Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2023 – 03:28 pm GMT

PDB ID	:	8BDF
Title	:	Tubulin-taxane-2a complex
Authors	:	Prota, A.E.; Lucena-Agell, D.; Ma, Y.; Estevez-Gallego, J.; Li, S.; Bargsten, K.; Altmann, K.H.; Gaillard, N.; Kamimura, S.; Muehlethaler, T.; Gago, F.; Oliva, M.A.; Steinmetz, M.O.; Fang, W.S.; Diaz, J.F.
Deposited on	:	2022-10-19
Resolution	:	1.95 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:

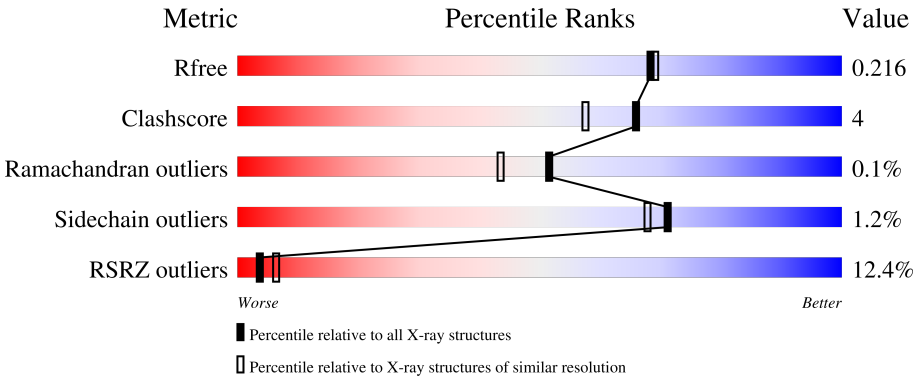
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	451	8% 90% 8%
1	C	451	4% 88% 9%
2	B	445	7% 84% 12%
2	D	445	14% 83% 12%

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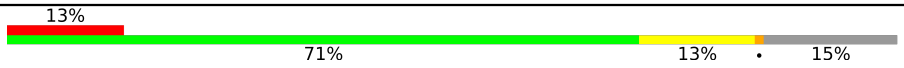
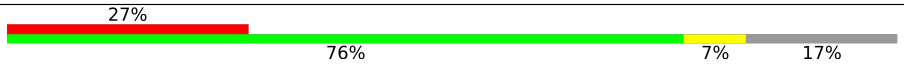
Mol	Chain	Length	Quality of chain
3	E	143	
4	F	384	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18392 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
1	A	441	Total	C	N	O	S	0	0	0
			3446	2179	585	660	22			
1	C	440	Total	C	N	O	S	0	2	0
			3447	2181	585	659	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3359	2110	575	647	27			
2	D	426	Total	C	N	O	S	0	1	0
			3354	2104	574	649	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	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

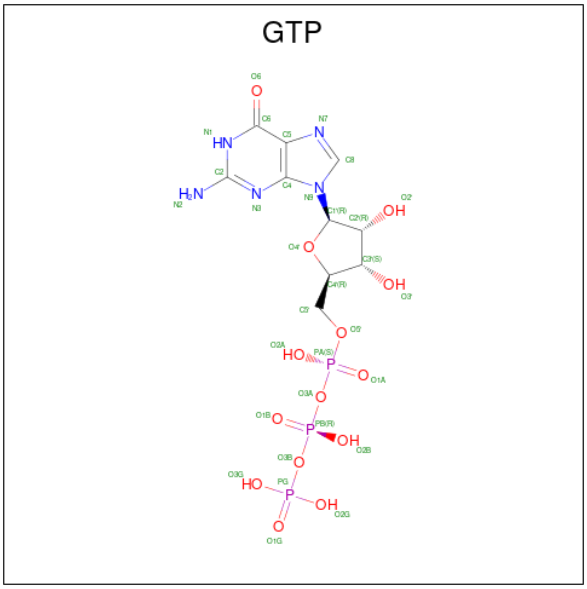
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	319	Total	C	N	O	S	0	0	0
			2614	1687	441	472	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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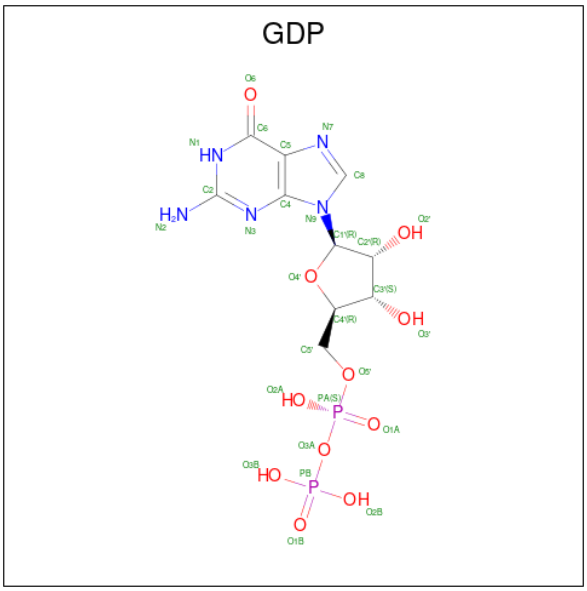
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

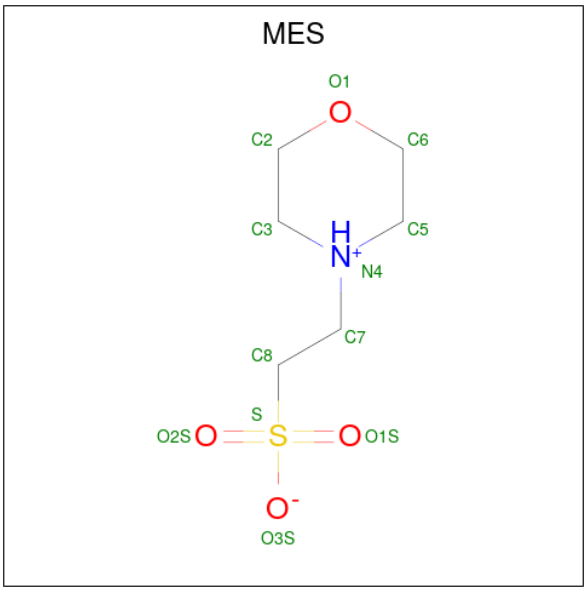
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



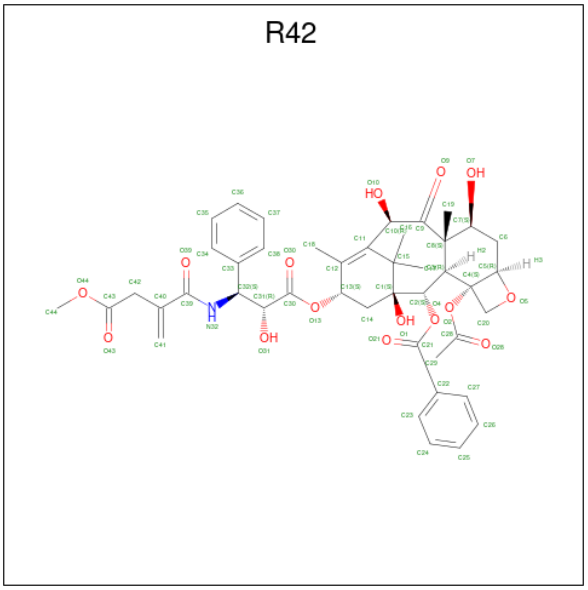
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

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



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

- Molecule 10 is [(1 {S},2 {S},3 {R},4 {S},7 {R},9 {S},10 {S},12 {R},15 {S})-4-acetyloxy-15-[(2 {R},3 {S})-3-[(4-methoxy-2-methylidene-4-oxidanylidene-butanoyl)amino]-2-oxidanyl-3-phenyl-propanoyl]oxy-10,14,16,16-tetramethyl-1,9,12-tris(oxidanyl)-11-oxidanylidene-6-oxatetracyclo[11.3.1.0^{3,10}.0^{4,7}]heptadec-13-en-2-yl] benzoate (three-letter code: R42) (formula: $C_{44}H_{51}NO_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			60	44	1	15		

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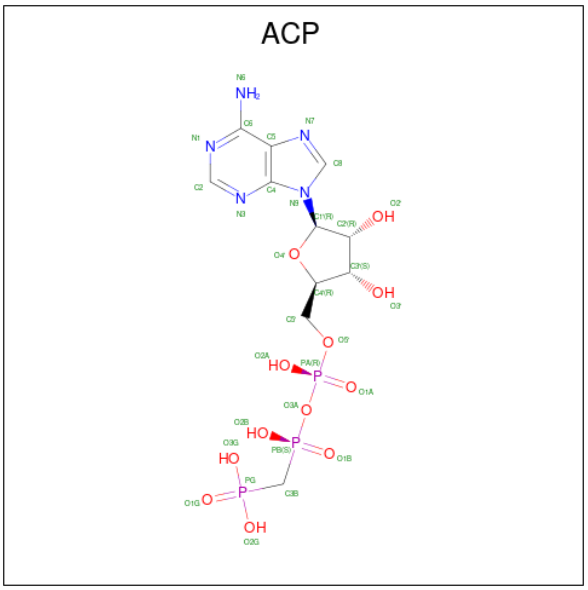
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			60	44	1	15		

- 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	C	N	O	P	0	0
			31	11	5	12	3		

