



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 07:13 pm BST

PDB ID : 8B7A
Title : Tubulin - maytansinoid - 4 complex
Authors : Boiarska, Z.; Perez-Pena, H.; Abel, A.-C.; Marzullo, P.; Alvarez-Bernad, B.; Bonato, F.; Santini, B.; Horvath, D.; Lucena-Agell, D.; Vasile, F.; Sironi, M.; Diaz, F.J.; Steinmetz, M.O.; Prota, A.E.; Piaraccini, S.; Passarella, D.
Deposited on : 2022-09-29
Resolution : 2.25 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

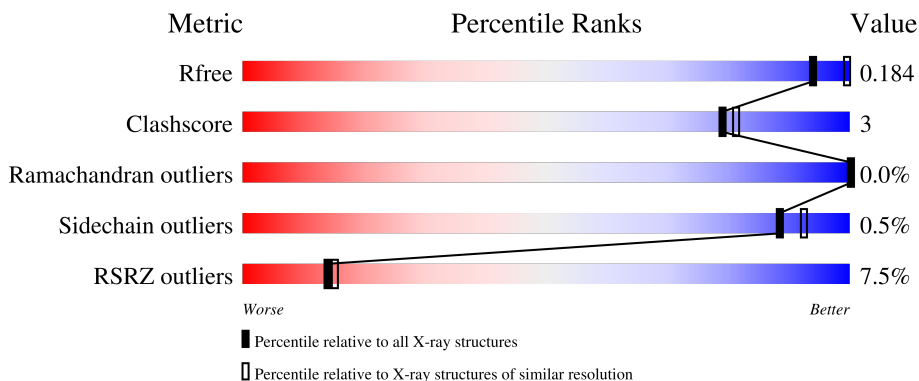
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

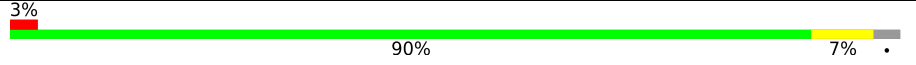
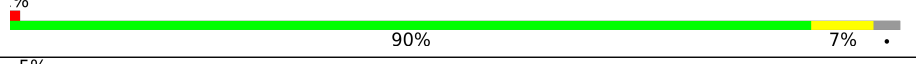


The reported resolution of this entry is 2.25 Å.

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.



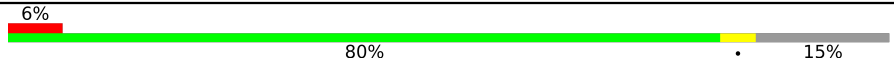

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	 3% 90% 7%
1	C	451	 0% 90% 7%
2	B	445	 5% 86% 10%
2	D	445	 3% 88% 6%

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Mol	Chain	Length	Quality of chain
3	E	143	 <p>6% 80% 15%</p>
4	F	384	 <p>26% 81% 6% 13%</p>

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 18429 atoms, of which 0 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
			Total	C	N	O	S			
1	A	437	Total	C	N	O	S	0	1	0
			3419	2165	581	650	23			
1	C	439	Total	C	N	O	S	0	10	0
			3482	2202	588	667	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	424	Total	C	N	O	S	0	1	0
			3350	2105	573	645	27			
2	D	420	Total	C	N	O	S	0	1	0
			3312	2082	565	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	1	0
			1005	620	182	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

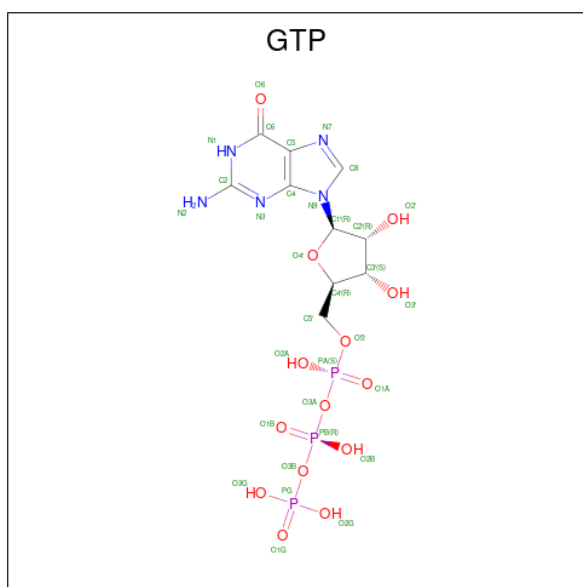
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	334	Total	C	N	O	S	0	1	0
			2748	1767	468	498	15			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
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		
6	F	1	Total	Mg	0	0
			1	1		

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

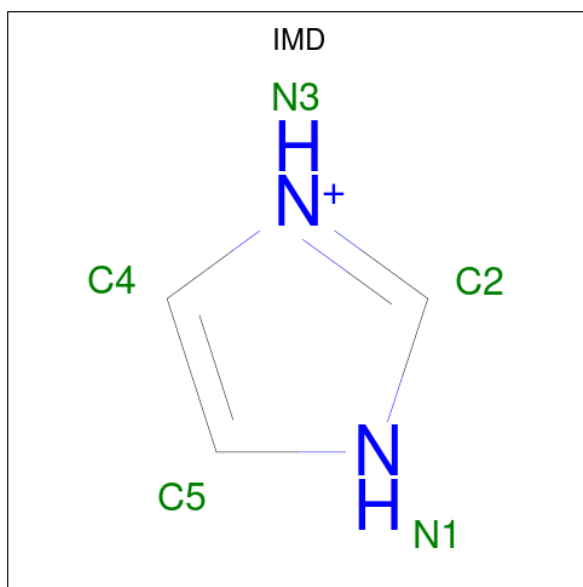
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0

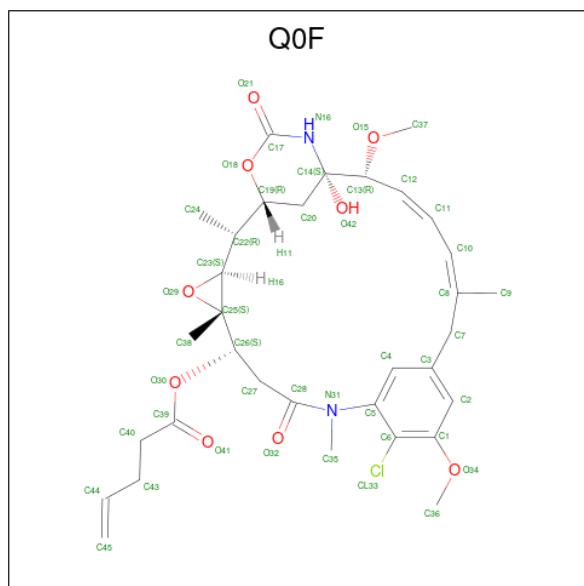
- Molecule 8 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N 5 3 2	0	0

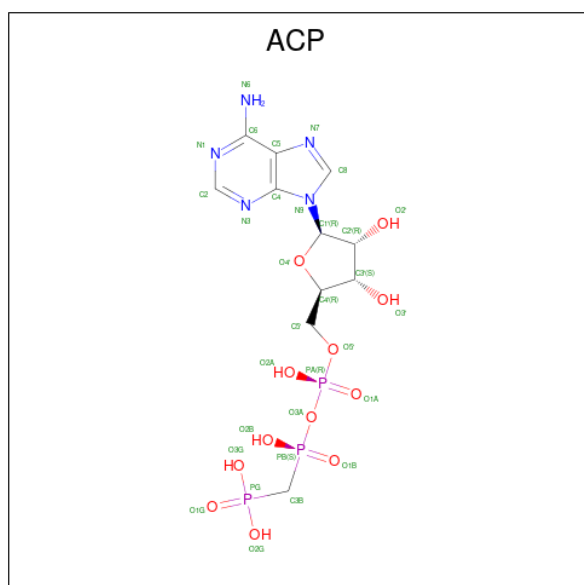
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

- Molecule 11 is [(1 {R},2 {R},3 {S},5 {S},6 {S},16 {E},18 {E},20 {R},21 {S})-11-chloranyl-12,20-dimethoxy-2,5,9,16-tetramethyl-21-oxidanyl-8,23-bis(oxidanylidene)-4,24-dioxo-9,22-diazatetracyclo[19.3.1.1[^]{10,14}.0[^]{3,5}]hexacos-10(26),11,13,16,18-pentaen-6-yl] pent-4-enoate (three-letter code: Q0F) (formula: C₃₃H₄₃ClN₂O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
11	D	1	45	33	1	2	9	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	F	1	31	11	5	12	3	0	0

