wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 01:59 PM JST

PDB ID	:	7CLD
Title	:	Crystal structure of T2R-TTL-Cevipabulin complex
Authors	:	Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on	:	2020-07-20
Resolution	:	2.61 Å(reported)

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

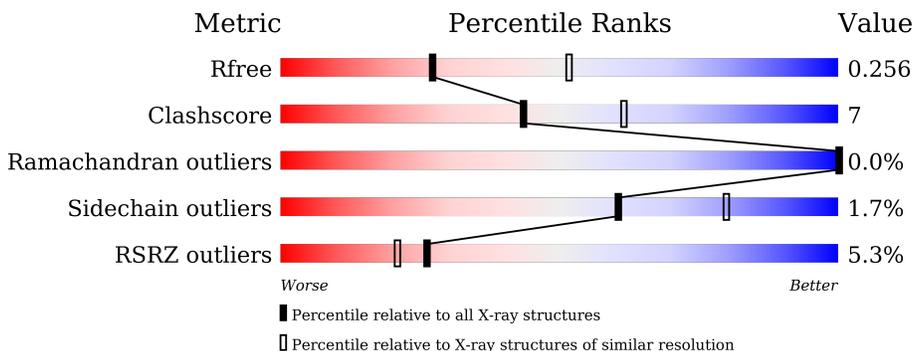|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.61 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		0.256
Clashscore		7
Ramachandran outliers		0.0%
Sidechain outliers		1.7%
RSRZ outliers		5.3%

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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 <=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	450	2% / 85% / 12% / •
1	C	450	85% / 12% / •
2	B	445	3% / 80% / 14% / 6%
2	D	445	5% / 77% / 19% / •
3	E	143	8% / 69% / 14% / • / 14%
4	F	384	15% / 68% / 22% / • / 9%

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 35069 atoms, of which 17070 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 6802	C 2182	H 3351	N 588	O 657	S 24	0	4	0
1	C	440	Total 6827	C 2196	H 3361	N 587	O 660	S 23	0	7	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	418	Total 6491	C 2077	H 3184	N 566	O 636	S 28	0	3	0
2	D	426	Total 6563	C 2100	H 3217	N 570	O 649	S 27	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total 2053	C 629	H 1031	N 185	O 203	S 5	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	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	351	Total 5696	C 1838	H 2824	N 491	O 528	S 15	0	1	0

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: $C_{10}H_{16}N_5O_{14}P_3$).
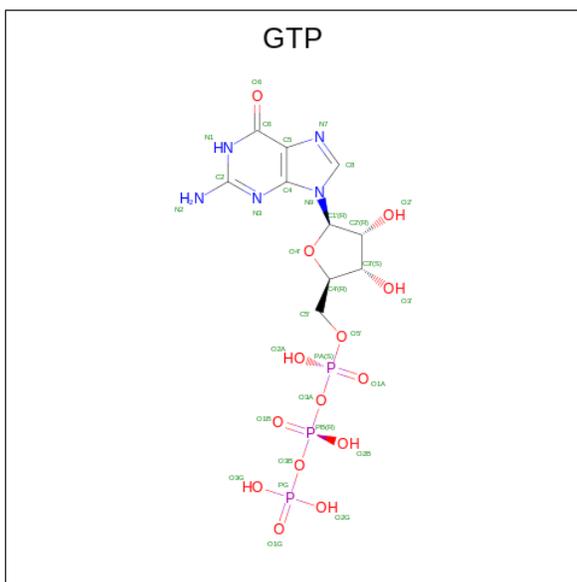
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

- 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		

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

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

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
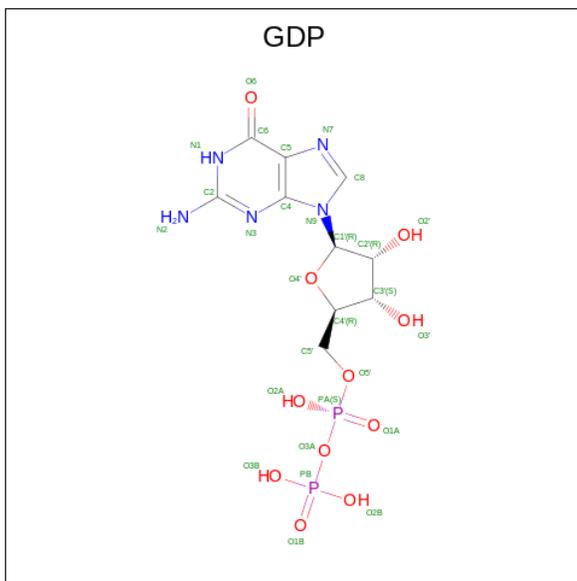
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
8	B	1	38	10	10	5	11	2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

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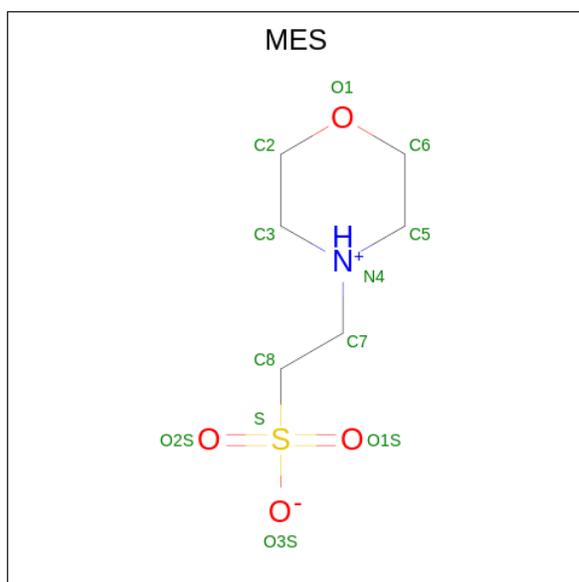
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 10 is 6-[2,6-bis(fluoranyl)-4-[3-(methylamino)propoxy]phenyl]-5-chloranyl-N-[(2S)-1,1,1-tris(fluoranyl)propan-2-yl]-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (three-letter code: G2X) (formula: $C_{18}H_{18}ClF_5N_6O$) (labeled as "Ligand of Interest" by depositor).
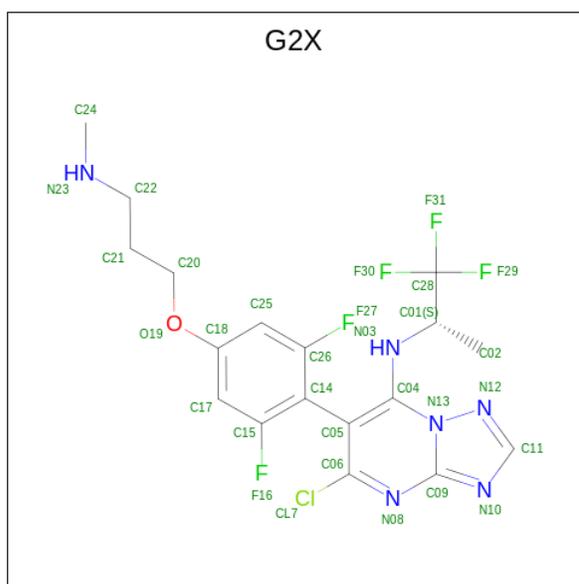
G2X

