



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:15 AM UTC

PDB ID : 7EMJ / pdb_00007emj
Title : Crystal structure of T2R-TTL-Barbigerone complex
Authors : Yang, J.H.; Yan, W.
Deposited on : 2021-04-14
Resolution : 2.33 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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

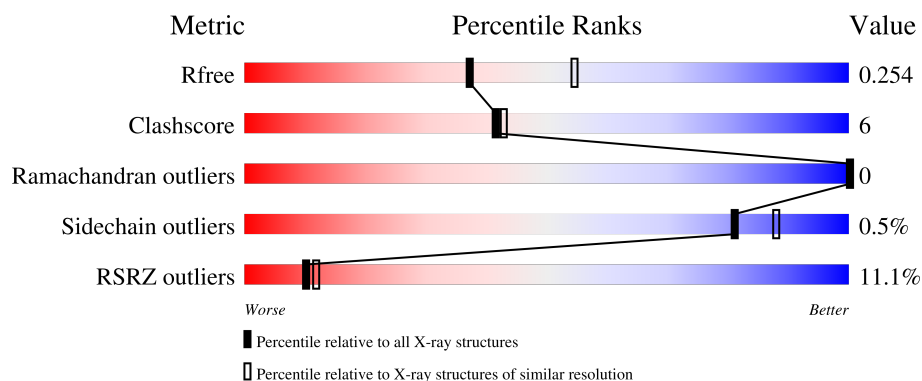
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	
1	C	451	
2	B	445	
2	D	445	
3	E	189	

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Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 35500 atoms, of which 17027 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	438	Total	C	H	N	O	S	0	8	0
			6817	2187	3361	586	658	25			
1	C	440	Total	C	H	N	O	S	0	9	0
			6826	2189	3365	586	662	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	426	Total	C	H	N	O	S	0	1	0
			6528	2101	3184	573	644	26			
2	D	422	Total	C	H	N	O	S	0	1	0
			6481	2084	3167	563	641	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	5	0
			2079	637	1044	188	205	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	350	Total	C	H	N	O	S	0	1	0
			5682	1834	2818	490	525	15			

There are 6 discrepancies between the modelled and reference sequences:

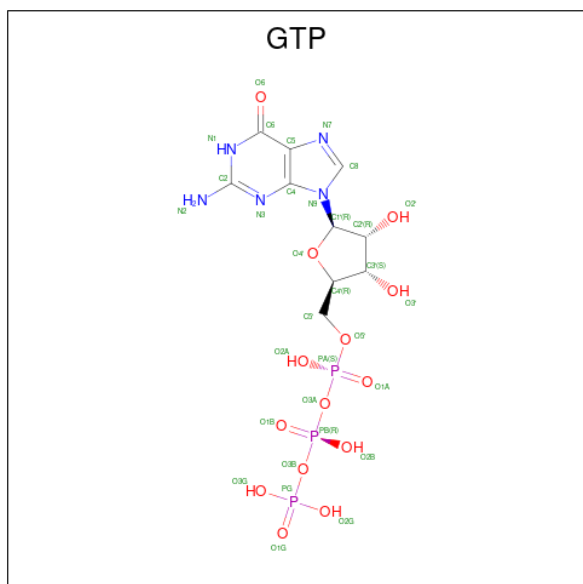
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		

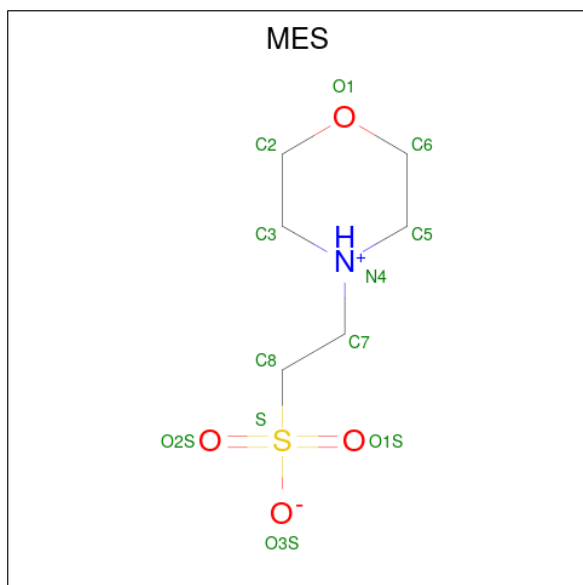
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

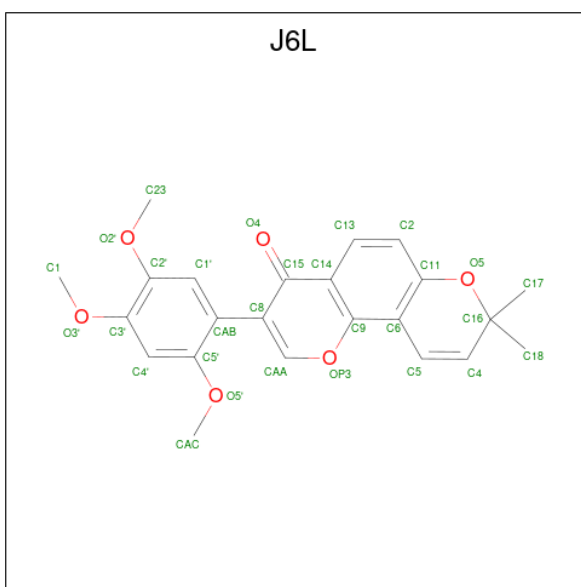
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	Ca 2	2	0
7	B	2	Total 2	Ca 2	2	0
7	C	1	Total 1	Ca 1	1	0
7	D	1	Total 1	Ca 1	1	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



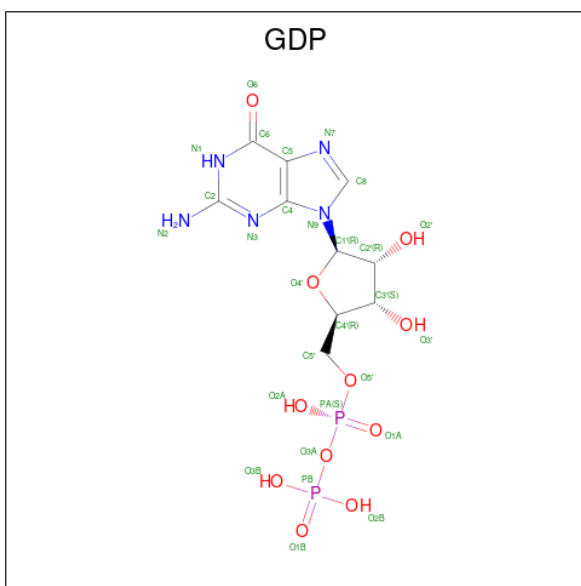
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	24	0
			24	6	12	1	4	1		