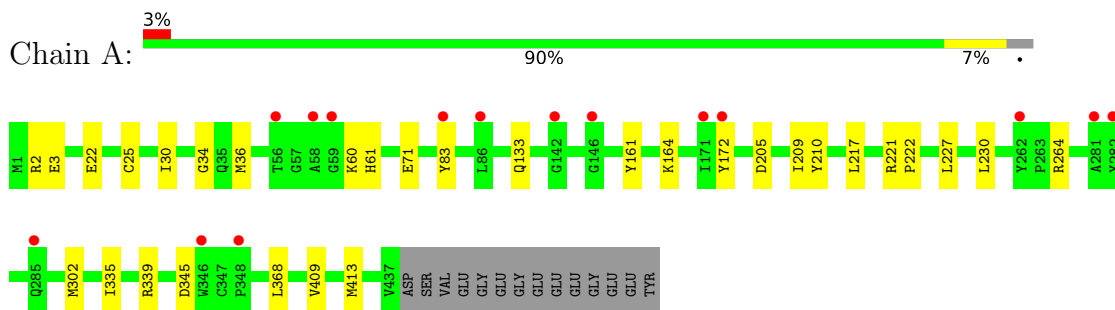
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	166	Total 166	O 166	0	0
13	B	198	Total 198	O 198	0	0
13	C	325	Total 325	O 325	0	0
13	D	107	Total 107	O 107	0	0
13	E	36	Total 36	O 36	0	0
13	F	57	Total 57	O 57	0	0

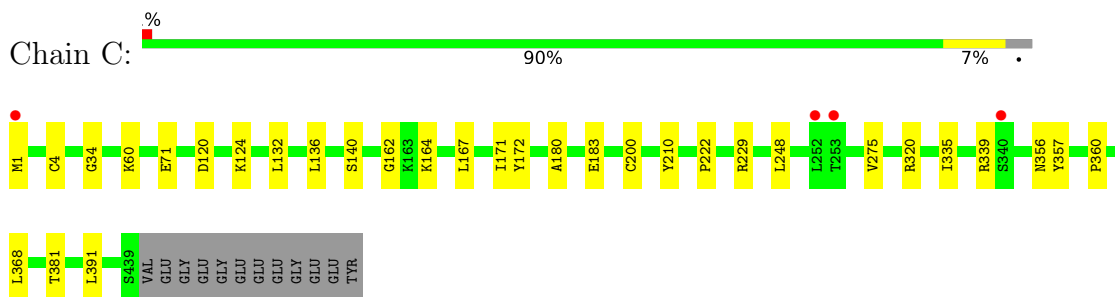
3 Residue-property plots [i](#)

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.

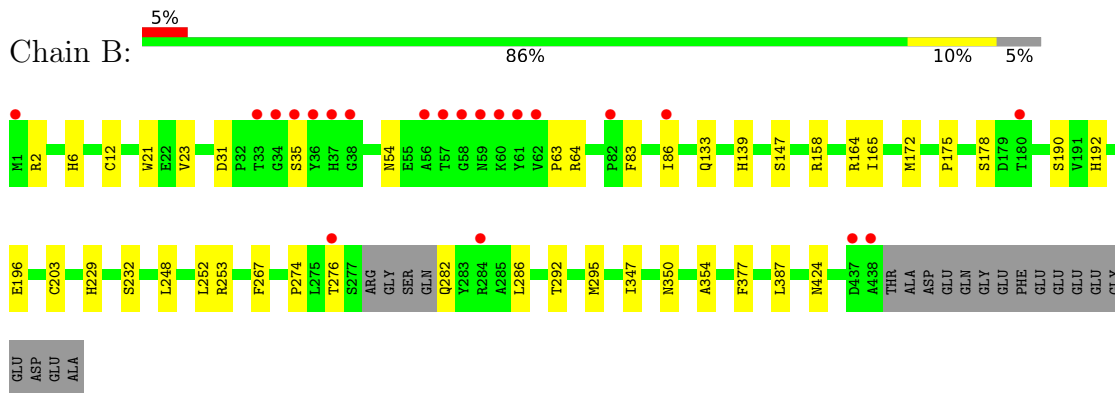
- Molecule 1: Tubulin alpha-1B chain



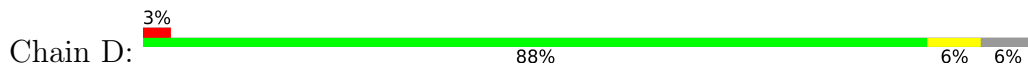
- Molecule 1: Tubulin alpha-1B chain

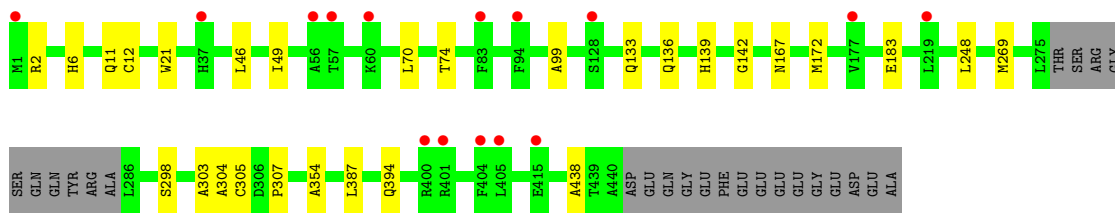


- Molecule 2: Tubulin beta-2B chain

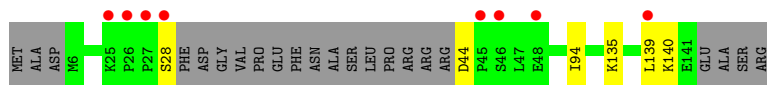
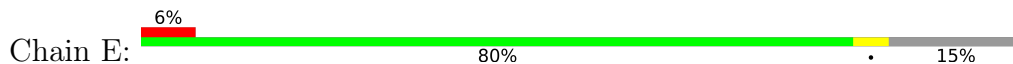


- Molecule 2: Tubulin beta-2B chain

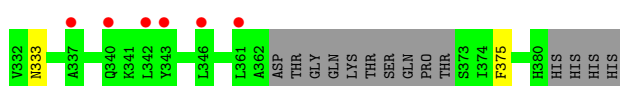
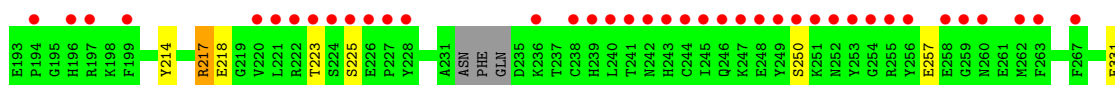
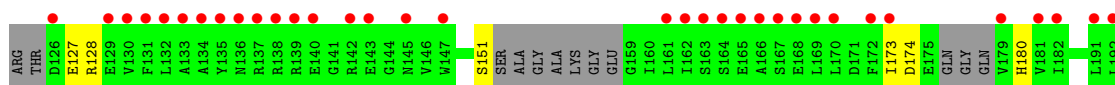
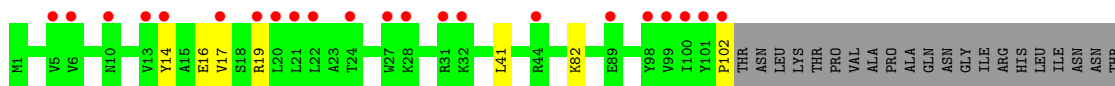
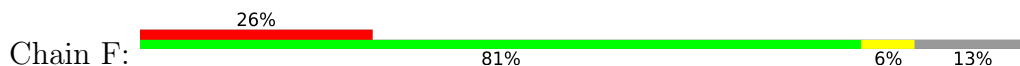




• Molecule 3: Stathmin-4



• 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	105.27Å 158.55Å 181.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.15 – 2.25 48.17 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.15-2.25) 99.9 (48.17-2.25)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.181 , 0.223 0.180 , 0.184	Depositor DCC
R_{free} test set	7225 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtrriage
Anisotropy	0.132	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18429	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: GDP, GTP, Q0F, IMD, CA, MG, MES, ACP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/3500	0.43	0/4751
1	C	0.26	0/3584	0.44	0/4866
2	B	0.26	0/3424	0.43	0/4636
2	D	0.25	0/3385	0.42	0/4584
3	E	0.24	0/1016	0.34	0/1348
4	F	0.24	0/2812	0.40	0/3794
All	All	0.25	0/17721	0.42	0/23979