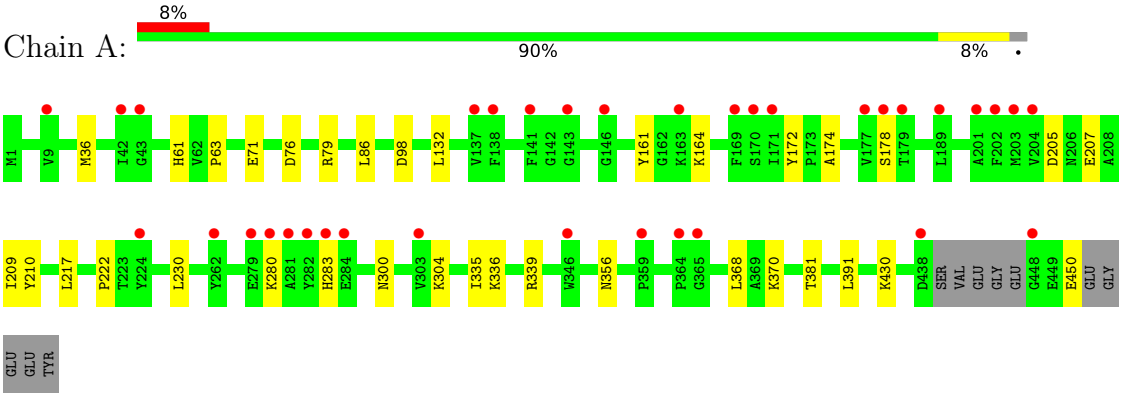
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	169	Total	O	0	0
			169	169		
12	B	156	Total	O	0	0
			156	156		
12	C	316	Total	O	0	0
			316	316		
12	D	122	Total	O	0	0
			122	122		
12	E	47	Total	O	0	0
			47	47		
12	F	73	Total	O	0	0
			73	73		

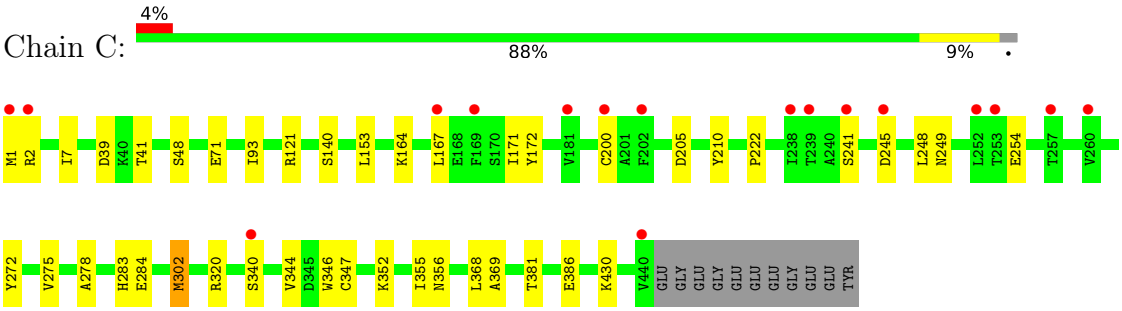
3 Residue-property plots (i)

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.

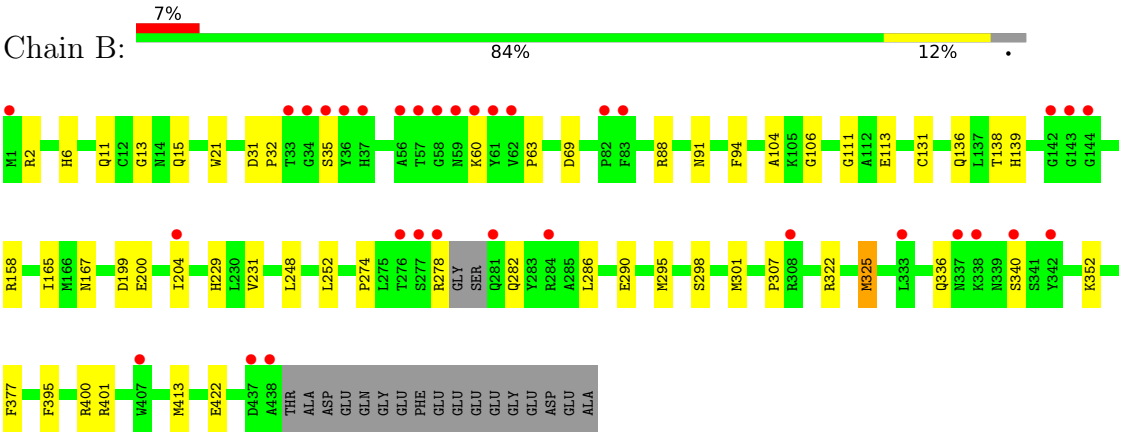
• Molecule 1: Tubulin alpha-1B chain



• Molecule 1: Tubulin alpha-1B chain

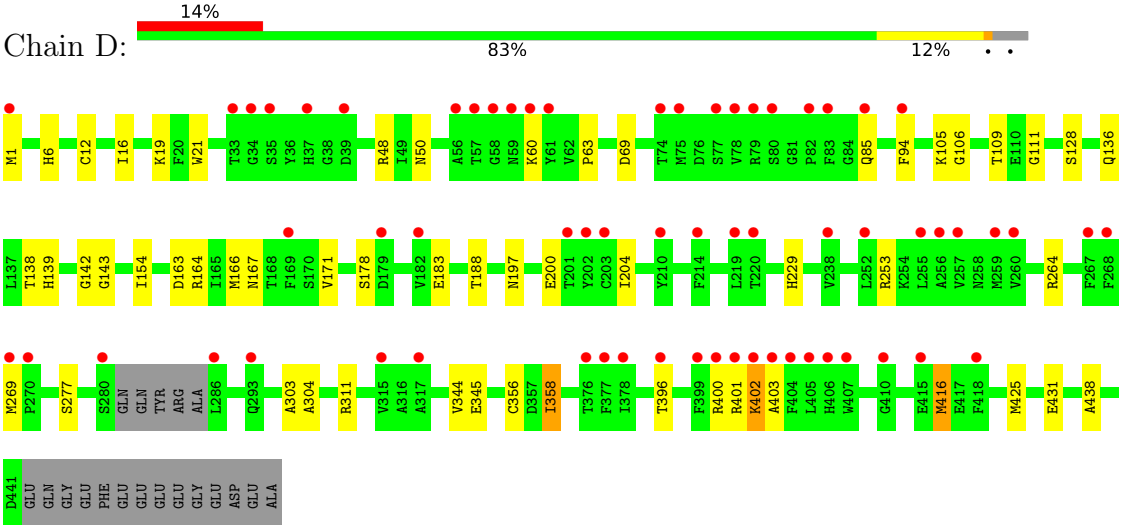


• Molecule 2: Tubulin beta-2B chain



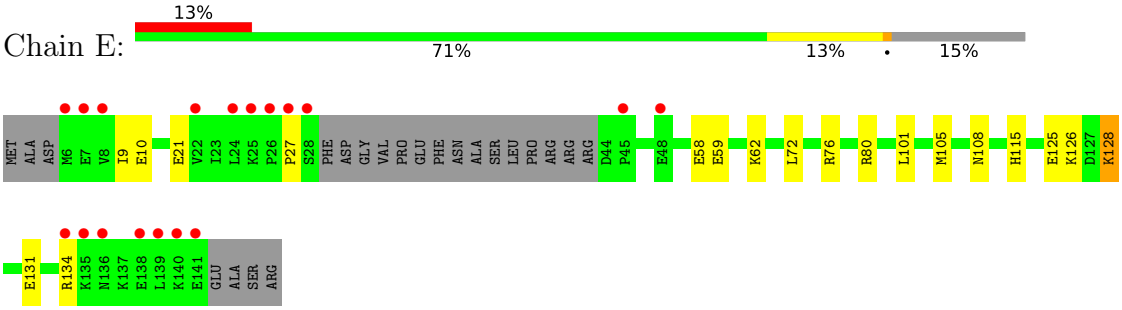
• Molecule 2: Tubulin beta-2B chain

Chain D:



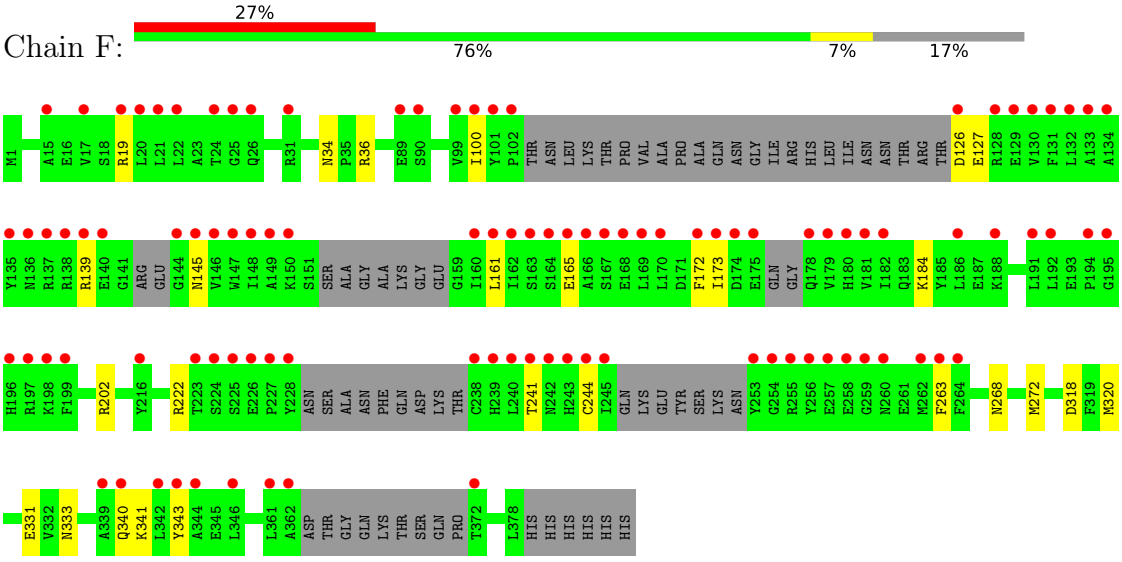
• Molecule 3: Stathmin-4

Chain E:



