W O R L D W I D E

wwPDB

P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Dec 9, 2023 – 05:28 pm GMT

PDB ID	:	8CLB
Title	:	Colchicine bound to tubulin (T2R-TTL) complex
Authors	:	Wranik, M.; Kepa, M.W.; Bertrand, Q.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on	:	2023-02-16
Resolution	:	3.00 Å(reported)

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

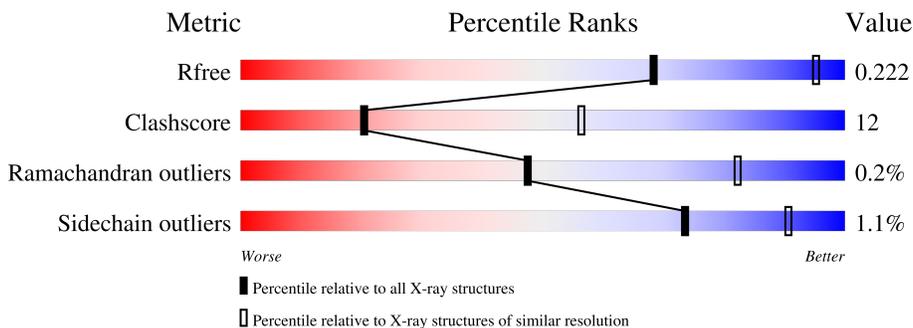|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.222
Clashscore		12
Ramachandran outliers		0.2%
Sidechain outliers		1.1%

Worse | Better

█ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	440	72% 27%
1	C	440	77% 22%
2	B	431	76% 23%
2	D	431	68% 30%
3	E	121	79% 21%
4	F	320	70% 28%

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 34597 atoms, of which 17054 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	439	Total 6913	C 2214	H 3431	N 582	O 661	S 25	0	13	0
1	C	440	Total 6893	C 2205	H 3412	N 587	O 665	S 24	0	10	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	423	Total 6646	C 2126	H 3271	N 569	O 653	S 27	1	9	0
2	D	421	Total 6533	C 2091	H 3211	N 561	O 642	S 28	5	4	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total 2032	C 621	H 1026	N 182	O 198	S 5	0	1	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	320	Total 5281	C 1711	H 2641	N 437	O 478	S 14	13	5	0

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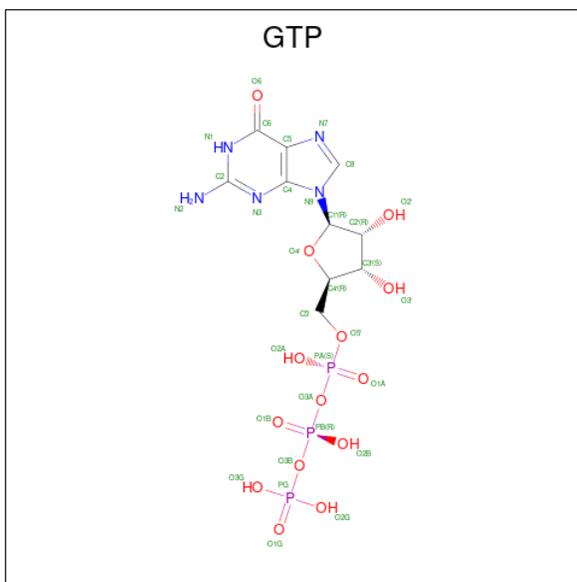
GTP

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			44	10	12	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 GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
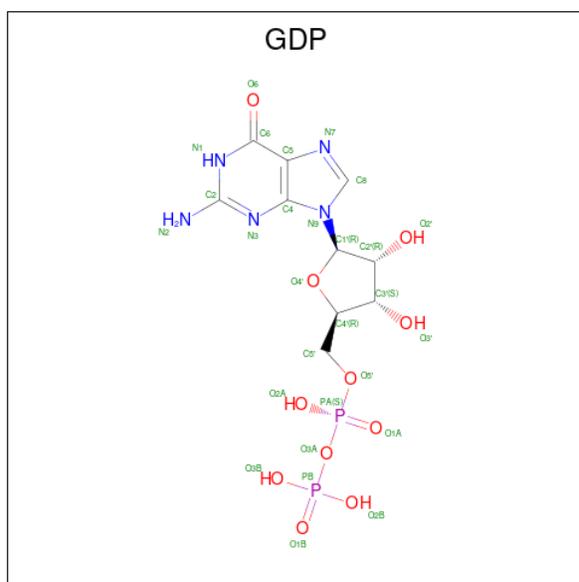
GDP

