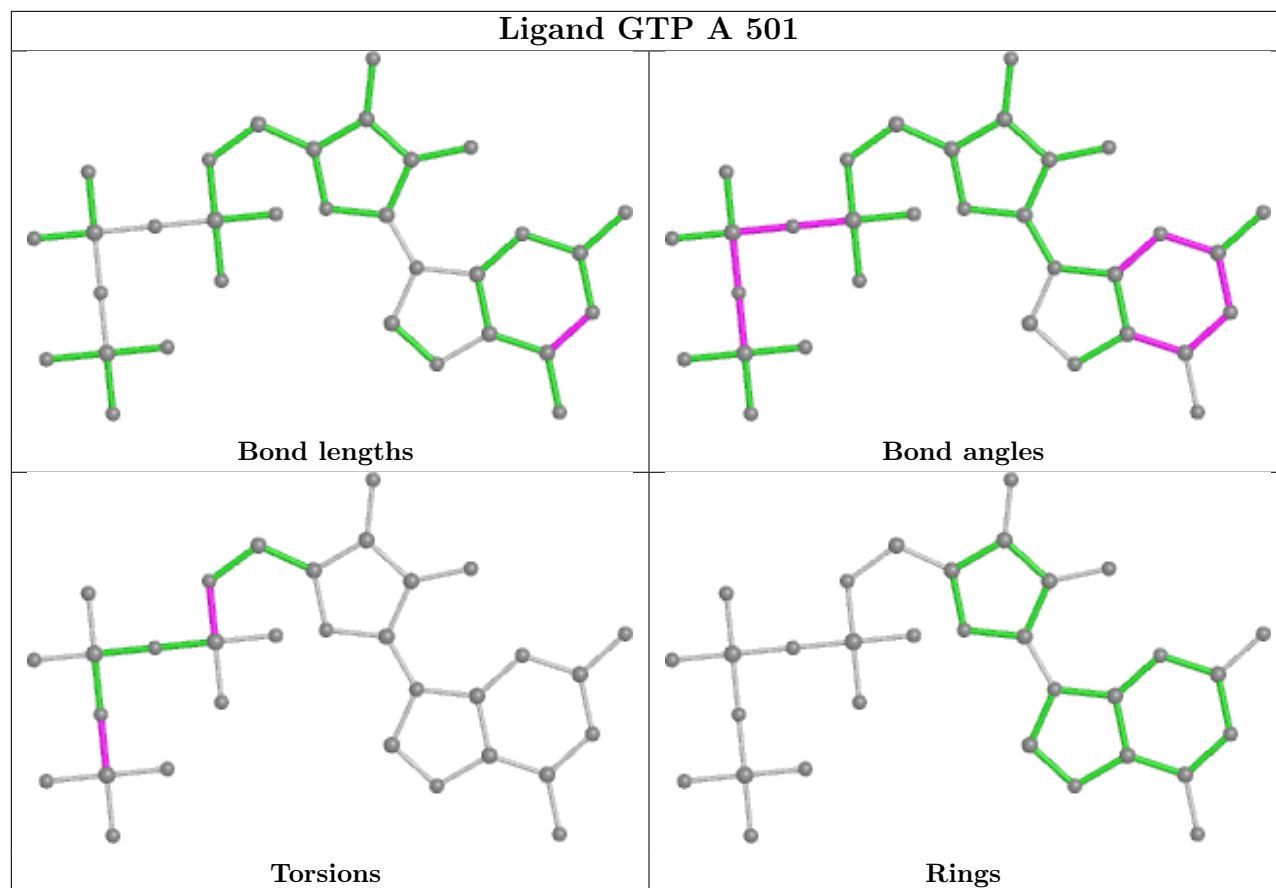
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