• Molecule 4: Tubulin beta-2B chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.84Å 157.89Å 179.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 1.95 49.28 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.28-1.95) 100.0 (49.28-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.189 , 0.216 0.189 , 0.216	Depositor DCC
R_{free} test set	10797 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.4	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	0.97	EDS
Total number of atoms	18392	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GDP, R42, MES, MG, ACP, GTP, 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	0.26	0/3523	0.46	0/4780
1	C	0.28	0/3528	0.48	0/4790
2	B	0.26	0/3433	0.45	0/4648
2	D	0.25	0/3427	0.45	0/4640
3	E	0.24	0/1008	0.36	0/1337
4	F	0.24	0/2670	0.41	0/3603
All	All	0.26	0/17589	0.45	0/23798

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	284	GLU	Peptide

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	3446	0	3348	21	0
1	C	3447	0	3360	24	1
2	B	3359	0	3241	32	1
2	D	3354	0	3234	33	0
3	E	1000	0	1018	11	0
4	F	2614	0	2597	19	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	12	2	0
10	B	60	0	0	1	0
10	D	60	0	0	1	0
11	F	31	0	14	4	0
12	A	169	0	0	3	0
12	B	156	0	0	1	0
12	C	316	0	0	4	0
12	D	122	0	0	4	0
12	E	47	0	0	3	0
12	F	73	0	0	1	0
All	All	18392	0	16872	137	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (137) 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:248:LEU:HD21	2:B:352:LYS:HB3	1.68	0.75
1:A:370:LYS:NZ	12:A:601:HOH:O	2.20	0.72
1:C:241:SER:HA	1:C:249:ASN:HD21	1.53	0.72
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.76	0.68
3:E:10:GLU:OE2	12:E:201:HOH:O	2.11	0.68
4:F:100:ILE:HD11	4:F:173:ILE:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.67
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.29	0.64
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.79	0.63
1:C:340:SER:O	12:C:601:HOH:O	2.14	0.63
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.80	0.62
2:D:19:LYS:NZ	12:D:606:HOH:O	2.32	0.62
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.64	0.61
2:D:438:ALA:O	12:D:601:HOH:O	2.16	0.60
1:C:1:MET:O	12:C:602:HOH:O	2.16	0.60
2:B:158:ARG:CZ	9:B:503:MES:H21	2.32	0.59
2:D:188:THR:HG23	2:D:425:MET:HE3	1.85	0.58
2:B:199:ASP:OD2	9:B:503:MES:H52	2.04	0.58
2:B:278:ARG:HH21	2:B:282:GLN:HE22	1.53	0.55
3:E:80:ARG:NH1	12:E:205:HOH:O	2.39	0.55
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.40	0.55
1:A:280:LYS:HB2	1:A:283:HIS:NE2	2.20	0.55
4:F:139:ARG:HB2	4:F:145:ASN:HD21	1.72	0.55
2:D:396:THR:O	2:D:400:ARG:HB2	2.07	0.54
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.54
2:D:277:SER:OG	12:D:602:HOH:O	2.18	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
2:D:229:HIS:NE2	10:D:503:R42:O39	2.34	0.53
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.90	0.53
1:C:272:TYR:HB2	1:C:302:MET:HE1	1.91	0.52
1:C:2:ARG:HB2	1:C:2:ARG:HH11	1.73	0.52
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.28	0.52
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.92	0.52
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.91	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.74	0.51
2:D:311[B]:ARG:HH21	2:D:344:VAL:HA	1.75	0.51
2:D:401:ARG:HG3	2:D:403:ALA:HB2	1.92	0.51
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.93	0.50
2:D:128:SER:O	2:D:128:SER:OG	2.29	0.50
2:D:142:GLY:O	2:D:183:GLU:HG2	2.11	0.50
4:F:36:ARG:NH1	12:F:504:HOH:O	2.43	0.50
1:C:320:ARG:HA	1:C:356:ASN:O	2.12	0.50
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.30	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.49
1:A:280:LYS:HB2	1:A:283:HIS:CE1	2.47	0.49
1:C:386:GLU:OE2	12:C:603:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:131:GLU:HG3	3:E:134:ARG:HH21	1.77	0.49
1:C:272:TYR:CB	1:C:302:MET:HE1	2.43	0.48
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.48
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.95	0.48
2:B:301:MET:HE1	2:B:307:PRO:HD3	1.95	0.48
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.48
4:F:139:ARG:HB2	4:F:145:ASN:ND2	2.29	0.47
3:E:108:ASN:ND2	12:E:206:HOH:O	2.44	0.47
2:B:295:MET:CG	2:B:377:PHE:HB2	2.45	0.47
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.96	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
2:B:422:GLU:HG3	12:B:615:HOH:O	2.15	0.47
2:B:69:ASP:O	2:B:94:PHE:HA	2.15	0.47
1:C:48:SER:OG	1:C:245:ASP:HB2	2.15	0.47
2:D:197:ASN:HD21	3:E:126:LYS:HE2	1.80	0.47
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.51	0.46
1:C:39:ASP:OD1	1:C:41:THR:OG1	2.33	0.46
2:D:311[B]:ARG:NH2	2:D:345:GLU:OE2	2.45	0.46
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.98	0.46
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.96	0.46
4:F:222:ARG:NH1	11:F:401:ACP:O2G	2.49	0.46
2:B:11:GLN:O	2:B:15:GLN:HG3	2.15	0.46
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.46
2:D:106:GLY:O	2:D:111:GLY:HA3	2.15	0.46
2:B:2:ARG:NH1	2:B:131:CYS:SG	2.88	0.46
4:F:145:ASN:HA	4:F:184:LYS:HE2	1.97	0.46
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.16	0.45
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.81	0.45
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.45
4:F:161:LEU:HD12	4:F:172:PHE:CG	2.52	0.45
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.45
3:E:125:GLU:O	3:E:128:LYS:HG3	2.17	0.45
2:D:163:ASP:O	2:D:253:ARG:NH2	2.50	0.45
2:D:178:SER:OG	2:D:183:GLU:OE2	2.27	0.45
2:B:298:SER:HA	2:B:301:MET:HE2	1.98	0.44
3:E:101:LEU:O	3:E:105:MET:HG2	2.17	0.44
1:C:430:LYS:HE2	1:C:430:LYS:HB3	1.75	0.44
2:D:416:MET:HA	2:D:416:MET:CE	2.46	0.44
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.99	0.44
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.00	0.44
2:D:356:CYS:SG	2:D:358:ILE:HG23	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:164:LYS:NZ	2.50	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.44
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.52	0.44
1:A:430:LYS:HB3	1:A:430:LYS:HE2	1.55	0.44
1:A:300:ASN:ND2	12:A:610:HOH:O	2.50	0.44
12:C:623:HOH:O	3:E:115:HIS:HE1	2.01	0.44
1:A:450:GLU:OE1	4:F:333:ASN:HB3	2.18	0.43
2:B:274:PRO:HB3	2:B:286:LEU:HD22	2.01	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.84	0.43
1:A:207:GLU:OE2	1:A:304:LYS:HE2	2.19	0.43
1:A:174:ALA:O	1:A:178:SER:HB3	2.19	0.43
1:A:356:ASN:ND2	12:A:608:HOH:O	2.47	0.43
2:B:340:SER:HB3	4:F:34:ASN:HD21	1.84	0.43
2:D:402:LYS:O	2:D:402:LYS:HD2	2.19	0.43
2:D:16:ILE:HD11	2:D:138:THR:HB	2.01	0.42
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.42
2:B:229:HIS:HB3	10:B:504:R42:C25	2.49	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.02	0.42
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.20	0.42
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.42
2:B:104:ALA:HB2	2:B:413:MET:SD	2.59	0.42
4:F:161:LEU:HA	4:F:161:LEU:HD23	1.80	0.42
4:F:318:ASP:OD2	11:F:401:ACP:O3G	2.37	0.42
3:E:9:ILE:HG12	3:E:21:GLU:HB3	2.01	0.42
2:D:1:MET:HE1	2:D:48:ARG:HG2	2.02	0.41
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.02	0.41
1:C:302:MET:N	1:C:302:MET:SD	2.93	0.41
2:B:322:ARG:HD3	2:B:322:ARG:HA	1.87	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.55	0.41
2:B:88:ARG:HD2	2:B:91:ASN:OD1	2.19	0.41
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.03	0.41
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.02	0.41
2:B:35:SER:OG	2:B:60:LYS:NZ	2.54	0.41
4:F:202:ARG:HB2	4:F:222:ARG:NH2	2.36	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
2:D:171:VAL:HA	2:D:204:ILE:O	2.21	0.41
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.21	0.41
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.03	0.41
2:B:13:GLY:HA2	2:B:138:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:126:ASP:OD1	4:F:127:GLU:N	2.55	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	2.21	0.40
4:F:263:PHE:CE2	4:F:341:LYS:HE2	2.56	0.40
2:B:325:MET:H	2:B:325:MET:CE	2.34	0.40
4:F:320:MET:HE2	4:F:320:MET:HB3	1.87	0.40
2:D:164:ARG:NH1	12:D:607:HOH:O	2.55	0.40
2:D:105:LYS:HA	2:D:109:THR:OG1	2.22	0.40
4:F:268:ASN:O	4:F:272:MET:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLU:OE2	1:C:283:HIS:NE2[4_555]	2.19	0.01