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	B	1	Total	C	Cl	F	H	N	O	0	0
			49	18	1	5	18	6	1		
10	C	1	Total	C	Cl	F	H	N	O	0	0
			49	18	1	5	18	6	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).
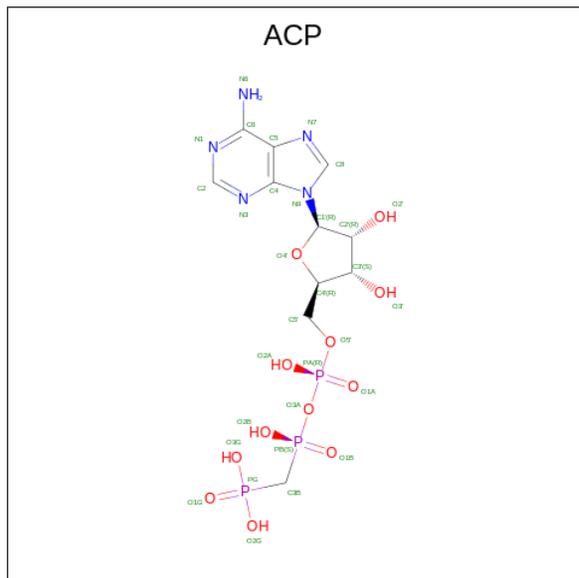
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
11	F	1	45	11	14	5	12	3	0	0

- Molecule 12 is water.

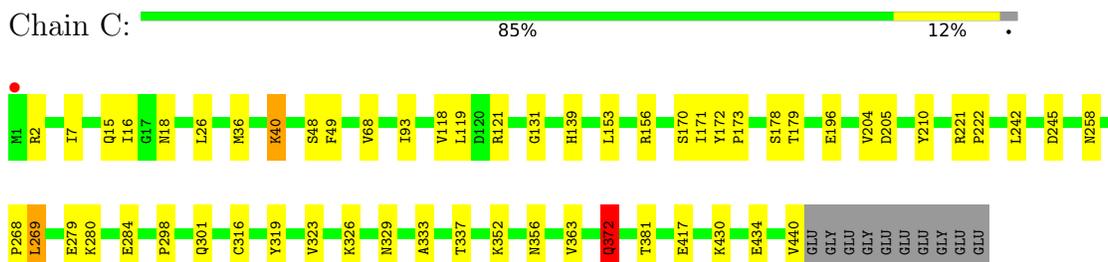| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	72	Total 72	O 72	0	0
12	B	53	Total 53	O 53	0	0
12	C	104	Total 104	O 104	0	0
12	D	32	Total 32	O 32	0	0
12	E	13	Total 13	O 13	0	0
12	F	20	Total 20	O 20	0	0

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.
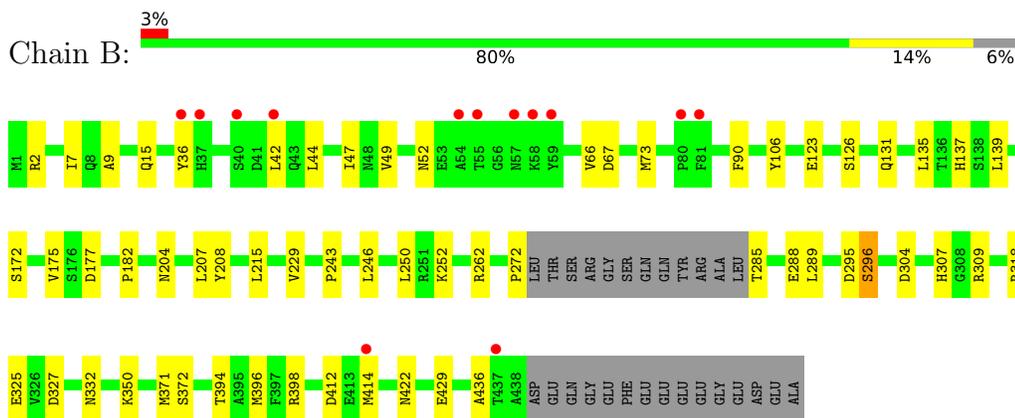
- Molecule 1: Tubulin alpha-1B chain
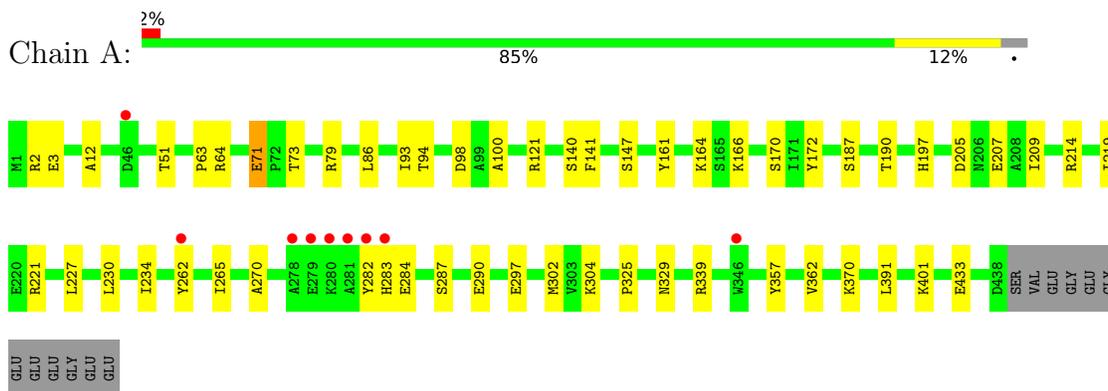
- Molecule 1: Tubulin alpha-1B chain

- Molecule 2: Tubulin beta chain

- Molecule 2: Tubulin beta chain

Chain D:

5%

77%

19%

M1 R2 Q11 Q15 V23 G29 I30 D31 P32 T33 Y36 H37 G38 L42 Q43 L44 I47 N48 V49 A54 T55 C56 N57 K58 Y59 V60 D67 L68 G71 T72 M73 I84 P87 F90 V91 F92 G93 Q94 N100 W101 A102 K103 G104 H105 Y106 T107

