



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:34 PM UTC

PDB ID : 5XLT / pdb_00005xlt
Title : The crystal structure of tubulin in complex with 4'-demethylepipodophyllotoxin
Authors : Yu, Y.; Chen, Q.
Deposited on : 2017-05-11
Resolution : 2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

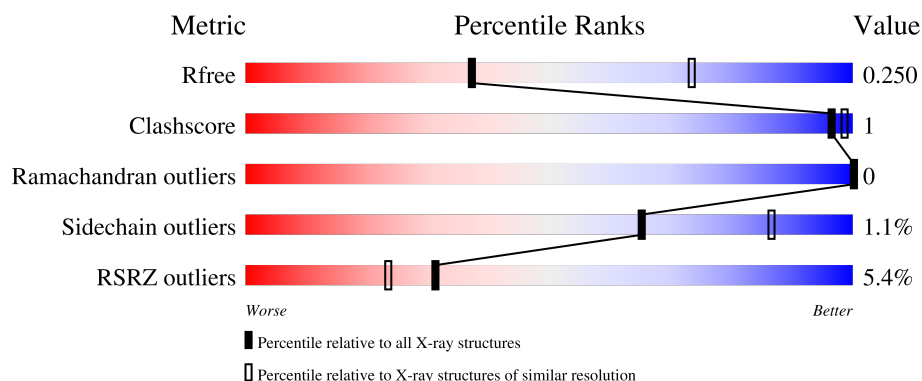
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	450	2% 95% ..
1	C	450	% 96% ..
2	B	445	2% 92% ..
2	D	445	8% 91% 5%
3	E	143	5% 83% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	14% 83% • 13%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 34508 atoms, of which 16893 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	H	N	O	S	0	0	0
			6734	2163	3318	581	650	22			
1	C	440	Total	C	H	N	O	S	0	1	0
			6789	2180	3344	585	657	23			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	1	0
			6604	2115	3235	577	650	27			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2014	617	1014	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 P63043
E	4	ALA	-	expression tag	UNP P63043

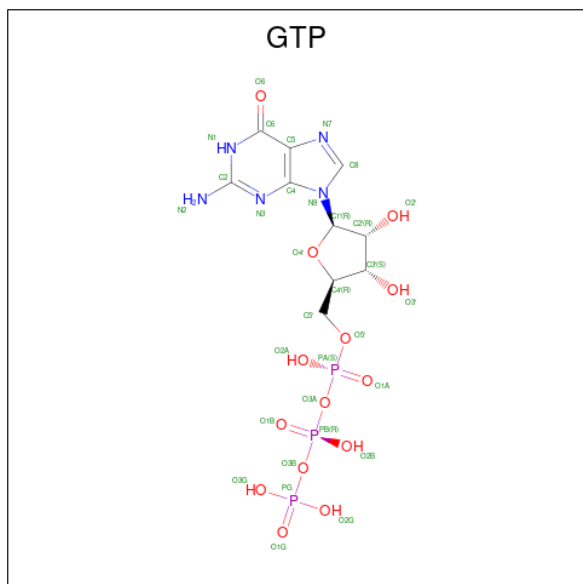
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	0	0
			5442	1761	2698	470	499	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 (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	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		

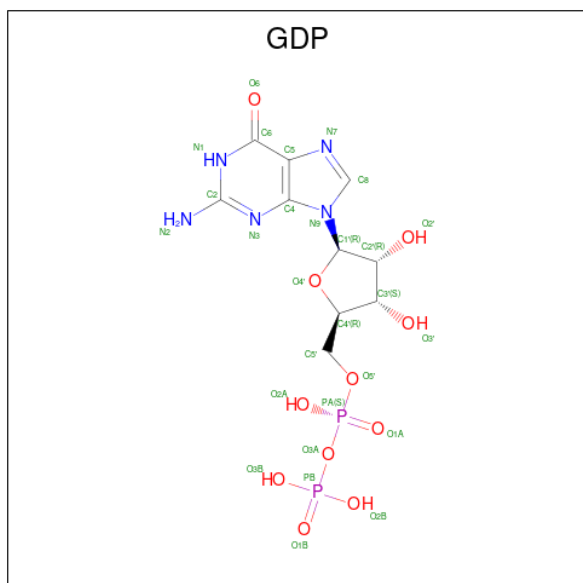
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

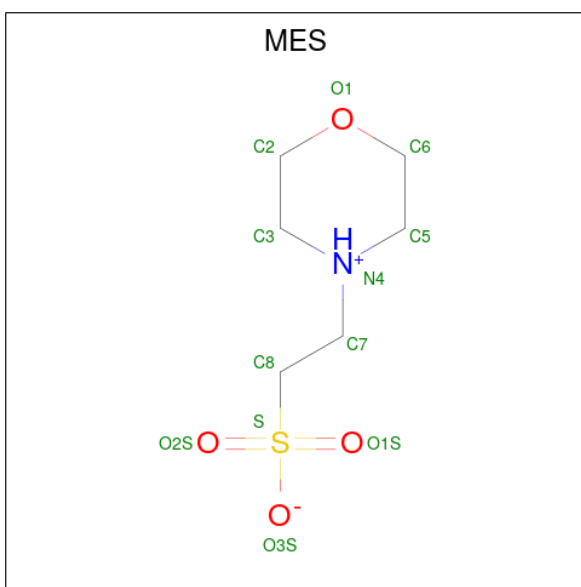
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: 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		

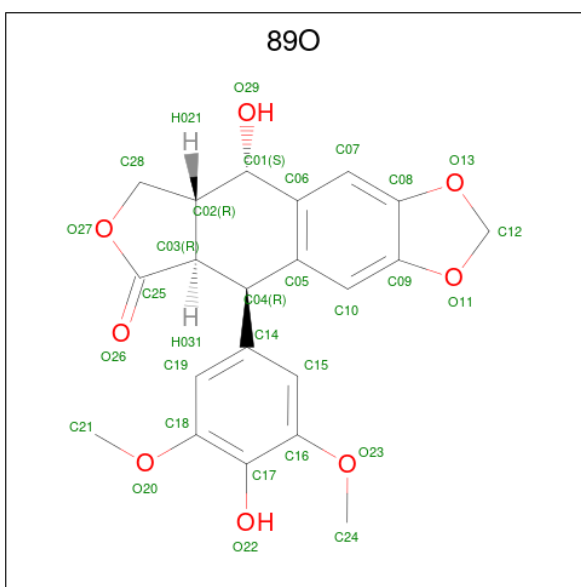
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		
9	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 10 is (5S,5aR,8aR,9R)-9-(3,5-dimethoxy-4-oxidanyl-phenyl)-5-oxidanyl-5a,6,8a,9-tetrahydro-5H-[2]benzofuro[6,5-f][1,3]benzodioxol-8-one (CCD ID: 89O) (formula: C₂₁H₂₀O₈).



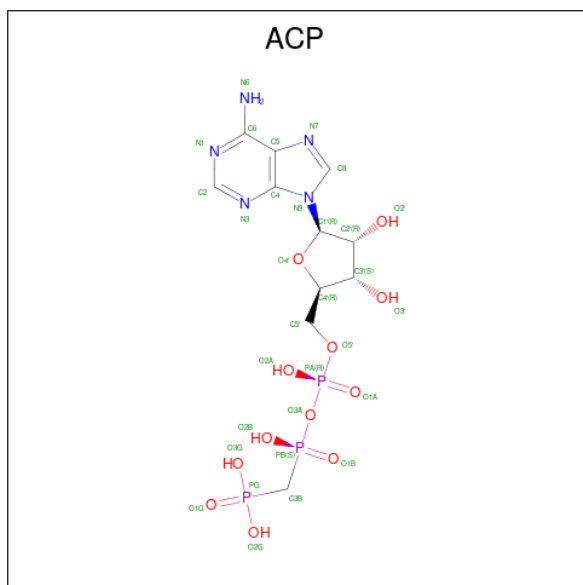
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			49	21	20	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	H	O	0	0
			49	21	20	8		

- 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	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	25	Total	O	0	0
			25	25		
12	B	16	Total	O	0	0
			16	16		
12	C	37	Total	O	0	0
			37	37		
12	D	9	Total	O	0	0
			9	9		
12	E	2	Total	O	0	0
			2	2		
12	F	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