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	437/451 (97%)	431 (99%)	6 (1%)	0	100 100
1	C	440/451 (98%)	430 (98%)	10 (2%)	0	100 100
2	B	422/445 (95%)	415 (98%)	7 (2%)	0	100 100
2	D	423/445 (95%)	415 (98%)	7 (2%)	1 (0%)	47 38
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	17 8
4	F	303/384 (79%)	296 (98%)	7 (2%)	0	100 100
All	All	2142/2319 (92%)	2102 (98%)	38 (2%)	2 (0%)	51 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27	PRO
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	371/379 (98%)	368 (99%)	3 (1%)	81	80
1	C	373/379 (98%)	369 (99%)	4 (1%)	73	71
2	B	369/383 (96%)	366 (99%)	3 (1%)	81	80
2	D	369/383 (96%)	362 (98%)	7 (2%)	57	50
3	E	109/127 (86%)	107 (98%)	2 (2%)	59	53
4	F	287/342 (84%)	284 (99%)	3 (1%)	76	74
All	All	1878/1993 (94%)	1856 (99%)	22 (1%)	71	68

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	336	LYS
1	A	381	THR
2	B	139	HIS
2	B	325	MET
2	B	336	GLN
1	C	71	GLU
1	C	302	MET
1	C	347	CYS
1	C	381	THR
2	D	50	ASN
2	D	60	LYS
2	D	85	GLN
2	D	139	HIS
2	D	358	ILE
2	D	402	LYS
2	D	416	MET

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Mol	Chain	Res	Type
3	E	59	GLU
3	E	128	LYS
4	F	19	ARG
4	F	165	GLU
4	F	244	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	15	GLN
2	B	50	ASN
2	B	167	ASN
2	B	424	ASN
2	B	434	GLN
1	C	249	ASN
2	D	59	ASN
2	D	167	ASN
2	D	197	ASN
2	D	426	ASN
3	E	84	GLN
3	E	108	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 14 ligands modelled in this entry, 6 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	R42	D	503	-	65,65,65	0.89	2 (3%)	100,101,101	2.04	24 (24%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.37	5 (15%)
8	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.12	3 (10%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.31	6 (18%)
10	R42	B	504	-	65,65,65	0.89	3 (4%)	100,101,101	2.00	24 (24%)
11	ACP	F	401	6	27,33,33	1.37	5 (18%)	32,52,52	1.43	4 (12%)
8	GDP	B	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.08	4 (13%)
9	MES	B	503	-	12,12,12	2.23	1 (8%)	14,16,16	1.86	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	R42	D	503	-	-	6/42/129/129	0/6/6/6
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
10	R42	B	504	-	-	3/42/129/129	0/6/6/6
11	ACP	F	401	6	-	5/15/38/38	0/3/3/3
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
9	MES	B	503	-	-	2/6/14/14	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.48	1.66	1.77
5	C	501	GTP	C5-C6	-4.01	1.39	1.47
5	A	501	GTP	C5-C6	-3.97	1.39	1.47
10	D	503	R42	O39-C39	3.43	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	R42	O39-C39	3.41	1.30	1.23
11	F	401	ACP	PG-O3G	2.88	1.61	1.54
11	F	401	ACP	PG-O2G	2.86	1.61	1.54
11	F	401	ACP	PB-O3A	2.63	1.61	1.58
11	F	401	ACP	C5-C4	2.53	1.47	1.40
8	B	501	GDP	C6-N1	-2.33	1.34	1.37
8	D	501	GDP	C6-N1	-2.27	1.34	1.37
11	F	401	ACP	PB-O2B	2.16	1.61	1.56
5	A	501	GTP	C2-N3	2.12	1.38	1.33
5	C	501	GTP	C2-N3	2.08	1.38	1.33
10	B	504	R42	C4-C3	2.03	1.59	1.54
10	D	503	R42	C4-C3	2.01	1.59	1.54
10	B	504	R42	O13-C13	-2.01	1.42	1.45

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	503	R42	C32-N32-C39	9.75	138.04	122.32
10	B	504	R42	C40-C39-N32	6.78	126.88	117.63
10	D	503	R42	O4-C28-C29	6.06	121.70	110.68
10	B	504	R42	O4-C28-C29	6.02	121.63	110.68
10	B	504	R42	C32-N32-C39	5.75	131.60	122.32
10	B	504	R42	C2-O2-C21	5.53	128.26	117.79
10	D	503	R42	C2-O2-C21	5.50	128.19	117.79
9	B	503	MES	C5-N4-C3	4.93	119.92	108.83
10	D	503	R42	C31-C32-N32	4.90	121.71	109.31
11	F	401	ACP	PB-O3A-PA	-3.77	120.61	132.56
10	D	503	R42	C8-C9-C10	3.75	128.27	122.69
10	B	504	R42	C17-C15-C16	-3.73	95.27	106.26
10	B	504	R42	C31-C32-N32	3.73	118.74	109.31
10	B	504	R42	C18-C12-C11	-3.66	120.86	125.30
10	D	503	R42	C40-C39-N32	3.65	122.61	117.63
10	B	504	R42	C8-C9-C10	3.61	128.06	122.69
10	D	503	R42	O4-C28-O28	-3.60	117.00	123.61
10	D	503	R42	C17-C15-C16	-3.58	95.73	106.26
10	B	504	R42	O4-C28-O28	-3.57	117.05	123.61
10	D	503	R42	C18-C12-C11	-3.57	120.98	125.30
10	B	504	R42	O44-C43-C42	3.35	117.47	111.27
10	B	504	R42	C33-C32-N32	3.34	118.66	112.11
11	F	401	ACP	C3'-C2'-C1'	3.30	105.94	100.98
5	A	501	GTP	C5-C6-N1	3.16	119.54	113.95
11	F	401	ACP	N3-C2-N1	-3.12	123.80	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	R42	C10-C11-C12	-3.11	115.94	120.65
10	D	503	R42	O10-C10-C11	-3.10	106.48	111.48
10	B	504	R42	O10-C10-C9	3.08	114.63	109.51
5	C	501	GTP	C8-N7-C5	3.04	108.78	102.99
10	D	503	R42	O44-C43-C42	3.02	116.87	111.27
10	D	503	R42	O10-C10-C9	3.01	114.53	109.51
5	C	501	GTP	C5-C6-N1	3.00	119.25	113.95
10	B	504	R42	O10-C10-C11	-2.99	106.66	111.48
10	B	504	R42	C4-O4-C28	2.97	126.74	119.06
10	B	504	R42	C4-C3-C2	2.96	117.46	111.66
5	A	501	GTP	C8-N7-C5	2.91	108.54	102.99
10	D	503	R42	O13-C30-C31	2.90	115.90	111.15
10	D	503	R42	C4-O4-C28	2.88	126.52	119.06
10	D	503	R42	C4-C3-C2	2.86	117.26	111.66
10	B	504	R42	C20-O5-C5	2.84	94.65	91.39
8	D	501	GDP	PA-O3A-PB	-2.74	123.42	132.83
10	D	503	R42	C20-O5-C5	2.69	94.47	91.39
5	A	501	GTP	C2-N1-C6	-2.64	120.24	125.10
10	B	504	R42	O39-C39-N32	-2.64	118.45	123.08
5	C	501	GTP	C2-N1-C6	-2.64	120.24	125.10
10	D	503	R42	C33-C32-C31	2.63	118.13	111.36
11	F	401	ACP	C4-C5-N7	-2.63	106.66	109.40
9	B	503	MES	O3S-S-C8	2.60	109.98	105.77
10	D	503	R42	C10-C11-C12	-2.58	116.75	120.65
8	B	501	GDP	C5-C6-N1	2.49	118.35	113.95
5	A	501	GTP	PB-O3B-PG	-2.45	124.43	132.83
5	A	501	GTP	PA-O3A-PB	-2.44	124.45	132.83
8	D	501	GDP	C8-N7-C5	2.36	107.48	102.99
5	C	501	GTP	PB-O3B-PG	-2.36	124.74	132.83
8	B	501	GDP	O6-C6-C5	-2.30	119.88	124.37
9	B	503	MES	C7-N4-C5	2.28	117.07	111.23
10	D	503	R42	C1-C2-C3	-2.28	114.70	118.18
5	C	501	GTP	PA-O3A-PB	-2.25	125.12	132.83
10	B	504	R42	O13-C30-C31	2.25	114.83	111.15
10	D	503	R42	O1-C1-C2	2.24	110.40	105.49
8	D	501	GDP	C5-C6-N1	2.23	117.90	113.95
10	B	504	R42	C1-C2-C3	-2.23	114.78	118.18
10	B	504	R42	O9-C9-C10	-2.21	114.85	117.37
10	B	504	R42	C42-C40-C41	-2.19	121.30	123.09
8	B	501	GDP	PA-O3A-PB	-2.15	125.44	132.83
10	D	503	R42	O9-C9-C10	-2.15	114.92	117.37
8	B	501	GDP	C8-N7-C5	2.15	107.08	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	R42	O5-C20-C4	-2.13	89.54	91.95
10	B	504	R42	O1-C1-C2	2.13	110.17	105.49
10	D	503	R42	O13-C30-O30	-2.10	120.02	123.94
5	C	501	GTP	O6-C6-C5	-2.06	120.34	124.37
10	D	503	R42	C17-C15-C1	2.01	115.61	111.11
10	D	503	R42	O5-C20-C4	-2.00	89.69	91.95

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
10	B	504	R42	C42-C43-O44-C44
10	B	504	R42	O43-C43-O44-C44
10	D	503	R42	C42-C43-O44-C44
10	D	503	R42	O43-C43-O44-C44
10	D	503	R42	C39-C40-C42-C43
10	D	503	R42	O31-C31-C32-N32
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	503	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3B-PG-O1G
10	B	504	R42	C30-C31-C32-C33
10	D	503	R42	C30-C31-C32-N32
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
10	D	503	R42	C40-C42-C43-O44

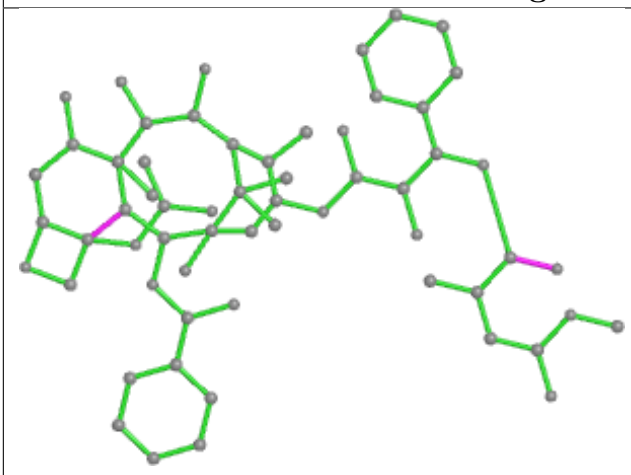
There are no ring outliers.