- Molecule 9 is 8,8-dimethyl-3-(2,4,5-trimethoxyphenyl)pyrano[2,3-f]chromen-4-one (CCD ID: J6L) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



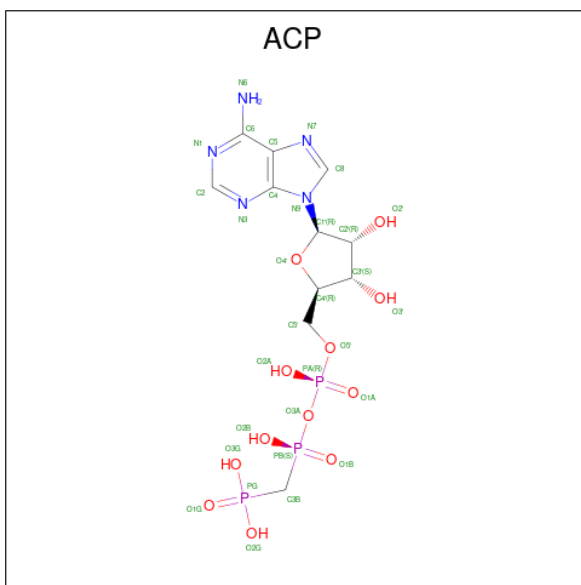
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			51	23	22	6		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	B	1	Total	C	H	N	O	P	38	0
			38	10	10	5	11	2		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		

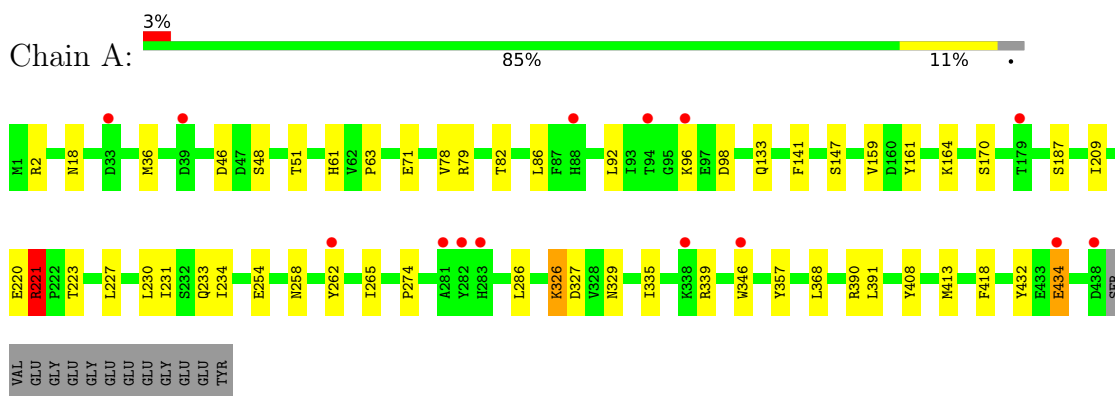
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	170	Total O 170 170	0	0
12	B	139	Total O 139 139	0	0
12	C	277	Total O 277 277	0	0
12	D	101	Total O 101 101	0	0
12	E	41	Total O 41 41	0	0
12	F	64	Total O 64 64	0	0

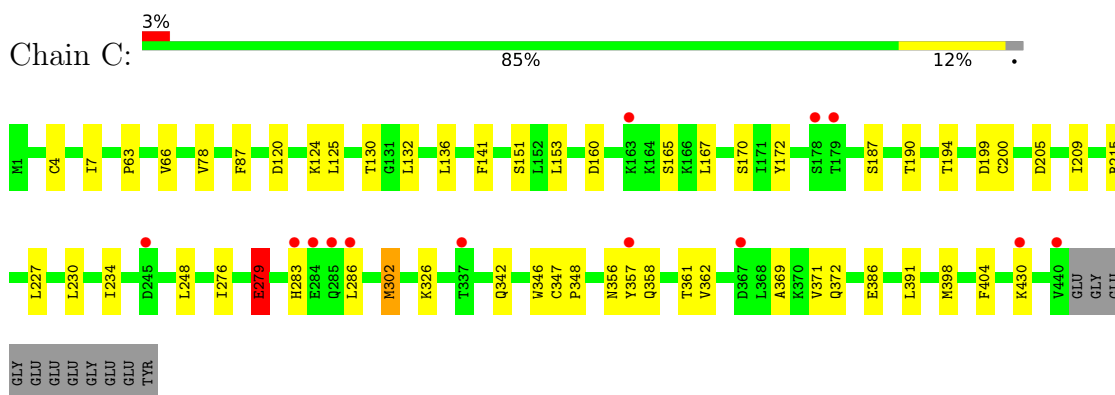
3 Residue-property plots

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.