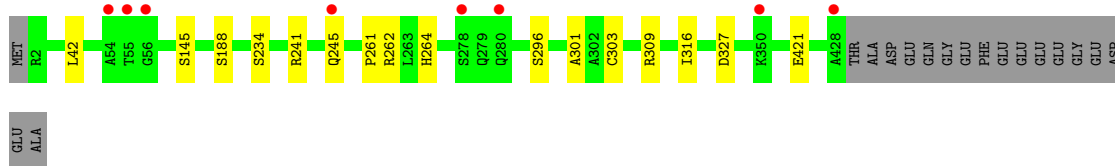
- Molecule 1: Tubulin alpha-1B chain



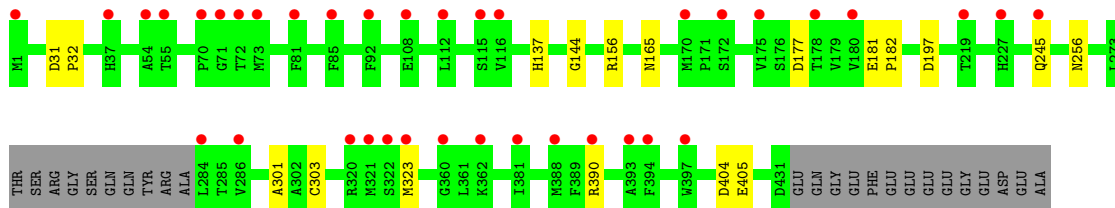
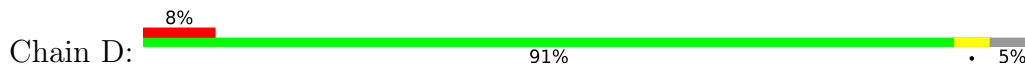
- Molecule 1: Tubulin alpha-1B chain



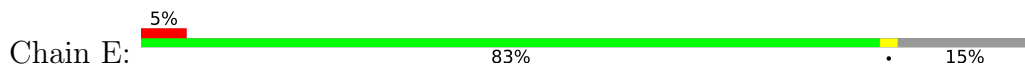
- Molecule 2: Tubulin beta-2B chain

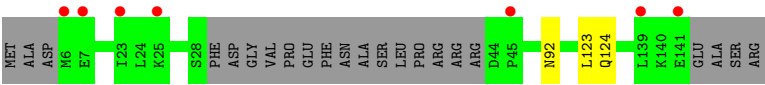


- Molecule 2: Tubulin beta-2B chain

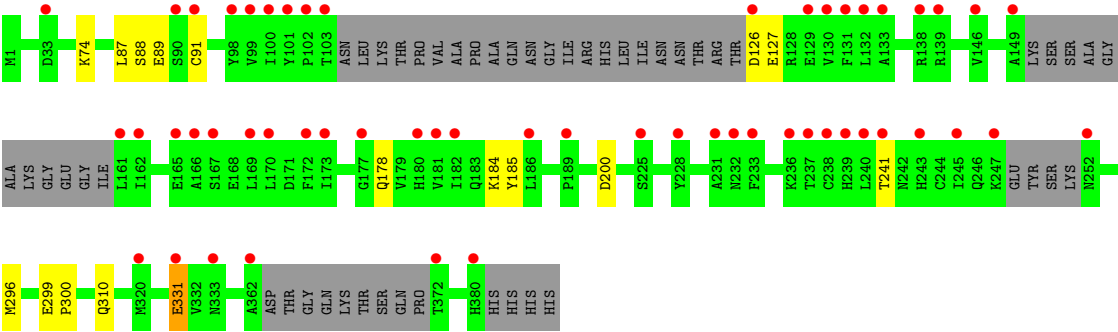
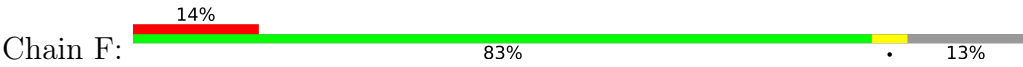


- Molecule 3: Stathmin-4





● Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.47Å 156.93Å 180.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.81 46.86 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.86-2.81) 96.4 (46.86-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.206 , 0.249 0.209 , 0.250	Depositor DCC
R_{free} test set	1044 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34508	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 89O, ACP, MG, GDP, GTP, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/3494	0.61	0/4743
1	C	0.29	0/3523	0.61	0/4782
2	B	0.29	0/3444	0.60	0/4664
2	D	0.29	0/3382	0.61	0/4581
3	E	0.27	0/1008	0.58	0/1337
4	F	0.26	0/2806	0.57	0/3791
All	All	0.29	0/17657	0.60	0/23898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3318	3330	4	0
1	C	3445	3344	3356	2	0
2	B	3369	3235	3246	8	0
2	D	3309	3179	3189	11	0
3	E	1000	1014	1018	1	0
4	F	2744	2698	2709	9	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
8	D	28	10	12	0	0
9	B	24	25	25	1	0
10	B	29	20	0	1	0
10	D	29	20	0	2	0
11	F	31	0	14	2	0
12	A	25	0	0	0	0
12	B	16	0	0	1	0
12	C	37	0	0	0	0
12	D	9	0	0	1	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17615	16893	16935	35	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 1.

All (35) 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)
10:B:505:89O:C25	10:B:505:89O:O27	1.65	1.32
10:D:502:89O:C25	10:D:502:89O:O27	1.65	1.28
1:A:221:ARG:NH2	2:B:327:ASP:OD2	2.35	0.60
2:D:404:ASP:OD1	2:D:405:GLU:N	2.36	0.58
4:F:178:GLN:N	4:F:178:GLN:OE1	2.38	0.57
2:B:145:SER:HG	2:B:188:SER:HG	1.51	0.55
4:F:126:ASP:OD1	4:F:127:GLU:N	2.39	0.55
2:B:296:SER:N	9:B:504:MES:O3S	2.39	0.54
2:B:309:ARG:NH1	12:B:604:HOH:O	2.39	0.54
1:C:245:ASP:N	1:C:245:ASP:OD1	2.41	0.53
2:B:234:SER:O	2:B:241:ARG:NH2	2.41	0.53
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.42	0.51
2:B:261:PRO:O	2:B:264:HIS:ND1	2.41	0.50
2:D:256:ASN:ND2	10:D:502:89O:O29	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ASN:ND2	12:D:603:HOH:O	2.46	0.48
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.24	0.47
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.36	0.46
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.33	0.46
4:F:87:LEU:O	4:F:88:SER:OG	2.28	0.46
2:D:301:ALA:O	2:D:303:CYS:N	2.50	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.32	0.45
4:F:184:LYS:NZ	4:F:185:TYR:O	2.47	0.44
2:D:137:HIS:ND1	2:D:144:GLY:O	2.32	0.44
2:D:323:MET:HE3	2:D:323:MET:HA	1.99	0.44
2:D:177:ASP:OD1	2:D:177:ASP:N	2.51	0.43
4:F:331:GLU:CD	11:F:401:ACP:H3B2	2.43	0.43
2:B:301:ALA:O	2:B:303:CYS:N	2.48	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.81	0.43
2:B:262:ARG:NE	2:B:421:GLU:OE2	2.52	0.42
4:F:331:GLU:OE2	11:F:401:ACP:H3B2	2.18	0.42
4:F:299:GLU:N	4:F:300:PRO:HD2	2.35	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.84	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.03	0.40
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.03	0.40
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

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	435/450 (97%)	419 (96%)	16 (4%)	0	100	100
1	C	439/450 (98%)	430 (98%)	9 (2%)	0	100	100
2	B	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	324/384 (84%)	314 (97%)	10 (3%)	0	100	100
All	All	2158/2317 (93%)	2100 (97%)	58 (3%)	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	368/378 (97%)	364 (99%)	4 (1%)	65	86
1	C	372/378 (98%)	367 (99%)	5 (1%)	61	85
2	B	370/383 (97%)	367 (99%)	3 (1%)	73	90
2	D	364/383 (95%)	362 (100%)	2 (0%)	81	93
3	E	109/127 (86%)	107 (98%)	2 (2%)	51	80
4	F	301/342 (88%)	296 (98%)	5 (2%)	53	81
All	All	1884/1991 (95%)	1863 (99%)	21 (1%)	65	86

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	A	256	GLN
1	A	279	GLU
1	A	420	GLU
2	B	42	LEU
2	B	245	GLN
2	B	316	ILE
1	C	2	ARG
1	C	177	VAL
1	C	178	SER
1	C	245	ASP
1	C	251	ASP