L112 Q134 L135 T136 H137 G140 G141 G146 L150 K154 I155 R162 I163 M164 N165 T166 F167 S168 V169 M170 S176 D177 N184 S188 V189 T196 I202 T219 S230 S234 G235 T238 C239 P243 G244 Q245 L246 N247 L253 P261

H264 S278 GLN GLN TYR ARG ALA L284 T285 V286 P287 E288 M293 R309 Y310 A314 K324 K350 T351 A352 F375 I376 K400 M411 M414 E415 F416 M423 A436 D439 GLU GLN GLY GLU PHE GLU GLU GLU GLU GLY GLU ASP GLU ALA

• Molecule 3: Stathmin-4

Chain E:

8%

69%

14%

14%

MET ALA ASP M6 Q18 S19 P27 S28 PHE ASP GLY VAL PRO GLU PHE ASN SER LEU PRO ARG ARG D44 P45 E48 E49 K52 K53 E67 H71 R80 E81 V82 K85 E89 I94 K95 R112 L116 A117 A118 M119 R122 L123 Q124 E125

K126 D127 K128 E131 R134 A143 SER ARG

• Molecule 4: Tubulin tyrosine ligase

Chain F:

15%

68%

22%

9%

M1 R7 D8 E9 Y14 A15 E16 V17 S18 R19 L20 L21 T24 R31 K32 N38 L39 M40 L41 R44 N45 R46 F49 L52 G53 H54 Q60 K70 R73 K74 A75 S76 L77 V78 K79 K82 S88 E89 S90 C91 Y98 V99 I100 Y101 P102 T103

ASN LEU LYS THR PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG T125 D126 E127 R128 E129 V130 F131 L132 Y135 R138 R139 E140 E143 G144 N145 A149 K150 S151 S152 A153 G154 A155 K156 G157 E158 G159 I160 L161 I162 S163 S164 E165 L169 L170

D171 F172 I173 D174 E175 Q176 G177 Q178 V179 H180 V181 I182 Q183 K184 Y185 L186 P189 R197 K198 F199 D200 Y211 R217 L221 R222 T223 S224 S230 A231 N232 F233 Q234 D235 K236 T237 C238 H239 L240 T241 N242 H243 C244 I245 Q246 K247 E248 Y249 S250 K251 N252 Y253 E257 E258

G259 F263 L295 M296 C297 I298 K305 H308 D322 N333 G334 A335 P336 A337 C338 A339 Q348 A362 D363 THR GLY GLN LYS THR SER GLN PRO T372 S373 H380 HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.42Å 160.78Å 174.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.03 – 2.61 50.03 – 2.61	Depositor EDS
% Data completeness (in resolution range)	93.4 (50.03-2.61) 93.5 (50.03-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.207 , 0.258 0.207 , 0.256	Depositor DCC
R_{free} test set	1761 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.0	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	0.92	EDS
Total number of atoms	35069	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 6.17% 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: MG, G2X, CA, GTP, ACP, GDP, 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	0.36	0/3532	0.49	0/4794
1	C	0.50	3/3568 (0.1%)	0.56	2/4846 (0.0%)
2	B	0.35	0/3386	0.51	0/4584
2	D	0.34	0/3422	0.48	0/4634
3	E	0.58	3/1030 (0.3%)	0.65	3/1367 (0.2%)
4	F	0.34	0/2937	0.50	0/3967
All	All	0.40	6/17875 (0.0%)	0.52	5/24192 (0.0%)

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	C	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	372	GLN	CD-NE2	-13.98	0.97	1.32
3	E	95	LYS	CE-NZ	-9.52	1.25	1.49
3	E	95	LYS	CG-CD	-8.74	1.22	1.52
1	C	279	GLU	CD-OE2	-7.32	1.17	1.25
1	C	372	GLN	CD-OE1	-5.45	1.11	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	95	LYS	CD-CE-NZ	-12.69	82.52	111.70
1	C	372	GLN	CB-CG-CD	-9.65	86.50	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	80	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	C	372	GLN	N-CA-CB	-6.54	98.82	110.60
3	E	95	LYS	CB-CG-CD	-5.92	96.21	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	372	GLN	Sidechain

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	3451	3351	3362	42	0
1	C	3466	3361	3376	35	0
2	B	3307	3184	3193	38	1
2	D	3346	3217	3227	49	0
3	E	1022	1031	1034	19	1
4	F	2872	2824	2835	63	0
5	A	32	10	12	0	0
5	C	32	10	12	1	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	2	0	0	0	0
7	D	1	0	0	0	0
8	B	28	10	12	1	0
9	B	12	12	12	0	0
10	B	31	18	0	0	0
10	C	31	18	0	1	0
11	F	31	14	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	72	0	0	2	0
12	B	53	0	0	2	0
12	C	104	0	0	5	0
12	D	32	0	0	6	0
12	E	13	0	0	2	0
12	F	20	0	0	0	0
All	All	17999	17070	17101	234	1

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 7.

The worst 5 of 234 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:A:79:ARG:NH1	12:A:601:HOH:O	2.03	0.89
3:E:95:LYS:HD3	3:E:95:LYS:N	1.91	0.86
4:F:296[B]:MET:SD	4:F:380:HIS:ND1	2.51	0.83
4:F:140:GLU:O	4:F:140:GLU:OE1	2.04	0.76
2:B:285:THR:N	2:B:288:GLU:OE1	2.19	0.75

All (1) 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:320:ARG:HH21	3:E:131:GLU:OE1[4_455]	1.46	0.14

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	440/450 (98%)	431 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	445/450 (99%)	432 (97%)	13 (3%)	0	100	100
2	B	417/445 (94%)	404 (97%)	13 (3%)	0	100	100
2	D	423/445 (95%)	408 (96%)	15 (4%)	0	100	100
3	E	120/143 (84%)	116 (97%)	4 (3%)	0	100	100
4	F	346/384 (90%)	337 (97%)	8 (2%)	1 (0%)	41	62
All	All	2191/2317 (95%)	2128 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU

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	373/378 (99%)	371 (100%)	2 (0%)	88	95
1	C	378/378 (100%)	371 (98%)	7 (2%)	57	78
2	B	364/383 (95%)	359 (99%)	5 (1%)	67	84
2	D	369/383 (96%)	363 (98%)	6 (2%)	62	81
3	E	111/127 (87%)	108 (97%)	3 (3%)	44	69
4	F	314/342 (92%)	304 (97%)	10 (3%)	39	63
All	All	1909/1991 (96%)	1876 (98%)	33 (2%)	60	80