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	3419	0	3336	17	0
1	C	3482	0	3395	17	0
2	B	3350	0	3232	29	0
2	D	3312	0	3197	16	0
3	E	1005	0	1024	4	0
4	F	2748	0	2726	12	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	2	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	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	5	0	5	0	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	B	12	0	12	4	0
11	D	45	0	0	0	0
12	F	31	0	14	1	0
13	A	166	0	0	1	0
13	B	198	0	0	4	0
13	C	325	0	0	1	0
13	D	107	0	0	5	0
13	E	36	0	0	1	0
13	F	57	0	0	0	0
All	All	18429	0	16989	96	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 3.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:HIS:ND1	13:B:601:HOH:O	2.25	0.69
4:F:225:SER:HG	4:F:250:SER:HG	1.46	0.64
1:C:229:ARG:NH1	13:C:603:HOH:O	2.32	0.63
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.81	0.62
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.61
2:D:394:GLN:NE2	13:D:605:HOH:O	2.34	0.60
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.83	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.58
2:D:167:ASN:ND2	13:D:606:HOH:O	2.35	0.58
3:E:44:ASP:N	13:E:303:HOH:O	2.35	0.58
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.88	0.55
2:B:164:ARG:NH1	13:B:605:HOH:O	2.39	0.55
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.89	0.55
4:F:333:ASN:ND2	12:F:401:ACP:O3G	2.29	0.55
2:B:253[A]:ARG:NH1	10:B:504:MES:O3S	2.40	0.54
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.90	0.54
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.40	0.54
4:F:82:LYS:NZ	4:F:127:GLU:OE1	2.41	0.54
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.91	0.53
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.91	0.53
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.91	0.53
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.51
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.51
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.94	0.50
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.93	0.50
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.94	0.50
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.94	0.49
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.94	0.49
2:D:136:GLN:HA	2:D:167:ASN:O	2.11	0.49
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.47	0.49
2:B:424:ASN:HB3	13:B:604:HOH:O	2.13	0.49
1:A:264:ARG:NH1	13:A:604:HOH:O	2.39	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.49
2:B:147:SER:OG	2:B:190:SER:OG	2.28	0.48
2:B:253[A]:ARG:NH1	10:B:504:MES:O1S	2.33	0.48
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.48
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.26	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.96	0.47
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.97	0.47
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.50	0.47
2:B:175:PRO:HA	2:B:178:SER:HB2	1.97	0.47
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.50	0.47
2:D:46:LEU:HA	2:D:49:ILE:HB	1.97	0.47
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.98	0.46
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.97	0.46
1:C:132:LEU:HG	1:C:164:LYS:HD3	1.98	0.46
1:C:140:SER:HA	1:C:171:ILE:HB	1.98	0.46
2:B:192:HIS:ND1	13:B:604:HOH:O	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:NH1	2:B:196:GLU:O	2.48	0.46
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.47	0.45
2:B:276:THR:HG21	2:B:282:GLN:HA	1.99	0.45
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.49	0.45
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.99	0.44
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.44
4:F:102:PRO:HB3	4:F:173:ILE:HG22	1.98	0.44
2:B:295:MET:CG	2:B:377:PHE:HB2	2.48	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.44
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.33	0.44
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.53	0.44
2:B:31:ASP:OD1	2:B:35:SER:N	2.50	0.44
2:D:298:SER:HB3	2:D:307:PRO:HD2	1.99	0.44
9:D:501:GDP:O3B	13:D:601:HOH:O	2.21	0.44
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.17	0.44
2:D:11:GLN:HA	2:D:74:THR:HG21	2.00	0.44
2:B:253[A]:ARG:NH1	10:B:504:MES:S	2.86	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.43
1:C:180:ALA:O	1:C:183:GLU:HG3	2.18	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HD3	2.01	0.43
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.55	0.42
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.49	0.42
1:C:368:LEU:HD23	1:C:368:LEU:HA	1.86	0.42
2:D:303:ALA:O	2:D:305:CYS:N	2.53	0.42
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.02	0.42
2:D:142:GLY:O	2:D:183:GLU:HG2	2.19	0.42
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.55	0.42
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.59	0.42
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.02	0.42
4:F:14:TYR:HA	4:F:17:VAL:HB	2.02	0.41
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.55	0.41
3:E:135:LYS:HE2	3:E:139:LEU:HD11	2.02	0.41
1:A:3:GLU:O	1:A:133:GLN:HG2	2.19	0.41
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.56	0.41
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.54	0.41
2:D:438:ALA:O	13:D:602:HOH:O	2.21	0.41
2:B:83:PHE:O	2:B:86:ILE:HG22	2.21	0.41
10:B:504:MES:H81	10:B:504:MES:H51	1.84	0.41
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.51	0.41
9:D:501:GDP:O1A	13:D:603:HOH:O	2.22	0.41
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:CYS:HB3	1:A:30:ILE:O	2.21	0.41
1:A:2:ARG:O	1:A:133:GLN:NE2	2.54	0.40
2:B:292:THR:HA	2:B:295:MET:HE2	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	436/451 (97%)	426 (98%)	10 (2%)	0	100	100
1	C	447/451 (99%)	440 (98%)	7 (2%)	0	100	100
2	B	421/445 (95%)	411 (98%)	10 (2%)	0	100	100
2	D	417/445 (94%)	409 (98%)	7 (2%)	1 (0%)	47	55
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	323/384 (84%)	313 (97%)	10 (3%)	0	100	100
All	All	2162/2319 (93%)	2117 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	304	ALA

5.3.2 Protein sidechains [i](#)

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	369/379 (97%)	367 (100%)	2 (0%)	88	92
1	C	380/379 (100%)	377 (99%)	3 (1%)	81	88
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	95
2	D	364/383 (95%)	363 (100%)	1 (0%)	92	95
3	E	110/127 (87%)	109 (99%)	1 (1%)	78	86
4	F	302/342 (88%)	300 (99%)	2 (1%)	84	90
All	All	1893/1993 (95%)	1883 (100%)	10 (0%)	88	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
2	B	139	HIS
1	C	1	MET
1	C	71	GLU
1	C	381	THR
2	D	139	HIS
3	E	140	LYS
4	F	217	ARG
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	18	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry i

Of 19 ligands modelled in this entry, 11 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
10	MES	B	504	-	12,12,12	2.16	1 (8%)	14,16,16	1.95	5 (35%)
11	Q0F	D	503	-	46,48,48	1.35	5 (10%)	53,71,71	1.45	13 (24%)
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.35	5 (15%)
9	GDP	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.16	3 (10%)
12	ACP	F	401	6	27,33,33	1.99	7 (25%)	32,52,52	1.17	3 (9%)
8	IMD	A	504	-	3,5,5	0.41	0	4,5,5	0.58	0
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.39	5 (15%)
9	GDP	D	501	6	24,30,30	0.96	1 (4%)	30,47,47	1.17	4 (13%)

