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 ⓘ

Mar 3, 2024 – 08:23 AM EST

PDB ID	:	6BRF
Title	:	Tubulin-RB3_SLD-TTL in complex with heterocyclic pyrimidine compound 4b
Authors	:	Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on	:	2017-11-30
Resolution	:	2.50 Å(reported)

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	:	2.36
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 2.50 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.
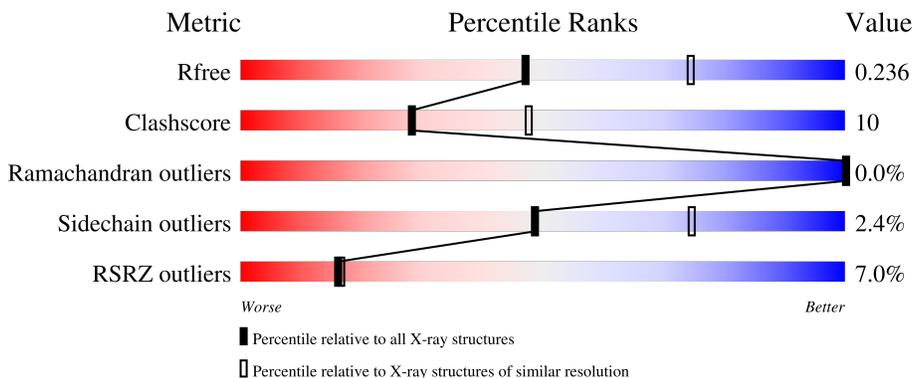
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% / 81% / 15% / · ·
1	C	450	83% / 15% / ·
2	B	445	3% / 78% / 17% / · ·
2	D	445	9% / 66% / 27% / · 5%
3	E	143	4% / 67% / 15% / · / 15%

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Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 17963 atoms, of which 14 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	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2724	1749	468	493	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: $C_{10}H_{16}N_5O_{14}P_3$).
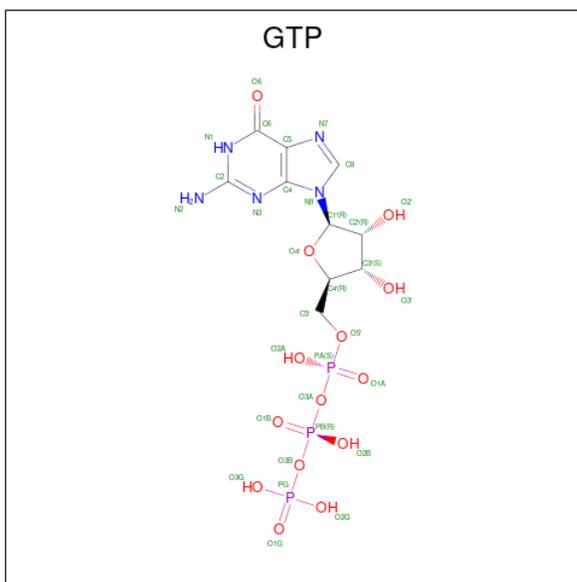
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
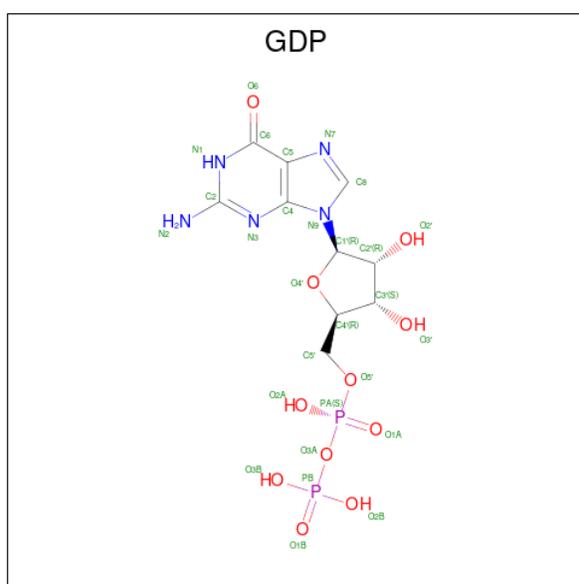
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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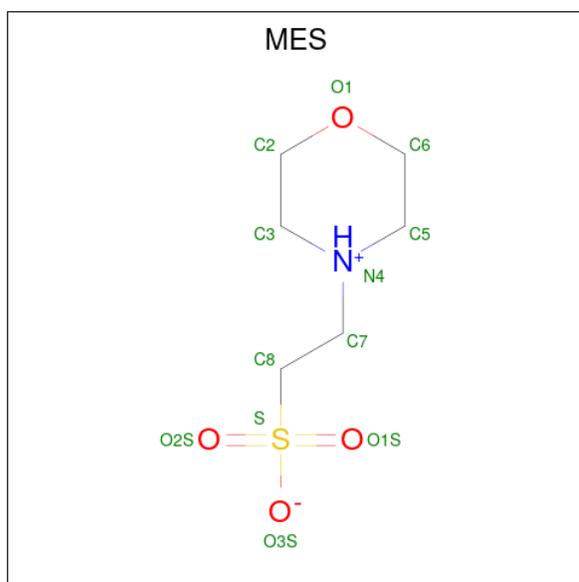
MES

C_2 \quad C_6 \quad O_1 \quad C_3 \quad C_5 \quad N_4 \quad C_7 \quad C_8 \quad S \quad O_{2S} \quad O_{1S} \quad O_{3S}