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	230	SER
4	F	249	TYR
4	F	348	GLN
1	C	269	LEU
1	C	268	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	18	GLN
4	F	60	GLN
4	F	310	GLN
4	F	183	GLN
4	F	252	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 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	1.13	2 (7%)	32,54,54	1.47	6 (18%)
10	G2X	C	504	-	28,33,33	2.80	10 (35%)	30,48,48	1.83	4 (13%)
9	MES	B	503	-	12,12,12	2.11	1 (8%)	14,16,16	1.77	4 (28%)
5	GTP	C	501	6	26,34,34	1.21	3 (11%)	32,54,54	1.45	6 (18%)
10	G2X	B	506	-	28,33,33	2.66	9 (32%)	30,48,48	1.38	2 (6%)
5	GTP	D	503	6	26,34,34	1.11	2 (7%)	32,54,54	1.63	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	GDP	B	501	-	24,30,30	0.97	2 (8%)	30,47,47	1.43	7 (23%)
11	ACP	F	402	6	27,33,33	2.54	8 (29%)	32,52,52	1.83	7 (21%)

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
10	G2X	C	504	-	-	3/20/20/20	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
10	G2X	B	506	-	-	3/20/20/20	0/3/3/3
5	GTP	D	503	6	-	5/18/38/38	0/3/3/3
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
11	ACP	F	402	6	-	2/15/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O4'-C1'	7.73	1.51	1.41
10	C	504	G2X	C28-C01	7.45	1.60	1.51
10	C	504	G2X	C06-N08	7.24	1.37	1.30
9	B	503	MES	C8-S	-7.02	1.67	1.77
10	B	506	G2X	C28-C01	6.99	1.60	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	504	G2X	C05-C06-CL7	-5.99	115.29	119.27
11	F	402	ACP	C3'-C2'-C1'	5.02	108.54	100.98
10	C	504	G2X	C14-C05-C04	4.60	128.00	121.41
9	B	503	MES	C5-N4-C3	4.13	118.11	108.83
11	F	402	ACP	N3-C2-N1	-4.03	122.38	128.68

There are no chirality outliers.

5 of 29 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-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

There are no ring outliers.
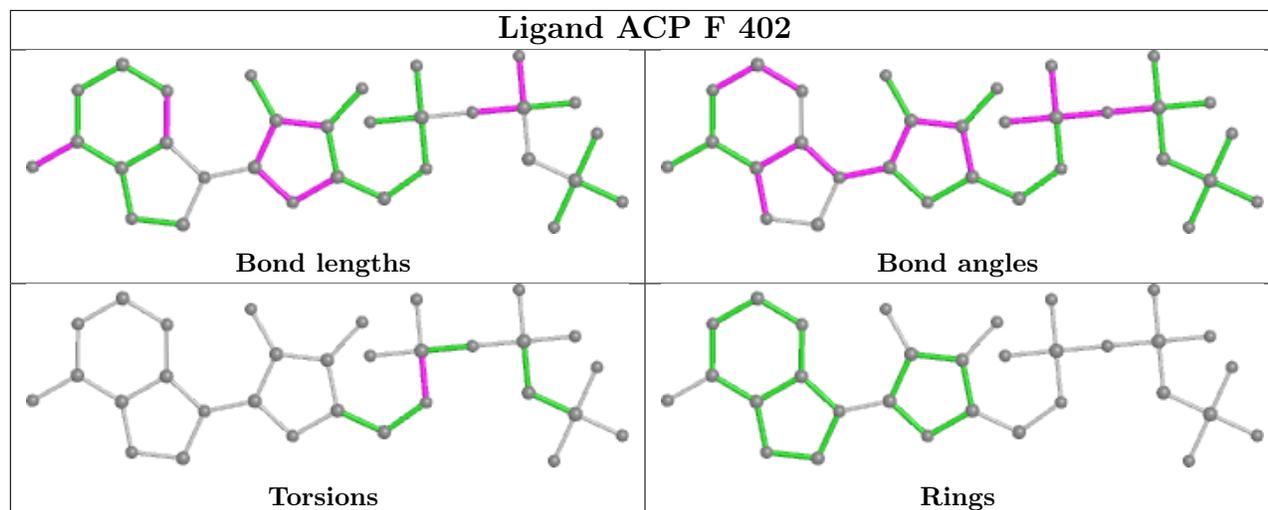
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	504	G2X	1	0
5	C	501	GTP	1	0
8	B	501	GDP	1	0
11	F	402	ACP	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 G2X C 504