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
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
11	Q0F	D	503	-	-	11/49/76/76	0/2/4/4
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
12	ACP	F	401	6	-	5/15/38/38	0/3/3/3
8	IMD	A	504	-	-	-	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.22	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PG-O1G	5.65	1.62	1.50
12	F	401	ACP	PB-O1B	4.13	1.61	1.51
11	D	503	Q0F	O21-C17	4.10	1.29	1.21
5	C	501	GTP	C5-C6	-3.92	1.39	1.47
5	A	501	GTP	C5-C6	-3.85	1.39	1.47
11	D	503	Q0F	O29-C23	-3.80	1.40	1.45
11	D	503	Q0F	C28-N31	3.58	1.42	1.35
12	F	401	ACP	PB-O2B	-3.46	1.48	1.56
12	F	401	ACP	PB-O3A	3.26	1.62	1.58
12	F	401	ACP	PG-O2G	-2.82	1.48	1.54
12	F	401	ACP	PG-O3G	2.79	1.61	1.54
11	D	503	Q0F	O18-C19	-2.45	1.43	1.46
9	D	501	GDP	C6-N1	-2.42	1.34	1.37
12	F	401	ACP	C5-C4	2.40	1.47	1.40
9	B	501	GDP	C6-N1	-2.32	1.34	1.37
5	A	501	GTP	C2-N3	2.20	1.38	1.33
5	C	501	GTP	C2-N3	2.09	1.38	1.33
11	D	503	Q0F	O18-C17	2.03	1.38	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	503	Q0F	C6-C5-N31	3.93	124.74	120.71
10	B	504	MES	C5-N4-C3	3.66	117.07	108.83
10	B	504	MES	O1S-S-C8	3.56	111.20	106.92
11	D	503	Q0F	C25-O29-C23	3.39	62.83	60.79
5	C	501	GTP	C8-N7-C5	3.19	109.06	102.99
5	A	501	GTP	C5-C6-N1	3.16	119.53	113.95
9	B	501	GDP	PA-O3A-PB	-3.06	122.31	132.83
5	A	501	GTP	C8-N7-C5	3.01	108.72	102.99
5	C	501	GTP	C5-C6-N1	2.99	119.23	113.95
11	D	503	Q0F	O29-C25-C23	-2.99	57.37	59.38
5	C	501	GTP	PA-O3A-PB	-2.97	122.63	132.83
12	F	401	ACP	C3'-C2'-C1'	2.94	105.40	100.98
12	F	401	ACP	N3-C2-N1	-2.91	124.13	128.68
9	D	501	GDP	PA-O3A-PB	-2.80	123.23	132.83
5	A	501	GTP	PA-O3A-PB	-2.78	123.27	132.83
5	A	501	GTP	C2-N1-C6	-2.76	120.01	125.10
12	F	401	ACP	PB-O3A-PA	-2.75	123.83	132.56
5	C	501	GTP	PB-O3B-PG	-2.73	123.45	132.83
11	D	503	Q0F	O29-C25-C38	2.60	117.89	114.17
10	B	504	MES	C6-C5-N4	-2.58	106.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N1-C6	-2.58	120.36	125.10
11	D	503	Q0F	O18-C17-O21	-2.45	114.31	117.87
10	B	504	MES	C7-N4-C5	2.44	117.49	111.23
9	B	501	GDP	C5-C6-N1	2.44	118.26	113.95
11	D	503	Q0F	O30-C26-C25	2.39	110.88	105.48
10	B	504	MES	O3S-S-C8	2.36	109.59	105.77
9	D	501	GDP	C8-N7-C5	2.36	107.49	102.99
9	D	501	GDP	C3'-C2'-C1'	2.33	104.49	100.98
9	B	501	GDP	C8-N7-C5	2.32	107.42	102.99
11	D	503	Q0F	O34-C1-C6	2.30	118.26	115.53
9	D	501	GDP	C5-C6-N1	2.27	117.97	113.95
5	A	501	GTP	PB-O3B-PG	-2.24	125.15	132.83
11	D	503	Q0F	O34-C1-C2	-2.19	120.36	124.12
11	D	503	Q0F	C4-C5-C6	-2.15	119.79	122.53
11	D	503	Q0F	C27-C28-N31	-2.15	116.47	118.89
11	D	503	Q0F	O30-C39-C40	2.11	116.04	111.50
11	D	503	Q0F	C5-C6-CL33	2.10	122.33	120.09
11	D	503	Q0F	C24-C22-C23	-2.05	108.12	112.55

There are no chirality outliers.

All (38) 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	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	PA-O3A-PB-O2B
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O1S
11	D	503	Q0F	C12-C13-O15-C37
11	D	503	Q0F	C6-C1-O34-C36
11	D	503	Q0F	C20-C19-C22-C23
11	D	503	Q0F	C20-C19-C22-C24
11	D	503	Q0F	O18-C19-C22-C24
12	F	401	ACP	C5'-O5'-PA-O3A
11	D	503	Q0F	C40-C39-O30-C26
11	D	503	Q0F	C2-C1-O34-C36

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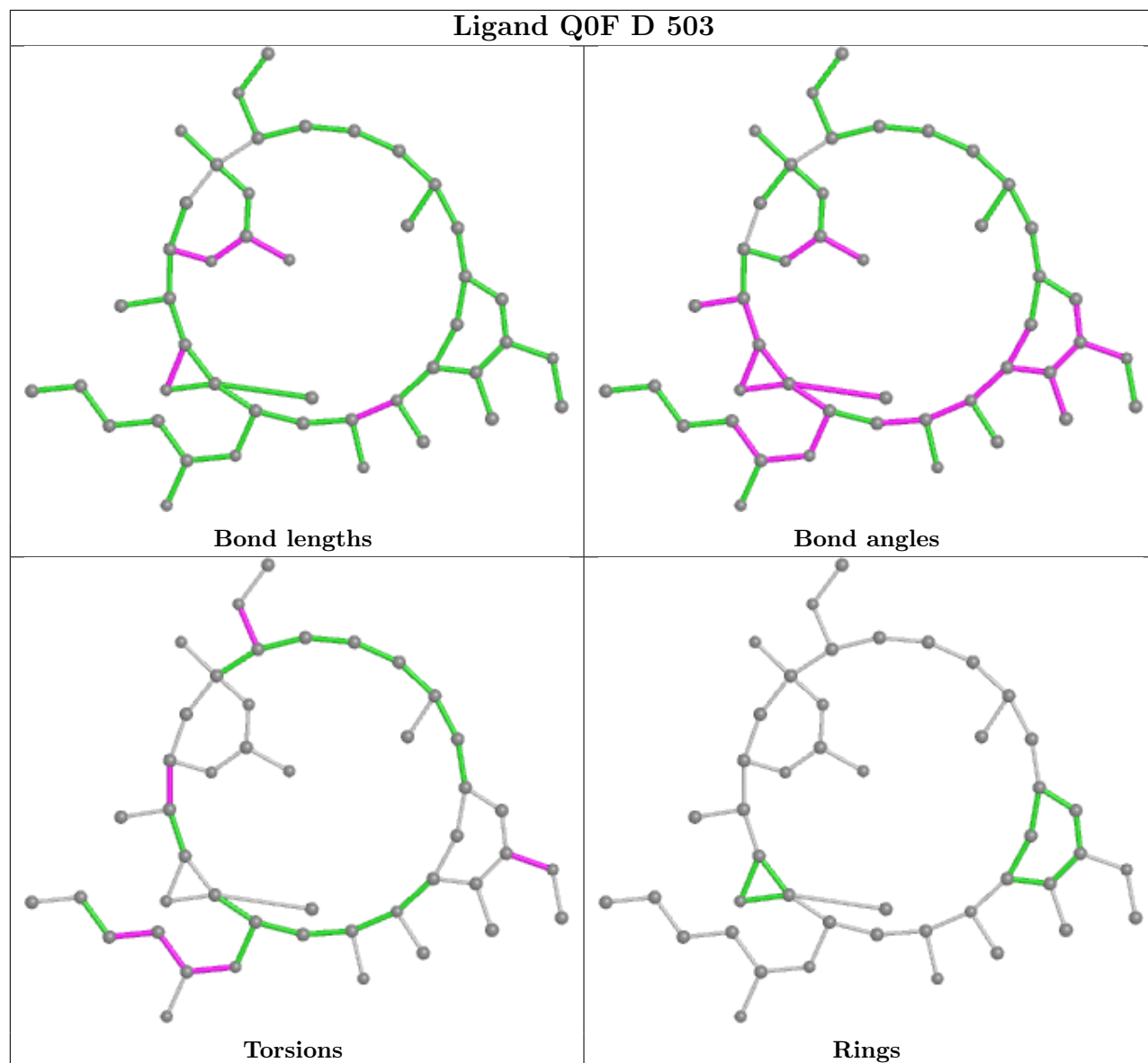
Mol	Chain	Res	Type	Atoms
11	D	503	Q0F	O41-C39-O30-C26
10	B	504	MES	C7-C8-S-O3S
11	D	503	Q0F	O18-C19-C22-C23
11	D	503	Q0F	C39-C40-C43-C44
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
12	F	401	ACP	O4'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
12	F	401	ACP	C3'-C4'-C5'-O5'
11	D	503	Q0F	O30-C39-C40-C43