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
8	D	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 9 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$) (labeled as "Ligand of Interest" by depositor).
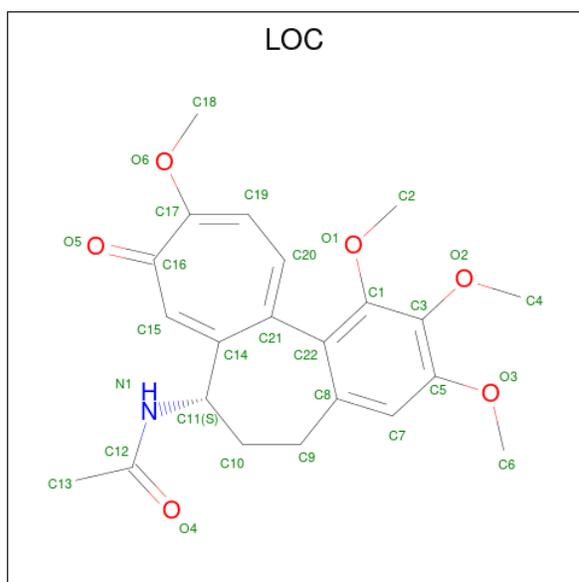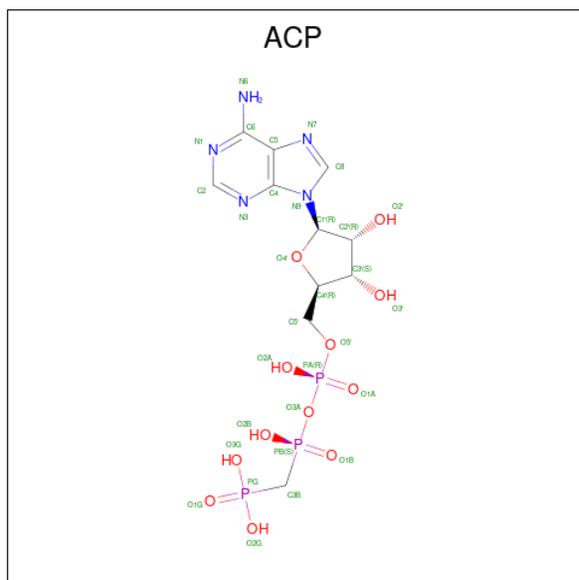

LOC

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			29	22	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	D	1	29	22	1	6	0	0

- Molecule 10 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
			Total	C	H	N	O	P		
10	F	1	45	11	14	5	12	3	0	0

- Molecule 11 is water.

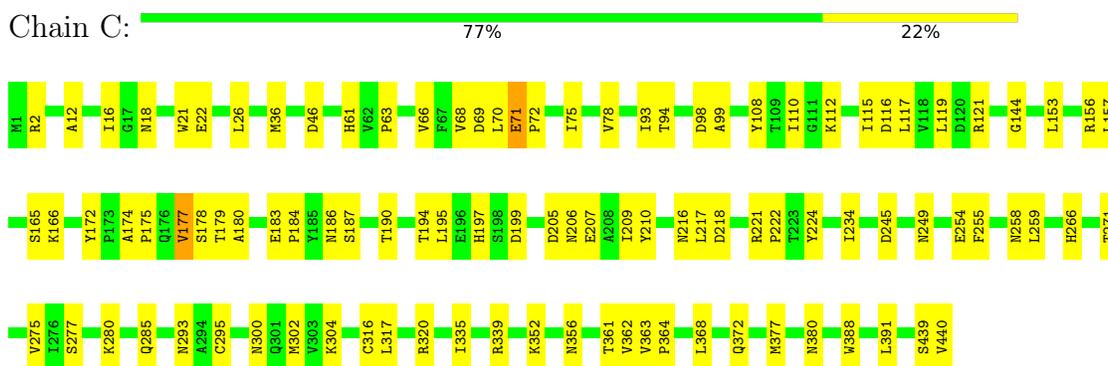| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	7	Total	O	0	0
			7	7		
11	B	5	Total	O	0	0
			5	5		
11	C	6	Total	O	0	0
			6	6		
11	D	1	Total	O	0	0
			1	1		
11	E	1	Total	O	0	0
			1	1		
11	F	2	Total	O	0	0
			2	2		

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. 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. 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.
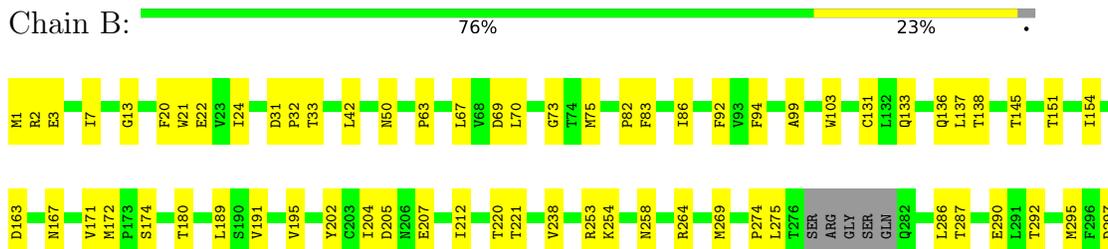
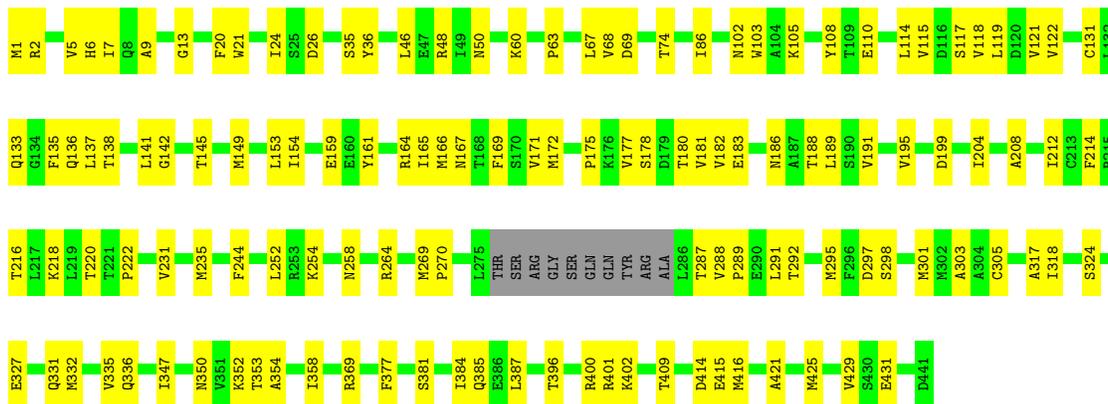• Molecule 1: Tubulin alpha-1B chain
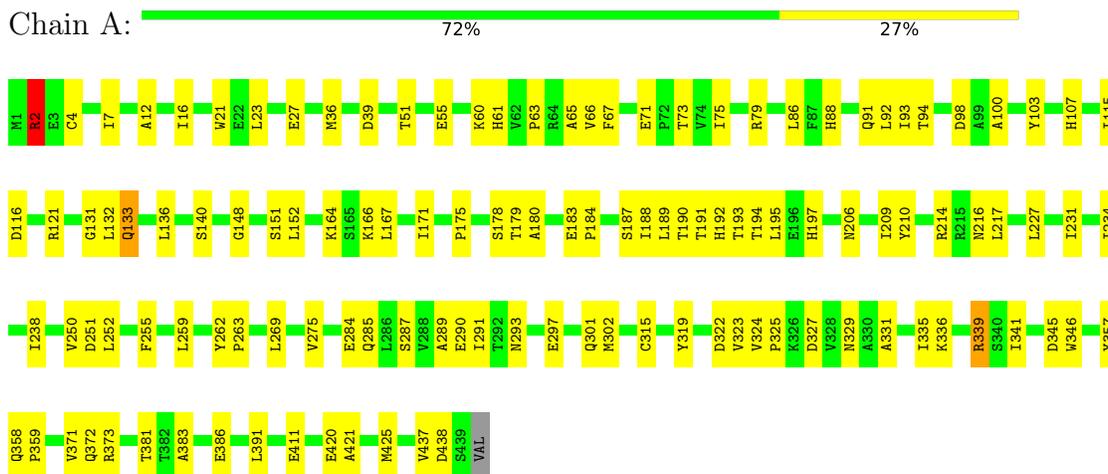
Chain A:

• Molecule 1: Tubulin alpha-1B chain

Chain C:

• Molecule 2: Tubulin beta-2B chain

Chain B:

S298 M301 M302 A303 A304 C305 D306 P307 R308 H309 Y312 A317 I318 F319 V335 N339 Y342 W346 K352 D357 I358 P359 G370 L371 A375 T376 F377 I378 Q385 E386 L387 F388 K389 R400 M425 V429 A438 THR ALA ASP

• Molecule 2: Tubulin beta-2B chain

Chain D: 68%   30%

M1 R2 V5 H6 I7 Q8 A9 G13 F20 W21 I24 S25 D26 S35 Y36 L46 E47 R48 I49 N50 K60 P63 L67 V68 D69 T74 I86 N102 W103 A104 K105 Y108 T109 E110 L114 V115 D116 S117 V118 L119 D120 V121 V122 C131 L132

Q133 G134 F135 Q136 L137 T138 L141 G142 T145 M149 L153 I154 E159 E160 Y161 R164 I165 M166 N167 T168 F169 S170 V171 M172 P175 K176 V177 S178 D179 T180 V181 V182 E183 N186 A187 T188 L189 S190 V191 V195 D199 I204 A208 I212 C213 F214 R215

T216 L217 K218 L219 T220 T221 P222 V231 M235 F244 L252 R253 K254 N258 R264 M269 P270 L275 THR SER ARG GLY SER GLN GLN TYR ARG ALA L286 T287 V288 P289 E290 L291 T292 M295 F296 D297 S298 M301 M302 A303 A304 C305 A317 I318 S324

E327 Q331 M332 V335 Q336 I347 N350 V351 K352 T353 A354 I358 R369 F377 S381 I384 Q385 E386 L387 T396 R400 R401 K402 T409 D414 E415 M416 A421 M425 V429 S430 E431 D441

• Molecule 3: Stathmin-4

Chain E: 79%   21%

M6 E7 V8 G17 L24 S28 L47 E48 Q51 K52 K53 L54 E55 R60 R61 K62 Y63 Q64 K75 R76 E79 M96 K100 Q103 L123 E132 V133 R134 K135 N136 K140 E141

• Molecule 4: Tubulin-Tyrosine Ligase

Chain F: 70%   28%

M1 Y2 T3 D8 Y14 S18 L21 L22 A23 T24 G25 Q26 W27 L30 R31 K32 D33 R36 F37 N38 L41 G42 E43 L52 L58 V59 Q60 R73 K74 A75 S76 K82 C91 T92 W93 F94 P95 E96 S97 P102 T125 D126 E127 R128 V146 W147

I148 A149 K150 S151 I162 S163 S164 E165 A166 S167 E168 L169 L170 D171 F172 I173 I182 Q183 L186 E187 G195 R202 V205 H209 L210 Y211 Y214 G219 V220 L221 H222 T223 S224 P227 C238 H239 L240 T241 Q246 Y249 S250 N252 Y253 G254 R255 Y256 E257 E258

G259 F264 F267 L279 E280 L284 I291 E299 P300 T304 S311 M320 E331 A339 Q340 K341 L342 Y343 I355 F359 P360 L361 I374 F375 L378

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.71Å 160.61Å 180.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.18 – 3.00 15.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.18-3.00) 69.5 (15.22-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.163 , 0.214 0.176 , 0.222	Depositor DCC
R_{free} test set	2000 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 72.7	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34597	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GTP, MG, LOC, CA, ACP, GDP

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	0.39	0/3599	0.54	0/4888
1	C	0.44	0/3589	0.56	0/4874
2	B	0.41	0/3473	0.57	0/4704
2	D	0.36	0/3407	0.53	0/4618
3	E	0.41	0/1017	0.51	0/1349
4	F	0.36	0/2712	0.54	0/3663
All	All	0.39	0/17797	0.55	0/24096