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Mol	Chain	Res	Type
2	D	245	GLN
2	D	390	ARG
3	E	92	ASN
3	E	124	GLN
4	F	89	GLU
4	F	91	CYS
4	F	296	MET
4	F	310	GLN
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	8	GLN
2	B	14	ASN
2	B	134	GLN
2	B	227	HIS
2	B	375	GLN
2	B	426	GLN
1	C	293	ASN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	48	ASN
2	D	165	ASN
2	D	204	ASN
2	D	347	ASN
3	E	90	ASN
3	E	136	ASN
4	F	180	HIS
4	F	269	GLN
4	F	306	HIS
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 [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 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	$\# Z > 2$
9	MES	B	503	-	12,12,12	2.37	1 (8%)	15,16,16	2.30	4 (26%)
10	89O	D	502	-	33,33,33	5.58	19 (57%)	50,50,50	3.54	17 (34%)
5	GTP	C	501	6	33,34,34	0.99	2 (6%)	50,54,54	1.52	8 (16%)
11	ACP	F	401	-	31,33,33	2.58	16 (51%)	47,52,52	4.22	23 (48%)
5	GTP	A	501	6	33,34,34	0.96	1 (3%)	50,54,54	1.49	8 (16%)
9	MES	B	504	-	12,12,12	2.29	1 (8%)	15,16,16	1.25	1 (6%)
8	GDP	B	501	6	29,30,30	1.19	3 (10%)	45,47,47	1.68	5 (11%)
8	GDP	D	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.71	5 (11%)
10	89O	B	505	-	33,33,33	5.52	19 (57%)	50,50,50	3.51	16 (32%)

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
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
10	89O	D	502	-	-	4/8/43/43	0/5/5/5
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	5/19/38/38	0/3/3/3
5	GTP	A	501	6	-	10/22/38/38	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
8	GDP	D	501	6	-	1/16/32/32	0/3/3/3
10	89O	B	505	-	-	4/8/43/43	0/5/5/5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	89O	O27-C25	14.27	1.65	1.35
10	B	505	89O	O27-C25	14.13	1.65	1.35
10	B	505	89O	C05-C04	12.30	1.68	1.51
10	D	502	89O	C05-C04	12.07	1.68	1.51
10	D	502	89O	C06-C05	11.64	1.61	1.40
10	B	505	89O	C06-C05	11.61	1.61	1.40
10	B	505	89O	C10-C09	11.49	1.58	1.38
10	D	502	89O	C10-C09	11.49	1.58	1.38
10	D	502	89O	C06-C01	11.18	1.67	1.51
10	D	502	89O	C07-C08	10.79	1.57	1.38
10	B	505	89O	C07-C08	10.52	1.56	1.38
10	B	505	89O	C06-C01	10.39	1.66	1.51
9	B	503	MES	C8-S	-7.95	1.66	1.77
9	B	504	MES	C8-S	-7.68	1.66	1.77
11	F	401	ACP	PB-O1B	5.95	1.65	1.51
11	F	401	ACP	PG-O1G	5.82	1.62	1.50
10	B	505	89O	C03-C02	4.39	1.63	1.54
10	D	502	89O	C03-C02	4.36	1.63	1.54
10	B	505	89O	C18-C17	4.22	1.46	1.40
10	D	502	89O	C18-C17	4.15	1.46	1.40
11	F	401	ACP	PB-O3A	3.96	1.62	1.58
10	D	502	89O	C16-C17	3.93	1.45	1.40
10	B	505	89O	C16-C17	3.90	1.45	1.40
11	F	401	ACP	PA-O3A	3.86	1.63	1.59
10	D	502	89O	C14-C04	3.81	1.57	1.52
10	B	505	89O	C14-C04	3.80	1.57	1.52
11	F	401	ACP	O4'-C1'	3.62	1.50	1.42
10	B	505	89O	C19-C18	3.57	1.44	1.38
10	B	505	89O	O20-C18	3.54	1.42	1.37
10	B	505	89O	C03-C25	-3.47	1.46	1.51
10	D	502	89O	C19-C18	3.47	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	C2-N1	3.41	1.40	1.33
11	F	401	ACP	C2-N3	3.39	1.39	1.33
10	D	502	89O	C15-C16	3.32	1.44	1.38
10	B	505	89O	C15-C16	3.29	1.44	1.38
10	D	502	89O	O20-C18	3.28	1.42	1.37
11	F	401	ACP	PG-O2G	3.18	1.62	1.55
10	D	502	89O	C03-C25	-3.14	1.47	1.51
8	D	501	GDP	C5-C4	3.11	1.47	1.38
11	F	401	ACP	C5-C4	-3.08	1.33	1.39
8	B	501	GDP	C5-C4	3.02	1.47	1.38
10	D	502	89O	O13-C08	3.00	1.43	1.38
10	D	502	89O	O11-C09	2.97	1.43	1.38
11	F	401	ACP	C5-N7	-2.96	1.33	1.39
10	B	505	89O	O23-C16	2.93	1.41	1.37
10	D	502	89O	O23-C16	2.89	1.41	1.37
10	B	505	89O	O11-C09	2.86	1.42	1.38
10	B	505	89O	O13-C08	2.82	1.42	1.38
8	B	501	GDP	C6-N1	-2.79	1.33	1.38
8	D	501	GDP	C6-N1	-2.73	1.33	1.38
11	F	401	ACP	PG-O3G	-2.72	1.48	1.55
10	D	502	89O	C02-C01	2.63	1.56	1.52
11	F	401	ACP	C5-C6	-2.56	1.33	1.41
10	D	502	89O	C19-C14	2.53	1.42	1.39
10	B	505	89O	C19-C14	2.51	1.42	1.39
11	F	401	ACP	C8-N9	-2.42	1.33	1.37
11	F	401	ACP	PB-O2B	-2.26	1.50	1.56
8	B	501	GDP	C5-N7	-2.26	1.34	1.39
8	D	501	GDP	C5-N7	-2.24	1.34	1.39
5	C	501	GTP	C2-N3	2.18	1.38	1.33
5	C	501	GTP	PA-O3A	2.15	1.61	1.59
5	A	501	GTP	C2-N3	2.14	1.38	1.33
11	F	401	ACP	C4-N9	-2.09	1.33	1.37
11	F	401	ACP	C2'-C3'	-2.04	1.47	1.53
10	B	505	89O	C15-C14	2.03	1.42	1.39