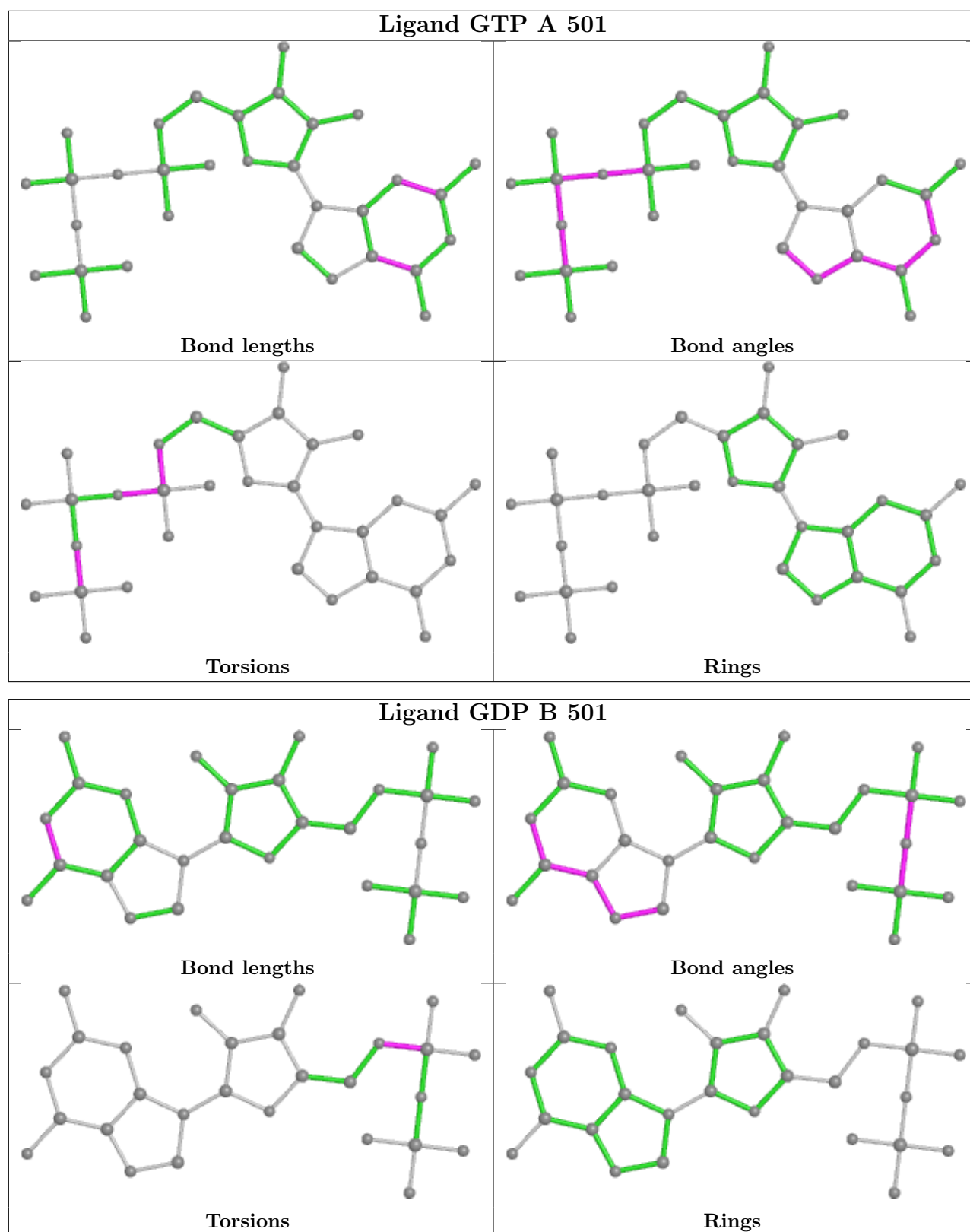
There are no ring outliers.

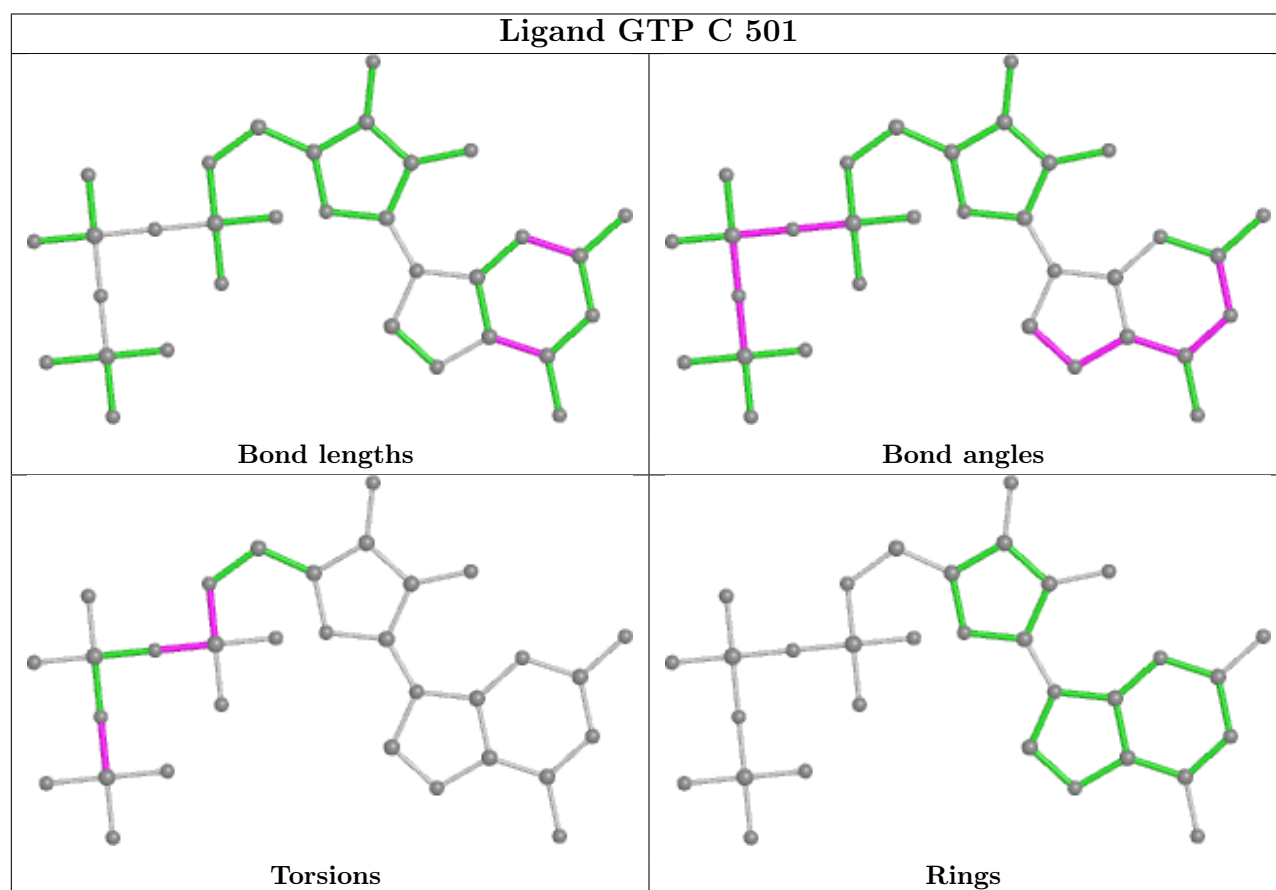
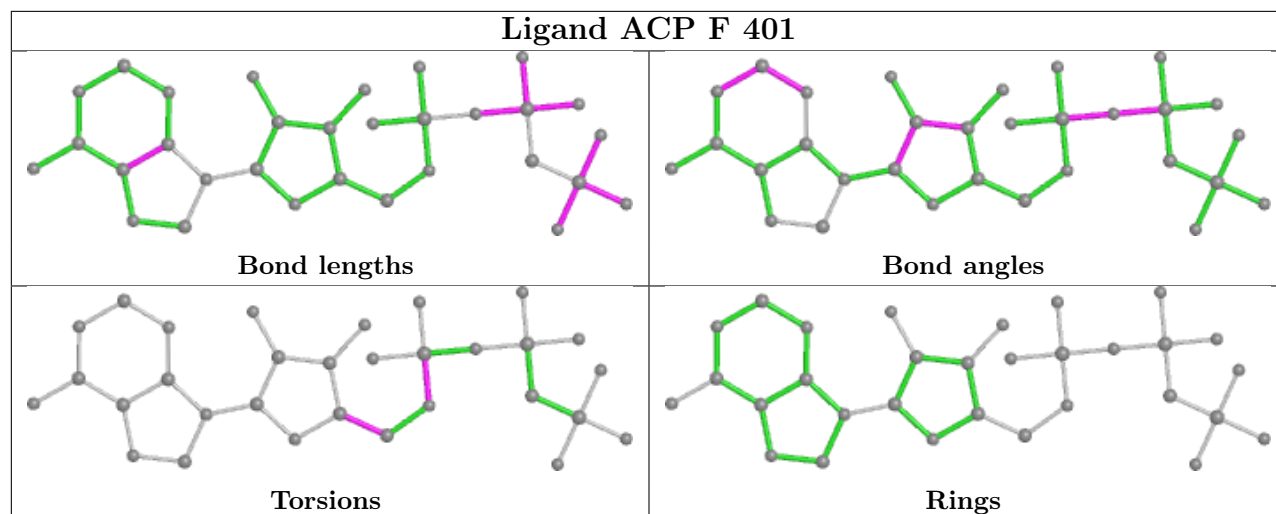
4 monomers are involved in 9 short contacts:

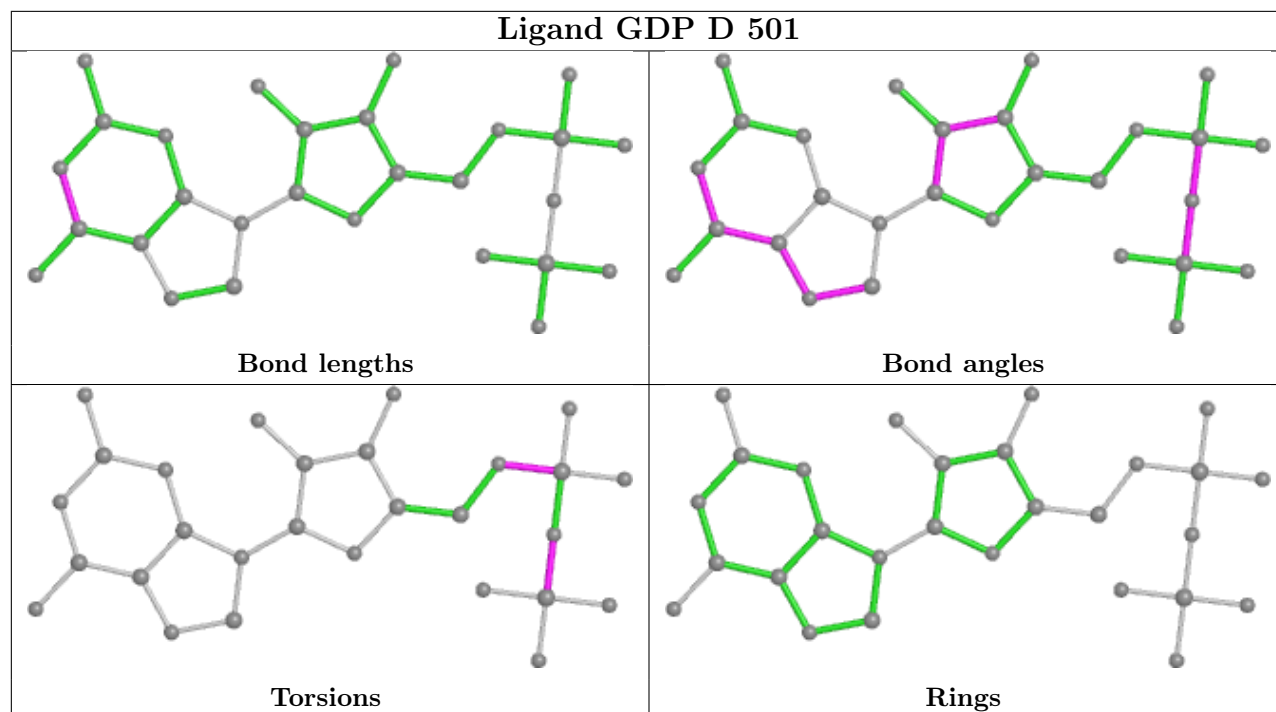
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	4	0
9	B	501	GDP	1	0
12	F	401	ACP	1	0
9	D	501	GDP	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	437/451 (96%)	0.14	15 (3%) 45 47	41, 61, 97, 164	0
1	C	439/451 (97%)	-0.16	4 (0%) 84 85	33, 47, 76, 103	0
2	B	424/445 (95%)	0.15	21 (4%) 28 31	37, 56, 97, 148	0
2	D	420/445 (94%)	0.07	15 (3%) 42 44	41, 72, 110, 145	0
3	E	121/143 (84%)	0.19	8 (6%) 18 20	47, 76, 113, 133	0
4	F	334/384 (86%)	1.22	101 (30%) 0 0	49, 85, 154, 199	0
All	All	2175/2319 (93%)	0.24	164 (7%) 14 15	33, 64, 114, 199	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	10.9
2	B	59	ASN	8.5
1	A	282	TYR	8.3
4	F	132	LEU	8.0
4	F	251	LYS	7.8
2	B	1	MET	7.7
4	F	135	TYR	7.5
2	B	57	THR	7.4
4	F	249	TYR	6.8
4	F	244	CYS	6.7
3	E	27	PRO	6.5
4	F	253	TYR	6.5
4	F	131	PHE	6.5
4	F	166	ALA	6.2
4	F	250	SER	6.1
4	F	139	ARG	5.8
4	F	240	LEU	5.8
4	F	130	VAL	5.7
4	F	161	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	5.6
4	F	252	ASN	5.5
3	E	139	LEU	5.4
4	F	20	LEU	5.4
2	D	1	MET	5.3
4	F	136	ASN	5.1
4	F	246	GLN	4.9
4	F	256	TYR	4.9
3	E	26	PRO	4.8
4	F	259	GLY	4.8
4	F	21	LEU	4.6
2	D	57	THR	4.6
4	F	133	ALA	4.6
1	A	346	TRP	4.6
1	C	340	SER	4.5
4	F	142	ARG	4.5
4	F	170	LEU	4.4
1	A	262	TYR	4.4
4	F	138	ARG	4.4
2	B	276	THR	4.4
2	D	56	ALA	4.3
4	F	248	GLU	4.3
4	F	145	ASN	4.3
4	F	129	GLU	4.2
2	D	400	ARG	4.2
2	B	438	ALA	4.2
4	F	165	GLU	4.2
2	B	60	LYS	4.1
4	F	143	GLU	4.1
4	F	101	TYR	4.1
4	F	243	HIS	4.0
4	F	17	VAL	4.0
4	F	99	VAL	3.8
4	F	31	ARG	3.8
2	B	36	TYR	3.6
2	B	38	GLY	3.6
4	F	239	HIS	3.5
4	F	225	SER	3.5
4	F	22	LEU	3.5
4	F	223	THR	3.5
2	D	37	HIS	3.5
4	F	182	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	167	SER	3.5
2	B	61	TYR	3.4
4	F	245	ILE	3.4
2	B	56	ALA	3.3
2	D	401	ARG	3.3
4	F	13	VAL	3.3
2	B	33	THR	3.3
1	A	59	GLY	3.2
4	F	254	GLY	3.2
2	B	37	HIS	3.2
2	B	437	ASP	3.2
2	D	83	PHE	3.1
4	F	192	LEU	3.1
4	F	340	GLN	3.1
4	F	194	PRO	3.1
4	F	247	LYS	3.1
3	E	28	SER	3.1
4	F	255	ARG	3.1
2	B	58	GLY	3.0
4	F	343	TYR	3.0
2	D	219	LEU	3.0
4	F	361	LEU	2.9
4	F	162	ILE	2.9
4	F	227	PRO	2.9
4	F	267	PHE	2.9
4	F	19	ARG	2.9
4	F	27	TRP	2.9
2	B	34	GLY	2.9
4	F	134	ALA	2.9
3	E	45	PRO	2.9
2	D	404	PHE	2.9
4	F	100	ILE	2.8
4	F	346	LEU	2.8
2	B	86	ILE	2.8
2	B	284	ARG	2.8
2	B	62	VAL	2.8
4	F	5	VAL	2.8
4	F	164	SER	2.8
2	D	415	GLU	2.8
1	A	171	ILE	2.8
1	A	86	LEU	2.8
4	F	221	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	241	THR	2.8
3	E	48	GLU	2.8
3	E	46	SER	2.7
1	C	1	MET	2.7
1	C	253	THR	2.7
4	F	191	LEU	2.7
4	F	147	TRP	2.7
2	B	82	PRO	2.6
4	F	140	GLU	2.6
4	F	197	ARG	2.6
4	F	6	VAL	2.6
4	F	222	ARG	2.6
4	F	163	SER	2.6
4	F	337	ALA	2.6
4	F	10	ASN	2.6
4	F	24	THR	2.6
4	F	226	GLU	2.5
4	F	236	LYS	2.5
4	F	242	ASN	2.5
4	F	258	GLU	2.5
1	A	281	ALA	2.5
1	C	252	LEU	2.5
2	D	128	SER	2.5
4	F	260	ASN	2.5
4	F	199	PHE	2.5
3	E	25	LYS	2.4
4	F	102	PRO	2.4
4	F	262	MET	2.4
1	A	56	THR	2.4
2	D	60	LYS	2.4
2	D	94	PHE	2.4
2	D	177	VAL	2.4
4	F	263	PHE	2.4
4	F	98	TYR	2.3
4	F	172	PHE	2.3
1	A	285	GLN	2.3
4	F	32	LYS	2.3
1	A	58	ALA	2.3
1	A	348	PRO	2.3
4	F	238	CYS	2.3
2	D	405	LEU	2.3
4	F	181	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	172	TYR	2.2
2	B	180	THR	2.2
4	F	89	GLU	2.2
4	F	179	VAL	2.2
4	F	220	VAL	2.2
4	F	126	ASP	2.2
4	F	44	ARG	2.2
2	B	35	SER	2.1
4	F	137	ARG	2.1
1	A	83	TYR	2.1
4	F	168	GLU	2.1
4	F	224	SER	2.1
4	F	196	HIS	2.1
4	F	14	TYR	2.1
1	A	146	GLY	2.1
1	A	142	GLY	2.1
4	F	228	TYR	2.0
4	F	342	LEU	2.0
4	F	28	LYS	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 monosaccharides 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.