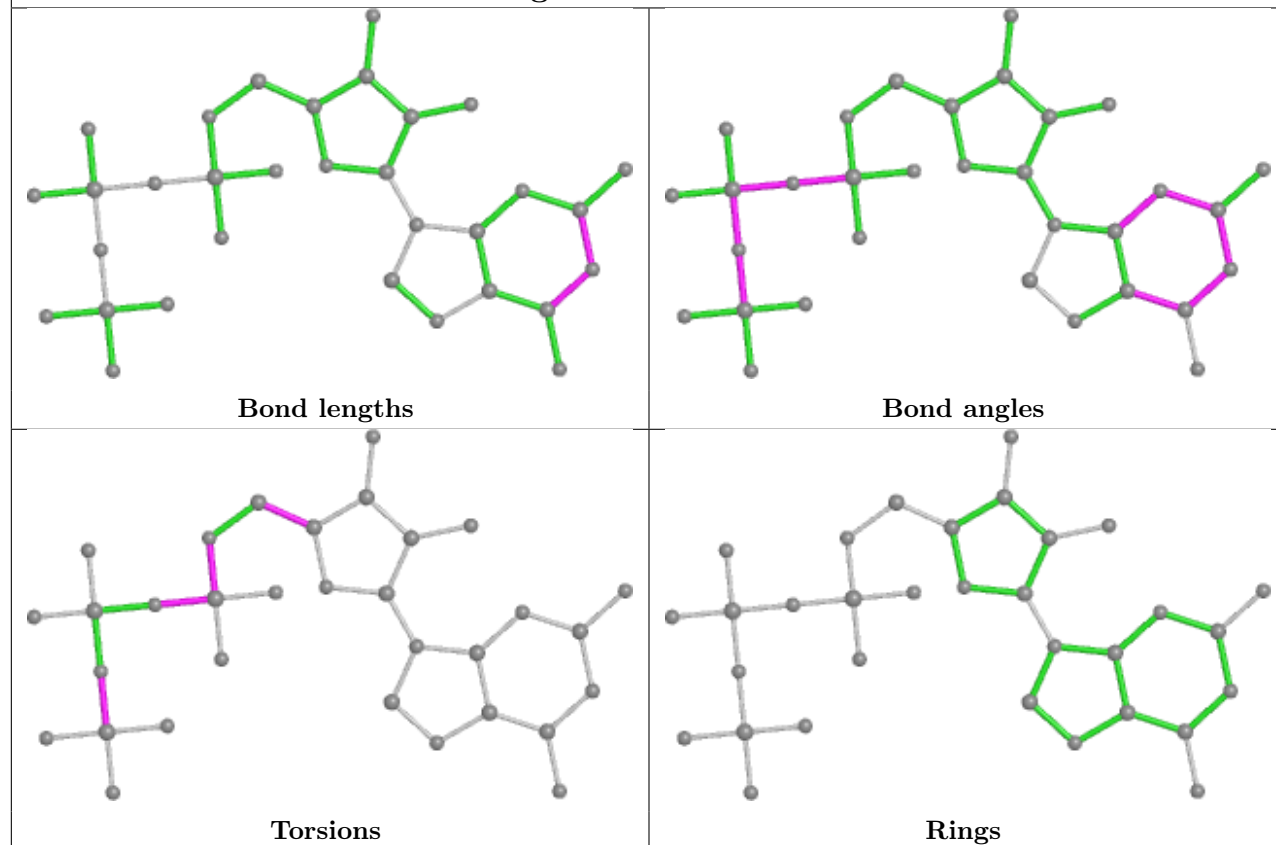
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	2	0
9	D	501	GDP	2	0
11	F	401	ACP	3	0
10	B	504	MES	1	0

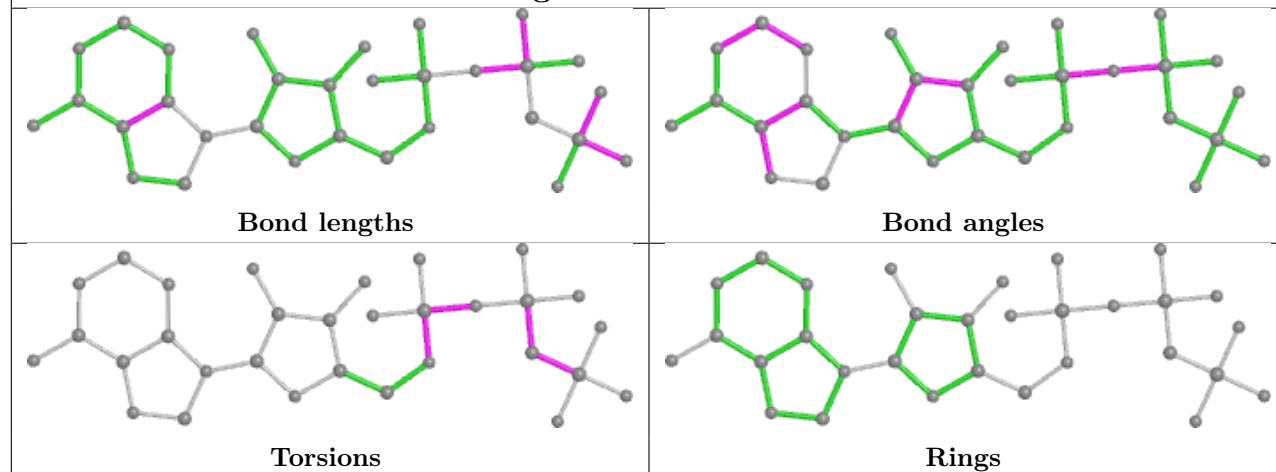
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