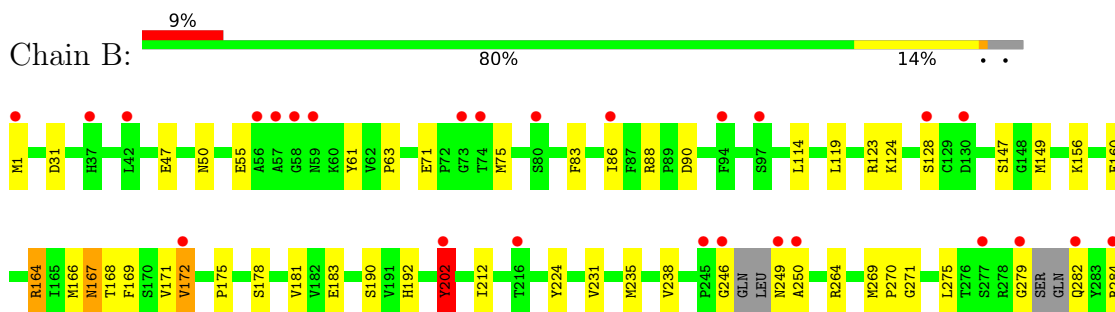
• Molecule 1: Tubulin alpha-1B chain

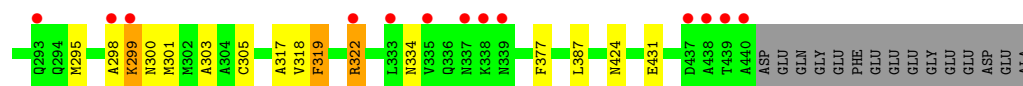


• Molecule 1: Tubulin alpha-1B chain

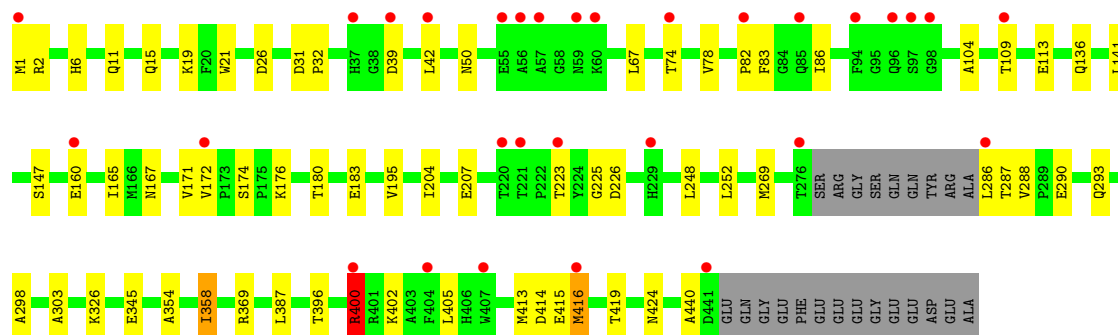
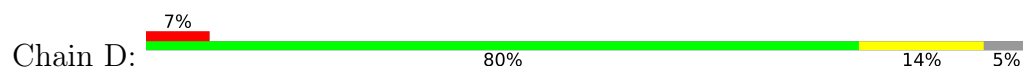


• Molecule 2: Tubulin beta chain

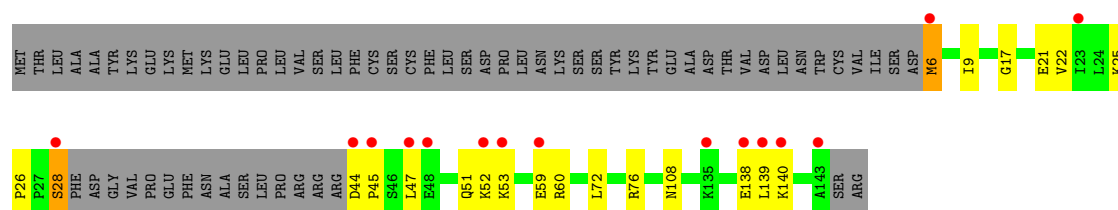




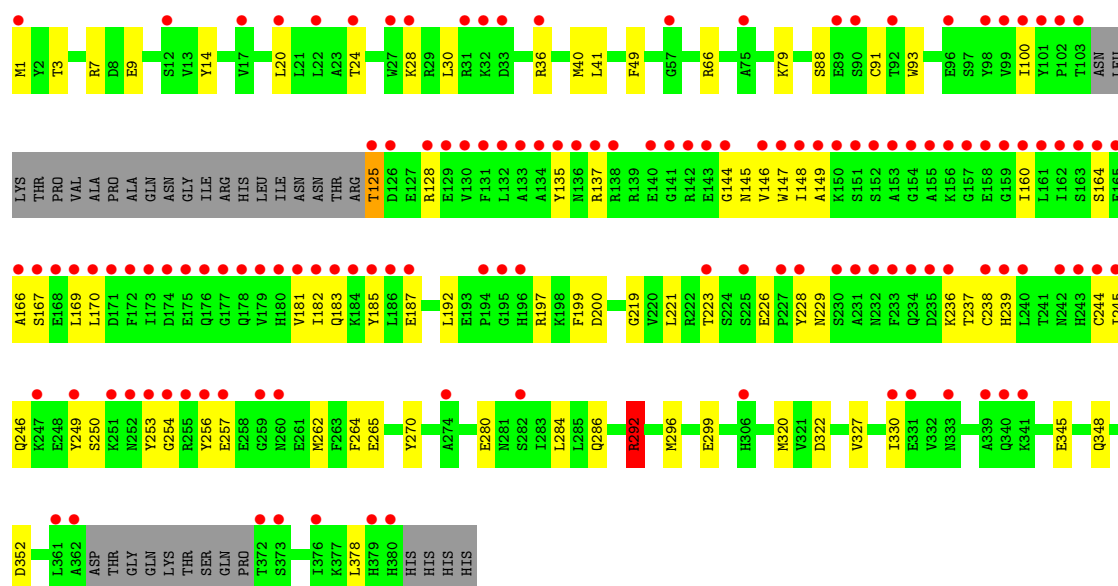
• Molecule 2: Tubulin beta chain



• 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	105.03Å 157.25Å 180.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 2.33 46.90 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.90-2.33) 99.2 (46.90-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.241 (Not available) , 0.254	Depositor DCC
R_{free} test set	6360 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35500	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, J6L, MES, MG, GTP, CA, ACP

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	0.38	3/3565 (0.1%)	0.61	9/4840 (0.2%)
1	C	0.50	8/3578 (0.2%)	0.58	4/4859 (0.1%)
2	B	0.79	22/3421 (0.6%)	0.70	8/4632 (0.2%)
2	D	0.57	10/3390 (0.3%)	0.80	10/4594 (0.2%)
3	E	0.69	2/1064 (0.2%)	0.73	2/1412 (0.1%)
4	F	0.41	1/2929 (0.0%)	0.65	6/3956 (0.2%)
All	All	0.56	46/17947 (0.3%)	0.67	39/24293 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
2	B	0	1
2	D	0	1
4	F	0	2
All	All	0	7

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	293	GLN	C-O	-13.83	1.07	1.24
2	B	183	GLU	C-O	-10.06	1.14	1.24
2	B	172	VAL	C-O	-9.86	1.11	1.24
2	B	171	VAL	C-O	-8.88	1.14	1.24
2	D	358	ILE	N-CA	8.61	1.52	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	ARG	NE-CZ-NH2	20.20	137.38	119.20
2	D	400	ARG	NE-CZ-NH1	-15.35	106.15	121.50
1	A	434	GLU	CG-CD-OE1	14.53	151.82	118.40
2	D	400	ARG	CB-CG-CD	11.70	138.20	111.30
1	A	434	GLU	CG-CD-OE2	-11.20	92.64	118.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	GLU	Sidechain
2	B	322	ARG	Sidechain
1	C	279	GLU	Sidechain
1	C	283	HIS	Mainchain
2	D	400	ARG	Sidechain

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	3456	3361	3342	38	0
1	C	3461	3365	3336	31	0
2	B	3344	3184	3221	42	2
2	D	3314	3167	3197	40	3
3	E	1035	1044	1023	14	1
4	F	2864	2818	2831	61	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	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	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	12	12	12	0	0
9	B	29	22	0	3	0
10	B	28	10	12	0	0
11	F	31	14	14	0	0
12	A	170	0	0	3	0
12	B	139	0	0	6	0
12	C	277	0	0	6	0
12	D	101	0	0	2	0
12	E	41	0	0	3	0
12	F	64	0	0	7	0
All	All	18473	17027	17024	221	3