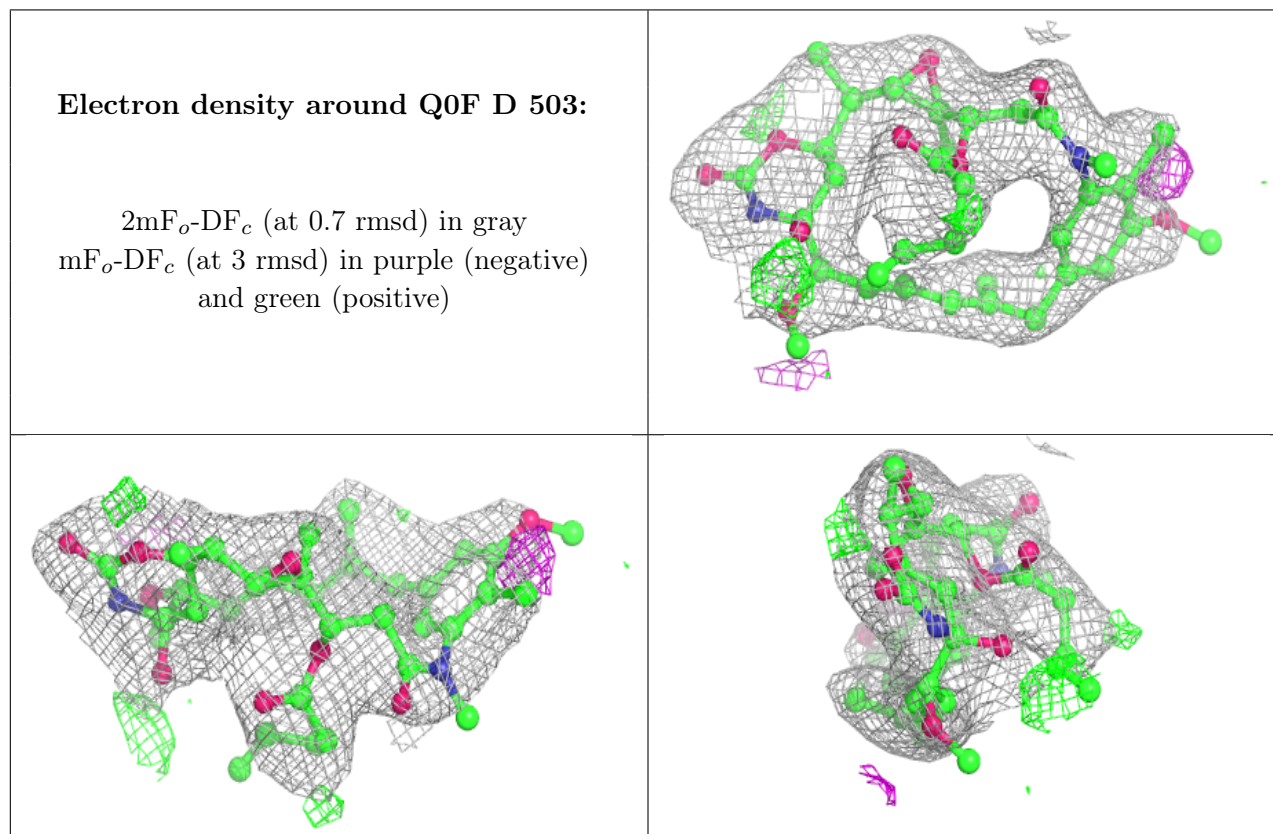
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	505	1/1	0.75	0.30	95,95,95,95	0
7	CA	E	201	1/1	0.84	0.08	112,112,112,112	0
7	CA	B	505	1/1	0.89	0.12	112,112,112,112	0
8	IMD	A	504	5/5	0.90	0.09	81,83,86,86	0

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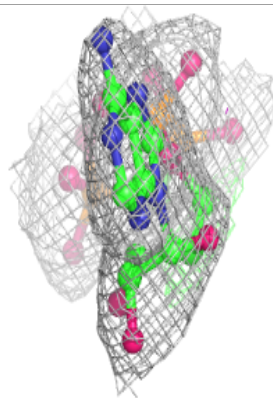
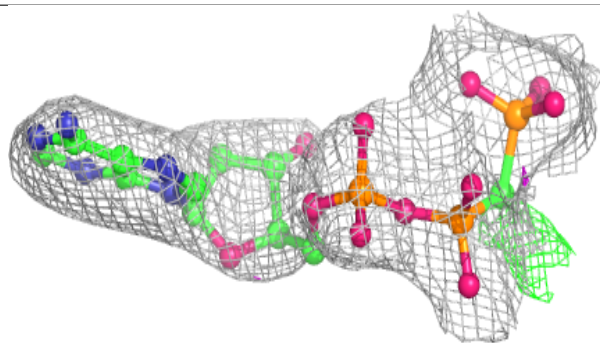
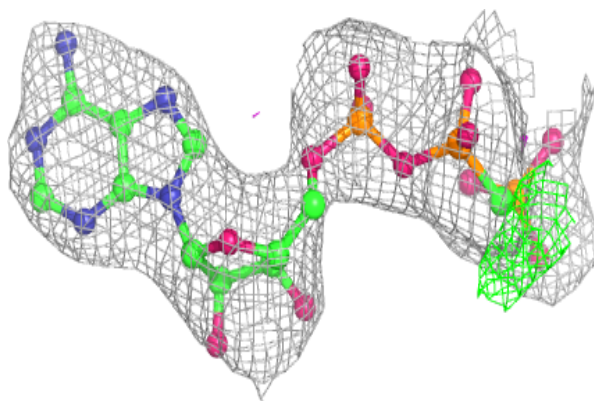
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	Q0F	D	503	45/45	0.91	0.24	55,93,108,127	0
12	ACP	F	401	31/31	0.92	0.14	104,112,125,128	0
7	CA	B	503	1/1	0.94	0.06	109,109,109,109	0
9	GDP	D	501	28/28	0.95	0.11	52,61,81,97	0
10	MES	B	504	12/12	0.95	0.14	52,61,89,89	0
7	CA	A	503	1/1	0.97	0.03	75,75,75,75	0
6	MG	A	502	1/1	0.97	0.14	44,44,44,44	0
6	MG	D	502	1/1	0.97	0.04	76,76,76,76	0
6	MG	F	402	1/1	0.98	0.10	95,95,95,95	0
5	GTP	A	501	32/32	0.98	0.20	31,45,49,62	0
7	CA	C	503	1/1	0.99	0.08	62,62,62,62	0
6	MG	C	502	1/1	0.99	0.11	39,39,39,39	0
5	GTP	C	501	32/32	0.99	0.15	31,38,44,47	0
9	GDP	B	501	28/28	0.99	0.20	33,44,49,53	0
6	MG	B	502	1/1	1.00	0.16	41,41,41,41	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.