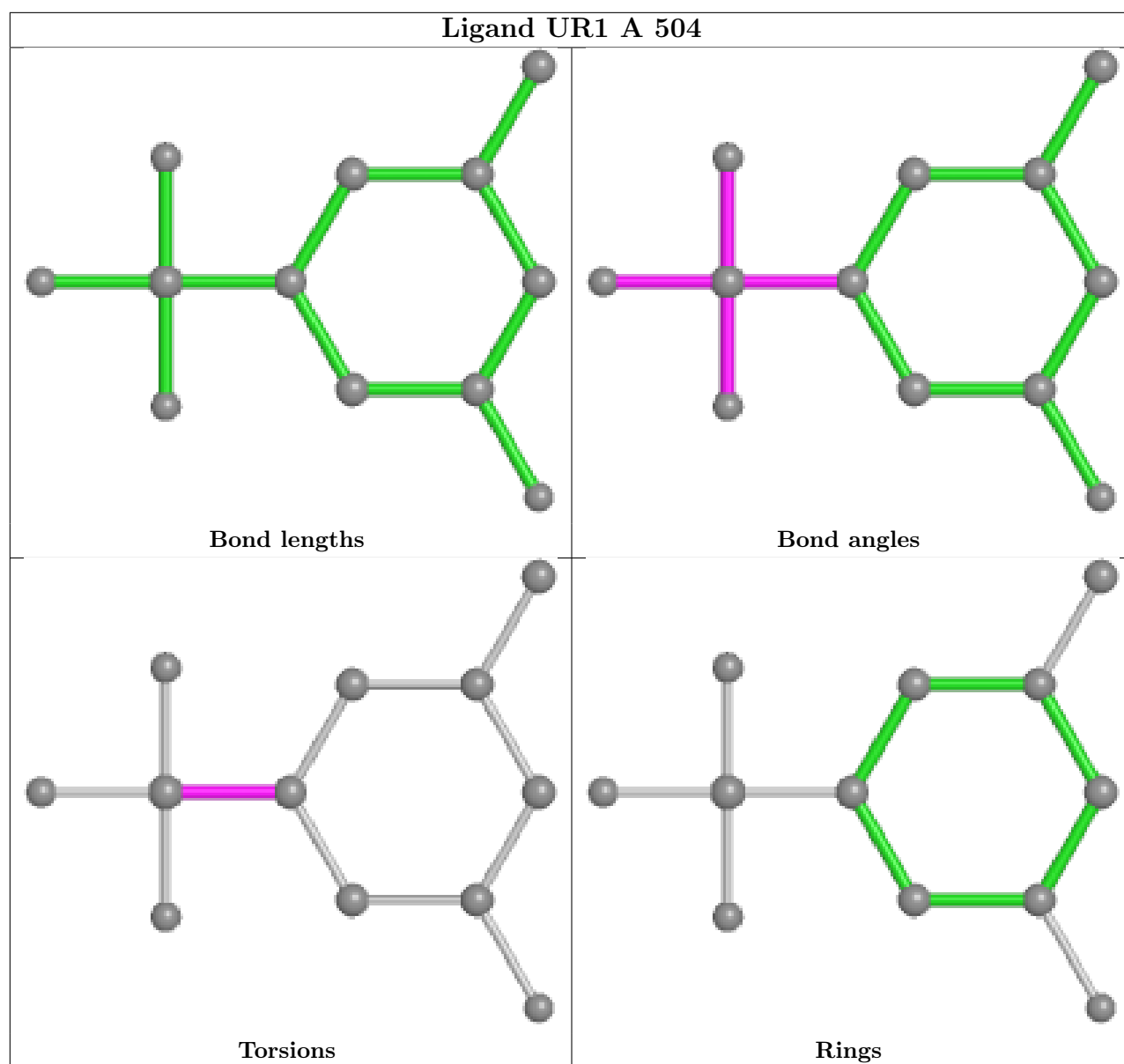


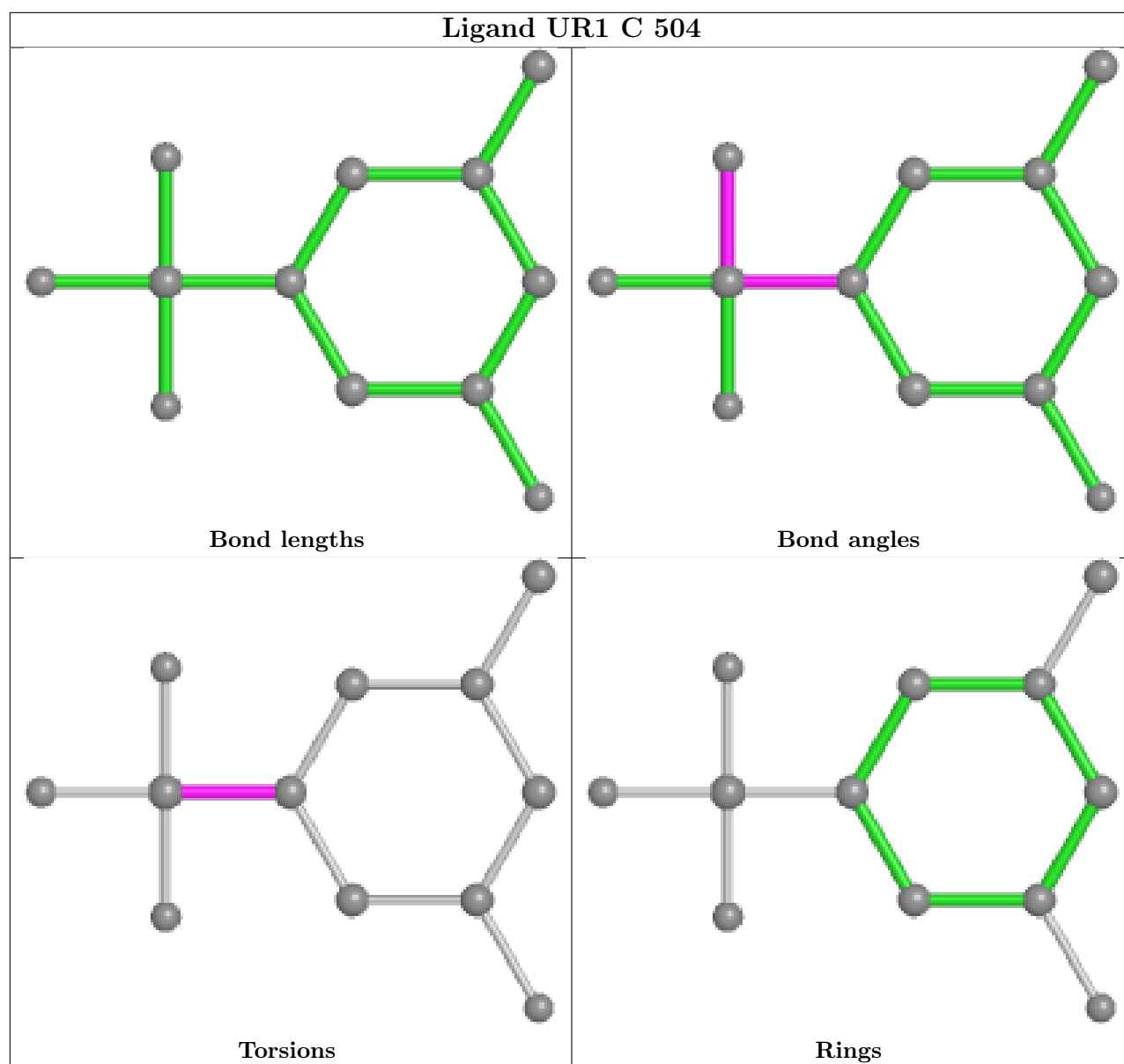
Ligand GTP C 501

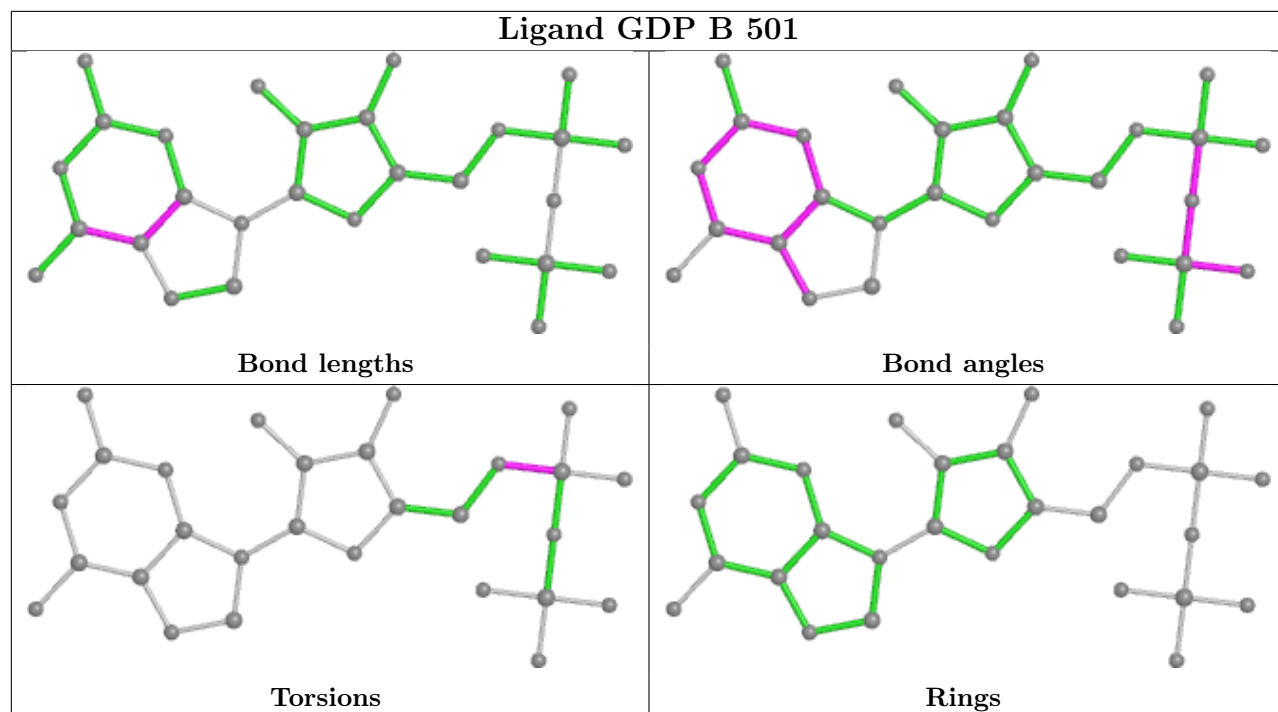


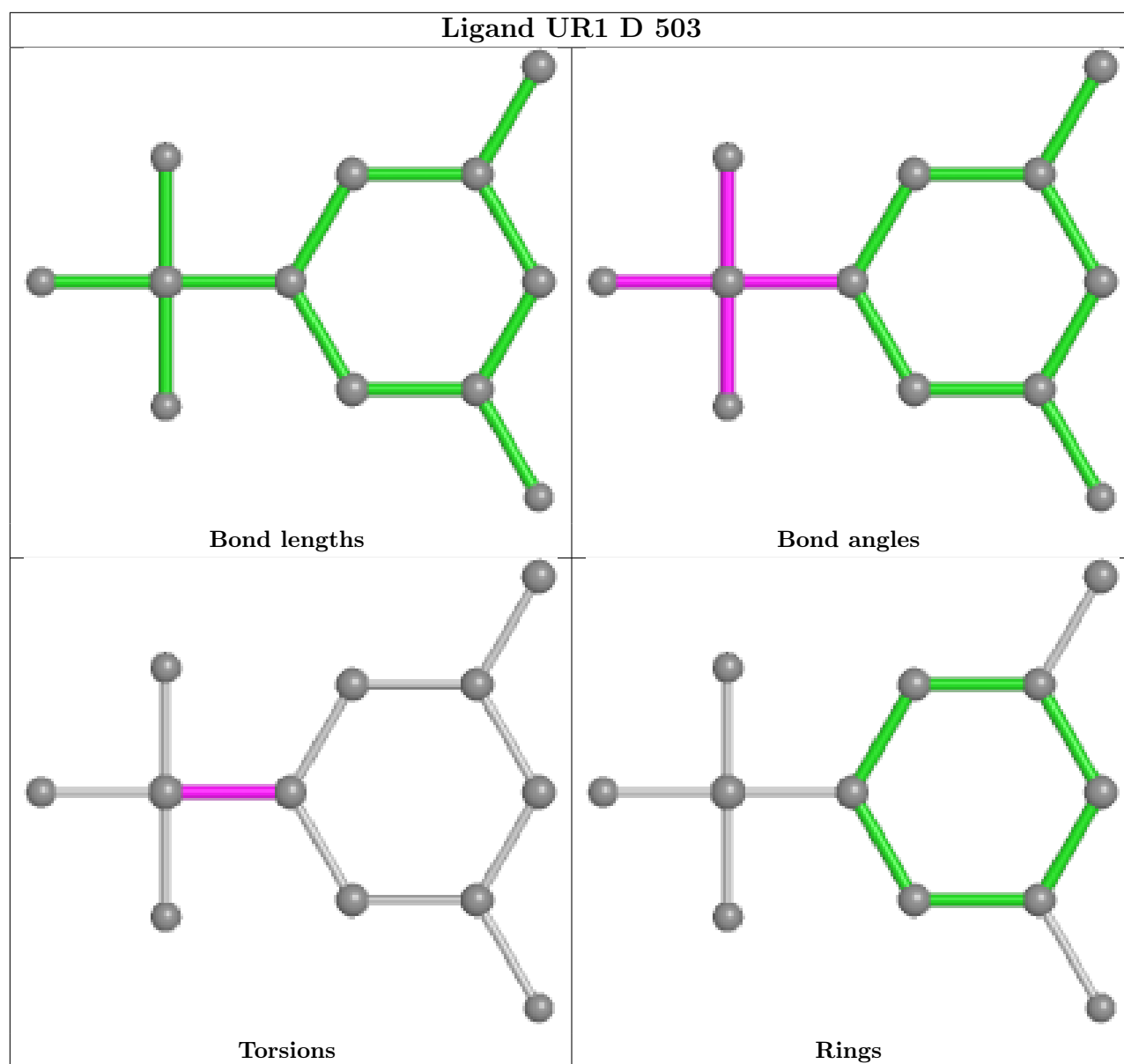
Ligand ACP F 401











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%)	0.45	20 (4%) 32 26	66, 87, 123, 200	0
1	C	440/451 (97%)	0.37	1 (0%) 95 95	59, 74, 105, 134	0
2	B	425/445 (95%)	0.41	9 (2%) 63 58	62, 84, 128, 163	2 (0%)
2	D	426/445 (95%)	0.35	23 (5%) 25 20	71, 97, 134, 174	4 (0%)
3	E	123/143 (86%)	0.65	14 (11%) 5 3	77, 100, 140, 182	0
4	F	349/384 (90%)	1.03	79 (22%) 0 0	82, 122, 178, 208	0