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 221 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)
2:B:167:ASN:HB3	9:B:505:J6L:C1	1.93	0.98
2:B:167:ASN:CB	9:B:505:J6L:C1	2.59	0.81
4:F:125:THR:OG1	12:F:501:HOH:O	2.04	0.75
2:B:202:TYR:CZ	2:B:270:PRO:HB3	2.21	0.75
4:F:345:GLU:O	12:F:502:HOH:O	2.09	0.69

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:NH2	2:D:160:GLU:OE2[4_455]	1.68	0.52
2:B:284:ARG:HH22	2:D:160:GLU:OE2[4_455]	1.25	0.35
2:D:39:ASP:OD2	3:E:59:GLU:OE2[4_455]	2.11	0.09

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	444/451 (98%)	435 (98%)	9 (2%)	0	100	100
1	C	447/451 (99%)	435 (97%)	12 (3%)	0	100	100
2	B	421/445 (95%)	411 (98%)	10 (2%)	0	100	100
2	D	419/445 (94%)	410 (98%)	9 (2%)	0	100	100
3	E	124/189 (66%)	124 (100%)	0	0	100	100
4	F	345/384 (90%)	333 (96%)	12 (4%)	0	100	100
All	All	2200/2365 (93%)	2148 (98%)	52 (2%)	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	377/379 (100%)	376 (100%)	1 (0%)	86	91
1	C	380/379 (100%)	380 (100%)	0	100	100
2	B	365/381 (96%)	363 (100%)	2 (0%)	81	88
2	D	364/381 (96%)	364 (100%)	0	100	100
3	E	115/171 (67%)	111 (96%)	4 (4%)	32	41
4	F	313/342 (92%)	311 (99%)	2 (1%)	78	86
All	All	1914/2033 (94%)	1905 (100%)	9 (0%)	81	88

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	125	THR
4	F	183	GLN
3	E	6	MET
3	E	28	SER
3	E	52	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	336	GLN
3	E	90	ASN
4	F	333	ASN
4	F	232	ASN
2	B	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 11 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	$\# Z > 2$
5	GTP	A	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
11	ACP	F	401	6	31,33,33	1.59	8 (25%)	47,52,52	1.90	11 (23%)
10	GDP	B	506	6	29,30,30	1.22	2 (6%)	45,47,47	1.97	7 (15%)
5	GTP	D	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
5	GTP	C	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.61	8 (16%)
8	MES	B	502	-	12,12,12	2.29	1 (8%)	15,16,16	1.92	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	J6L	B	505	-	32,32,32	4.07	13 (40%)	46,48,48	3.68	23 (50%)

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	-	8/22/38/38	0/3/3/3
11	ACP	F	401	6	-	2/19/38/38	0/3/3/3
10	GDP	B	506	6	-	3/16/32/32	0/3/3/3
5	GTP	D	501	6	-	7/22/38/38	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
8	MES	B	502	-	-	5/6/14/14	0/1/1/1
9	J6L	B	505	-	-	4/10/21/21	0/4/4/4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	505	J6L	OP3-C9	-15.45	1.22	1.37
9	B	505	J6L	O4-C15	-10.23	1.02	1.23
8	B	502	MES	C8-S	-7.66	1.66	1.77
9	B	505	J6L	C8-C15	-6.86	1.36	1.46
9	B	505	J6L	O5-C16	-4.81	1.38	1.47

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	505	J6L	OP3-C9-C6	10.95	127.16	115.29
9	B	505	J6L	C9-OP3-CAA	8.98	124.56	118.29
10	B	506	GDP	C5-C4-N3	-7.48	116.49	128.39
9	B	505	J6L	O3'-C3'-C2'	7.30	125.30	115.40
9	B	505	J6L	OP3-C9-C14	-7.27	114.86	121.30