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

- Molecule 10 is 2-chloro-4-(6-methoxy-3,4-dihydroquinolin-1(2H)-yl)pyrido[3,2-d]pyrimidine (three-letter code: E44) (formula: $C_{17}H_{15}ClN_4O$) (labeled as "Ligand of Interest" by depositor).
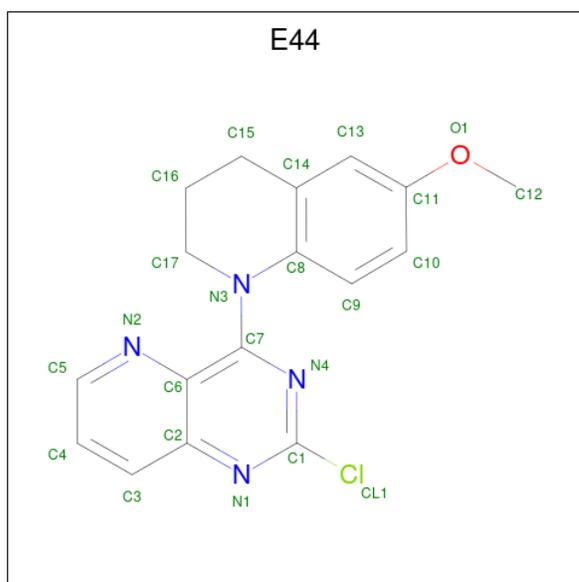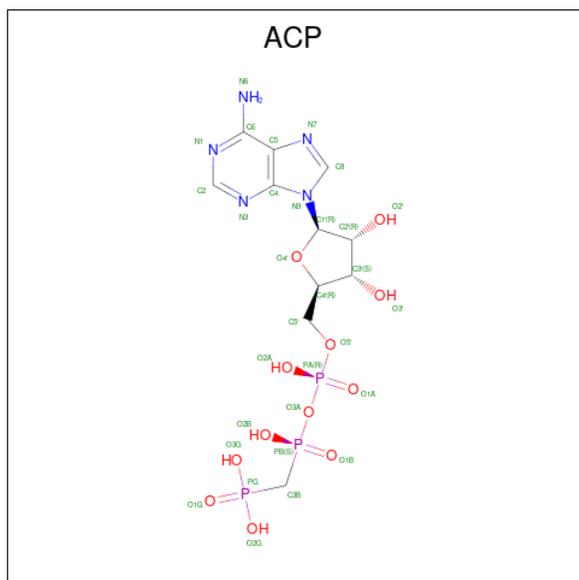
E44

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	Cl	N	O	0	0
			23	17	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total 23	C 17	Cl 1	N 4	O 1	0	0

- 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 45	C 11	H 14	N 5	O 12	P 3	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	102	Total 102	O 102	0	0
12	B	99	Total 99	O 99	0	0
12	C	191	Total 191	O 191	0	0
12	D	37	Total 37	O 37	0	0
12	E	22	Total 22	O 22	0	0
12	F	24	Total 24	O 24	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

Chain A:

- Molecule 1: Tubulin alpha-1B chain

Chain C:

- Molecule 2: Tubulin beta-2B chain

Chain B:

S296 A301 A302 C303 I316 K324 E325 V326 D327 E328 V333 K336 G360 L361 T366 T386 L377 T386 R390 M403 D404 E405 N414 D427 A428 THR ALA ASP GLU GLN GLY GLU PHE GLU GLU GLU GLY GLU ASP GLU ALA

• Molecule 2: Tubulin beta-2B chain

Chain D:

9%

66%   27%   5%

M1 R2 E3 I7 C12 Q15 I16 W21 D26 I30 G34 S35 Y36 H37 G38 L42 Q43 L44 E45 N48 A54 T55 G56 N57 K58 Y59 V60 P61 R62 A63 I64 L65 V66 D67 T72 M73 D74 S75 V76 R77 S78 G79 P80 F81 G82 Q83 I84 F85 R86

P87 F90 V91 F92 K103 G104 H105 Y106 T107 E108 G109 A110 V113 V116 L117 D118 V119 V120 R121 K122 E123 F133 Q134 L135 T136 H137 S138 L139 G140 G141 G142 T143 G144 S145 L150 L151 I152 S153 K154 I155 R156 P160 M164 N165 V169 M170 V175 S176 D177 T178

V179 V180 L192 V193 T196 I202 A206 L207 Y208 D209 I210 C211 F212 R213 T214 L215 K216 L217 T218 T219 P220 T221 D224 P243 G244 Q245 L246 N247 A248 F265 F266 M267 A271 P272 L273 THR SER ARG GLY SER GLN GLN TYR ARG ALA L284 T290 Q291 Q292 M293

N298 M299 R306 G319 R320 M321 S322 M323 K324 E328 V333 K336 Y340 E343 W344 I345 N348 P357 P358 R359 M363 F367 Q375 E376 L377 T386 F389 R390 R391 K392 A393 F394 L395 H396 W397 Y398 T399 G400 E401 D404 E405 M406 D417 L418

V419 S420 E421 A430 D431 GLU GLN GLY GLU PHE GLU GLU GLU GLY GLU ASP GLU ALA

• Molecule 3: Stathmin-4

Chain E:

4%

67%   15%   15%

MET ALA ASP M6 E7 V8 I9 G17 V22 I23 L24 K25 P26 P27 S28 PHE ASP GLY VAL PRO GLU PHE ASN ALA SER LEU PRO ARG ARG D44 P45 S46 L47 E48 E49 K52 K53 L54 E58 R61 L72 K75 R76 L120 K126 R134 K135 N136 K137

E138 L139 K140 E141 GLU ALA SER ARG

• Molecule 4: Tubulin tyrosine ligase

Chain F:

23%

59%   25%   14%

M1 Y2 T3 D8 E9 S12 V13 E16 V17 S18 R19 L20 L21 L22 A23 T24 G25 Q26 W27 R31 N34 P35 N38 L39 M40 R44 L47 H54 L61 V78 I81 E86 L87 S88 E89 S90 C91 E96 S97 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 THR ASP GLU R128 E129 V130 F131 L132 A133 A134 Y135 N136 R137 R138 R139 E140 G141 R142 E143 G144 N145 V146 W147 I148 A149 LYS SER SER ALA GLY ALA LYS GLY GLU ILE L161 I162 S163 S164

E165 A166 S167 E168 L169 L170 D171 F172 I173 D174 E175 Q176 G177 Q178 V179 H180 V181 I182 Q183 L186 E187 K188 P189 L190 L191 L192 E193 P194 G195 H196 R197 K198 F199 R202 V205 L206 Y211 Y216 R217 E218 G219 R222 T223 S224 S225 E226 P227 Y228 A231 N232 F233 Q234 D235