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	2
1	C	0	3
2	B	0	1
2	D	0	1
4	F	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
1	A	339	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	264	ARG	Sidechain
1	C	2	ARG	Sidechain
1	C	221	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	3482	3431	3430	99	0
1	C	3481	3412	3409	68	0
2	B	3375	3271	3268	86	0
2	D	3322	3211	3210	104	0
3	E	1006	1026	1026	20	0
4	F	2640	2641	2641	68	0
5	A	32	12	12	0	0
5	C	32	12	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	B	28	12	12	0	0
8	D	28	12	12	2	0
9	B	29	0	25	2	0
9	D	29	0	25	5	0
10	F	31	14	14	1	0
11	A	7	0	0	0	0
11	B	5	0	0	0	0
11	C	6	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	2	0	0	0	0
All	All	17543	17054	17096	430	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 12.

The worst 5 of 430 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:128:ARG:HE	4:F:170:LEU:HD22	1.37	0.88
1:A:381:THR:HG22	1:A:383:ALA:H	1.41	0.86
2:D:118:VAL:HG21	2:D:153:LEU:HD21	1.56	0.84
2:D:175:PRO:HA	2:D:178:SER:HB2	1.56	0.83
4:F:125:THR:HG22	4:F:126:ASP:HA	1.61	0.82

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	450/440 (102%)	431 (96%)	17 (4%)	2 (0%)	34	72
1	C	448/440 (102%)	432 (96%)	15 (3%)	1 (0%)	47	82
2	B	428/431 (99%)	406 (95%)	21 (5%)	1 (0%)	47	82
2	D	421/431 (98%)	400 (95%)	20 (5%)	1 (0%)	47	82
3	E	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
4	F	310/320 (97%)	288 (93%)	22 (7%)	0	100	100
All	All	2175/2183 (100%)	2073 (95%)	97 (4%)	5 (0%)	47	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	177	VAL
1	A	178	SER
2	D	74	THR
2	B	73	GLY
1	A	131	GLY

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	382/371 (103%)	379 (99%)	3 (1%)	81	93
1	C	381/371 (103%)	379 (100%)	2 (0%)	88	96
2	B	374/372 (100%)	374 (100%)	0	100	100
2	D	367/372 (99%)	367 (100%)	0	100	100
3	E	110/109 (101%)	106 (96%)	4 (4%)	35	70
4	F	294/289 (102%)	282 (96%)	12 (4%)	30	67
All	All	1908/1884 (101%)	1887 (99%)	21 (1%)	73	90

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	163	SER
4	F	222	ARG
4	F	311	SER
4	F	249	TYR
4	F	211	TYR

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	293	ASN
2	B	167	ASN
2	D	136	GLN
2	D	167	ASN
4	F	333	ASN

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 13 ligands modelled in this entry, 6 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	26,34,34	1.00	2 (7%)	32,54,54	0.72	1 (3%)
10	ACP	F	401	-	27,33,33	0.91	1 (3%)	32,52,52	0.97	3 (9%)
8	GDP	B	501	6	24,30,30	1.00	2 (8%)	30,47,47	0.65	1 (3%)
9	LOC	D	503	-	31,31,31	1.03	2 (6%)	44,44,44	1.60	5 (11%)
5	GTP	C	501	6	26,34,34	1.01	2 (7%)	32,54,54	0.69	1 (3%)
9	LOC	B	503	-	31,31,31	1.00	2 (6%)	44,44,44	1.48	6 (13%)
8	GDP	D	501	6	24,30,30	1.00	3 (12%)	30,47,47	0.68	1 (3%)

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	-	4/18/38/38	0/3/3/3
10	ACP	F	401	-	-	6/15/38/38	0/3/3/3
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
9	LOC	D	503	-	-	4/12/25/25	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LOC	B	503	-	-	2/12/25/25	0/3/3/3
8	GDP	D	501	6	-	5/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	LOC	C20-C21	3.66	1.42	1.37
9	B	503	LOC	C20-C21	3.44	1.42	1.37
9	D	503	LOC	C22-C21	-2.96	1.46	1.50
8	D	501	GDP	C5-C6	-2.78	1.41	1.47
5	C	501	GTP	C5-C6	-2.72	1.41	1.47

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	LOC	O6-C17-C16	7.19	116.57	109.56
9	B	503	LOC	O6-C17-C16	6.66	116.05	109.56
9	D	503	LOC	C14-C11-N1	-4.10	111.11	114.34
9	D	503	LOC	O6-C17-C19	-3.54	116.73	122.30
9	B	503	LOC	C14-C11-N1	-3.48	111.60	114.34

There are no chirality outliers.

5 of 30 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
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	503	LOC	C19-C17-O6-C18