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A

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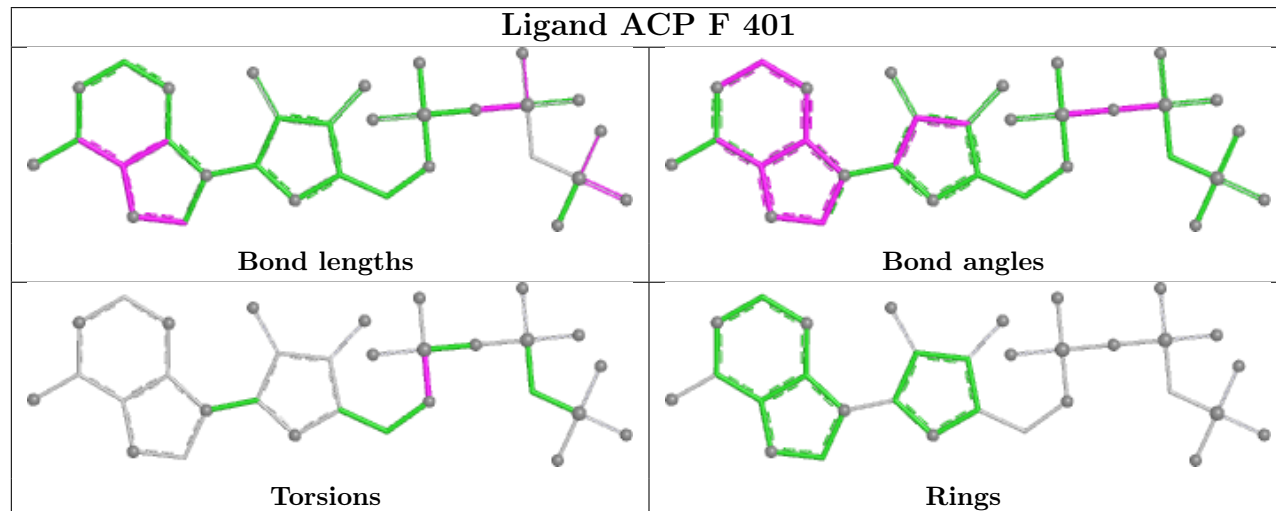
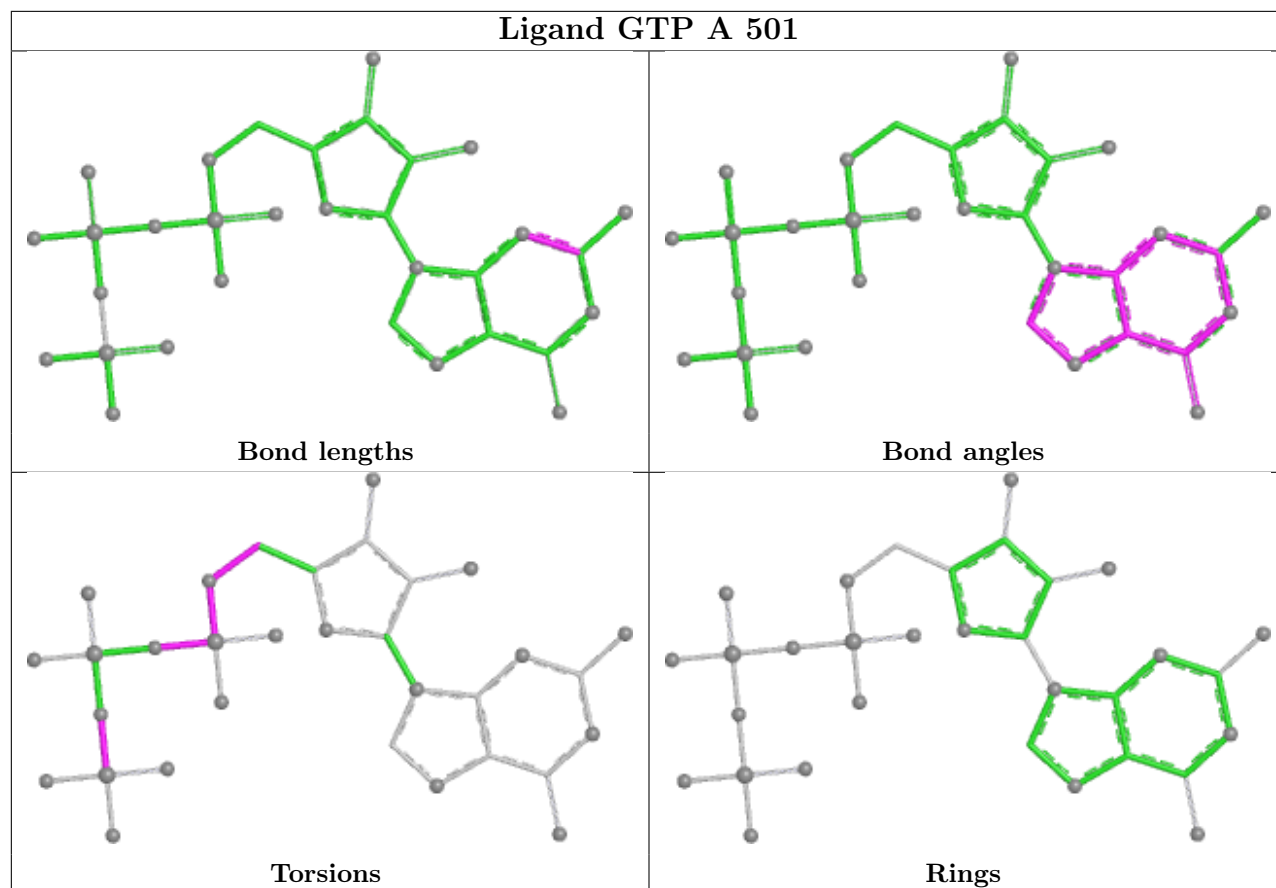
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G

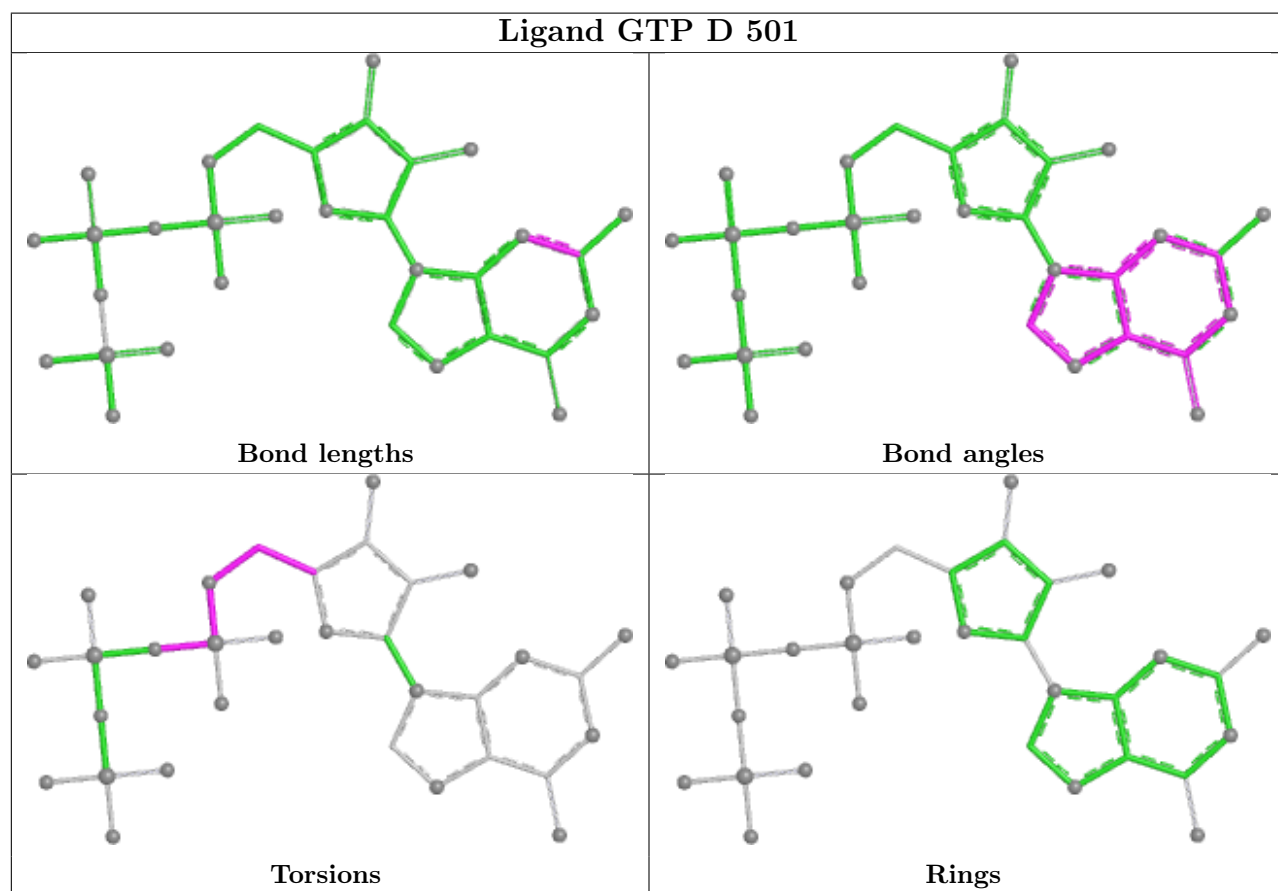
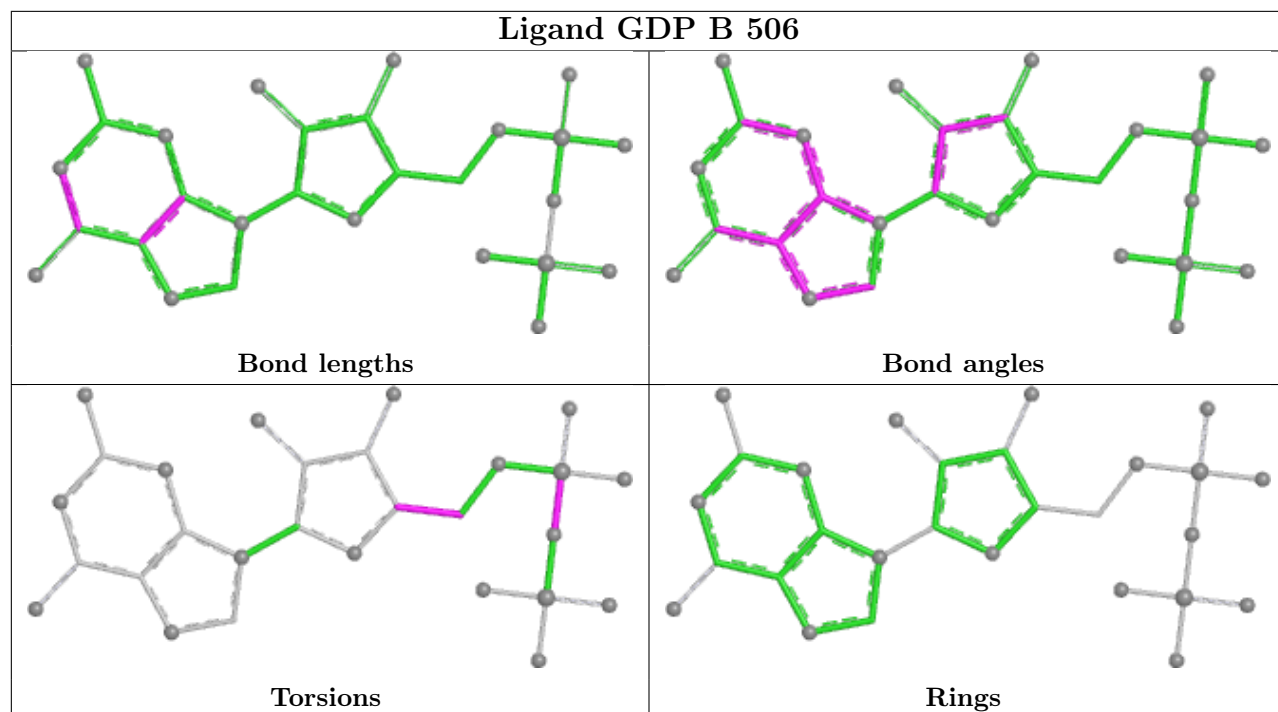
There are no ring outliers.