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand G2X B 506

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP F 402

Bond lengths

Bond angles

Torsions

Rings
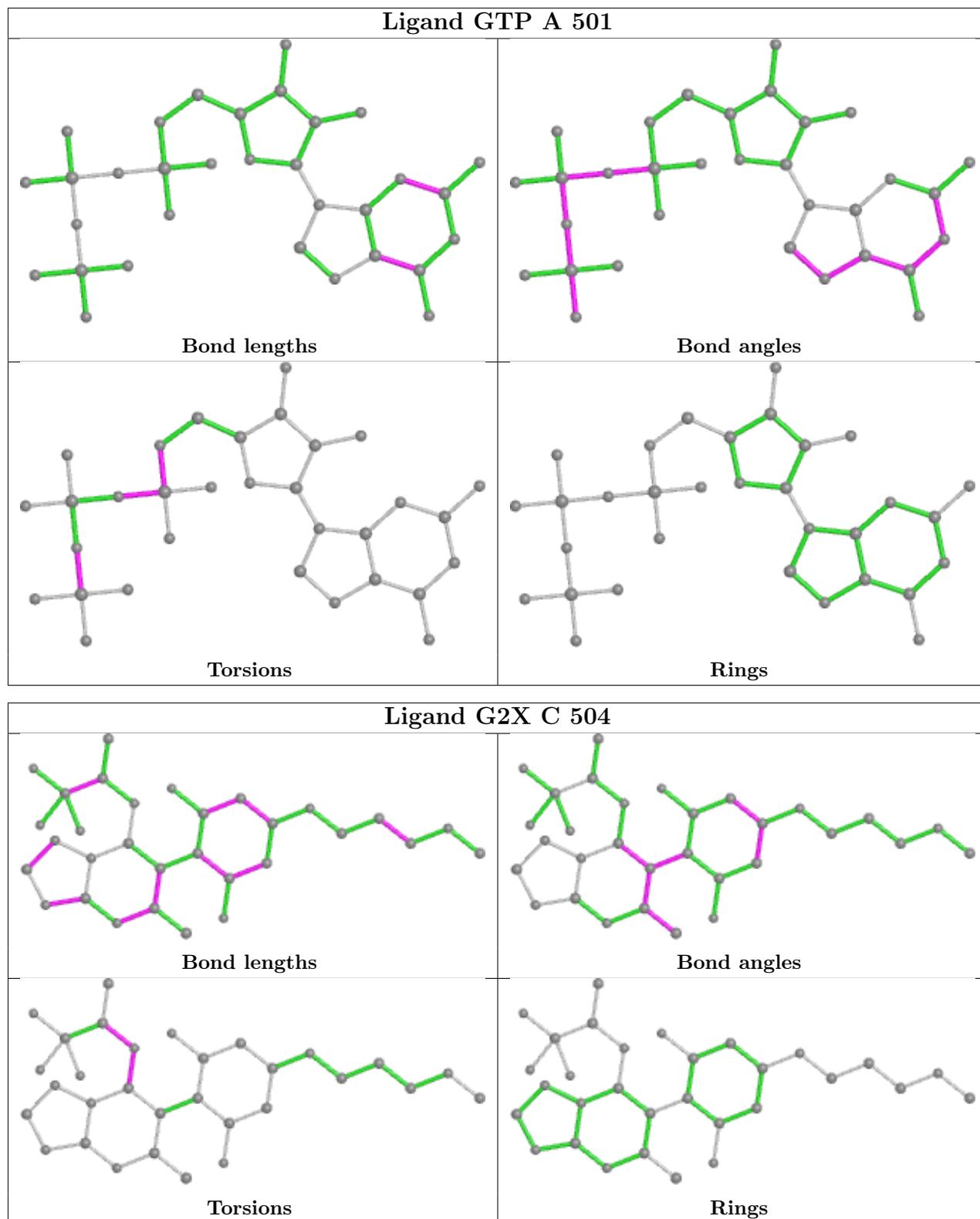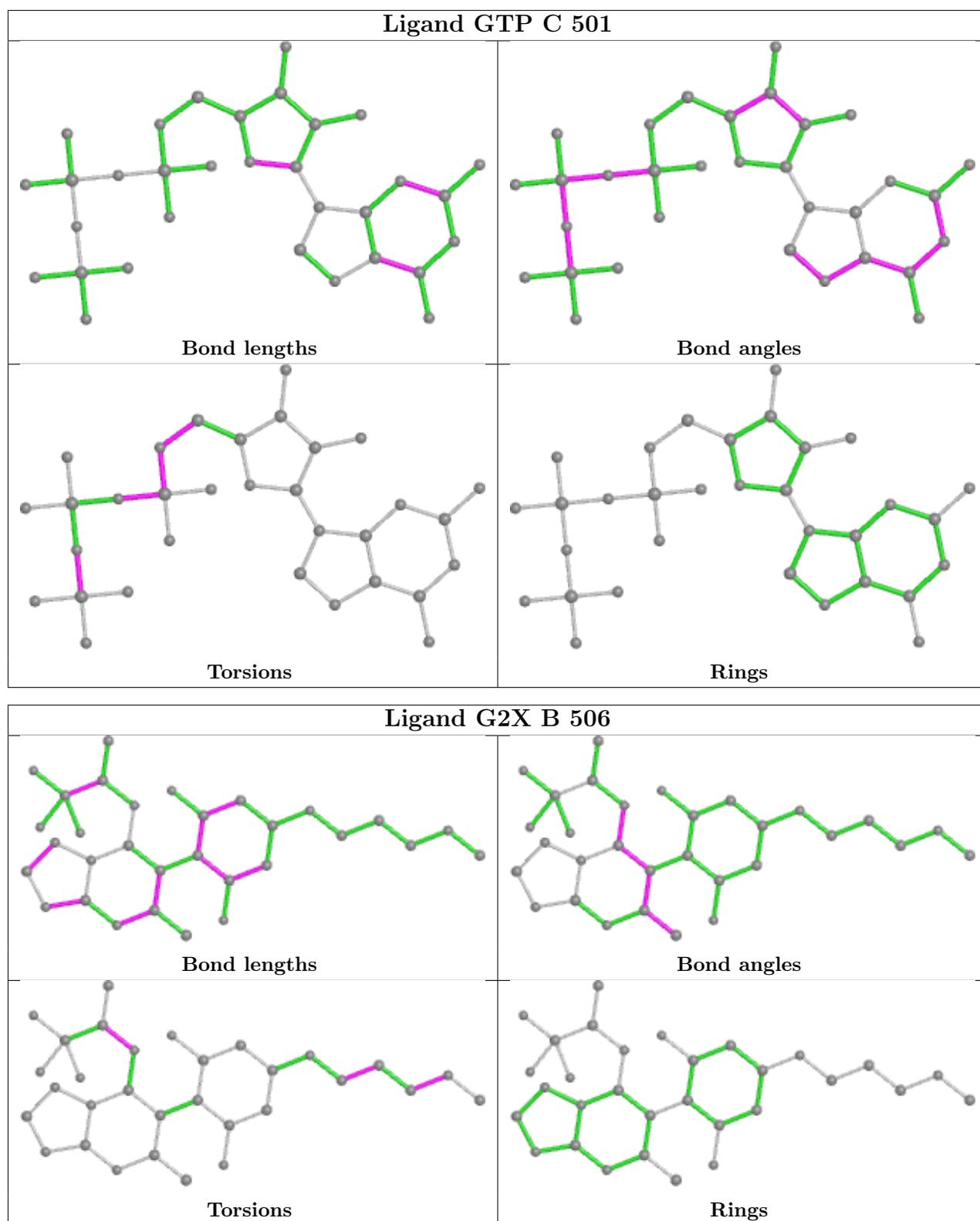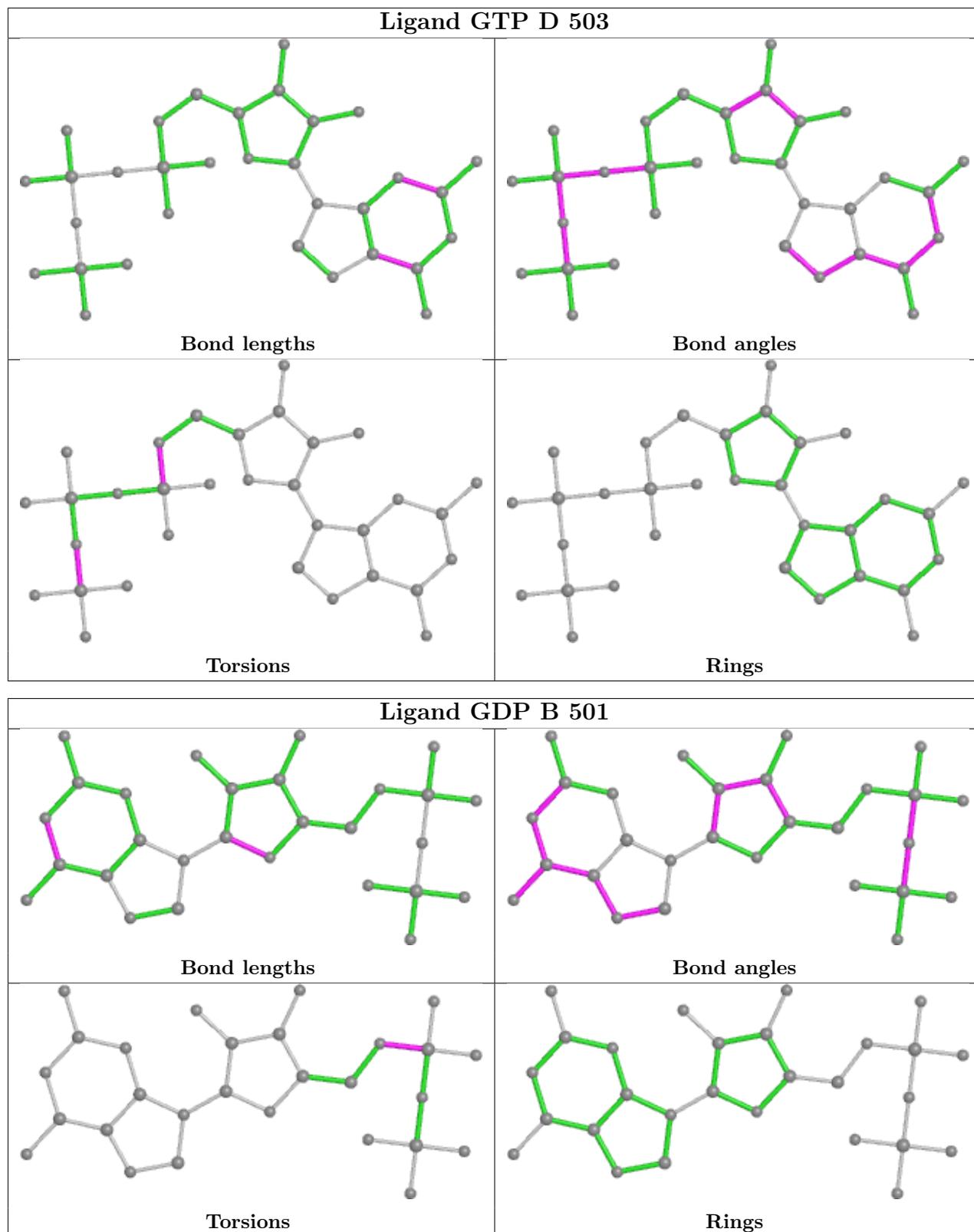
5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	438/450 (97%)	0.10	9 (2%)	63	58	14, 42, 77, 126	0
1	C	440/450 (97%)	-0.31	1 (0%)	95	95	9, 27, 53, 82	0
2	B	418/445 (93%)	-0.01	13 (3%)	49	42	8, 37, 76, 110	0
2	D	426/445 (95%)	0.38	23 (5%)	25	20	16, 52, 90, 116	0
3	E	123/143 (86%)	0.41	12 (9%)	7	5	19, 55, 96, 103	0
4	F	351/384 (91%)	0.76	58 (16%)	1	1	24, 68, 116, 130	0
All	All	2196/2317 (94%)	0.18	116 (5%)	26	21	8, 44, 93, 130	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	10.3
4	F	245	ILE	8.4
4	F	159	GLY	8.1
2	D	72	THR	7.4
1	A	282	TYR	6.5