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	401	ACP	1	0
9	D	503	LOC	5	0
9	B	503	LOC	2	0
8	D	501	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,
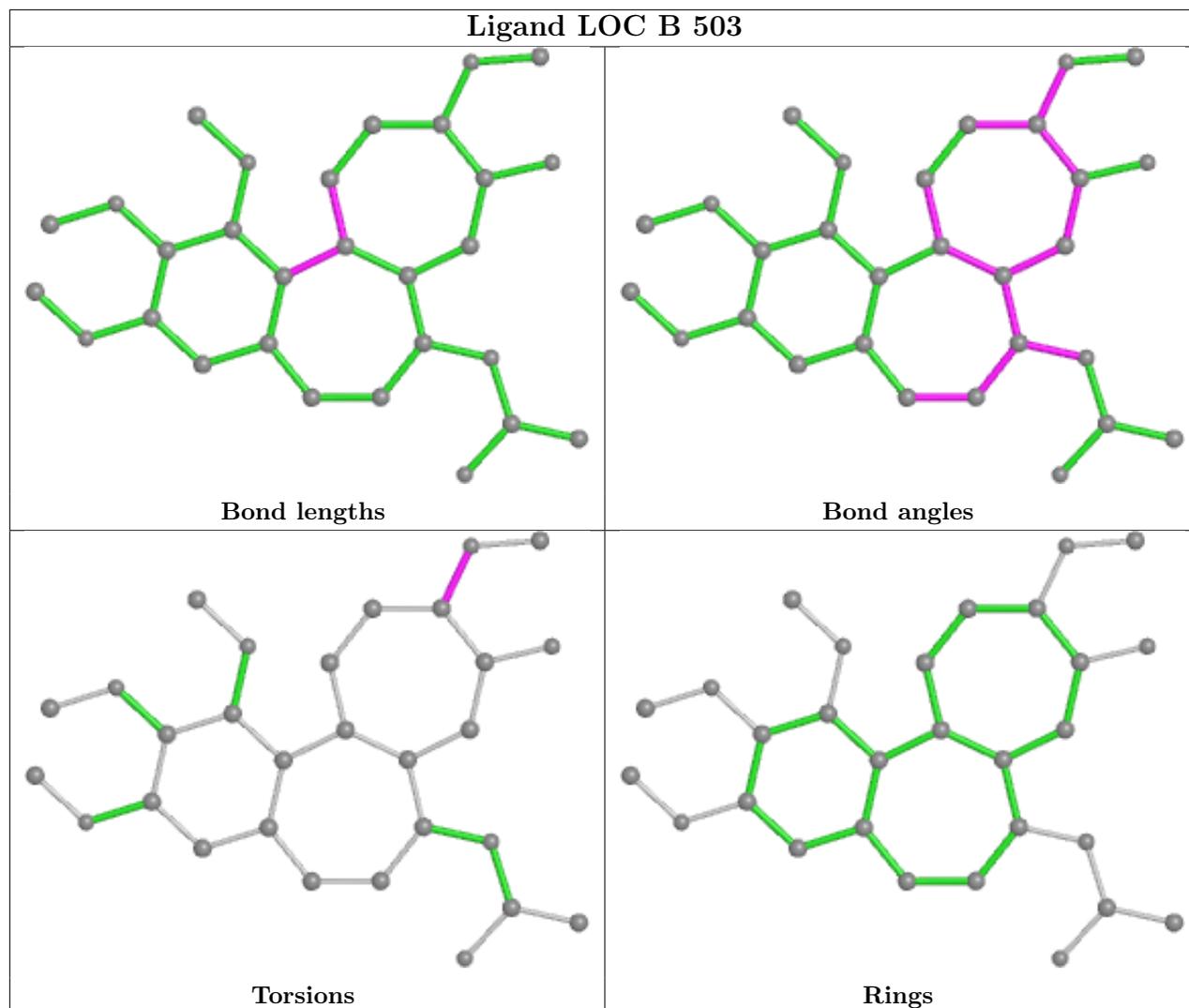
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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 501

Bond lengths   Bond angles

Torsions   Rings

Ligand ACP F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand LOC D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand LOC B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP D 501

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	6
3	E	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.70
1	F	362:ALA	C	373:SER	N	19.68
1	F	102:PRO	C	125:THR	N	12.42
1	F	151:SER	C	162:ILE	N	11.70
1	F	136:ASN	C	144:GLY	N	11.08

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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:

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

Electron density around GTP C 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
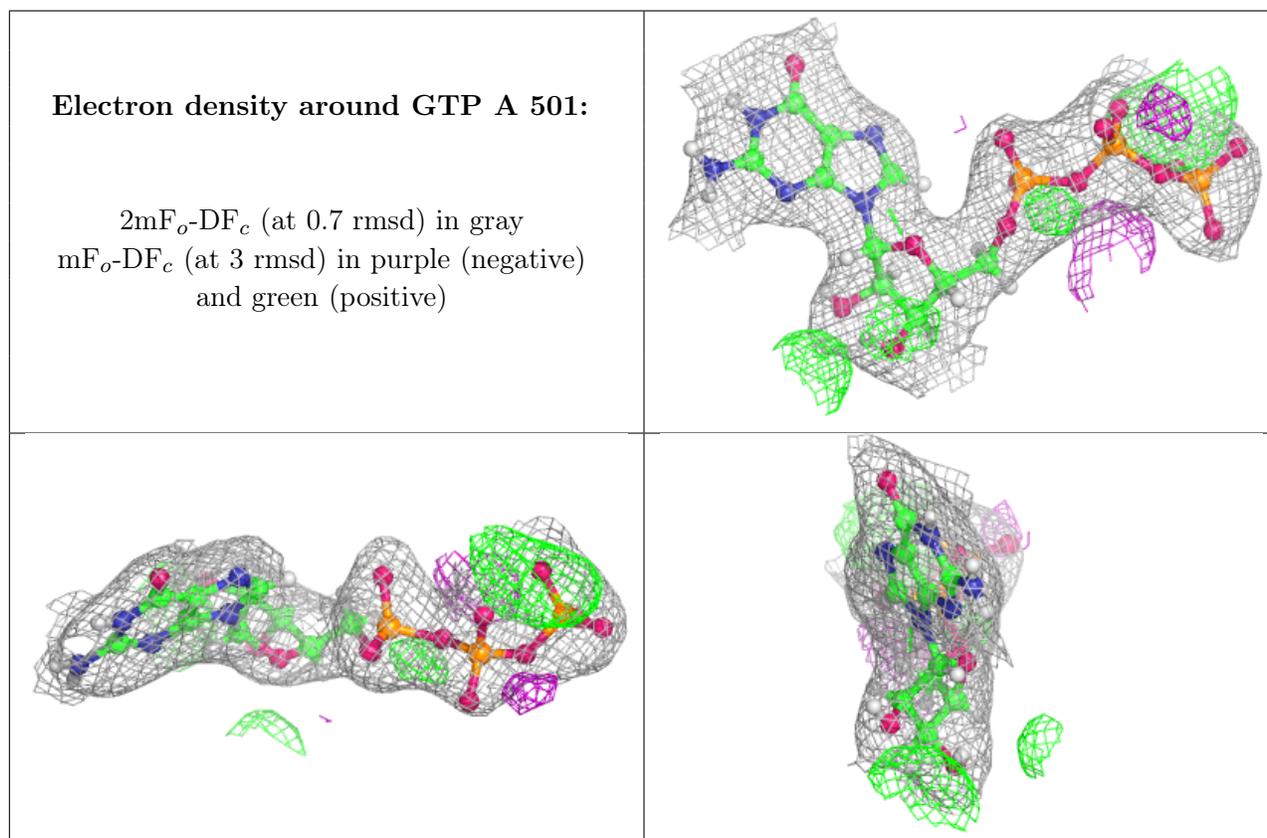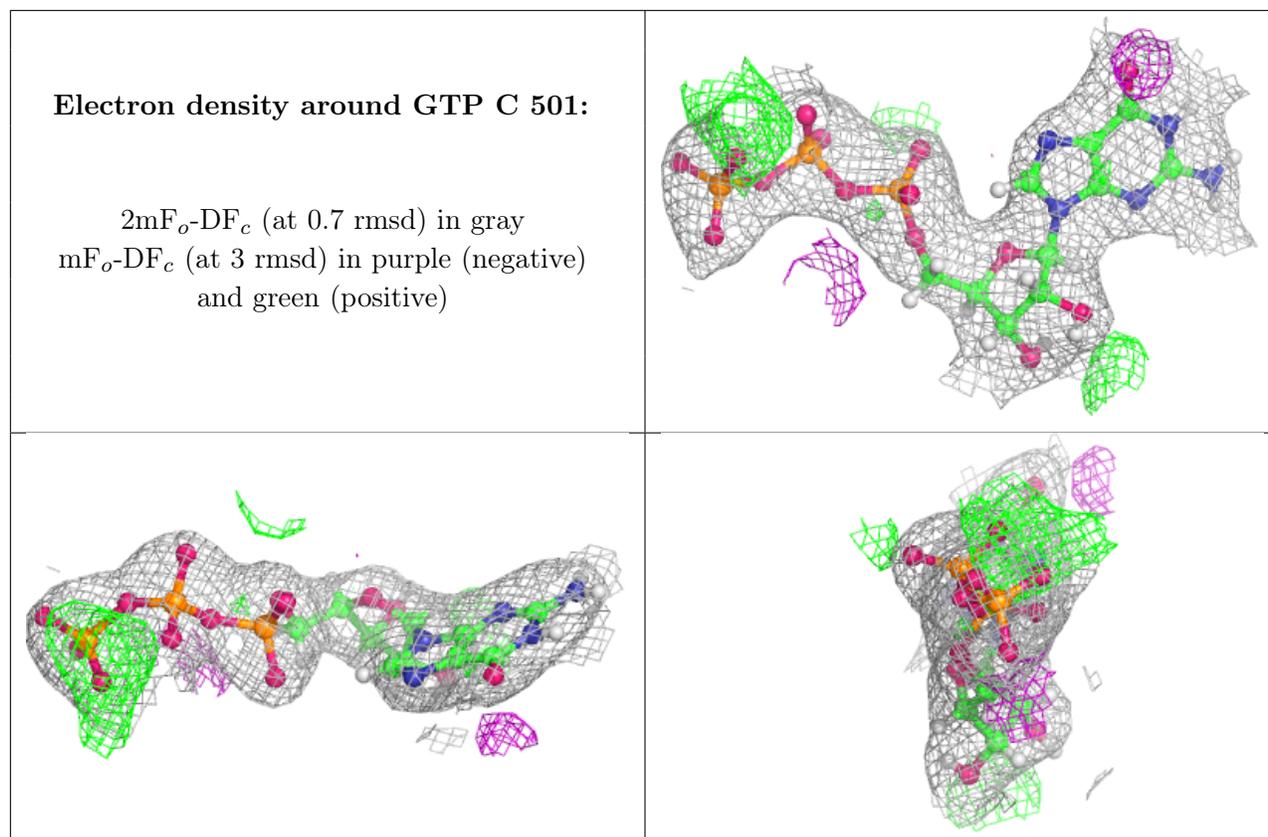
Electron density around GDP B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
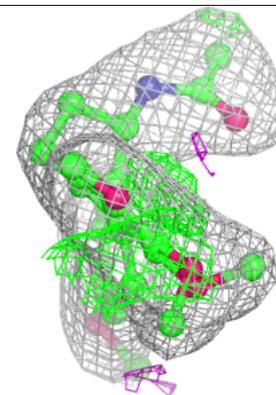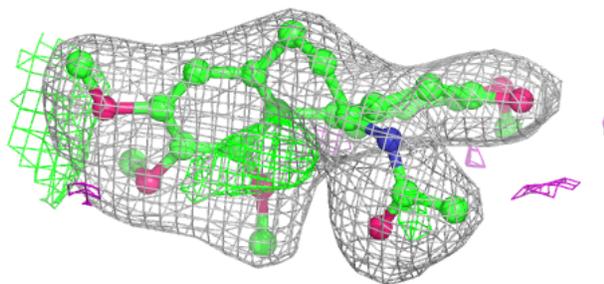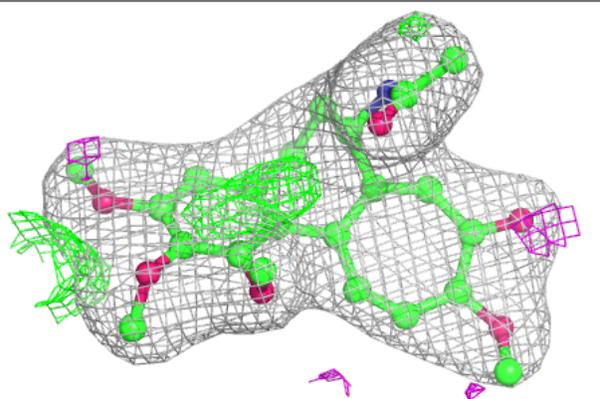