6 monomers are involved in 11 short contacts:

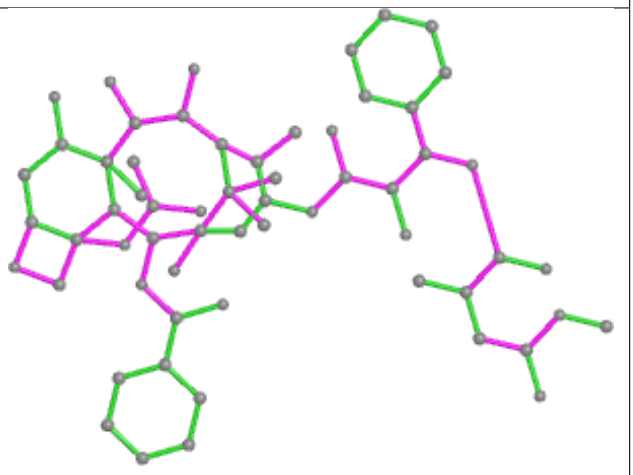
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	R42	1	0
5	A	501	GTP	1	0
8	D	501	GDP	2	0
10	B	504	R42	1	0
11	F	401	ACP	4	0
9	B	503	MES	2	0

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

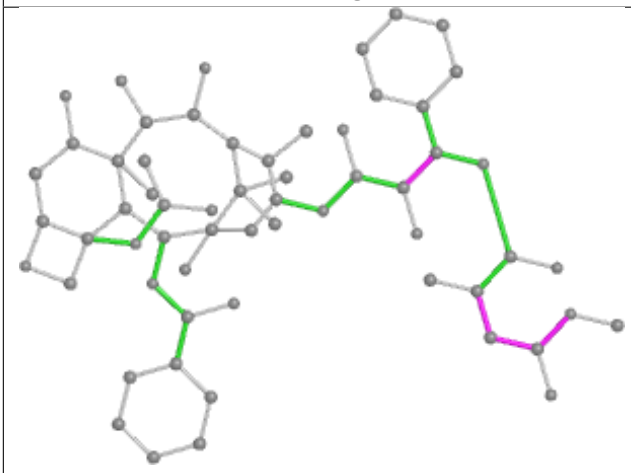
Ligand R42 D 503



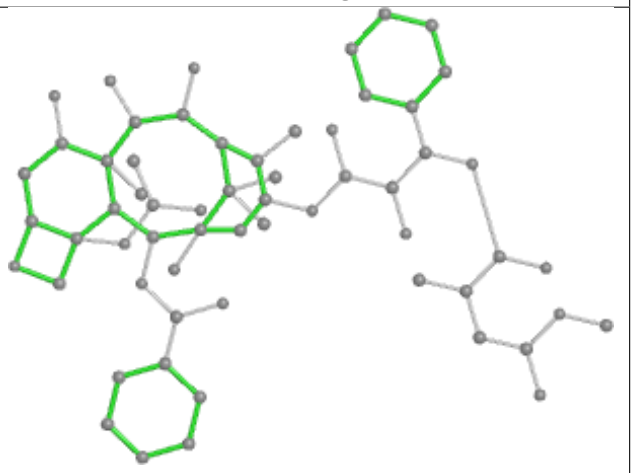
Bond lengths



Bond angles

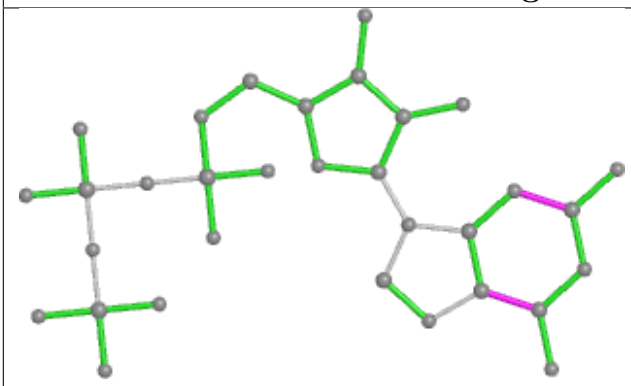


Torsions

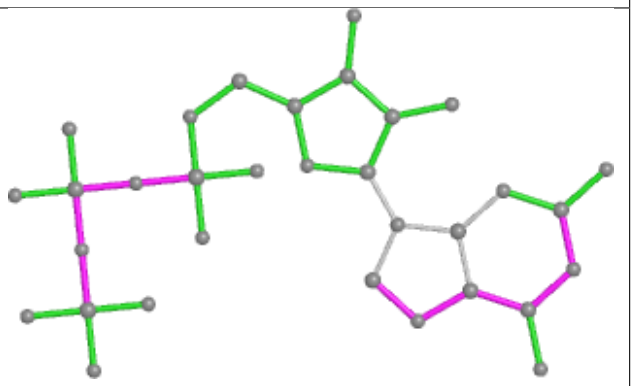


Rings

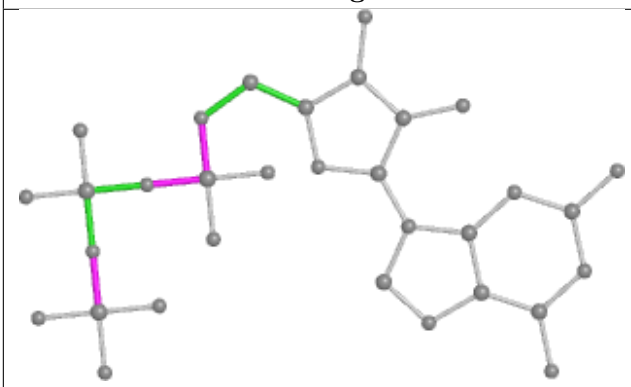
Ligand GTP A 501



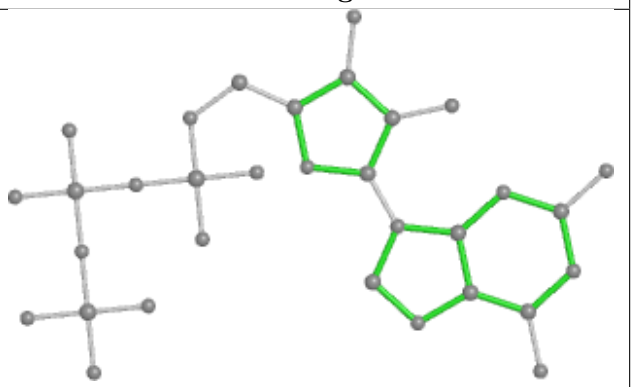
Bond lengths



Bond angles

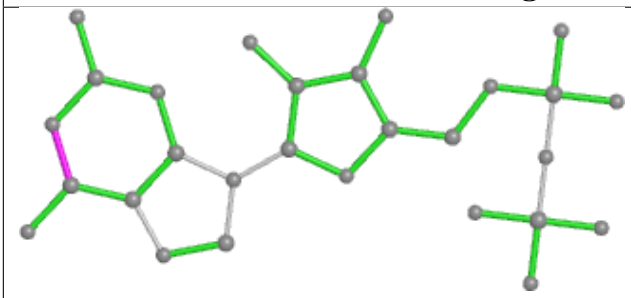


Torsions

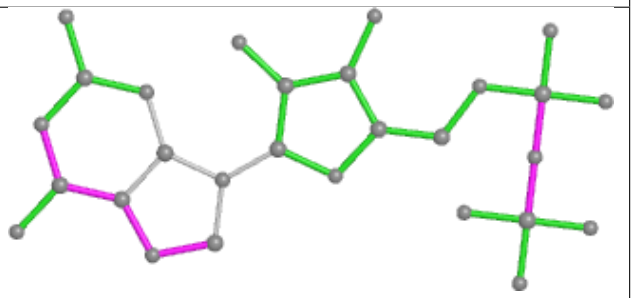


Rings

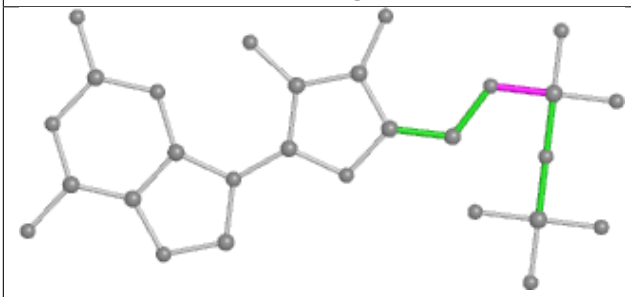
Ligand GDP D 501



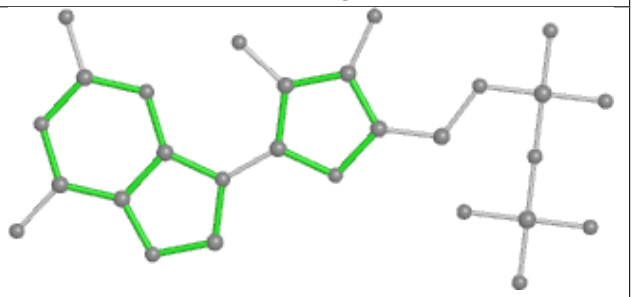
Bond lengths



Bond angles

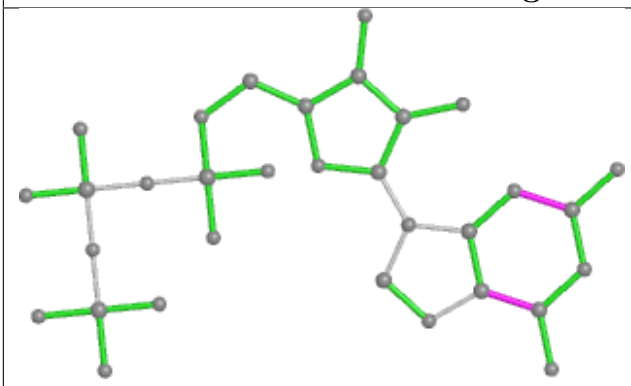


Torsions

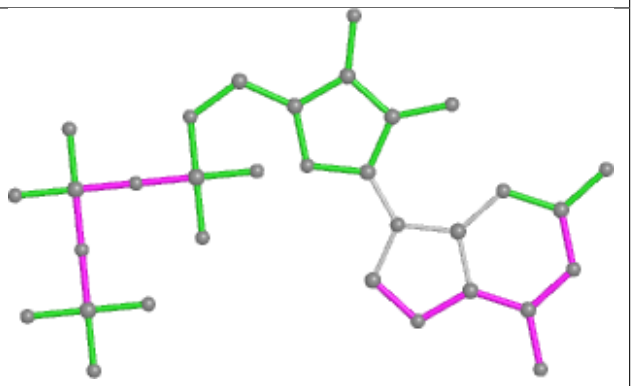


Rings

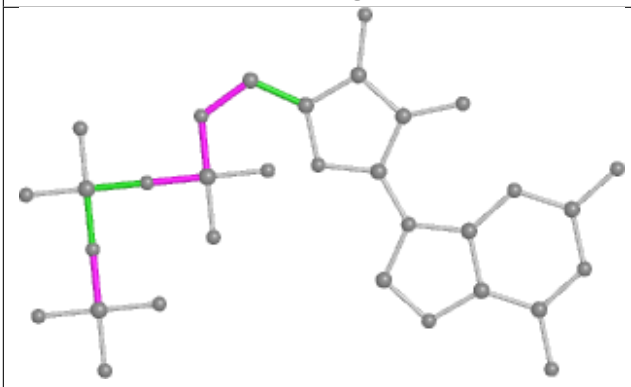
Ligand GTP C 501



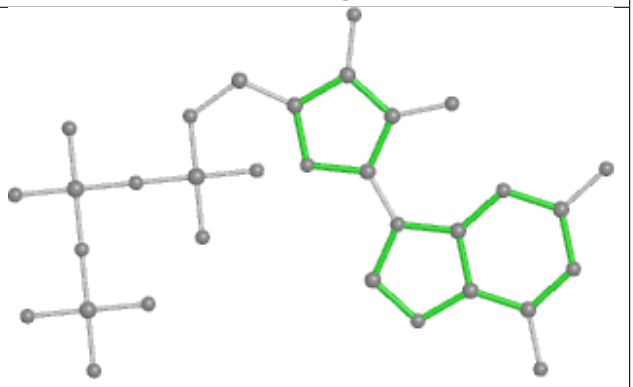
Bond lengths



Bond angles

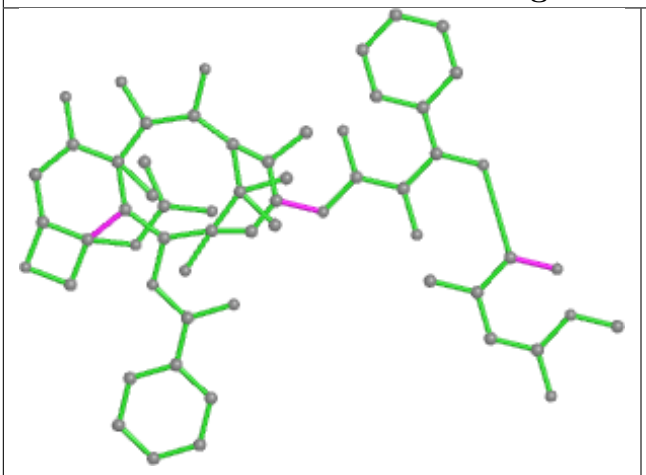


Torsions

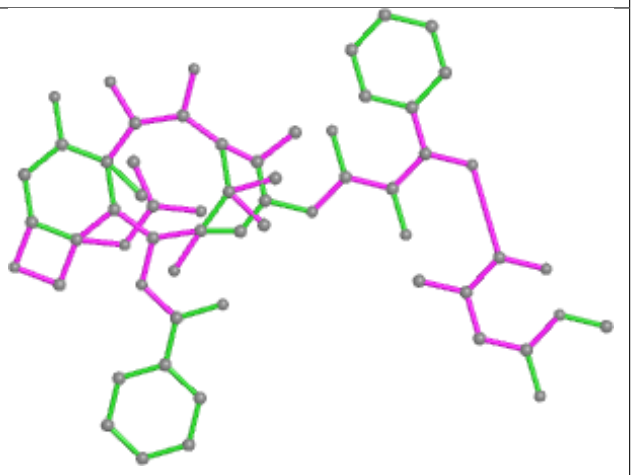


Rings

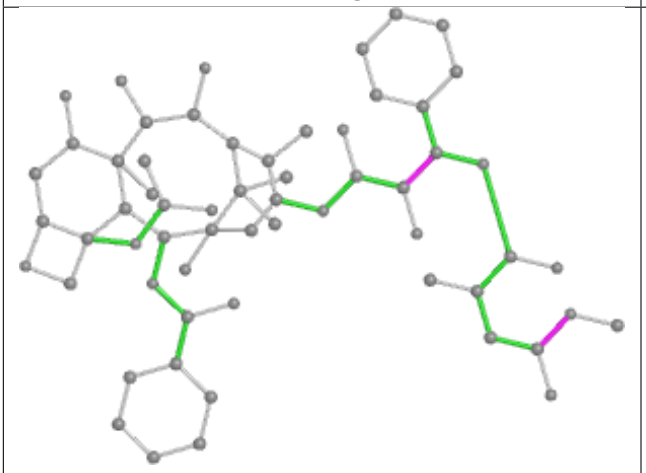
Ligand R42 B 504



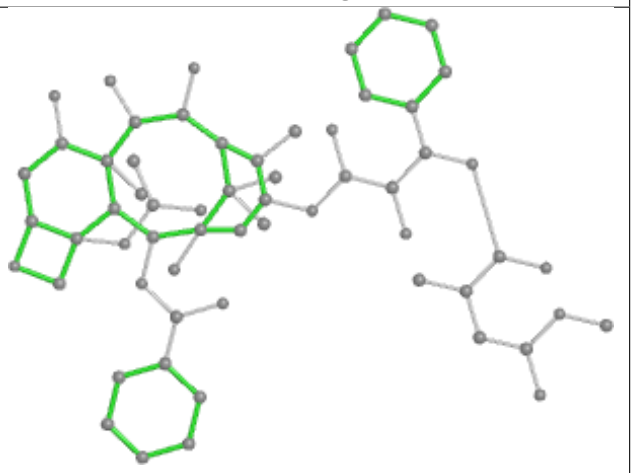
Bond lengths



Bond angles

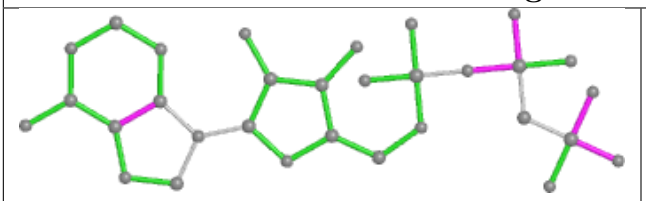


Torsions

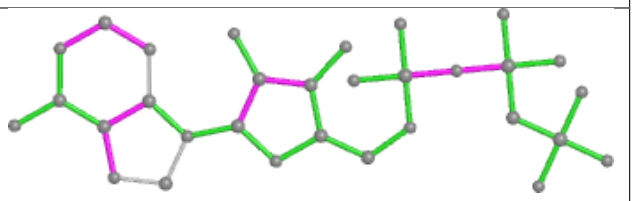


Rings

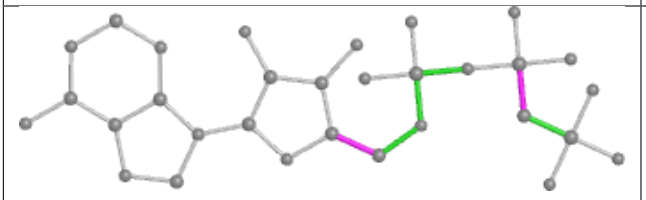
Ligand ACP F 401



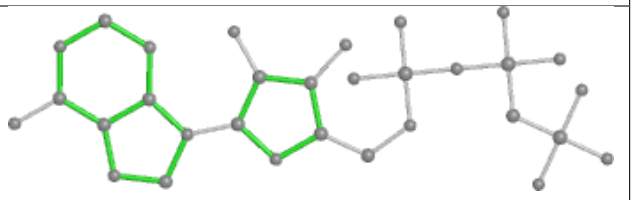
Bond lengths



Bond angles

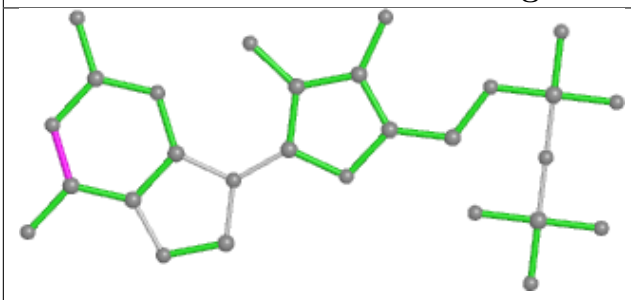


Torsions

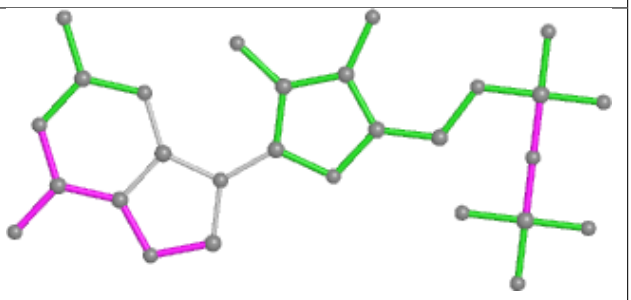


Rings

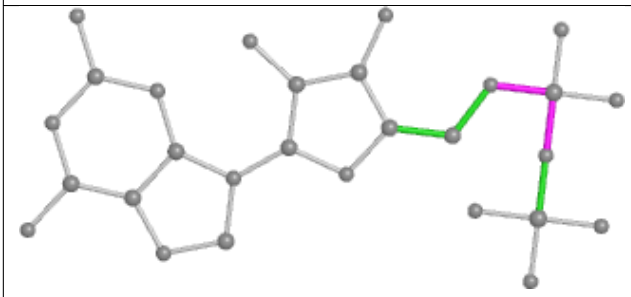
Ligand GDP B 501



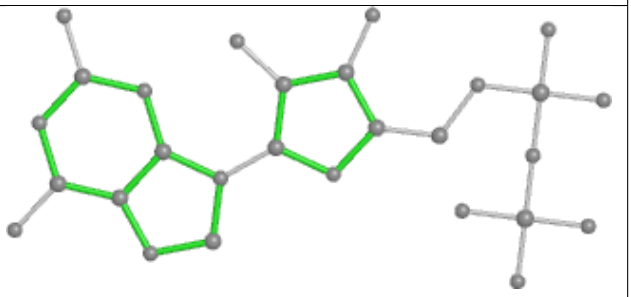
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	441/451 (97%)	0.61	35 (7%)	12	19	34, 54, 88, 148	0
1	C	440/451 (97%)	0.38	17 (3%)	39	49	30, 42, 73, 123	0
2	B	426/445 (95%)	0.63	33 (7%)	13	21	31, 53, 96, 149	0
2	D	426/445 (95%)	0.77	64 (15%)	2	3	37, 63, 99, 133	0
3	E	121/143 (84%)	0.65	18 (14%)	2	3	41, 68, 105, 130	0
4	F	319/384 (83%)	1.66	102 (31%)	0	0	45, 77, 149, 200	0
All	All	2173/2319 (93%)	0.76	269 (12%)	4	6	30, 57, 108, 200	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	12.5