K236 T237 C238 H239 N242 H243 C244 I245 Q246 K247 GLU TYR SER LYS N252 Y253 G254 R255 Y256 E257 E258 G259 N260 E261 M262 F263 F264 I287 I291 I298 E299 I302 K305 H306 L307 Q310 F315 G316 F317 D318 F319 E323 K326 V327 W328 E331 C338

K341 L342 Y343 Q348 D352 V353 A354 L361 A362 ASP THR GLY GLN LYS THR SER GLN PRO T372 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	105.13Å 157.75Å 181.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 2.50 49.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.78-2.50) 98.8 (49.78-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.237 0.187 , 0.236	Depositor DCC
R_{free} test set	5208 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.9	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	0.94	EDS
Total number of atoms	17963	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, E44, MG, ACP, MES, GDP, CA

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	0.34	0/3494	0.52	0/4743
1	C	0.38	0/3515	0.55	0/4772
2	B	0.35	0/3436	0.51	0/4654
2	D	0.31	0/3382	0.49	0/4581
3	E	0.31	0/1008	0.42	0/1337
4	F	0.30	0/2786	0.47	0/3764
All	All	0.34	0/17621	0.51	0/23851

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 ⓘ

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	3331	53	0
1	C	3437	0	3348	45	0
2	B	3361	0	3238	54	0
2	D	3309	0	3189	100	0
3	E	1000	0	1018	24	0
4	F	2724	0	2690	76	0
5	A	32	0	12	0	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	C	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	F	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	4	0
9	B	24	0	24	5	0
10	B	23	0	0	1	0
10	D	23	0	0	0	0
11	F	31	14	13	0	0
12	A	102	0	0	3	0
12	B	99	0	0	2	0
12	C	191	0	0	6	0
12	D	37	0	0	4	0
12	E	22	0	0	1	0
12	F	24	0	0	0	0
All	All	17949	14	16899	336	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 10.

The worst 5 of 336 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:OE2	1:C:73:THR:HB	1.67	0.94
4:F:226:GLU:HG3	4:F:237:THR:HG23	1.59	0.84
2:D:60:VAL:HG11	2:D:86:ARG:HG3	1.61	0.83
4:F:223:THR:HG21	4:F:257:GLU:OE2	1.82	0.79
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.16	0.79

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	435/450 (97%)	425 (98%)	10 (2%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	417/445 (94%)	409 (98%)	8 (2%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	322/384 (84%)	306 (95%)	15 (5%)	1 (0%)	41	61
All	All	2154/2317 (93%)	2101 (98%)	52 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	91	CYS

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	368/378 (97%)	362 (98%)	6 (2%)	62	84
1	C	371/378 (98%)	366 (99%)	5 (1%)	69	87
2	B	369/383 (96%)	362 (98%)	7 (2%)	57	80
2	D	364/383 (95%)	356 (98%)	8 (2%)	52	77
3	E	109/127 (86%)	106 (97%)	3 (3%)	43	70
4	F	298/342 (87%)	282 (95%)	16 (5%)	22	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1879/1991 (94%)	1834 (98%)	45 (2%)	49	74

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	136	ASN
4	F	197	ARG
4	F	12	SER
4	F	90	SER
4	F	211	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
2	B	99	ASN
1	C	356	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 15 ligands modelled in this entry, 6 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	7	26,34,34	1.16	1 (3%)	32,54,54	1.41	7 (21%)
11	ACP	F	402	7	27,33,33	4.72	10 (37%)	32,52,52	2.33	5 (15%)
10	E44	B	505	-	25,26,26	0.87	2 (8%)	30,37,37	1.32	2 (6%)
5	GTP	C	501	7	26,34,34	1.05	1 (3%)	32,54,54	1.41	7 (21%)
8	GDP	D	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.19	5 (16%)
8	GDP	B	501	7	24,30,30	0.98	1 (4%)	30,47,47	1.17	4 (13%)
9	MES	B	502	-	12,12,12	2.02	1 (8%)	14,16,16	2.16	4 (28%)
10	E44	D	502	-	25,26,26	0.89	2 (8%)	30,37,37	1.30	2 (6%)
9	MES	B	503	-	12,12,12	2.22	1 (8%)	14,16,16	1.91	5 (35%)

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	7	-	6/18/38/38	0/3/3/3
11	ACP	F	402	7	-	3/15/38/38	0/3/3/3
10	E44	B	505	-	-	2/5/16/16	0/4/4/4
5	GTP	C	501	7	-	7/18/38/38	0/3/3/3
8	GDP	D	501	-	-	5/12/32/32	0/3/3/3
8	GDP	B	501	7	-	3/12/32/32	0/3/3/3
9	MES	B	502	-	-	4/6/14/14	0/1/1/1
10	E44	D	502	-	-	2/5/16/16	0/4/4/4
9	MES	B	503	-	-	1/6/14/14	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O4'-C1'	15.13	1.62	1.41
11	F	402	ACP	C2'-C1'	-14.98	1.31	1.53
9	B	503	MES	C8-S	-7.32	1.67	1.77
11	F	402	ACP	PB-O3A	6.97	1.66	1.58
9	B	502	MES	C8-S	-6.69	1.68	1.77

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	402	ACP	C5-C6-N6	8.63	133.47	120.35
11	F	402	ACP	N6-C6-N1	-5.65	106.84	118.57
11	F	402	ACP	N3-C2-N1	-5.34	120.34	128.68
10	B	505	E44	N1-C1-N4	-5.10	125.48	130.62
10	D	502	E44	N1-C1-N4	-4.91	125.67	130.62

There are no chirality outliers.