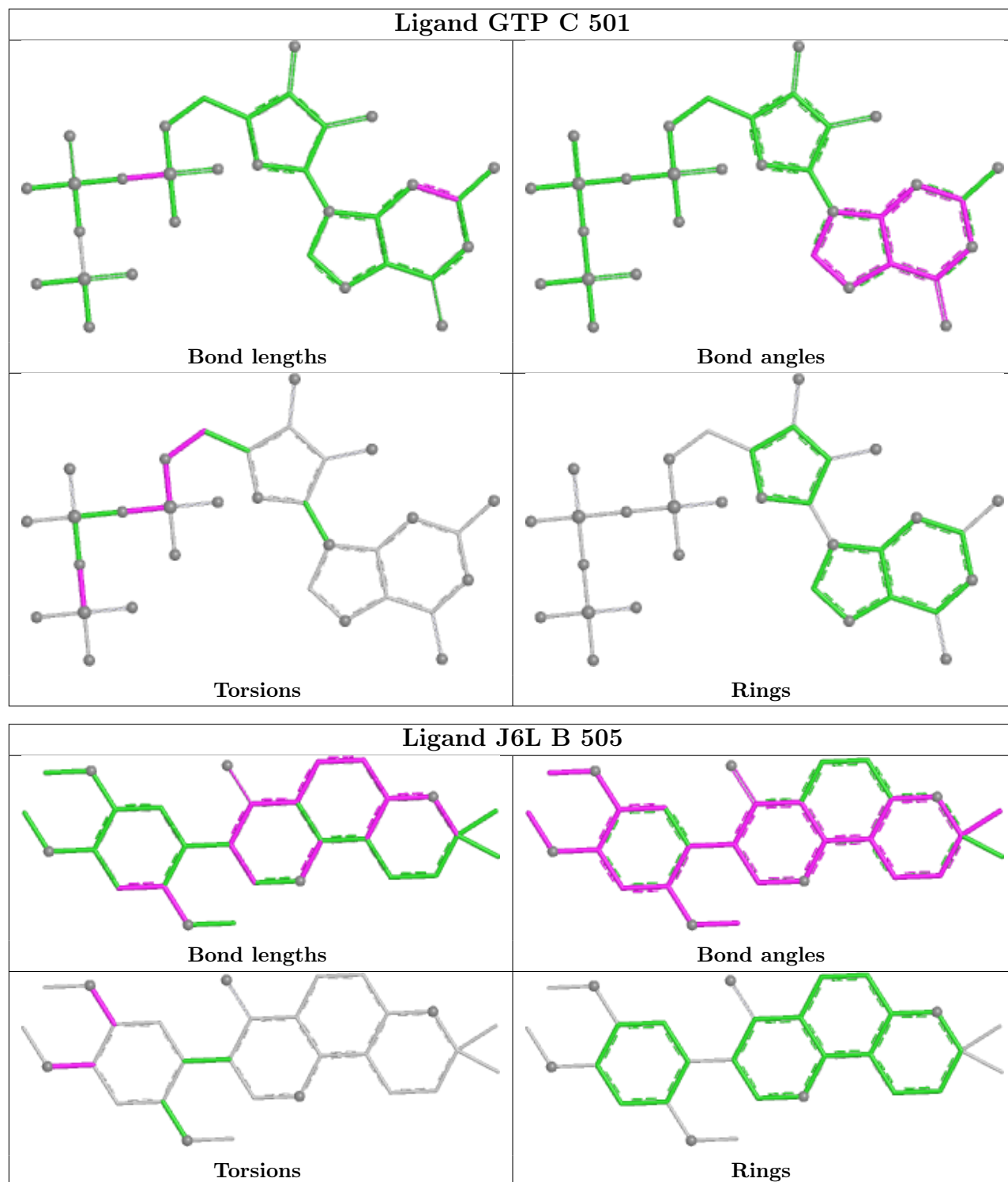
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	505	J6L	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	438/451 (97%)	0.03	14 (3%)	50	57	11, 35, 70, 97	5 (1%)
1	C	440/451 (97%)	-0.23	13 (2%)	52	59	9, 26, 57, 75	5 (1%)
2	B	426/445 (95%)	0.32	39 (9%)	14	18	16, 37, 75, 106	0
2	D	422/445 (94%)	0.45	30 (7%)	22	26	23, 46, 79, 108	1 (0%)
3	E	123/189 (65%)	0.79	15 (12%)	8	10	16, 54, 88, 106	3 (2%)
4	F	350/384 (91%)	1.73	132 (37%)	1	0	17, 68, 119, 131	1 (0%)
All	All	2199/2365 (92%)	0.43	243 (11%)	10	12	9, 40, 92, 131	15 (0%)