All	All	2200/2319 (94%)	0.51	146 (6%) 18 13	59, 91, 146, 208	6 (0%)

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	276	THR	7.4
4	F	240	LEU	6.6
4	F	142	ARG	6.2
2	D	277	SER	5.5
3	E	6	MET	5.4

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 ⓘ

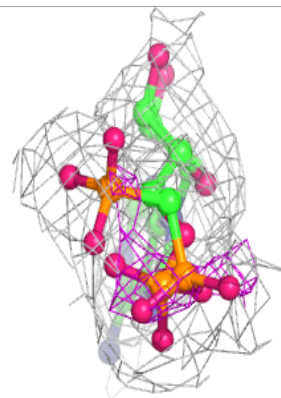
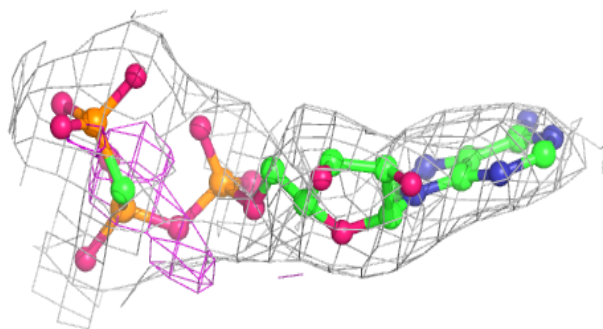
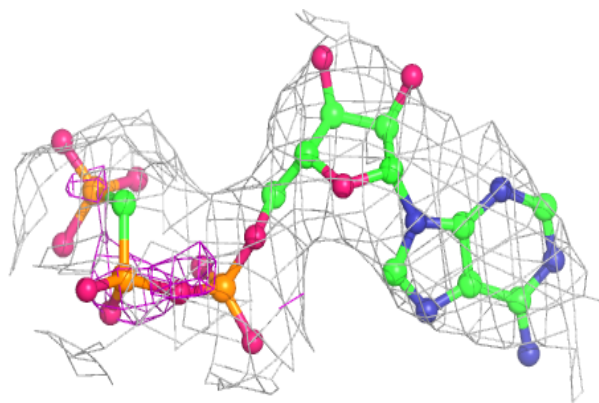
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	E	201	1/1	0.72	0.15	108,108,108,108	0
7	CA	B	503	1/1	0.73	0.17	131,131,131,131	0
11	ACP	F	401	31/31	0.88	0.22	118,128,139,141	0
6	MG	D	502	1/1	0.90	0.18	91,91,91,91	0
8	UR1	D	503	12/12	0.93	0.22	76,80,96,96	20
7	CA	A	503	1/1	0.93	0.11	126,126,126,126	0
9	GDP	D	501	28/28	0.94	0.17	87,90,99,100	0
10	MES	B	504	12/12	0.94	0.16	92,102,114,120	0
6	MG	B	502	1/1	0.94	0.15	75,75,75,75	0
8	UR1	C	504	12/12	0.95	0.21	61,73,86,88	20
8	UR1	A	504	12/12	0.96	0.30	72,80,96,96	20
7	CA	C	503	1/1	0.96	0.17	96,96,96,96	0
6	MG	A	502	1/1	0.97	0.17	74,74,74,74	0
6	MG	F	402	1/1	0.97	0.14	124,124,124,124	0
5	GTP	A	501	32/32	0.97	0.16	64,69,74,78	0
6	MG	C	502	1/1	0.97	0.17	68,68,68,68	0
9	GDP	B	501	28/28	0.98	0.19	57,68,73,78	0
5	GTP	C	501	32/32	0.98	0.20	58,65,76,80	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.