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	89O	O27-C25-O26	17.06	139.55	121.43
10	B	505	89O	O27-C25-O26	16.95	139.44	121.43
11	F	401	ACP	O4'-C1'-N9	-14.45	80.34	108.09
11	F	401	ACP	O4'-C4'-C3'	-13.96	77.44	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C2'-C1'-N9	9.06	135.82	113.30
11	F	401	ACP	O4'-C1'-C2'	-8.81	87.77	106.62
10	D	502	89O	O27-C25-C03	-8.78	96.40	109.50
10	B	505	89O	O27-C25-C03	-8.55	96.75	109.50
11	F	401	ACP	N3-C2-N1	-7.04	117.93	128.58
11	F	401	ACP	C2'-C3'-C4'	-6.15	90.73	102.61
10	B	505	89O	C28-O27-C25	5.82	116.10	110.31
8	D	501	GDP	C5-C4-N3	-5.76	119.22	128.39
8	B	501	GDP	C5-C4-N3	-5.50	119.64	128.39
10	B	505	89O	C02-C03-C25	5.31	110.98	103.14
10	D	502	89O	C02-C03-C25	5.11	110.68	103.14
9	B	503	MES	C5-N4-C3	4.98	119.56	108.84
5	C	501	GTP	C5-C4-N3	-4.96	120.49	128.39
5	A	501	GTP	C5-C4-N3	-4.85	120.67	128.39
10	D	502	89O	C28-O27-C25	4.84	115.12	110.31
8	B	501	GDP	C2-N3-C4	4.73	120.45	112.30
8	D	501	GDP	C2-N3-C4	4.71	120.42	112.30
10	D	502	89O	O20-C18-C17	4.70	119.45	114.53
9	B	503	MES	C7-N4-C5	4.61	123.52	111.24
5	C	501	GTP	C2-N3-C4	4.54	120.11	112.30
8	D	501	GDP	N9-C4-N3	4.52	134.99	125.95
5	A	501	GTP	C2-N3-C4	4.48	120.02	112.30
10	B	505	89O	C18-C19-C14	4.44	126.72	119.86
10	B	505	89O	O26-C25-C03	-4.41	123.77	129.38
10	B	505	89O	O20-C18-C17	4.39	119.12	114.53
10	D	502	89O	C18-C19-C14	4.36	126.59	119.86
11	F	401	ACP	N9-C8-N7	-4.35	107.77	113.94
11	F	401	ACP	C5-C4-N3	-4.30	120.79	126.72
8	B	501	GDP	N9-C4-N3	4.24	134.43	125.95
10	D	502	89O	O26-C25-C03	-4.22	124.01	129.38
10	D	502	89O	C03-C02-C01	4.11	116.47	109.67
10	B	505	89O	C06-C05-C04	3.97	124.71	114.39
11	F	401	ACP	C4-N9-C1'	-3.96	117.38	126.63
10	D	502	89O	C06-C05-C04	3.81	124.29	114.39
10	D	502	89O	O23-C16-C17	3.75	118.45	114.53
10	D	502	89O	C19-C14-C15	-3.65	113.13	118.09
10	B	505	89O	C19-C18-C17	-3.52	117.25	120.59
10	D	502	89O	C16-C15-C14	3.48	125.23	119.86
8	B	501	GDP	C6-C5-N7	3.46	136.59	130.29
10	D	502	89O	O11-C09-C10	3.45	132.44	127.86
10	B	505	89O	O11-C09-C10	3.41	132.39	127.86
10	B	505	89O	C19-C14-C15	-3.39	113.48	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C1'-N9-C8	3.38	134.59	127.09
9	B	503	MES	C6-C5-N4	-3.36	105.01	110.12
11	F	401	ACP	C2-N3-C4	3.32	119.95	111.83
10	B	505	89O	O23-C16-C17	3.32	118.00	114.53
8	D	501	GDP	C6-C5-N7	3.26	136.22	130.29
5	C	501	GTP	N9-C4-N3	3.23	132.41	125.95
10	B	505	89O	C03-C02-C01	3.18	114.94	109.67
11	F	401	ACP	C5-N7-C8	3.14	108.38	103.45
10	B	505	89O	C16-C15-C14	3.13	124.70	119.86
5	A	501	GTP	N9-C4-N3	3.13	132.22	125.95
11	F	401	ACP	O2B-PB-C3B	3.03	119.29	106.73
10	D	502	89O	C19-C18-C17	-3.01	117.73	120.59
11	F	401	ACP	O3G-PG-C3B	2.85	113.32	106.40
5	C	501	GTP	C2-N1-C6	-2.78	120.06	125.11
11	F	401	ACP	O5'-C5'-C4'	2.77	118.41	108.99
11	F	401	ACP	O2G-PG-O1G	-2.76	105.25	112.39
5	A	501	GTP	C2-N1-C6	-2.74	120.14	125.11
10	D	502	89O	C10-C09-C08	-2.74	118.60	122.03
11	F	401	ACP	C4-C5-N7	-2.73	107.46	110.58
11	F	401	ACP	C5-C6-N6	-2.70	116.59	123.29
10	B	505	89O	C10-C09-C08	-2.66	118.70	122.03
5	A	501	GTP	N9-C8-N7	-2.64	108.51	113.40
5	C	501	GTP	N9-C8-N7	-2.63	108.53	113.40
11	F	401	ACP	O1B-PB-C3B	2.52	115.68	109.05
5	C	501	GTP	C8-N7-C5	2.48	108.67	104.26
11	F	401	ACP	C6-C5-C4	2.46	120.54	117.18
5	A	501	GTP	C8-N7-C5	2.44	108.61	104.26
5	C	501	GTP	O6-C6-C5	-2.42	120.14	126.53
5	A	501	GTP	C5-C6-N1	2.40	119.37	113.25
5	C	501	GTP	C5-C6-N1	2.40	119.37	113.25
5	A	501	GTP	O6-C6-C5	-2.35	120.34	126.53
11	F	401	ACP	C5-C4-N9	2.34	108.36	105.81
8	D	501	GDP	C4-C5-N7	-2.33	106.98	110.67
8	B	501	GDP	C4-C5-N7	-2.31	107.01	110.67
11	F	401	ACP	C4-N9-C8	2.19	108.03	105.74
11	F	401	ACP	N3-C4-N9	2.16	130.85	127.17
10	D	502	89O	O27-C28-C02	-2.16	101.44	104.70
9	B	504	MES	C7-N4-C5	2.11	116.86	111.24
10	D	502	89O	C02-C03-C04	2.08	117.21	113.15
9	B	503	MES	C7-N4-C3	2.07	116.75	111.24
10	B	505	89O	C02-C03-C04	2.05	117.14	113.15

There are no chirality outliers.

All (40) 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
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-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	503	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
11	F	401	ACP	O4'-C4'-C5'-O5'
10	D	502	89O	C17-C18-O20-C21
10	D	502	89O	C19-C18-O20-C21
10	B	505	89O	C15-C16-O23-C24
10	D	502	89O	C17-C16-O23-C24
10	B	505	89O	C17-C16-O23-C24
9	B	504	MES	C7-C8-S-O3S
10	D	502	89O	C15-C16-O23-C24
10	B	505	89O	C17-C18-O20-C21
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
8	B	501	GDP	C5'-O5'-PA-O1A
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O2B
5	A	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	C4'-C5'-O5'-PA
10	B	505	89O	C19-C18-O20-C21
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A

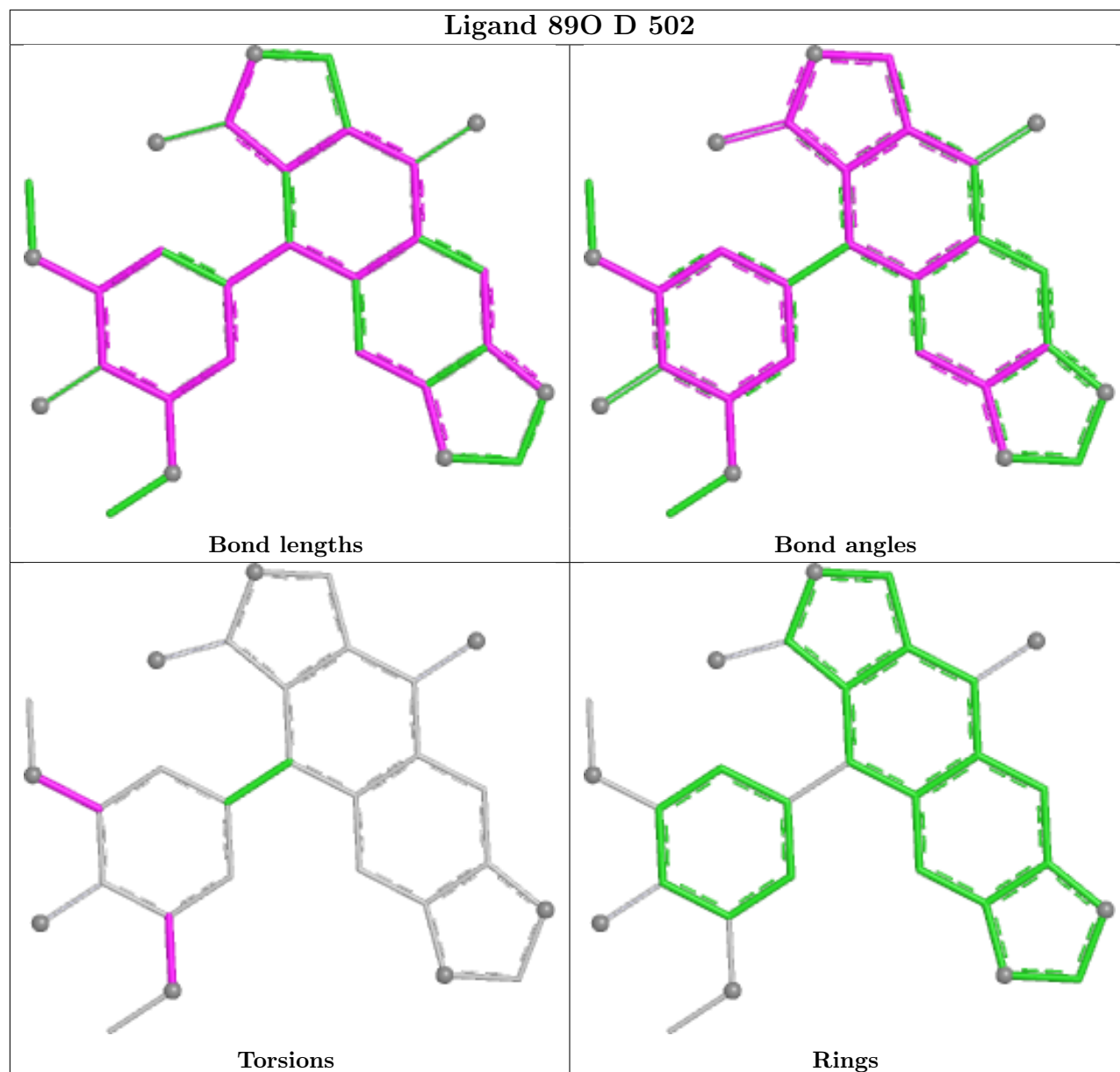
There are no ring outliers.