5 of 33 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	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	E44	1	0
8	D	501	GDP	4	0
8	B	501	GDP	1	0
9	B	502	MES	2	0
9	B	503	MES	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 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 402

Bond lengths

Bond angles

Torsions

Rings

Ligand E44 B 505

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand E44 D 502

Bond lengths

Bond angles

Torsions

Rings
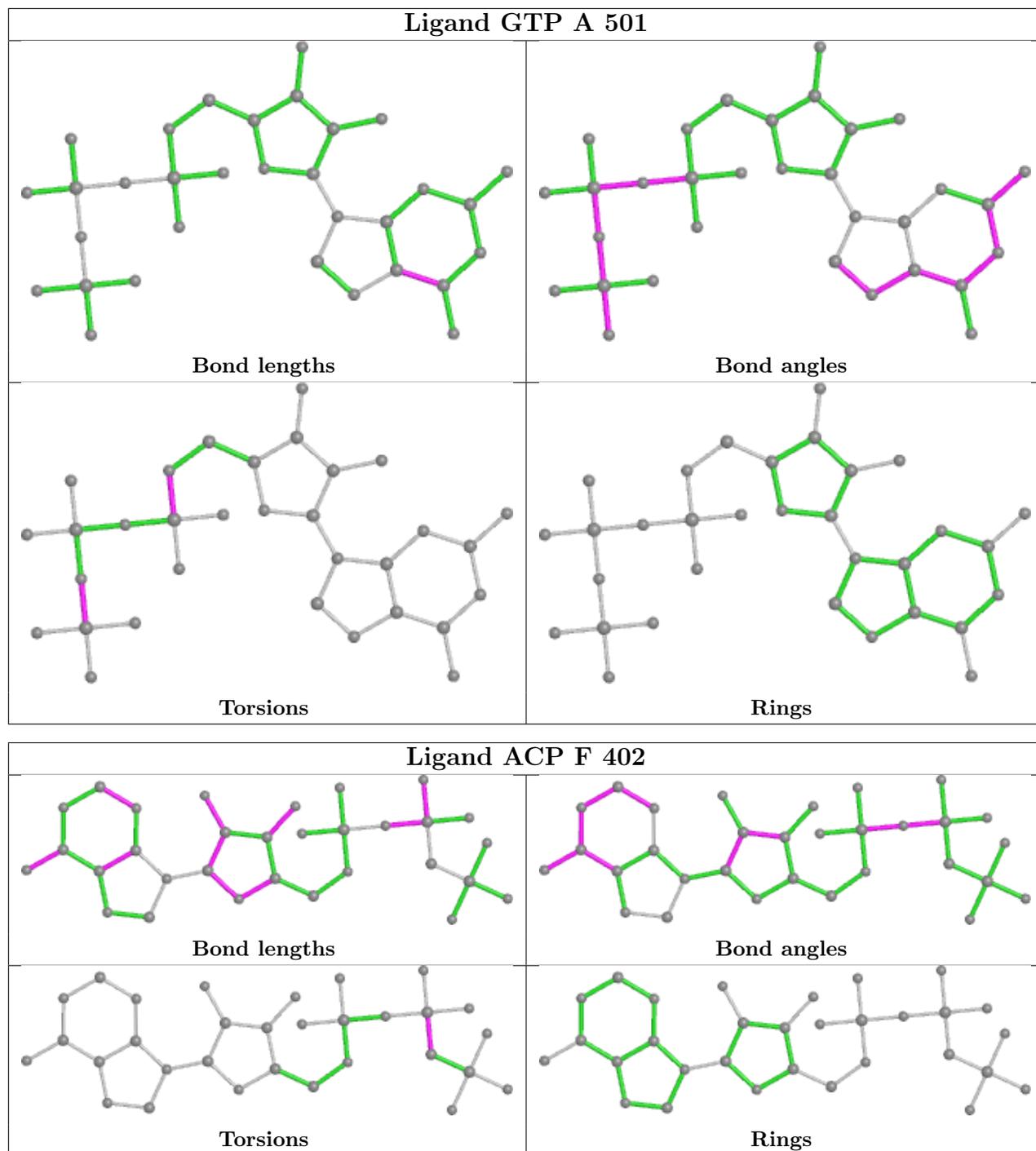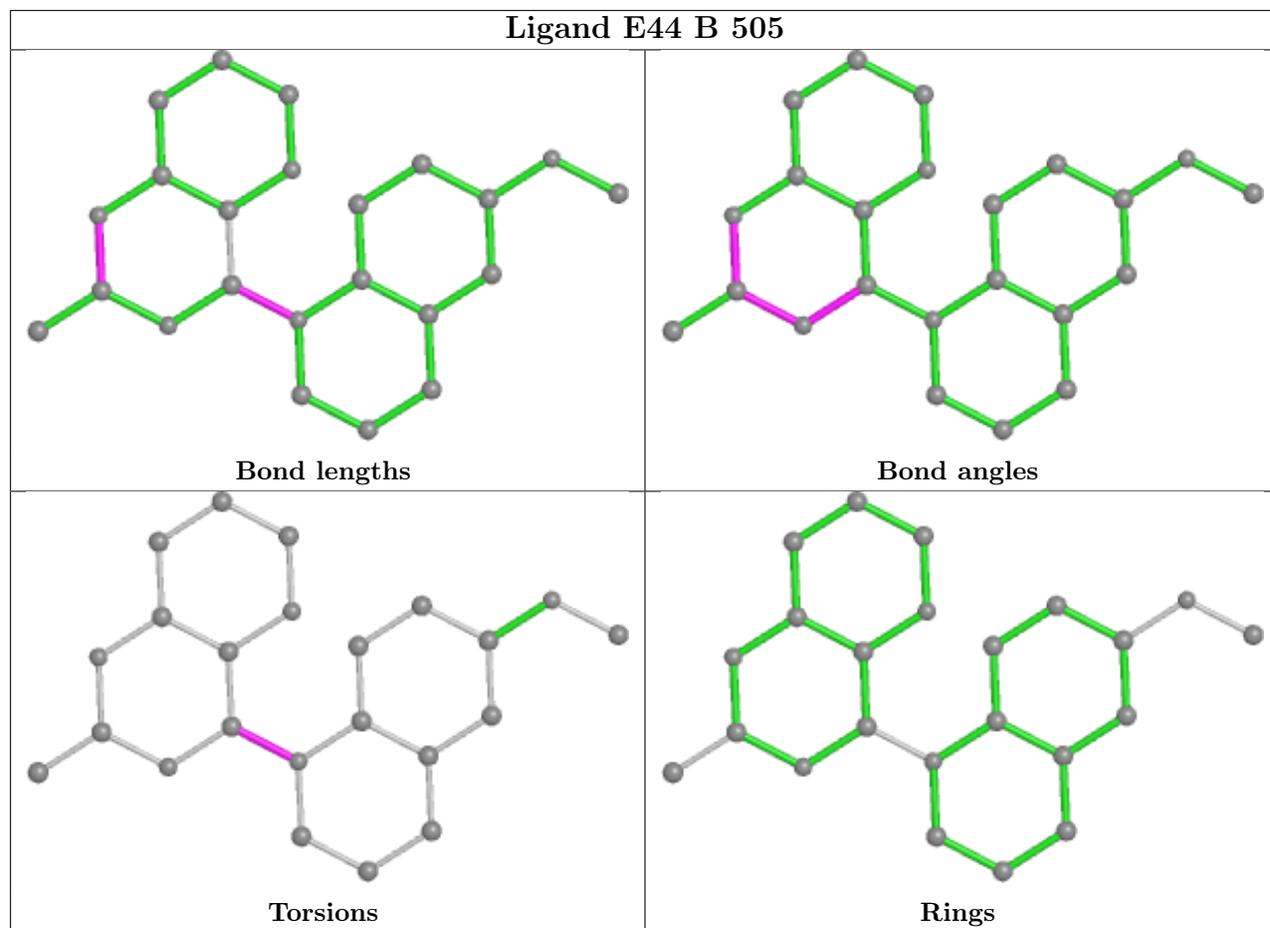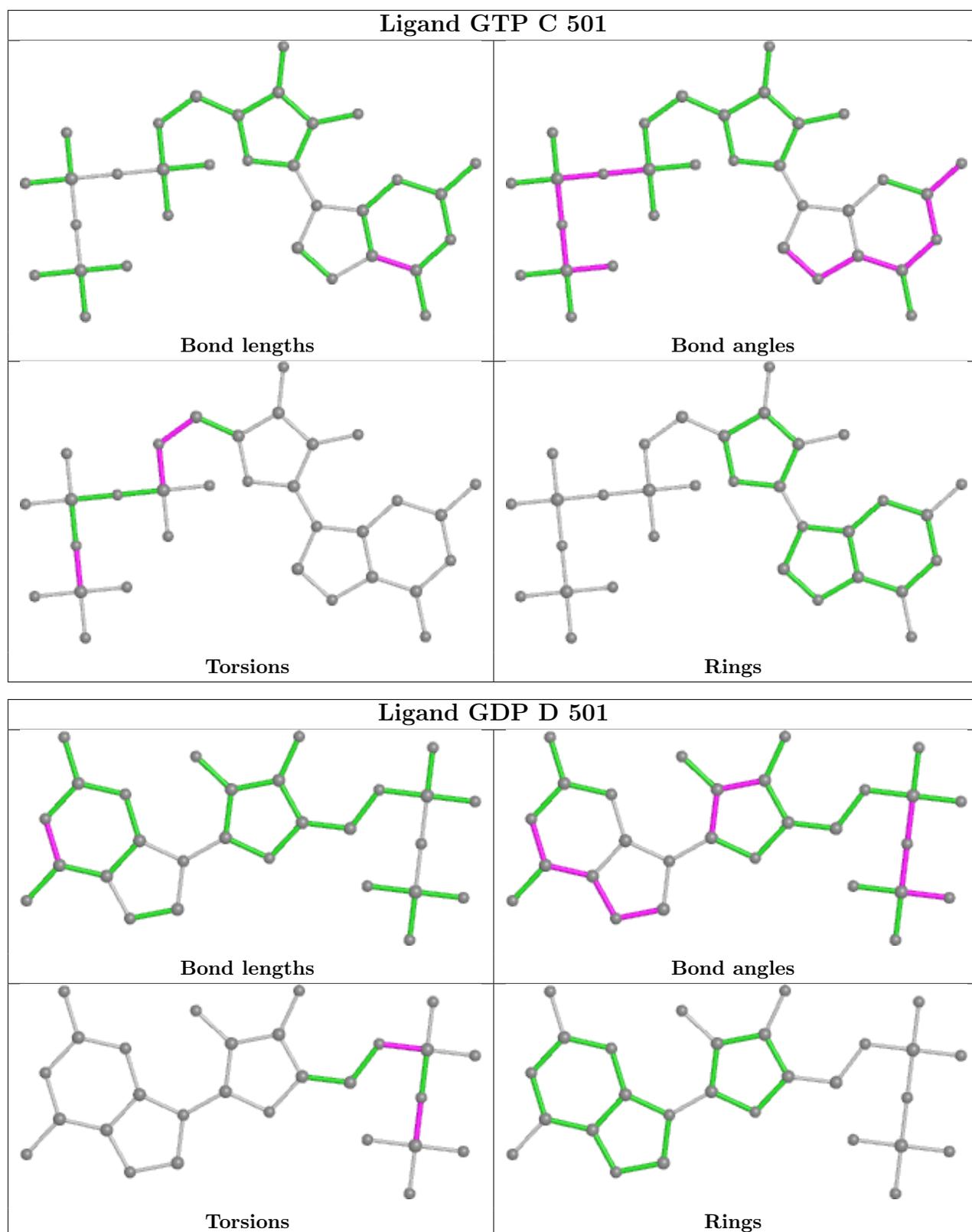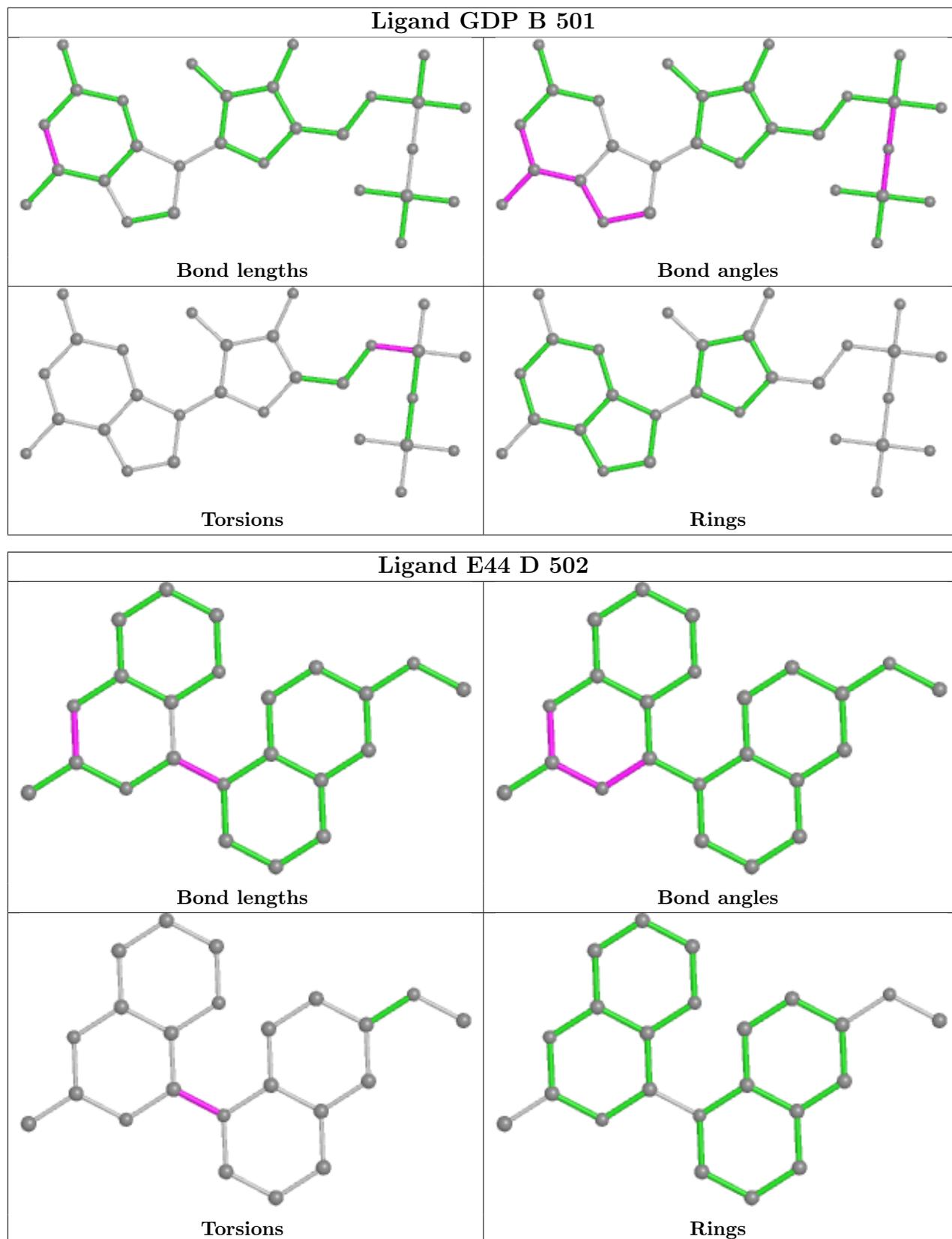
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	437/450 (97%)	-0.12	8 (1%)	68	71	24, 42, 73, 86	0
1	C	440/450 (97%)	-0.32	0	100	100	19, 31, 59, 84	0
2	B	427/445 (95%)	-0.13	14 (3%)	46	50	20, 39, 77, 126	0
2	D	421/445 (94%)	0.42	38 (9%)	9	9	29, 63, 102, 132	0
3	E	121/143 (84%)	0.16	6 (4%)	28	30	28, 56, 88, 105	0
4	F	332/384 (86%)	0.96	87 (26%)	0	0	30, 69, 130, 149	0
All	All	2178/2317 (94%)	0.12	153 (7%)	16	16	19, 47, 100, 149	0