4	F	253	TYR	9.3
4	F	240	LEU	9.2
4	F	161	LEU	9.0
4	F	169	LEU	7.8
1	A	283	HIS	7.8
4	F	166	ALA	7.7
4	F	241	THR	7.6
4	F	256	TYR	7.5
4	F	179	VAL	7.5
2	B	438	ALA	7.4
1	A	282	TYR	7.1
4	F	132	LEU	6.5
4	F	130	VAL	6.5
4	F	227	PRO	6.3
4	F	131	PHE	5.9
2	B	57	THR	5.8
4	F	259	GLY	5.8
4	F	182	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
4	F	162	ILE	5.6
3	E	26	PRO	5.5
4	F	133	ALA	5.5
4	F	167	SER	5.5
1	A	281	ALA	5.4
4	F	172	PHE	5.4
4	F	238	CYS	5.4
4	F	362	ALA	5.4
2	D	57	THR	5.4
3	E	139	LEU	5.2
2	B	1	MET	5.2
4	F	20	LEU	5.1
4	F	225	SER	5.1
4	F	160	ILE	5.0
4	F	17	VAL	5.0
4	F	134	ALA	5.0
4	F	342	LEU	5.0
3	E	6	MET	5.0
1	C	440	VAL	5.0
2	D	58	GLY	4.9
4	F	239	HIS	4.9
4	F	101	TYR	4.9
4	F	135	TYR	4.9
3	E	27	PRO	4.8
4	F	99	VAL	4.8
4	F	244	CYS	4.8
4	F	361	LEU	4.8
4	F	228	TYR	4.8
2	B	59	ASN	4.7
4	F	372	THR	4.7
4	F	147	TRP	4.7
2	B	33	THR	4.6
4	F	243	HIS	4.6
2	D	404	PHE	4.6
2	D	401	ARG	4.4
4	F	90	SER	4.4
4	F	263	PHE	4.4
1	A	346	TRP	4.4
4	F	175	GLU	4.4
4	F	255	ARG	4.3
4	F	25	GLY	4.3
4	F	226	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	448	GLY	4.2
4	F	170	LEU	4.2
2	D	37	HIS	4.2
1	A	42	ILE	4.1
4	F	254	GLY	4.0
1	A	280	LYS	4.0
4	F	258	GLU	4.0
4	F	196	HIS	3.9
2	D	286	LEU	3.8
1	A	171	ILE	3.8
2	B	37	HIS	3.8
4	F	139	ARG	3.8
1	A	179	THR	3.8
4	F	100	ILE	3.8
4	F	186	LEU	3.8
2	B	437	ASP	3.7
4	F	126	ASP	3.7
4	F	24	THR	3.7
4	F	163	SER	3.7
1	A	262	TYR	3.7
2	D	415	GLU	3.7
2	B	276	THR	3.7
2	D	202	TYR	3.6
2	D	94	PHE	3.6
2	B	36	TYR	3.6
4	F	102	PRO	3.6
4	F	242	ASN	3.6
4	F	197	ARG	3.6
2	D	400	ARG	3.5
4	F	223	THR	3.5
3	E	140	LYS	3.5
2	D	220	THR	3.5
4	F	165	GLU	3.5
2	B	337	ASN	3.4
2	B	62	VAL	3.4
2	B	83	PHE	3.4
4	F	174	ASP	3.4
4	F	129	GLU	3.4
4	F	192	LEU	3.4
2	D	407	TRP	3.4
4	F	128	ARG	3.4
4	F	26	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	1	MET	3.4
1	A	177	VAL	3.3
2	B	34	GLY	3.3
1	C	340	SER	3.3
2	D	82	PRO	3.3
2	D	33	THR	3.2
4	F	144	GLY	3.2
2	B	58	GLY	3.2
2	D	268	PHE	3.2
3	E	24	LEU	3.2
4	F	191	LEU	3.2
2	B	82	PRO	3.2
2	D	59	ASN	3.1
3	E	7	GLU	3.1
4	F	343	TYR	3.1
2	D	317	ALA	3.1
2	D	376	THR	3.1
2	D	56	ALA	3.0
4	F	21	LEU	3.0
1	A	202	PHE	3.0
2	D	256	ALA	3.0
2	B	60	LYS	3.0
4	F	194	PRO	3.0
2	B	144	GLY	3.0
1	C	252	LEU	3.0
2	D	260	VAL	3.0
4	F	89	GLU	3.0
4	F	146	VAL	3.0
4	F	260	ASN	3.0
2	D	399	PHE	2.9
4	F	164	SER	2.9
2	D	270	PRO	2.9
4	F	257	GLU	2.9
2	D	182	VAL	2.9