4 monomers are involved in 6 short contacts:

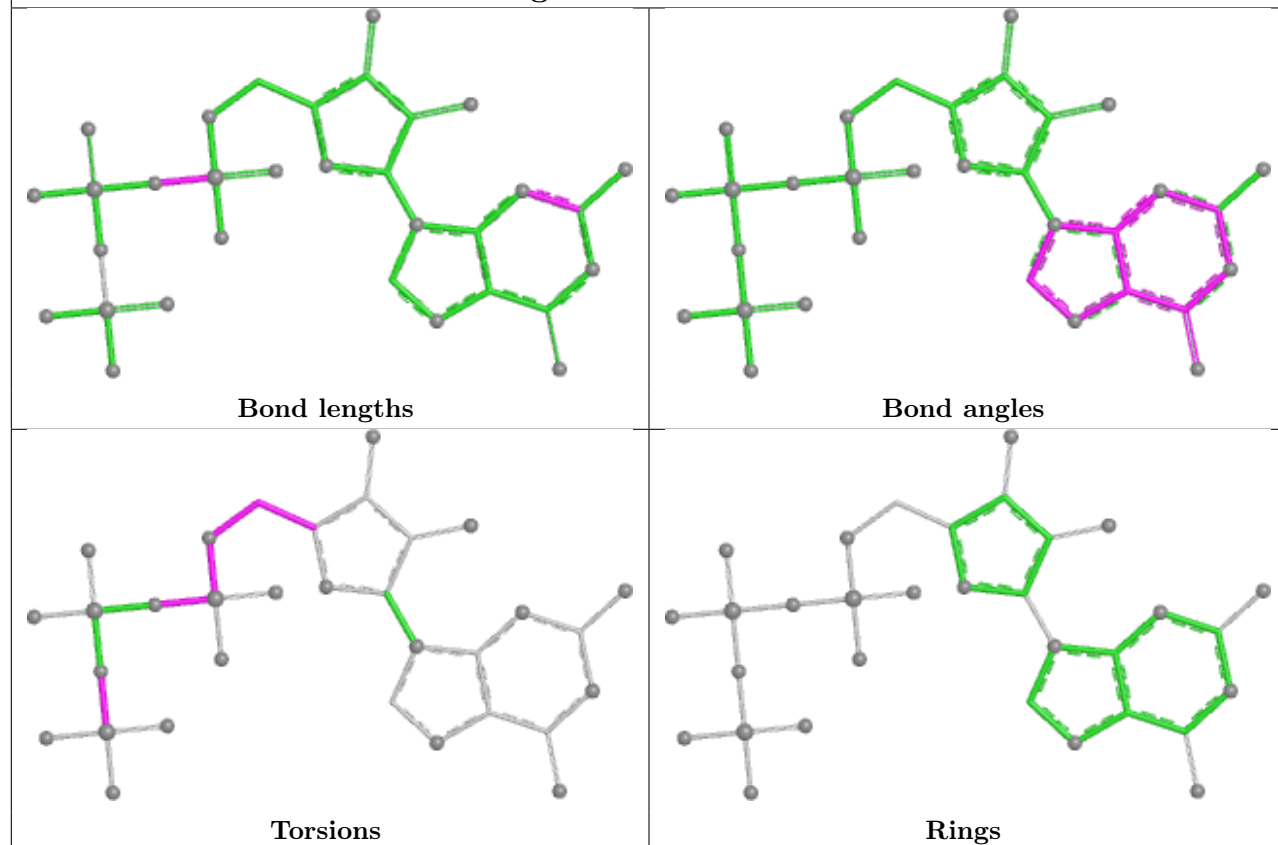
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	89O	2	0
11	F	401	ACP	2	0
9	B	504	MES	1	0
10	B	505	89O	1	0