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	8.5
4	F	173	ILE	7.6
4	F	134	ALA	6.1
4	F	130	VAL	5.7
4	F	167	SER	5.5

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
7	MG	F	401	1/1	0.83	0.14	104,104,104,104	0
11	ACP	F	402	31/31	0.88	0.19	79,102,130,151	0
8	GDP	D	501	28/28	0.93	0.13	50,58,65,70	0
10	E44	D	502	23/23	0.96	0.16	29,35,50,58	0
9	MES	B	503	12/12	0.96	0.18	69,70,82,82	0
9	MES	B	502	12/12	0.97	0.13	33,42,55,62	0
7	MG	B	504	1/1	0.97	0.19	26,26,26,26	0
10	E44	B	505	23/23	0.98	0.14	30,36,44,49	0
8	GDP	B	501	28/28	0.98	0.19	17,25,30,37	0
7	MG	A	503	1/1	0.98	0.12	26,26,26,26	0
5	GTP	C	501	32/32	0.99	0.15	24,26,30,31	0
7	MG	C	503	1/1	0.99	0.10	25,25,25,25	0
6	CA	A	502	1/1	0.99	0.03	66,66,66,66	0
6	CA	C	502	1/1	0.99	0.05	41,41,41,41	0
5	GTP	A	501	32/32	0.99	0.19	23,28,32,36	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
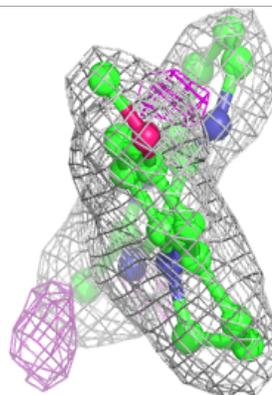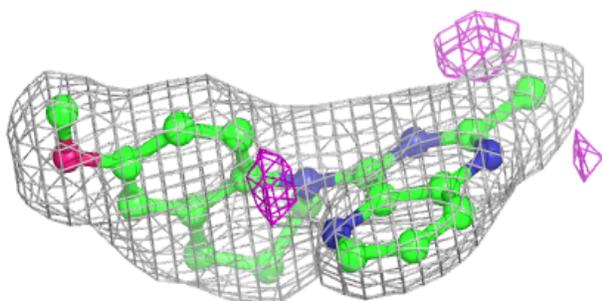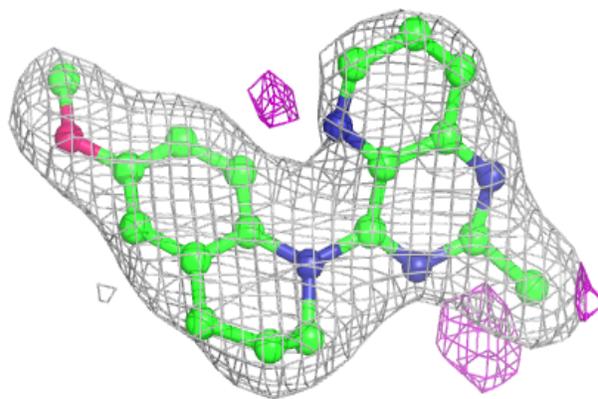mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
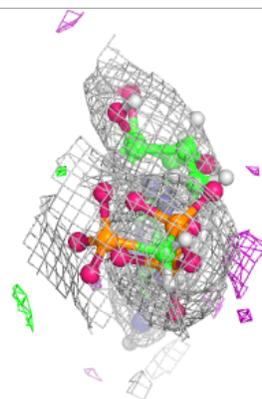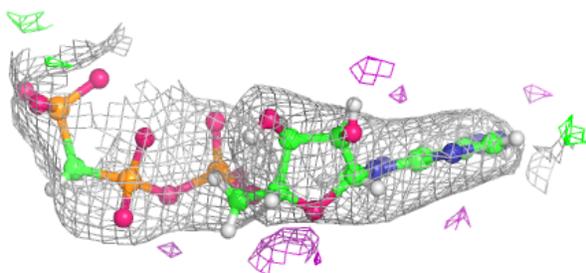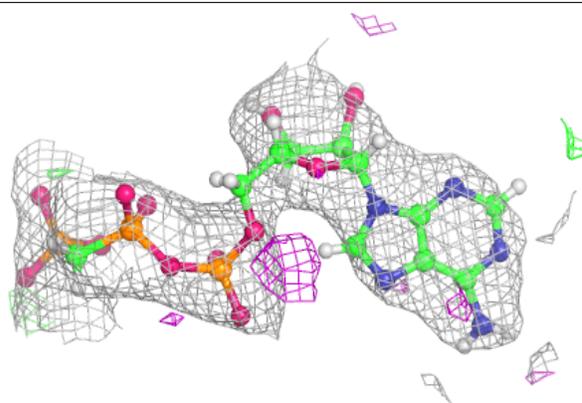
Electron density around GDP D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
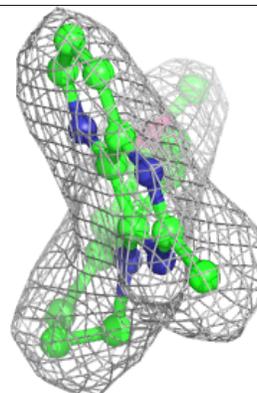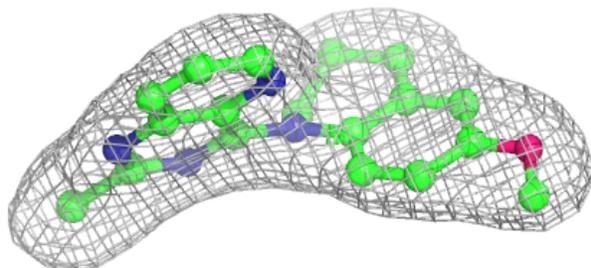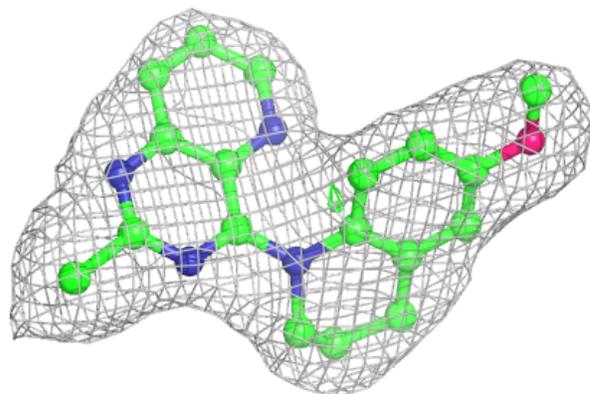mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
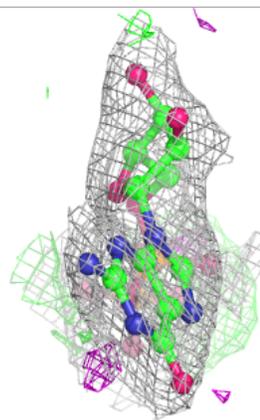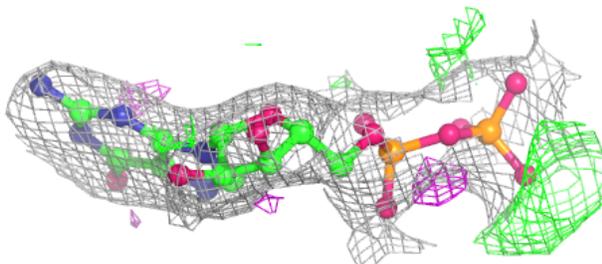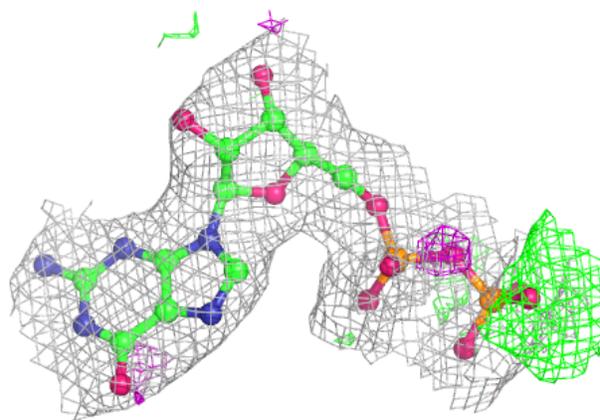
Electron density around E44 D 502:

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

**Electron density around E44 B 505:**

$2mF_o\text{-}DF_c$ (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:

$2mF_o\text{-}DF_c$ (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:

$2mF_o$-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)
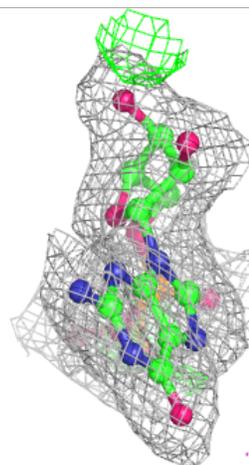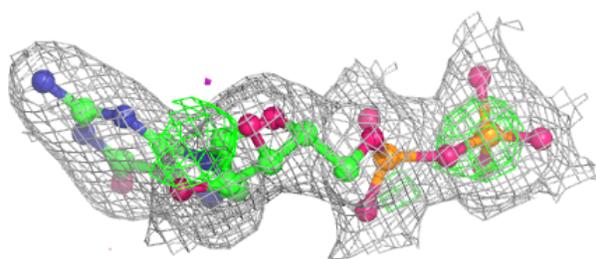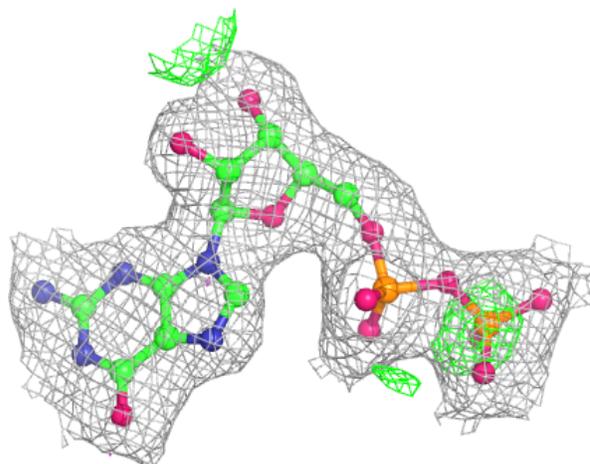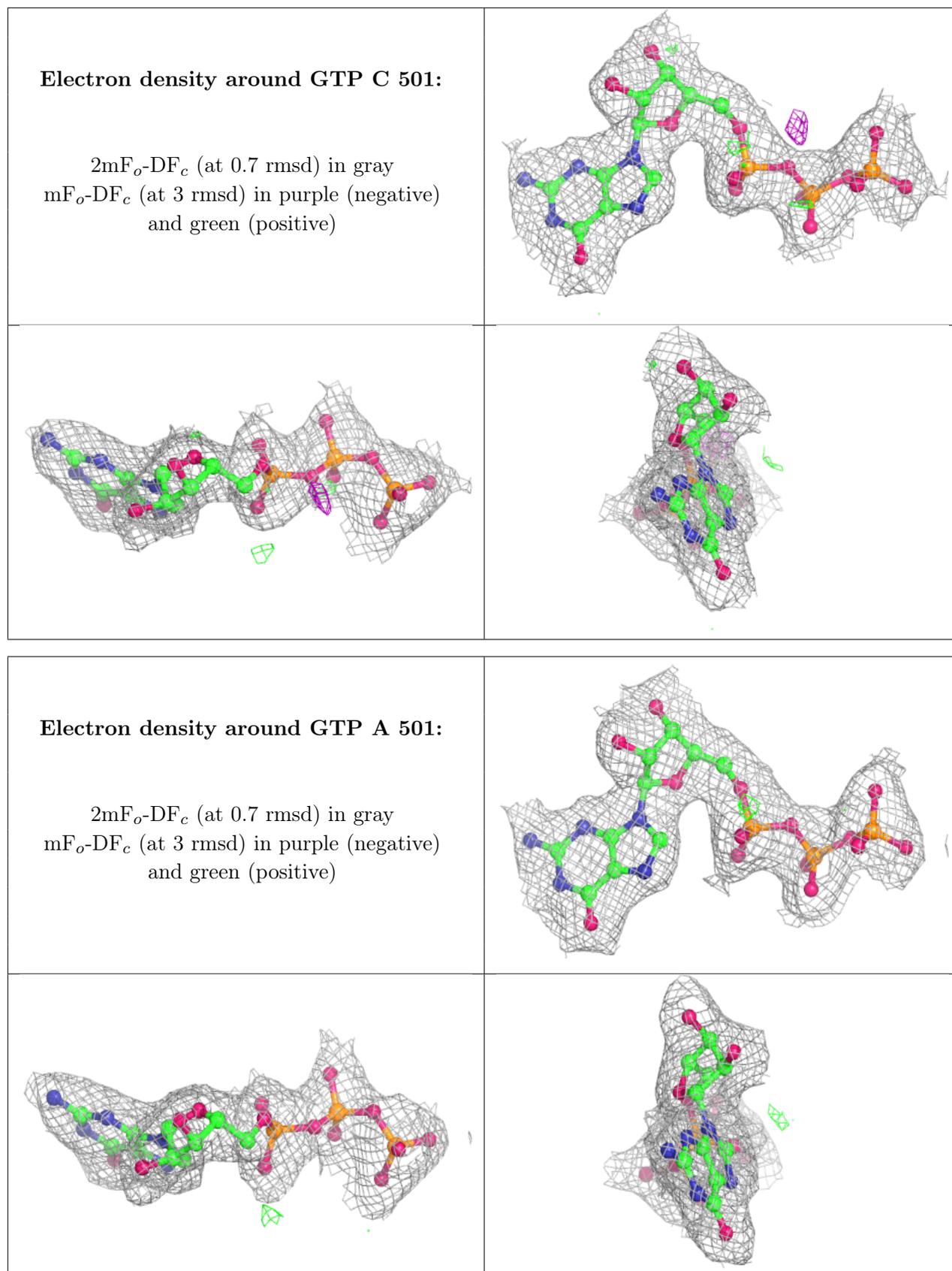
6.5 Other polymers (i)

There are no such residues in this entry.