The worst 5 of 243 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	57	ALA	7.8
4	F	150	LYS	7.0
4	F	169	LEU	6.5
4	F	362	ALA	6.2
2	B	1	MET	6.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

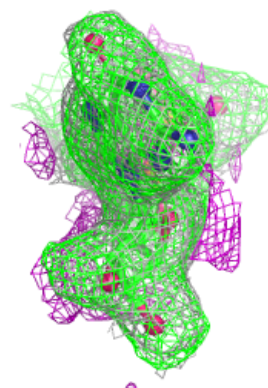
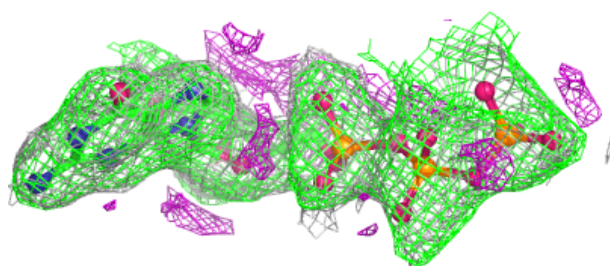
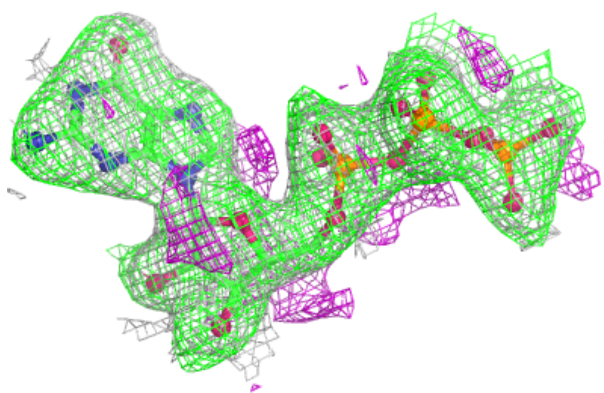
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	17,19,26,28	42
5	GTP	C	501	32/32	-	-	15,17,26,28	42
5	GTP	D	501	32/32	-	-	37,40,49,51	42
6	MG	A	502	1/1	-	-	23,23,23,23	1
6	MG	B	501	1/1	-	-	31,31,31,31	1
6	MG	C	502	1/1	-	-	17,17,17,17	1
6	MG	D	502	1/1	-	-	41,41,41,41	1
6	MG	F	402	1/1	-	-	67,67,67,67	1
7	CA	A	503	1/1	-	-	58,58,58,58	1
7	CA	A	504	1/1	-	-	37,37,37,37	1
7	CA	B	503	1/1	-	-	50,50,50,50	1
7	CA	B	504	1/1	-	-	68,68,68,68	1
7	CA	C	503	1/1	-	-	36,36,36,36	1
7	CA	D	503	1/1	-	-	49,49,49,49	1
8	MES	B	502	12/12	-	-	26,31,35,35	24
9	J6L	B	505	29/29	0.90	0.13	32,55,68,79	0
10	GDP	B	506	28/28	-	-	17,25,37,42	38
11	ACP	F	401	31/31	-	-	63,66,81,83	45

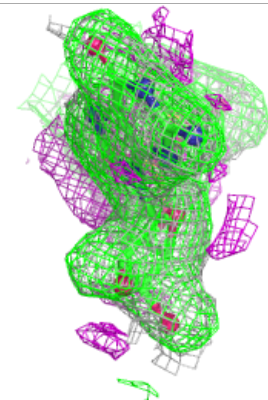
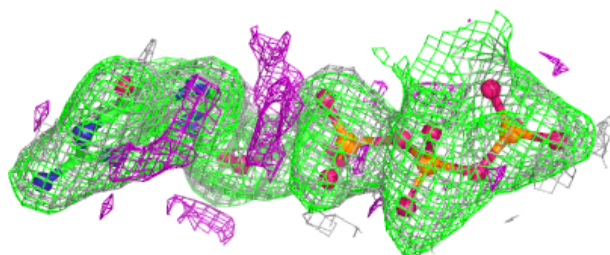
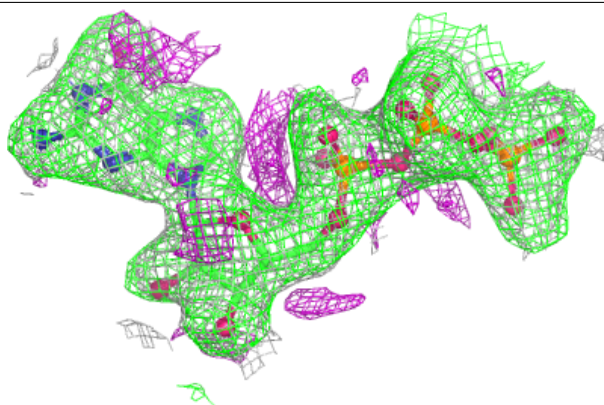
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