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

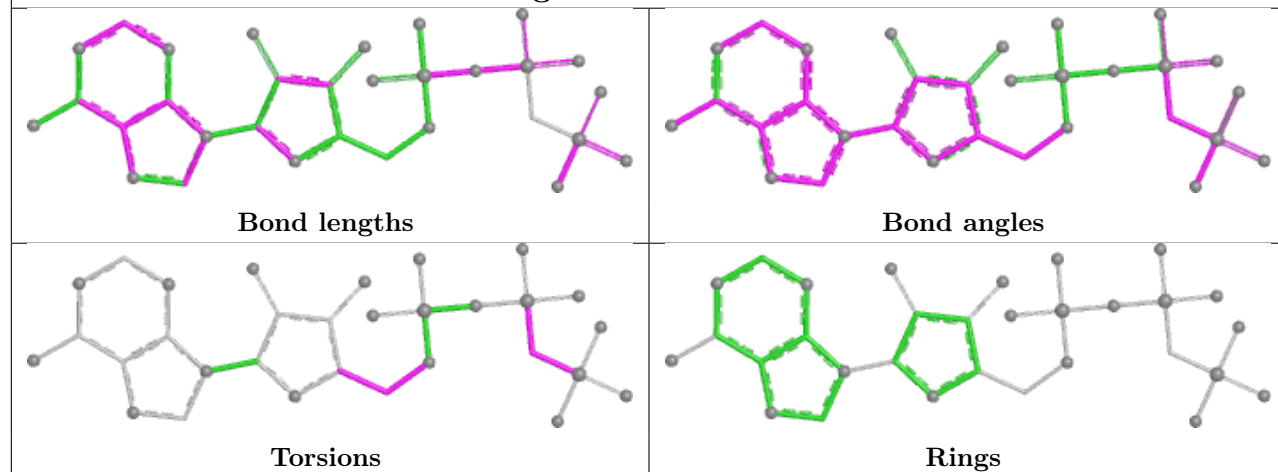
Ligand 89O D 502

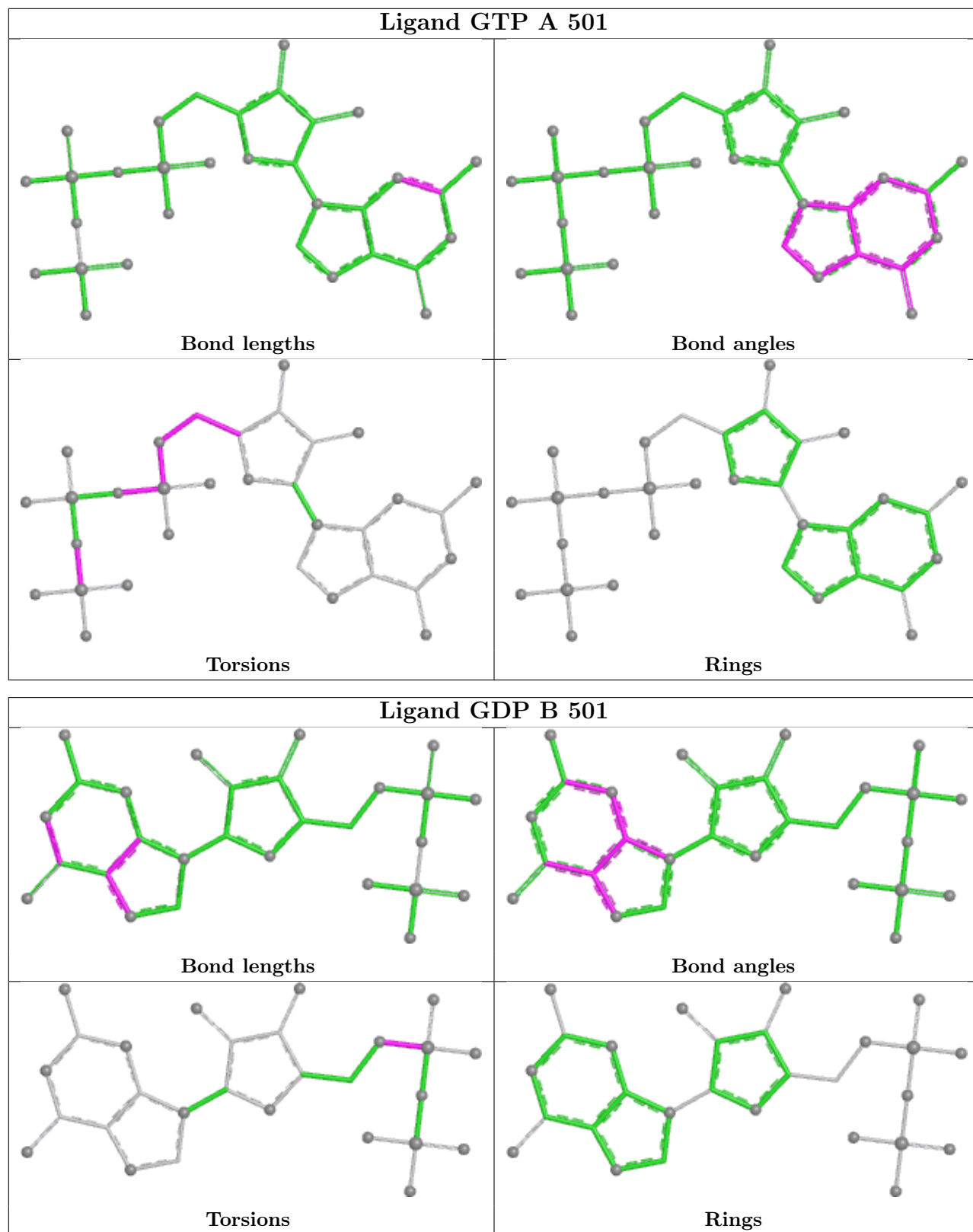


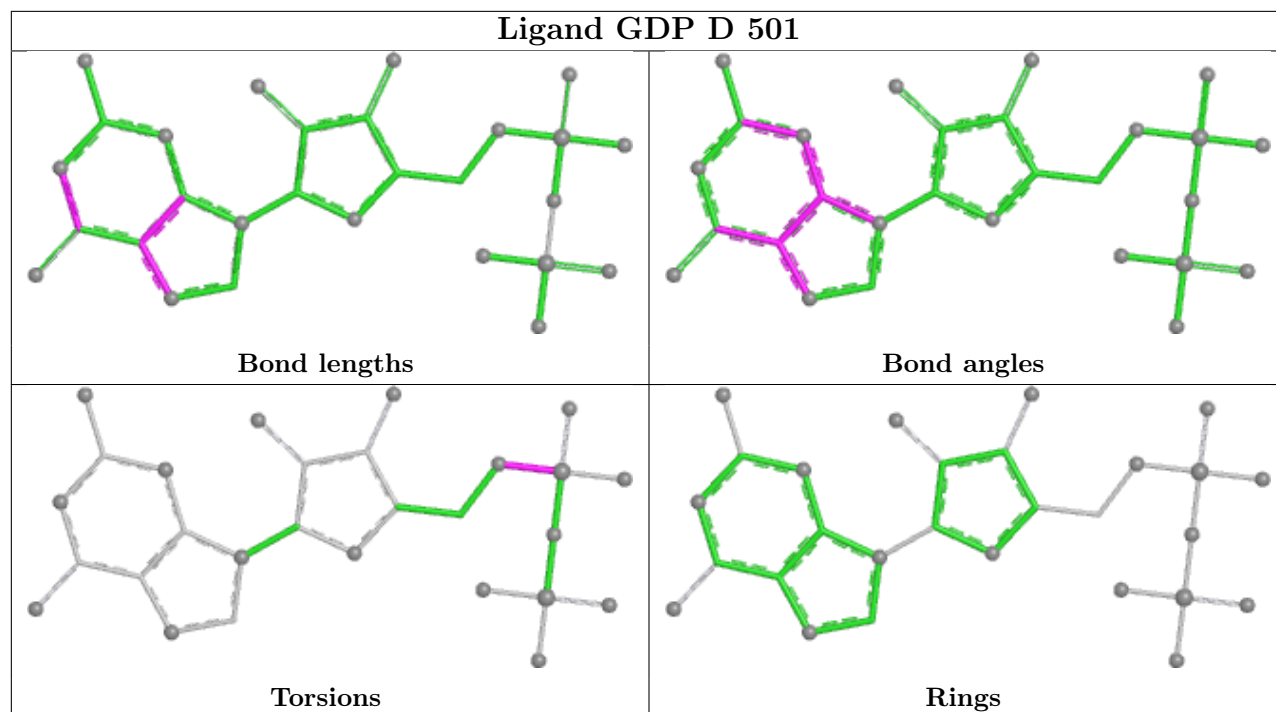
Ligand GTP C 501

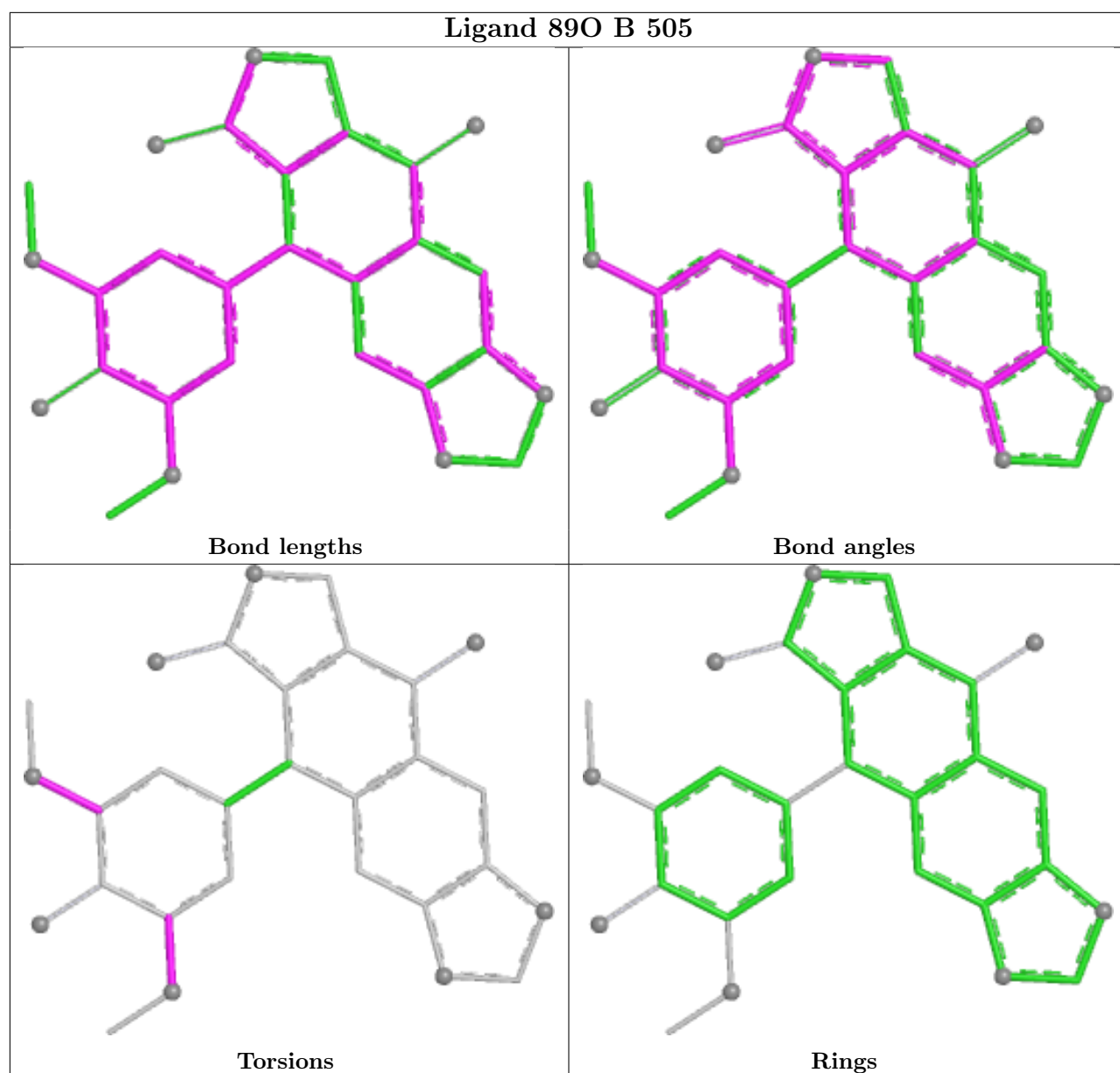


Ligand ACP F 401









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	437/450 (97%)	0.13	8 (1%) 67 58	25, 48, 82, 110	0
1	C	440/450 (97%)	-0.32	3 (0%) 84 78	18, 34, 66, 83	1 (0%)
2	B	427/445 (95%)	0.03	8 (1%) 66 57	17, 45, 85, 147	1 (0%)
2	D	421/445 (94%)	0.68	37 (8%) 15 11	31, 65, 106, 133	0
3	E	121/143 (84%)	0.52	7 (5%) 29 21	32, 65, 104, 117	0
4	F	334/384 (86%)	0.88	55 (16%) 4 3	35, 77, 146, 164	0
All	All	2180/2317 (94%)	0.26	118 (5%) 31 23	17, 53, 108, 164	2 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	4.8
4	F	149	ALA	4.7
4	F	233	PHE	4.4
1	A	179	THR	4.3
1	A	88	HIS	3.9
4	F	103	THR	3.9
2	D	180	VAL	3.9
2	D	284	LEU	3.8
4	F	182	ILE	3.7
2	D	394	PHE	3.7
2	D	323	MET	3.7
2	D	55	THR	3.6
1	A	178	SER	3.5
4	F	243	HIS	3.5
4	F	240	LEU	3.5
4	F	181	VAL	3.4
2	D	72	THR	3.4
4	F	372	THR	3.4
2	D	245	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	3.3
4	F	186	LEU	3.3
2	B	428	ALA	3.3
2	D	322	SER	3.2
4	F	133	ALA	3.2
4	F	231	ALA	3.2
3	E	6	MET	3.1
4	F	162	ILE	3.1
2	B	280	GLN	3.1
4	F	362	ALA	3.0
4	F	237	THR	3.0
2	B	54	ALA	3.0
4	F	252	ASN	3.0
2	B	55	THR	3.0
4	F	173	ILE	2.9
2	D	92	PHE	2.9
4	F	232	ASN	2.9
2	D	115	SER	2.9
4	F	167	SER	2.8
1	A	436	GLY	2.8
1	C	440	VAL	2.8
2	D	1	MET	2.8
1	A	437	VAL	2.7
2	D	73	MET	2.7
1	A	89	PRO	2.7
4	F	132	LEU	2.7
2	D	388	MET	2.6
4	F	91	CYS	2.6
4	F	238	CYS	2.6
4	F	320	MET	2.6
2	D	70	PRO	2.6
2	D	112	LEU	2.6
4	F	90	SER	2.5
2	B	56	GLY	2.5
4	F	130	VAL	2.5
2	D	81	PHE	2.5
4	F	170	LEU	2.5
4	F	225	SER	2.5
2	D	397	TRP	2.5
3	E	141	GLU	2.5
2	D	172	SER	2.5
2	D	54	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	139	LEU	2.4
1	C	341	ILE	2.4
2	D	362	LYS	2.4
4	F	172	PHE	2.4
4	F	100	ILE	2.4
2	D	360	GLY	2.4
4	F	138	ARG	2.4
3	E	7	GLU	2.4
2	D	170	MET	2.4