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

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

6.3 Carbohydrates ⓘ

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	501	1/1	0.74	0.19	59,59,59,59	0
7	CA	B	504	1/1	0.76	0.26	119,119,119,119	0
6	MG	F	401	1/1	0.85	0.17	89,89,89,89	0
7	CA	C	503	1/1	0.86	0.28	98,98,98,98	0
11	ACP	F	402	31/31	0.88	0.18	69,89,110,122	0
6	MG	B	502	1/1	0.89	0.48	44,44,44,44	0
7	CA	B	505	1/1	0.92	0.17	72,72,72,72	0
7	CA	A	504	1/1	0.93	0.14	98,98,98,98	0
5	GTP	D	503	32/32	0.94	0.15	38,48,61,69	0
7	CA	D	502	1/1	0.96	0.07	78,78,78,78	0
10	G2X	B	506	31/31	0.96	0.19	24,37,57,58	0
10	G2X	C	504	31/31	0.96	0.16	18,32,59,62	0
5	GTP	C	501	32/32	0.96	0.17	15,27,49,59	0
9	MES	B	503	12/12	0.97	0.17	36,43,51,54	0
6	MG	A	502	1/1	0.97	0.20	23,23,23,23	0
5	GTP	A	501	32/32	0.98	0.25	10,28,40,49	0
8	GDP	B	501	28/28	0.98	0.19	15,28,51,64	0
7	CA	A	503	1/1	0.98	0.06	75,75,75,75	0
6	MG	C	502	1/1	0.99	0.09	19,19,19,19	0
7	CA	C	505	1/1	0.99	0.09	30,30,30,30	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 402:

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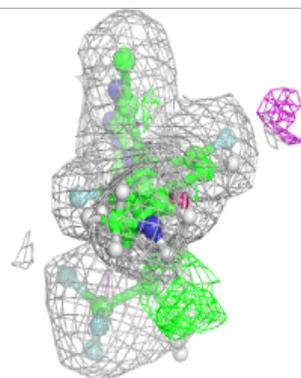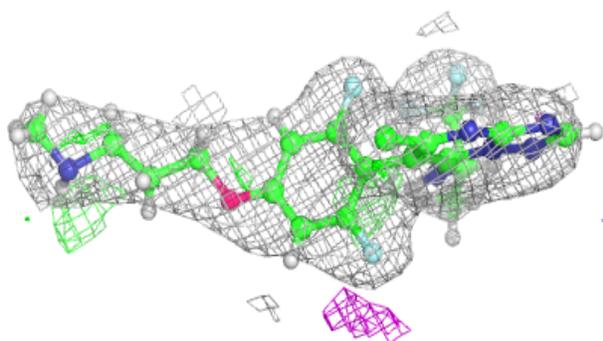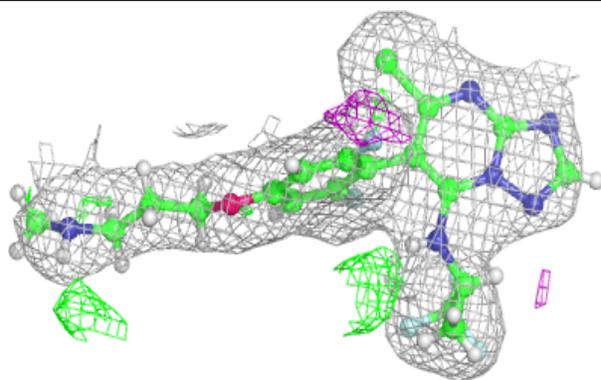mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
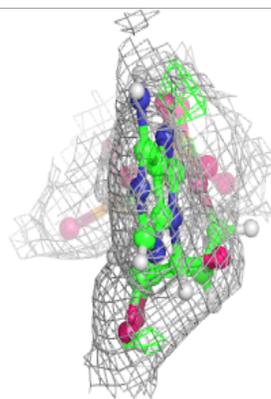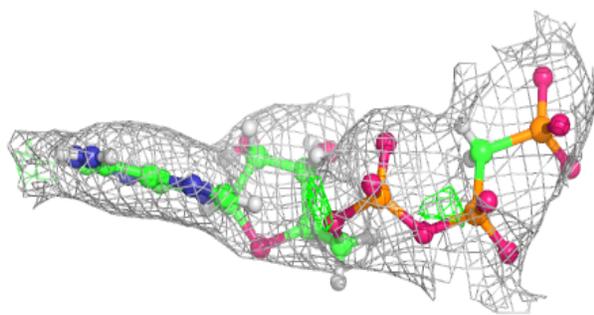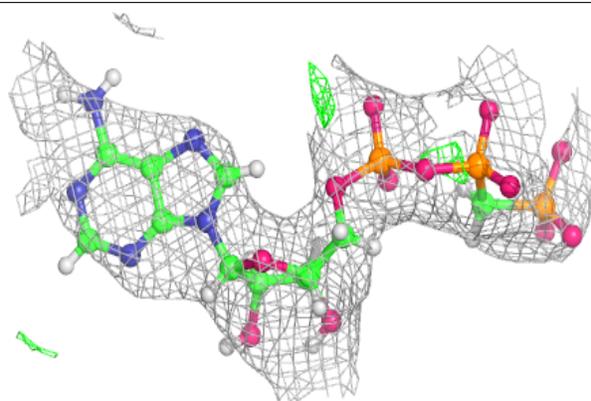
Electron density around GTP D 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
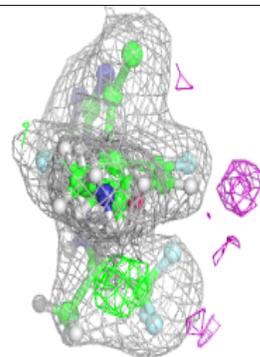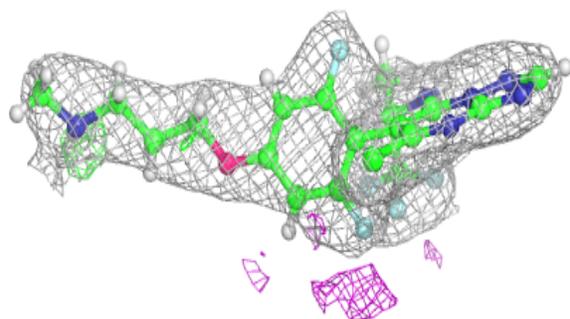mF_o-DF_c (at 3 rmsd) in purple (negative)