2	B	56	ALA	2.9
4	F	140	GLU	2.9
2	D	280	SER	2.9
4	F	148	ILE	2.9
2	B	284	ARG	2.9
1	A	178	SER	2.9
2	D	252	LEU	2.9
2	D	378	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	264	PHE	2.9
4	F	180	HIS	2.8
1	A	141	PHE	2.8
4	F	262	MET	2.8
2	B	340	SER	2.8
2	D	77	SER	2.8
4	F	137	ARG	2.8
2	B	61	TYR	2.8
2	D	403	ALA	2.8
2	D	396	THR	2.8
2	D	60	LYS	2.8
1	C	181	VAL	2.8
2	D	315	VAL	2.8
2	D	238	VAL	2.7
4	F	149	ALA	2.7
3	E	28	SER	2.7
2	D	39	ASP	2.7
2	D	83	PHE	2.7
1	C	238	ILE	2.7
4	F	199	PHE	2.7
4	F	31	ARG	2.7
2	D	267	PHE	2.6
4	F	145	ASN	2.6
1	C	253	THR	2.6
2	D	34	GLY	2.6
2	B	35	SER	2.6
3	E	136	ASN	2.6
3	E	138	GLU	2.6
1	C	260	VAL	2.6
1	A	201	ALA	2.6
4	F	339	ALA	2.6
2	D	80	SER	2.6
3	E	134	ARG	2.6
4	F	224	SER	2.6
4	F	195	GLY	2.6
2	D	169	PHE	2.5
2	D	418	PHE	2.5
1	C	257	THR	2.5
1	A	170	SER	2.5
1	A	364	PRO	2.5
2	D	402	LYS	2.5
1	C	167	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	201	THR	2.5
3	E	135	LYS	2.5
4	F	245	ILE	2.5
3	E	45	PRO	2.5
2	D	61	TYR	2.5
4	F	346	LEU	2.5
1	A	438	ASP	2.5
1	C	202	PHE	2.5
4	F	178	GLN	2.4
2	D	257	VAL	2.4
2	B	281	GLN	2.4
4	F	150	LYS	2.4
2	D	79	ARG	2.4
1	C	245	ASP	2.4
1	A	169	PHE	2.4
4	F	340	GLN	2.4
2	D	179	ASP	2.4
4	F	136	ASN	2.4
4	F	198	LYS	2.4
1	C	169	PHE	2.4
1	A	303	VAL	2.4
2	D	78	VAL	2.4
4	F	22	LEU	2.3
2	B	342	TYR	2.3
2	D	377	PHE	2.3
3	E	141	GLU	2.3
2	D	255	LEU	2.3
2	B	277	SER	2.3
1	A	203	MET	2.3
2	D	293	GLN	2.3
2	D	35	SER	2.3
1	C	200	CYS	2.3
2	B	143	GLY	2.2
1	A	189	LEU	2.2
2	D	85	GLN	2.2
2	D	259	MET	2.2
4	F	344	ALA	2.2
3	E	22	VAL	2.2
3	E	25	LYS	2.2
2	D	75	MET	2.2
1	C	241	SER	2.2
1	A	359	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	269	MET	2.2
1	A	163	LYS	2.2
4	F	188	LYS	2.2
4	F	216	TYR	2.2
2	B	142	GLY	2.2
1	A	9	VAL	2.2
1	A	204	VAL	2.2
2	D	219	LEU	2.2
2	D	74	THR	2.2
4	F	15	ALA	2.2
4	F	138	ARG	2.2
1	A	284	GLU	2.2
2	D	214	PHE	2.2
2	D	406	HIS	2.1
2	B	407	TRP	2.1
1	A	146	GLY	2.1
2	B	204	ILE	2.1
2	B	333	LEU	2.1
2	B	338	LYS	2.1
2	D	410	GLY	2.1
1	C	239	THR	2.1
1	C	2	ARG	2.1
2	D	203	CYS	2.1
3	E	48	GLU	2.1
4	F	168	GLU	2.1
2	D	210	TYR	2.1
1	C	1	MET	2.1
2	B	278	ARG	2.1
1	A	138	PHE	2.1
2	D	405	LEU	2.1
1	A	365	GLY	2.1
2	B	308	ARG	2.0
1	A	224	TYR	2.0
1	A	137	VAL	2.0
3	E	8	VAL	2.0
4	F	19	ARG	2.0
4	F	181	VAL	2.0
1	A	43	GLY	2.0
1	A	143	GLY	2.0
1	A	279	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 monosaccharides in this entry.