4	F	180	HIS	2.4
4	F	126	ASP	2.3
2	D	393	ALA	2.3
2	D	321	MET	2.3
4	F	228	TYR	2.3
4	F	241	THR	2.3
2	B	350	LYS	2.3
2	D	37	HIS	2.3
4	F	236	LYS	2.3
4	F	239	HIS	2.3
1	C	340	SER	2.3
1	A	94	THR	2.3
4	F	99	VAL	2.3
4	F	380	HIS	2.3
4	F	333	ASN	2.2
3	E	45	PRO	2.2
4	F	177	GLY	2.2
4	F	247	LYS	2.2
2	D	116	VAL	2.2
4	F	331	GLU	2.2
2	D	286	VAL	2.2
4	F	139	ARG	2.2
4	F	245	ILE	2.1
2	D	175	VAL	2.1
2	D	71	GLY	2.1
3	E	25	LYS	2.1
4	F	129	GLU	2.1
2	D	227	HIS	2.1
2	D	219	THR	2.1
4	F	131	PHE	2.1
2	D	390	ARG	2.1
2	B	245	GLN	2.1
2	D	85	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	33	ASP	2.1
3	E	23	ILE	2.1
4	F	101	TYR	2.1
2	B	278	SER	2.0
4	F	102	PRO	2.0
2	D	381	ILE	2.0
4	F	166	ALA	2.0
2	D	108	GLU	2.0
4	F	98	TYR	2.0
4	F	146	VAL	2.0
4	F	189	PRO	2.0
2	D	320	ARG	2.0
1	A	45	GLY	2.0
2	D	178	THR	2.0
4	F	165	GLU	2.0

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 [i](#)

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($\text{\AA}^2$)	Q<0.9
11	ACP	F	401	31/31	0.70	0.17	87,104,134,140	0
6	MG	D	503	1/1	0.72	0.16	53,53,53,53	0
9	MES	B	504	12/12	0.86	0.12	59,72,80,83	0
8	GDP	D	501	28/28	0.89	0.13	42,61,78,82	0
10	89O	D	502	29/29	0.90	0.14	37,55,69,73	0
10	89O	B	505	29/29	0.90	0.15	26,44,62,67	0
9	MES	B	503	12/12	0.93	0.11	27,46,67,75	0
7	CA	A	503	1/1	0.95	0.07	86,86,86,86	0

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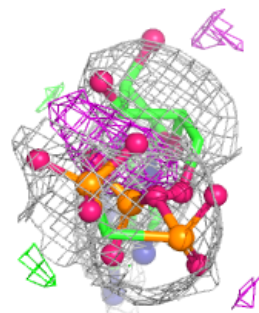
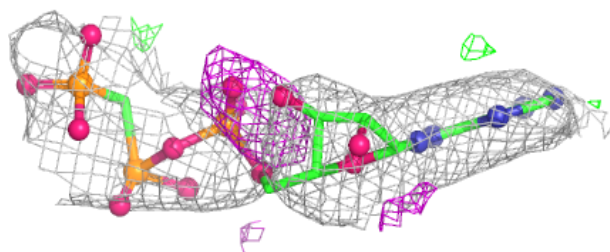
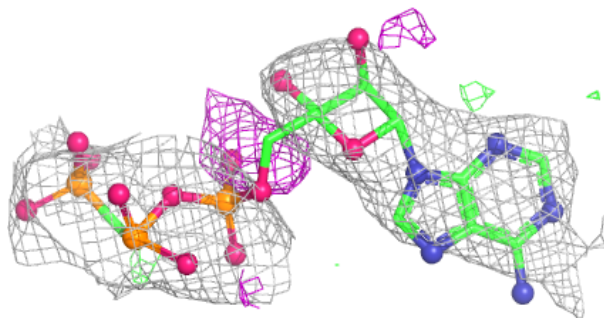
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GDP	B	501	28/28	0.95	0.09	14,26,36,49	0
6	MG	B	502	1/1	0.96	0.10	30,30,30,30	0
5	GTP	A	501	32/32	0.97	0.07	18,29,39,45	0
5	GTP	C	501	32/32	0.97	0.06	12,24,39,50	0
6	MG	A	502	1/1	0.98	0.04	22,22,22,22	0
7	CA	C	503	1/1	0.99	0.02	42,42,42,42	0
6	MG	C	502	1/1	0.99	0.07	22,22,22,22	0

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

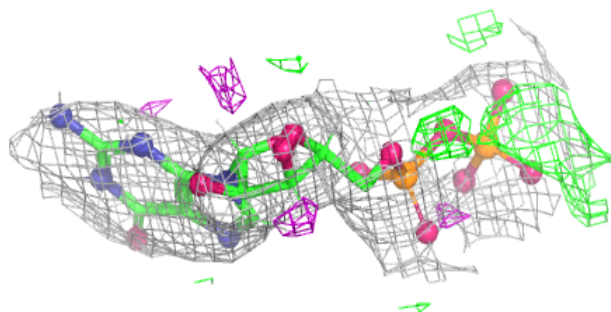
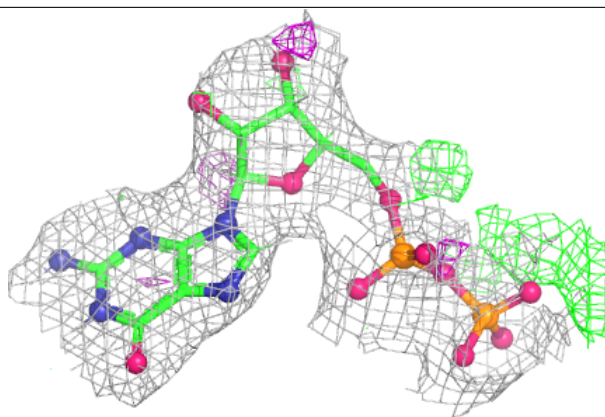
Electron density around ACP F 401:

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

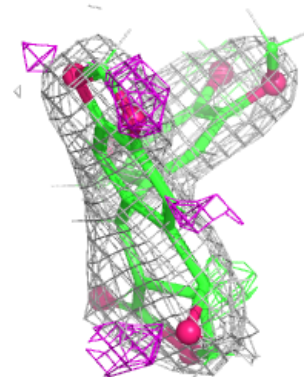
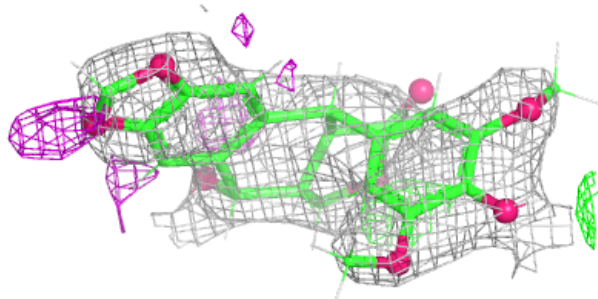
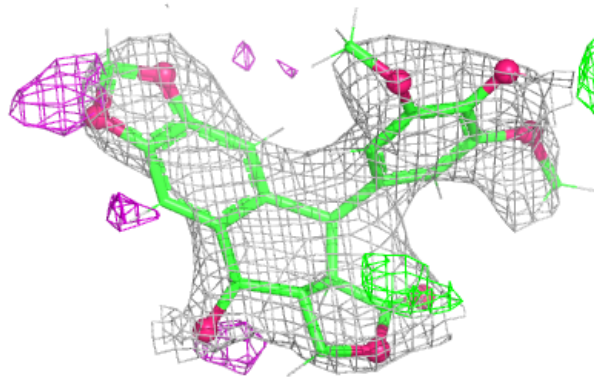


Electron density around GDP D 501:

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

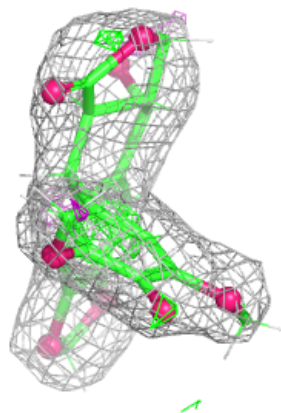
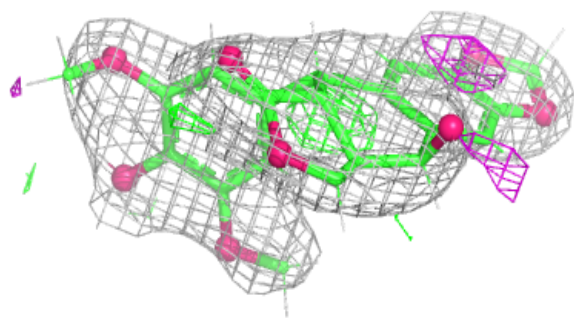
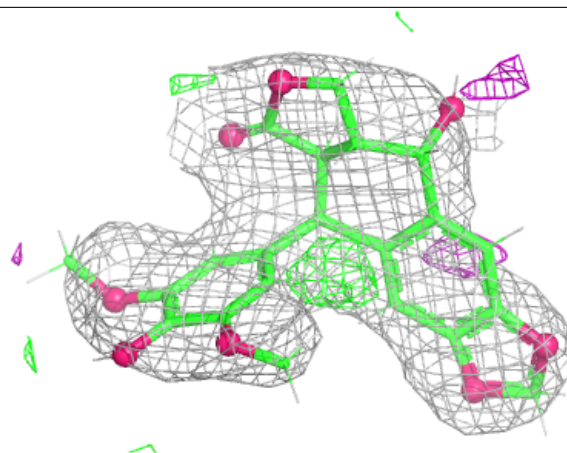
**Electron density around 89O D 502:**

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



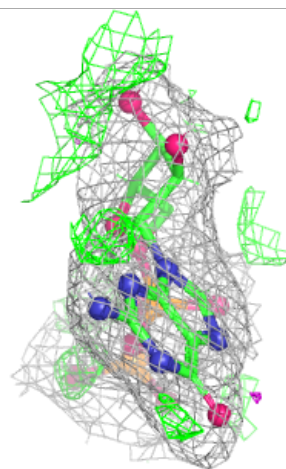
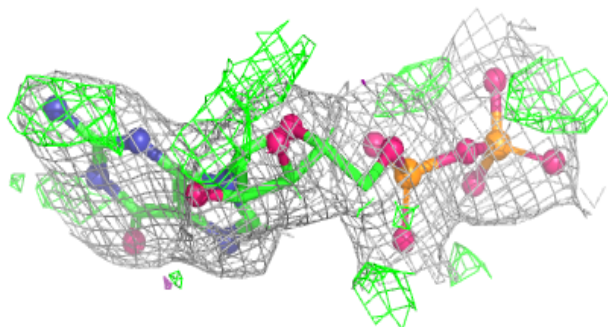
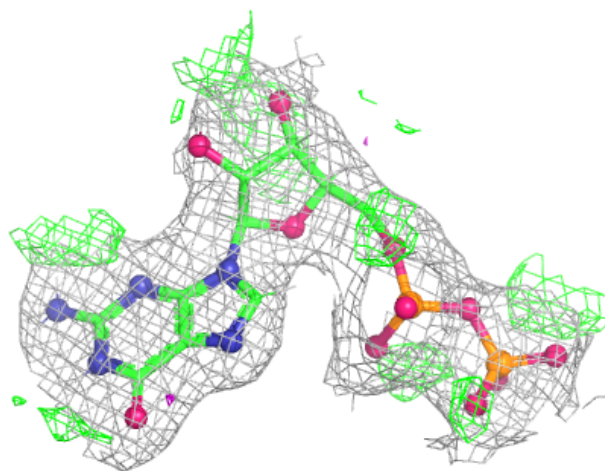
Electron density around 89O B 505:

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



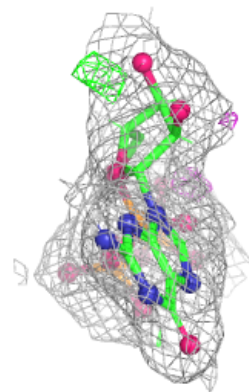
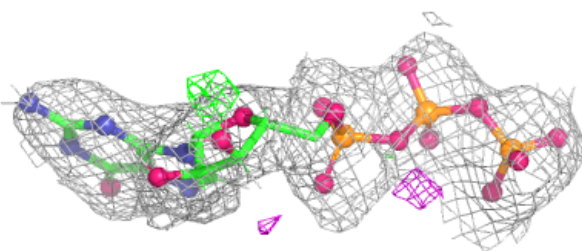
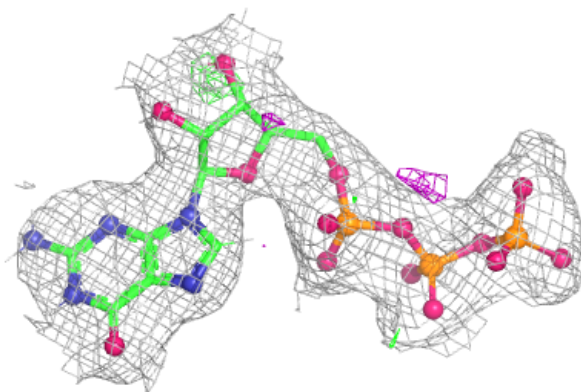
Electron density around GDP B 501:

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

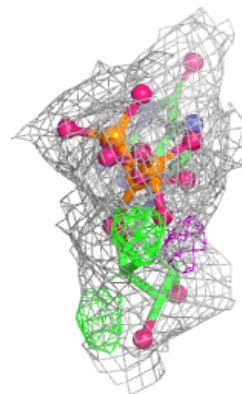
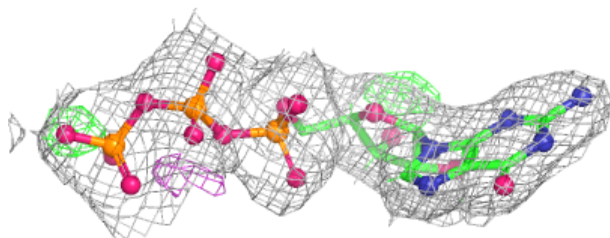
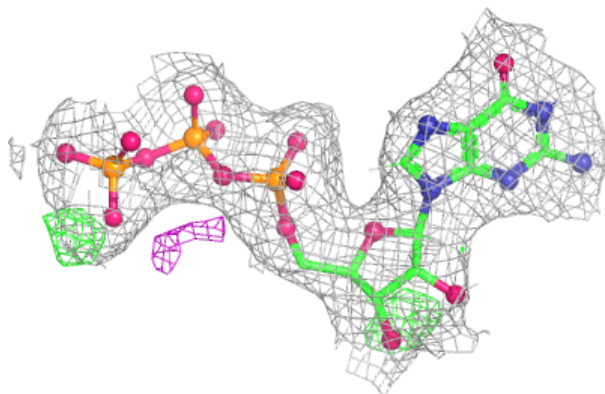


Electron density around GTP A 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.