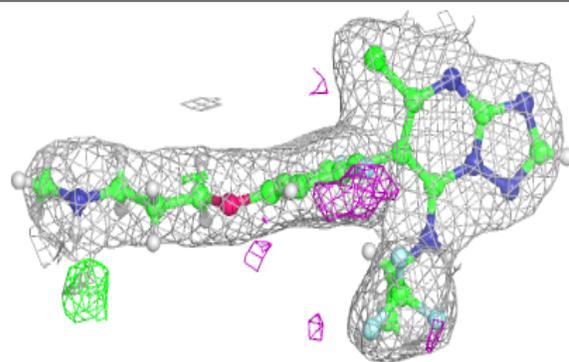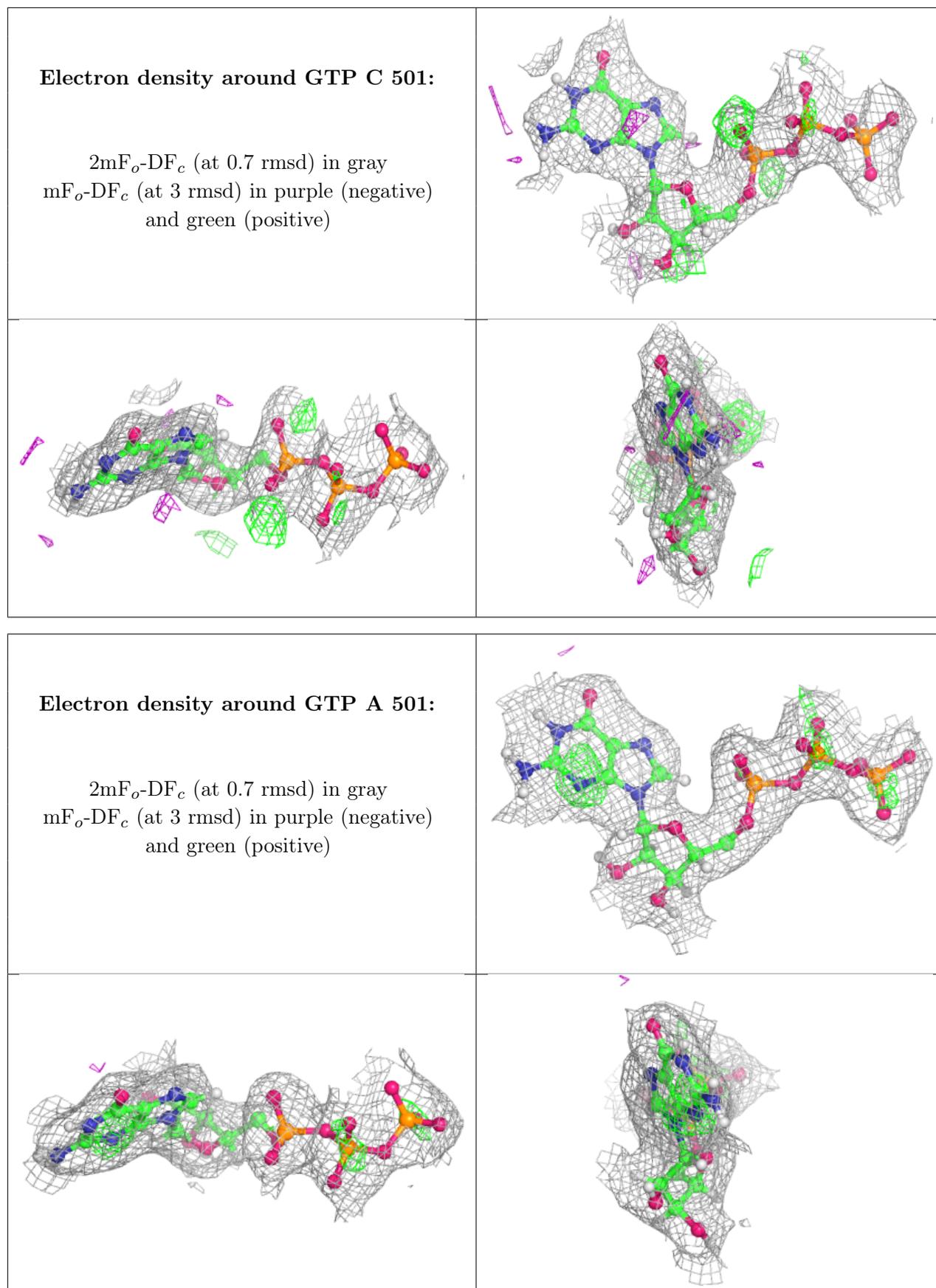and green (positive)
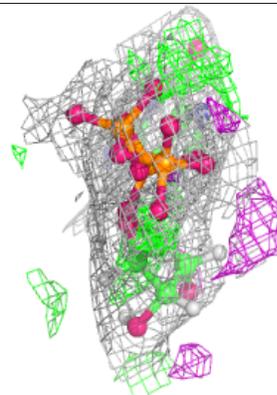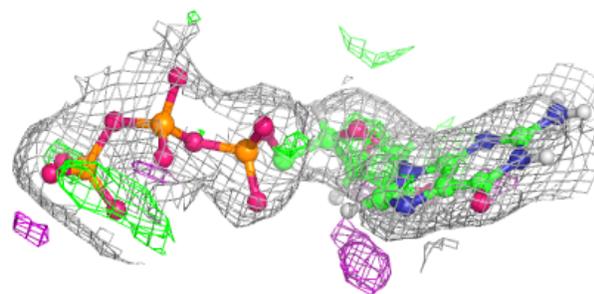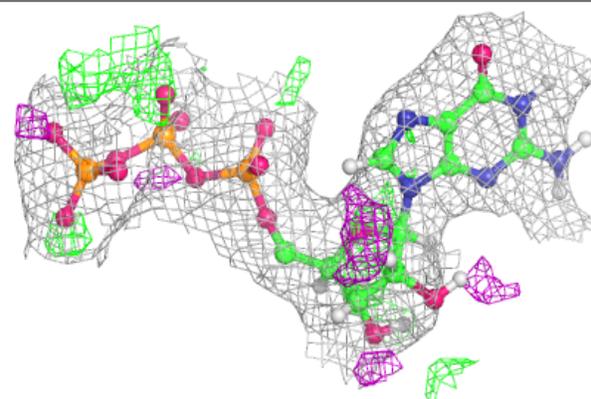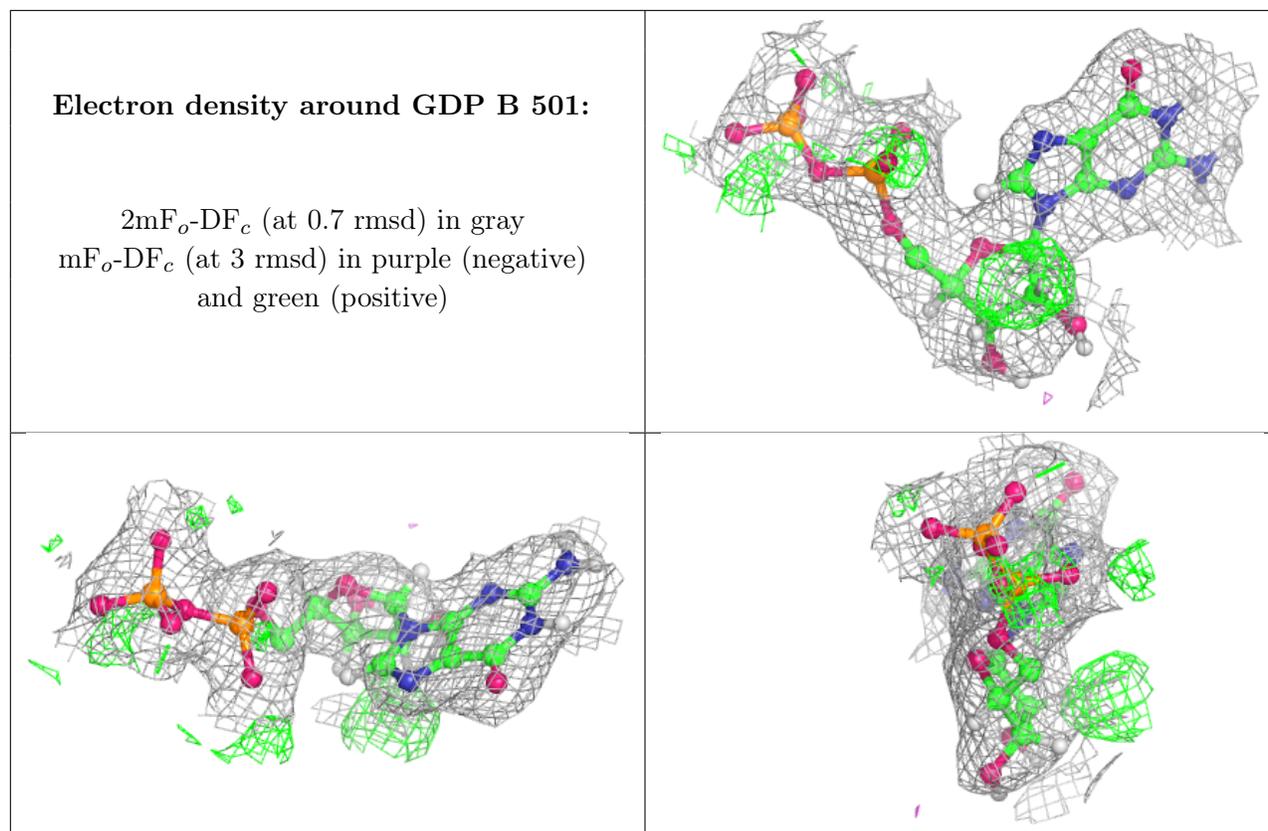
Electron density around G2X B 506:

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

Electron density around G2X 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 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 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 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 ⓘ

There are no such residues in this entry.