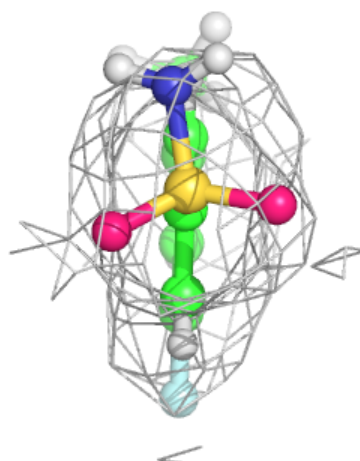
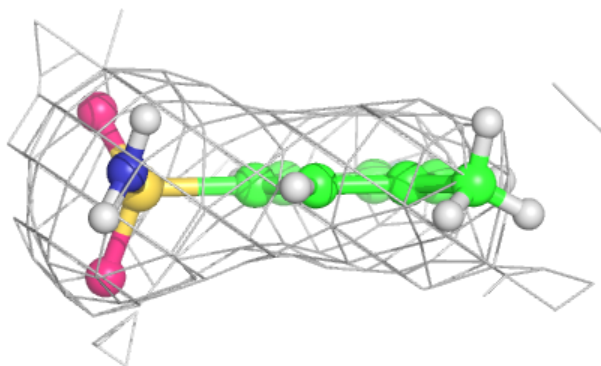
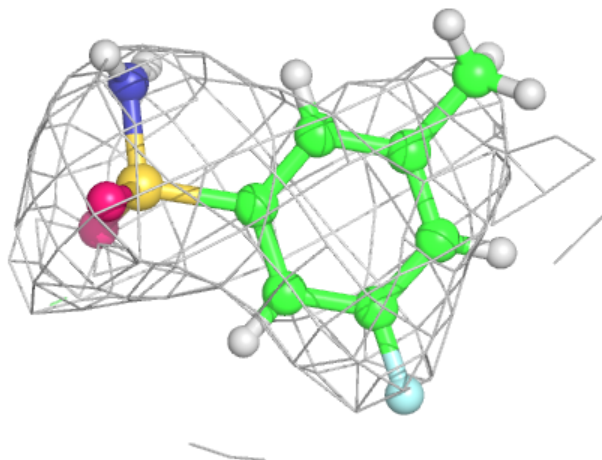
Electron density around ACP F 401:

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



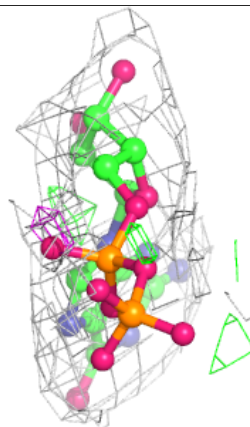
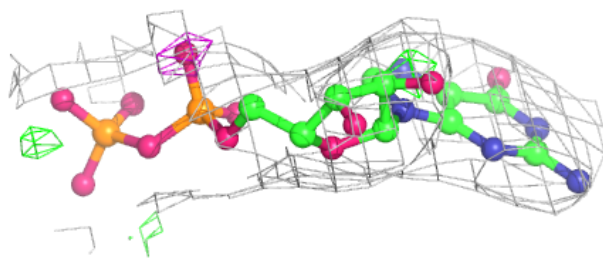
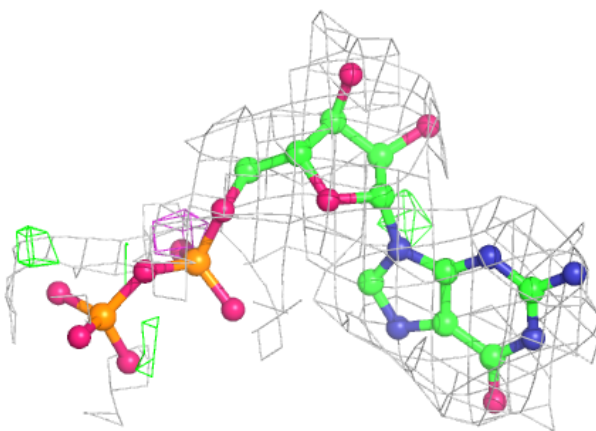
Electron density around UR1 D 503:

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



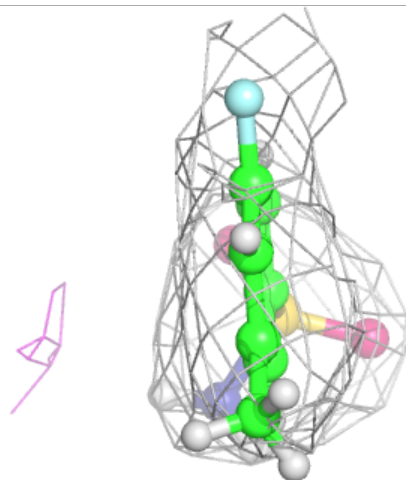
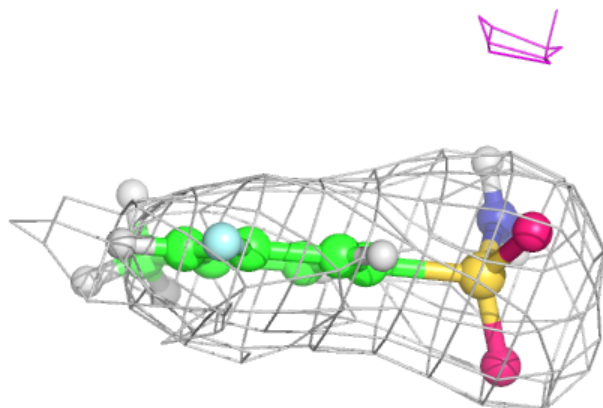
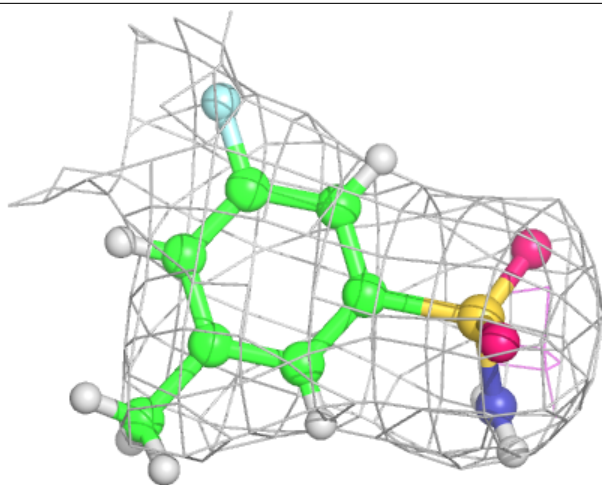
Electron density around GDP D 501:

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



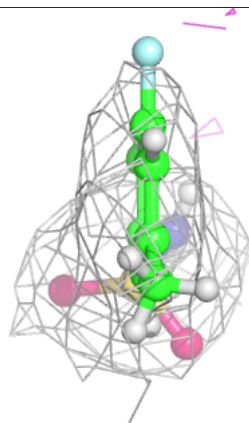
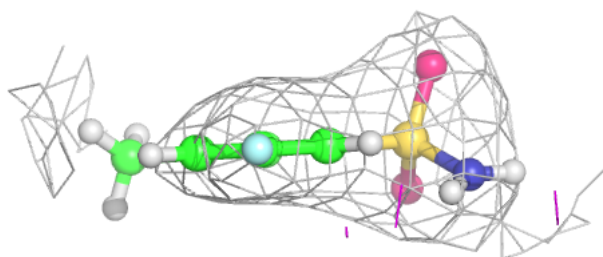
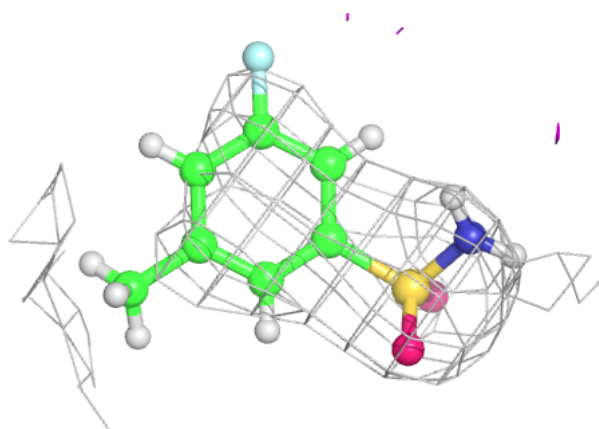
Electron density around UR1 C 504:

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



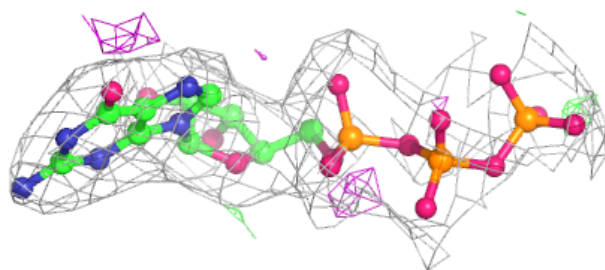
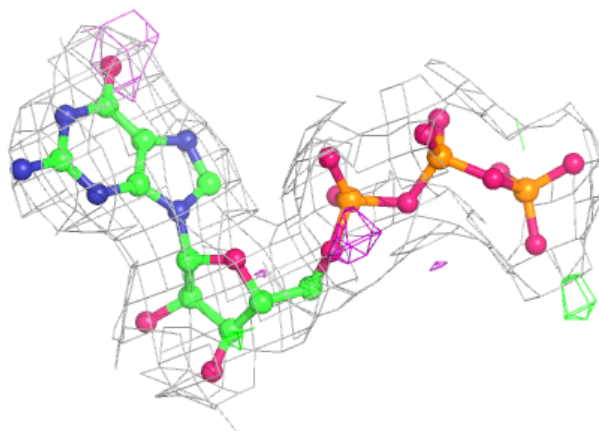
Electron density around UR1 A 504:

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



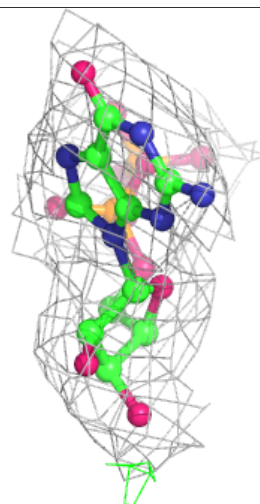
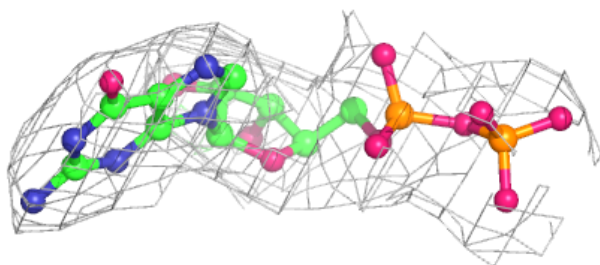
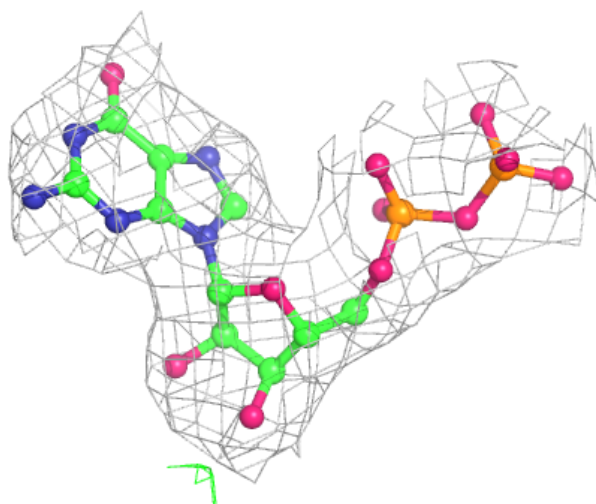
Electron density around GTP A 501:

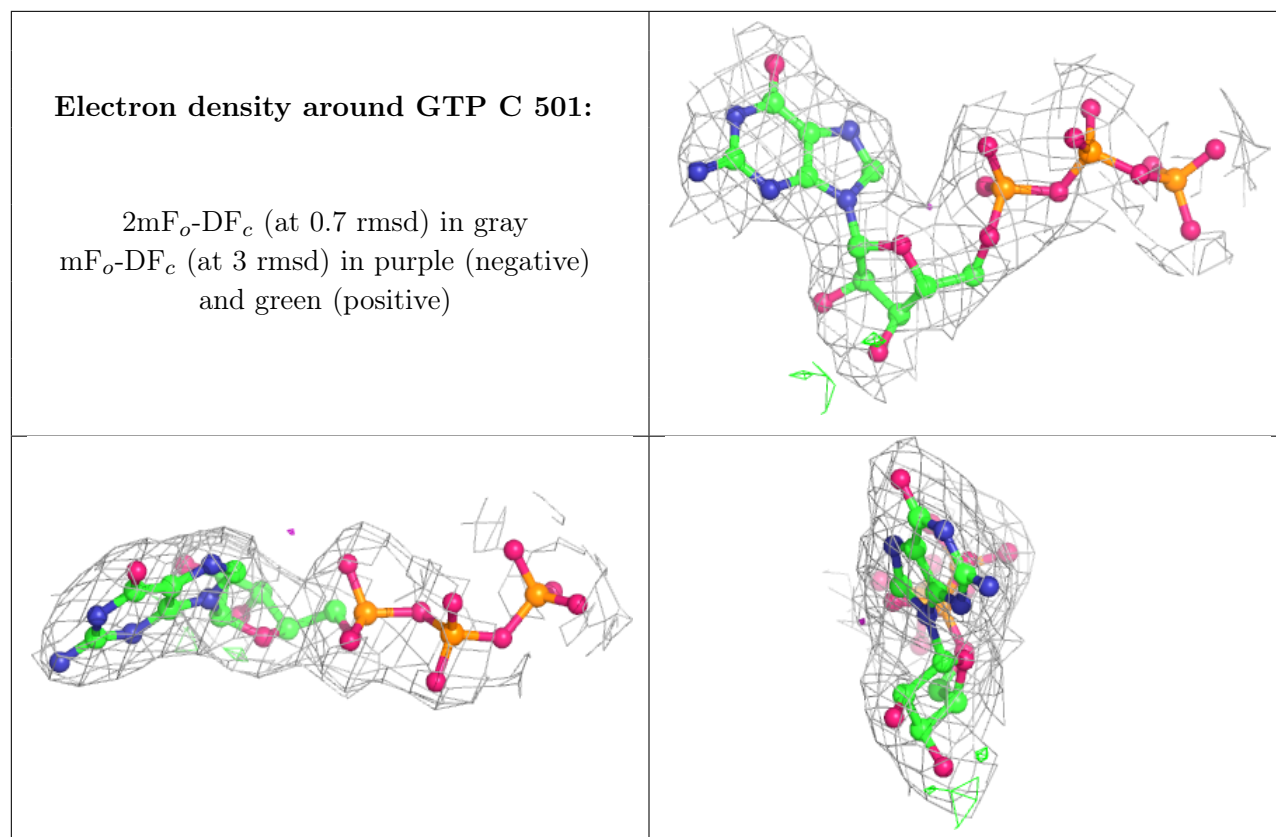
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.