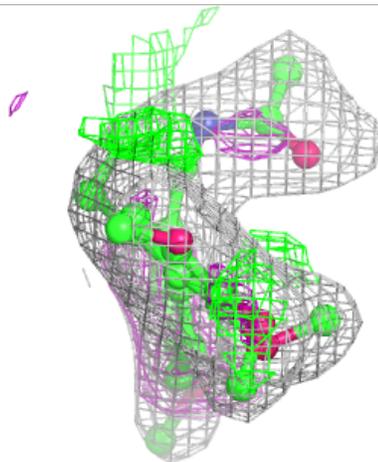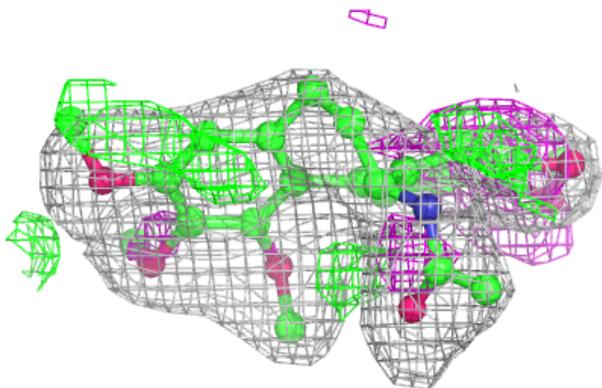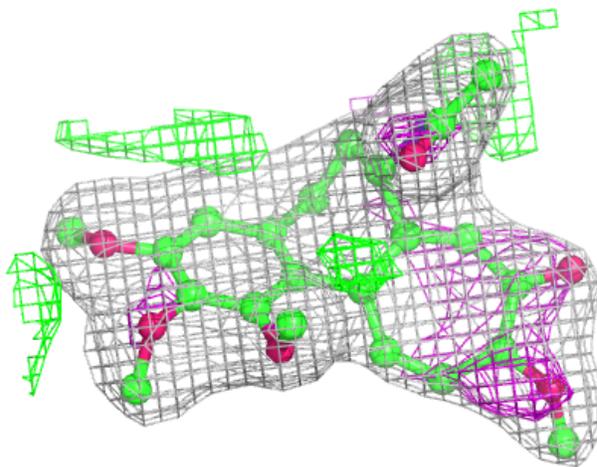mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
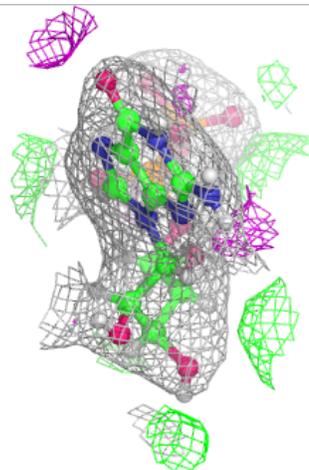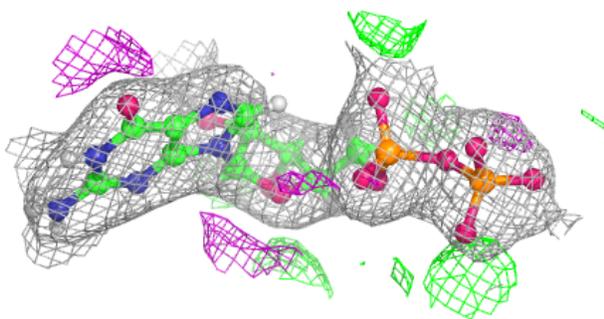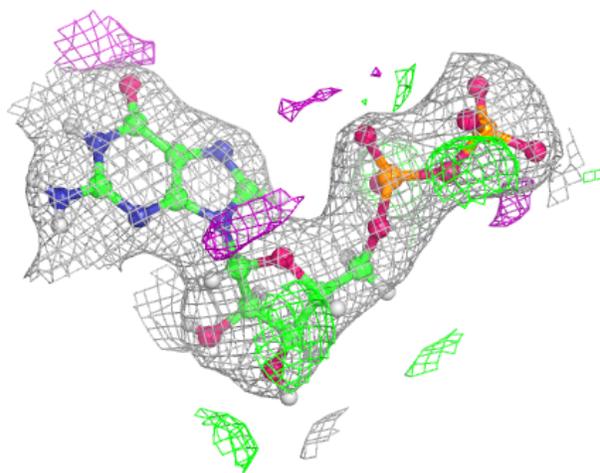
Electron density around GDP D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
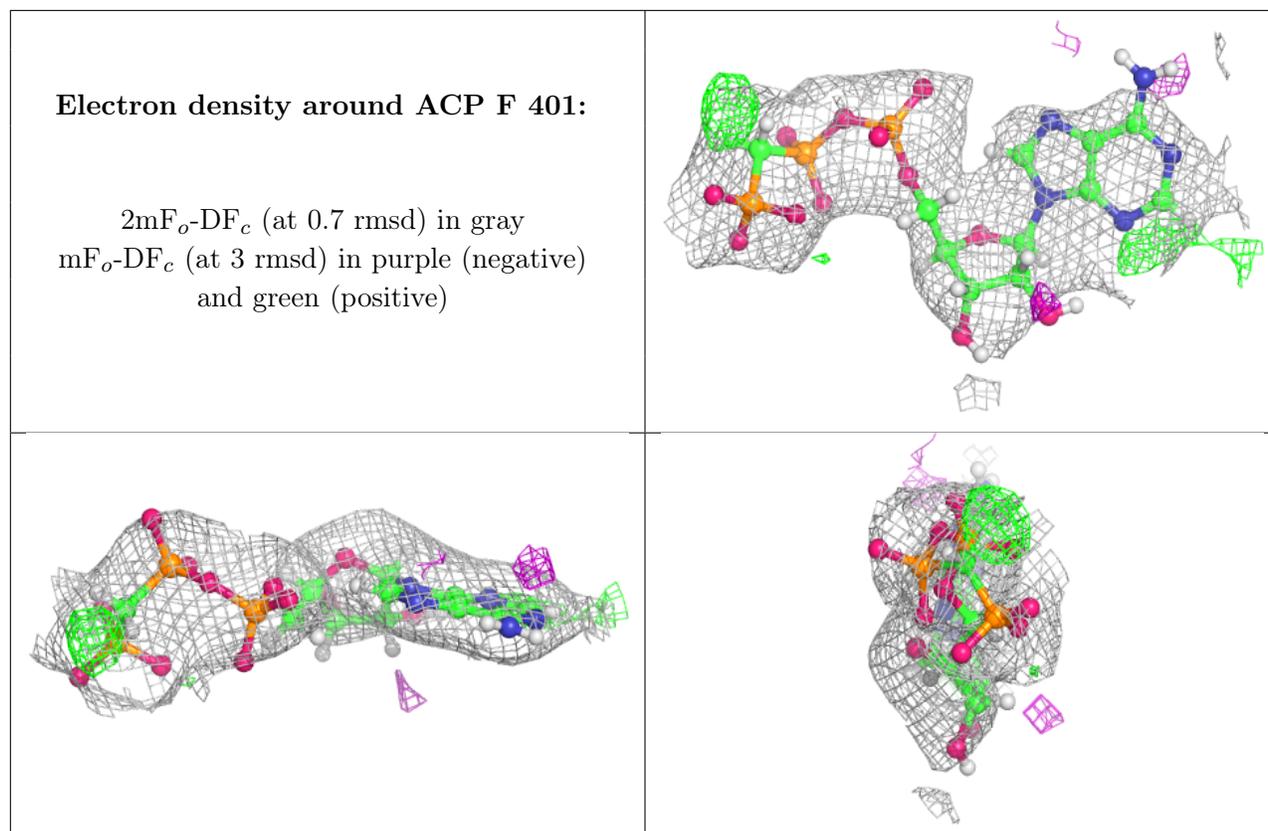and green (positive)