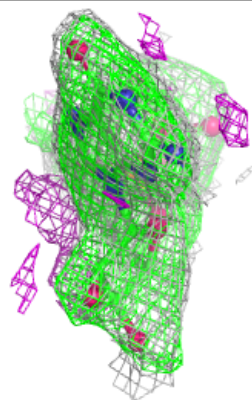
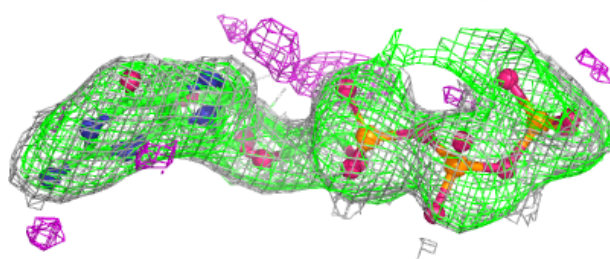
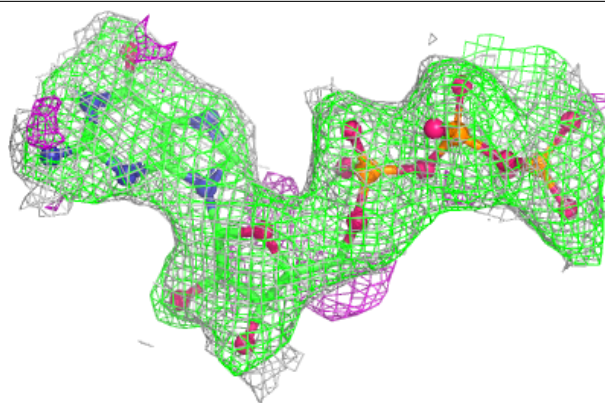
**Electron density around GTP C 501:**

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

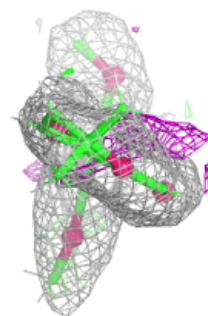
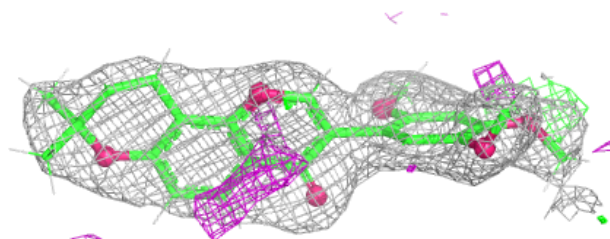
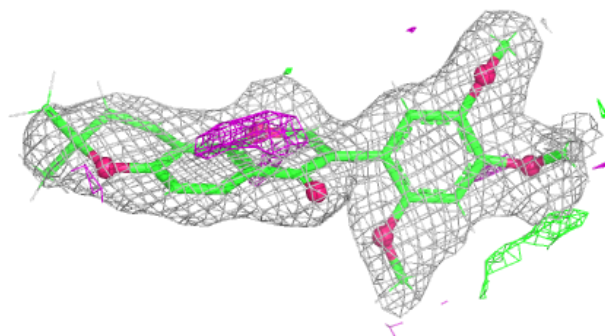


Electron density around GTP D 501:

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

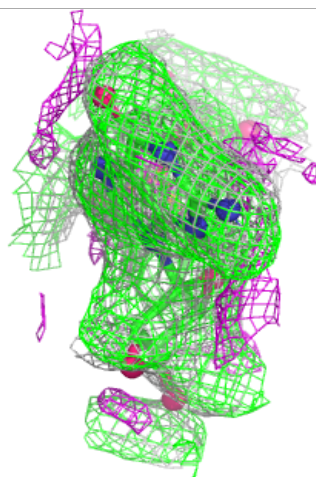
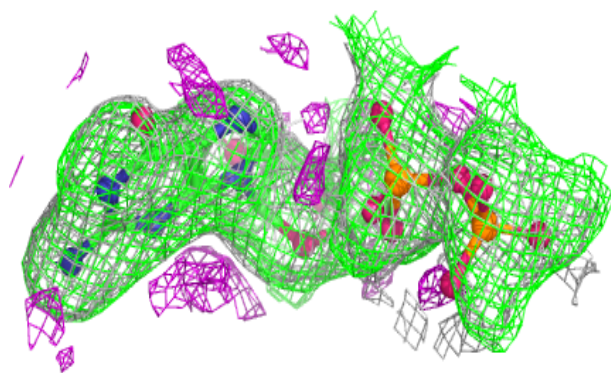
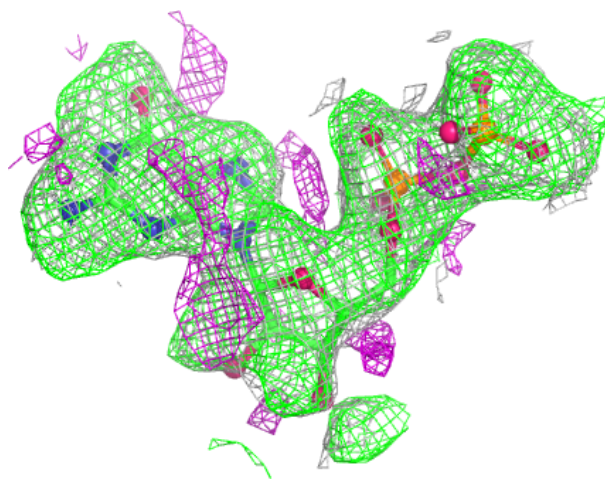
**Electron density around J6L B 505:**

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



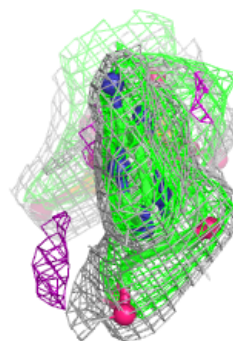
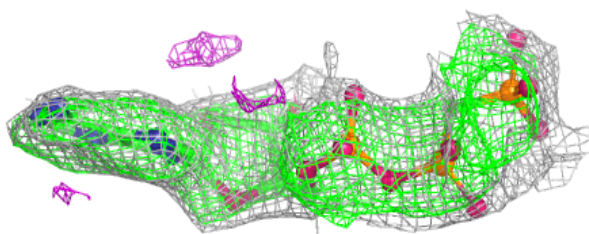
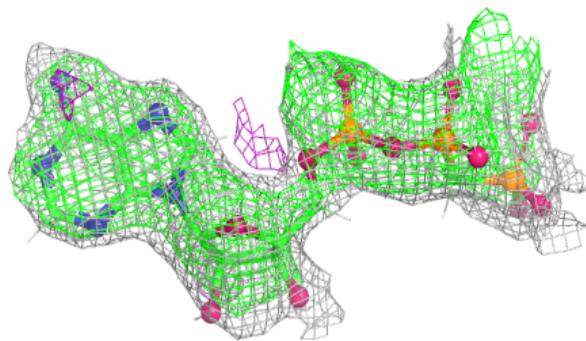
Electron density around GDP B 506:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.