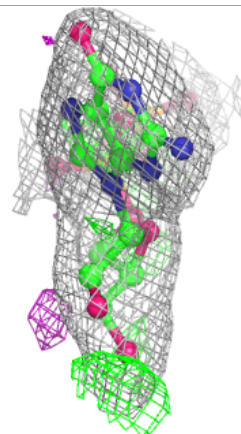
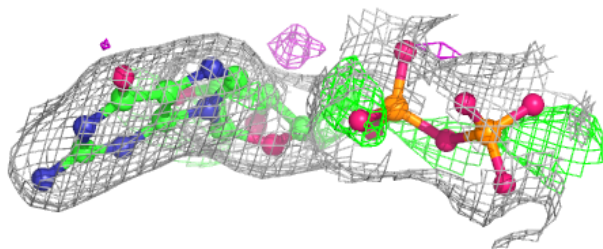
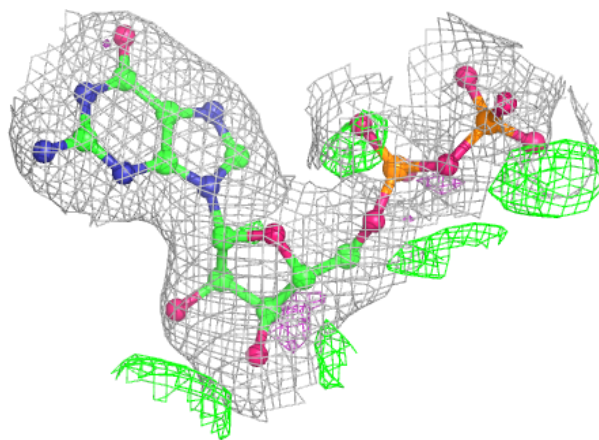


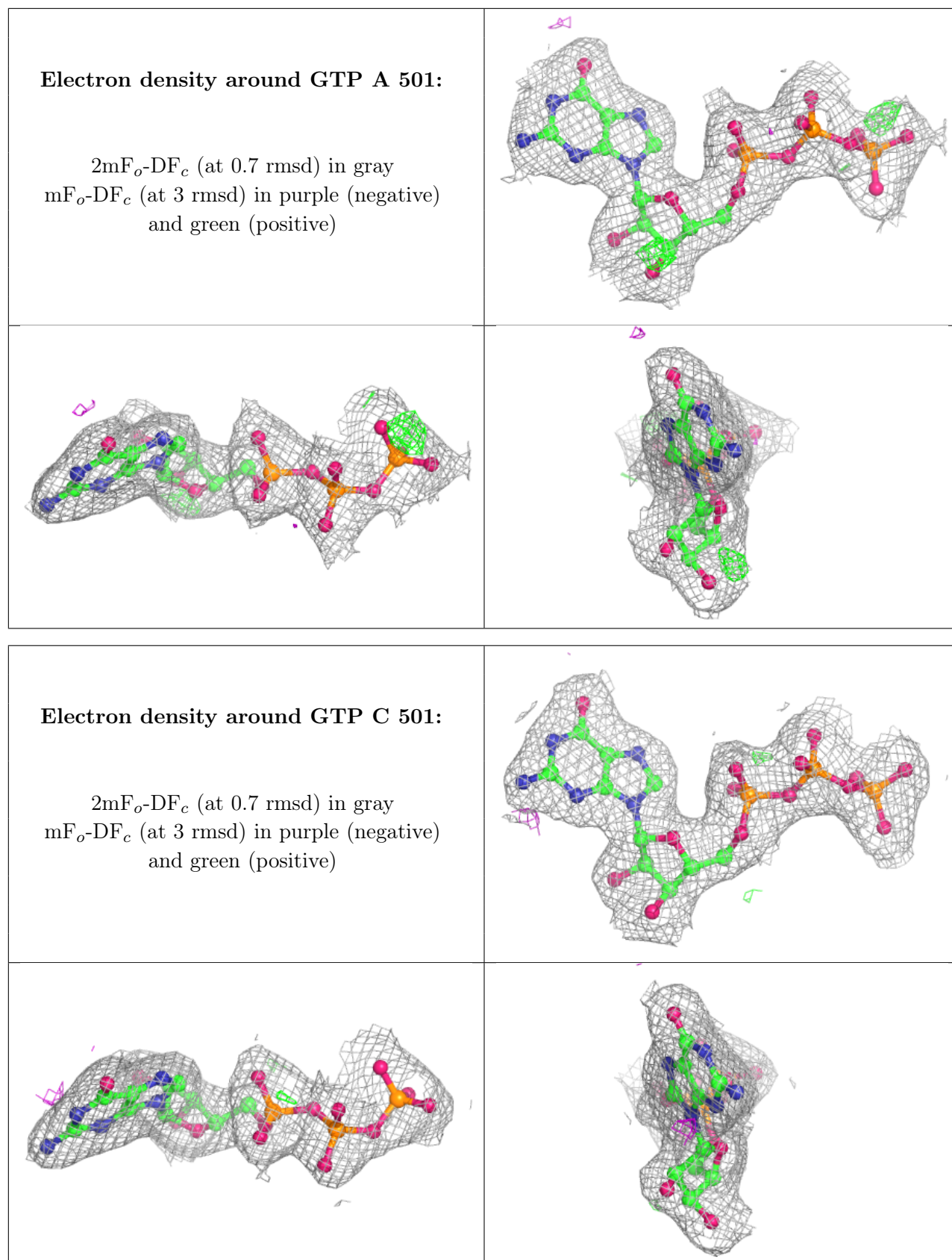
Electron density around ACP F 401:

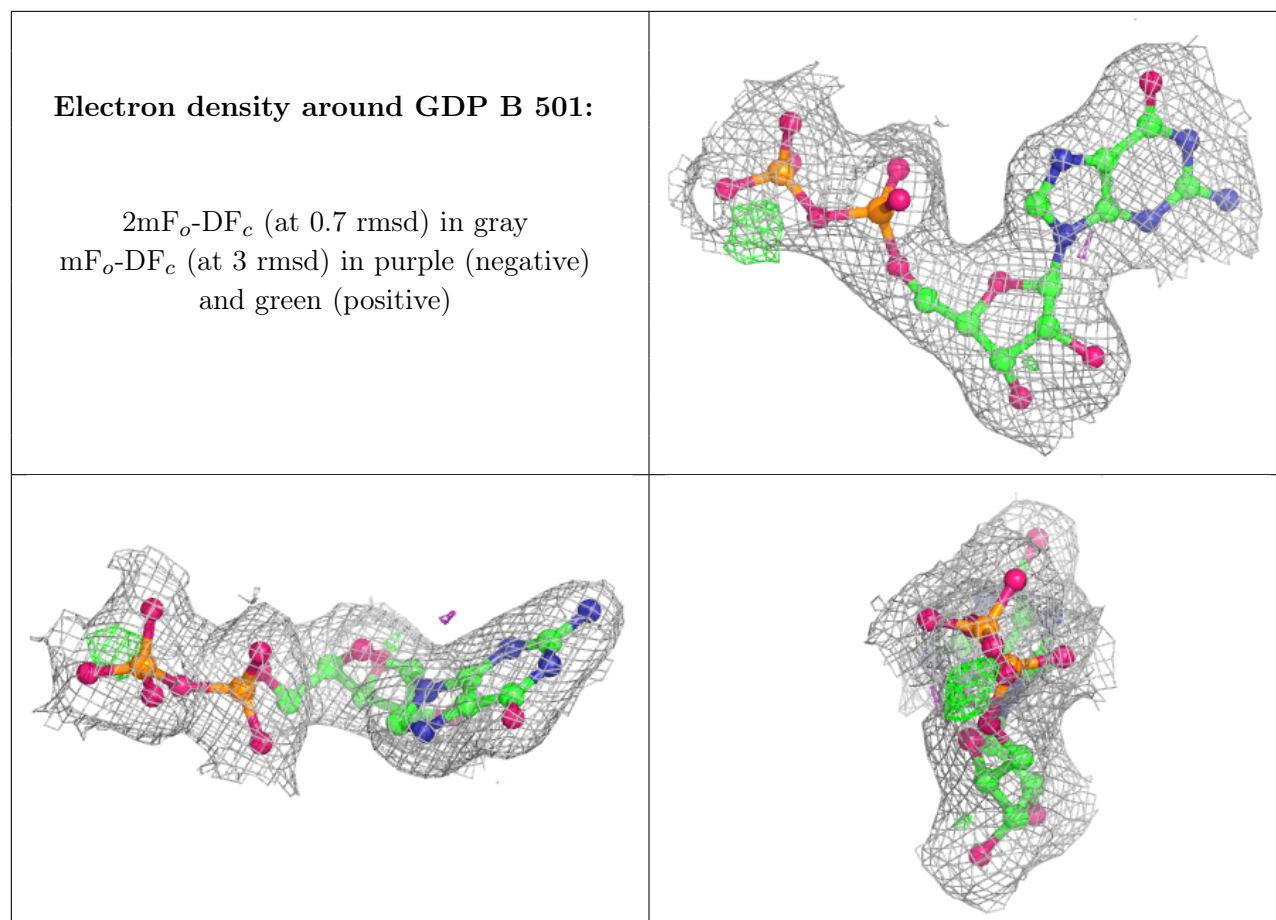
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**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)







6.5 Other polymers [i](#)

There are no such residues in this entry.