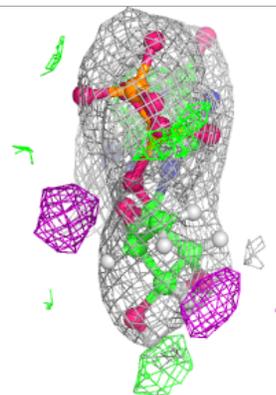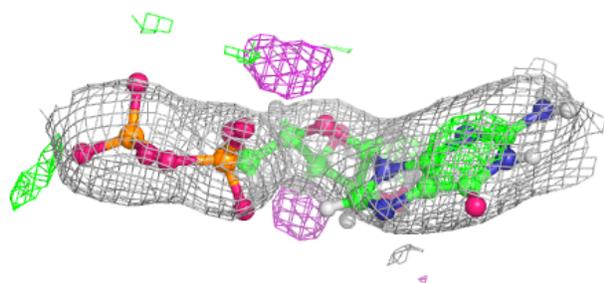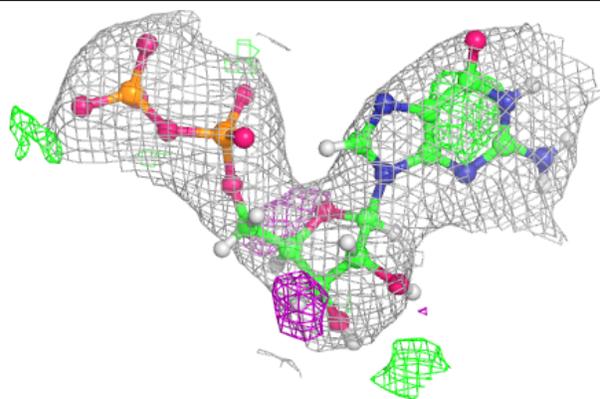
Electron density around LOC B 503:

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

Electron density around LOC 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 ACP F 401:

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

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.