6.4 Ligands (i)

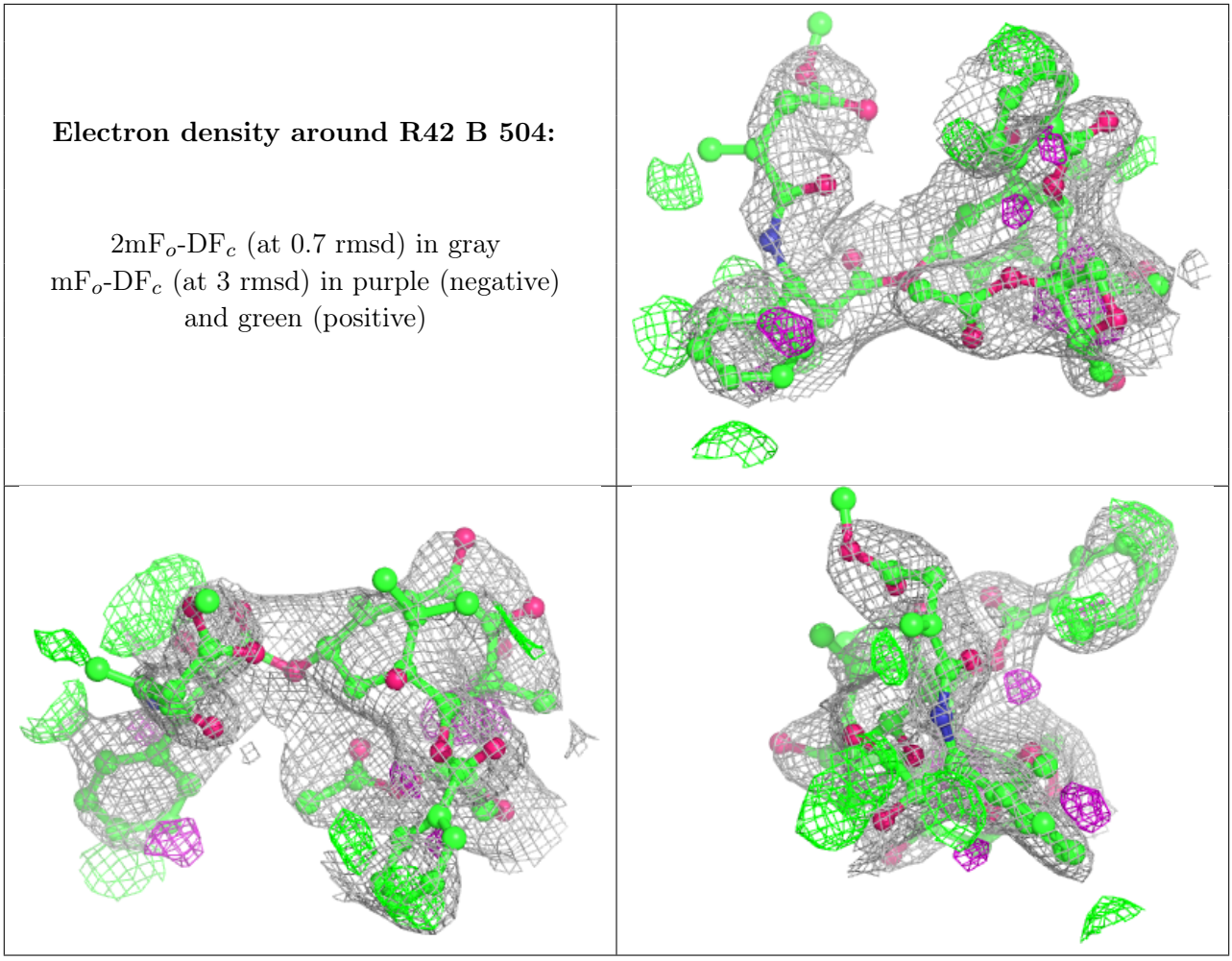
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	CA	A	503	1/1	0.76	0.19	117,117,117,117	0
10	R42	B	504	60/60	0.76	0.25	73,115,127,130	0
11	ACP	F	401	31/31	0.82	0.20	80,112,152,153	0
6	MG	F	402	1/1	0.86	0.17	81,81,81,81	0
10	R42	D	503	60/60	0.88	0.21	80,102,120,127	0
6	MG	A	502	1/1	0.92	0.16	40,40,40,40	0
9	MES	B	503	12/12	0.94	0.12	45,59,67,72	0
8	GDP	D	501	28/28	0.95	0.11	48,58,70,87	0
6	MG	D	502	1/1	0.97	0.12	61,61,61,61	0
5	GTP	A	501	32/32	0.97	0.18	31,37,42,45	0
8	GDP	B	501	28/28	0.98	0.17	30,36,41,41	0
6	MG	C	502	1/1	0.98	0.12	34,34,34,34	0
5	GTP	C	501	32/32	0.99	0.14	27,32,37,37	0
6	MG	B	502	1/1	1.00	0.26	28,28,28,28	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.

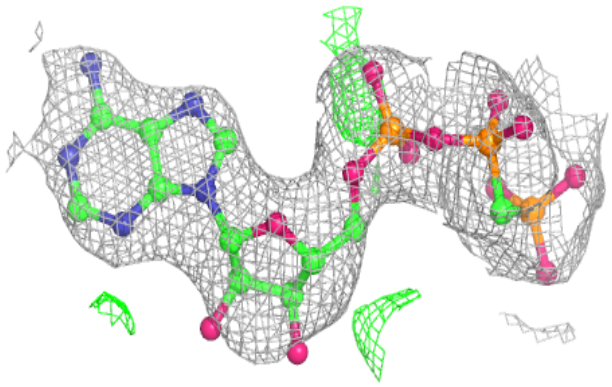
Electron density around R42 B 504:

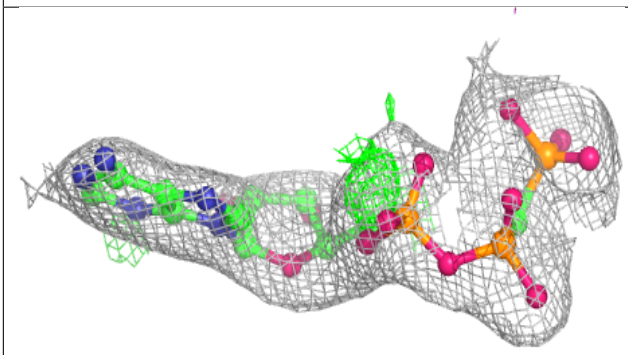
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

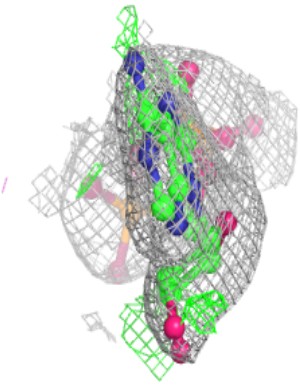


Electron density around ACP F 401:

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

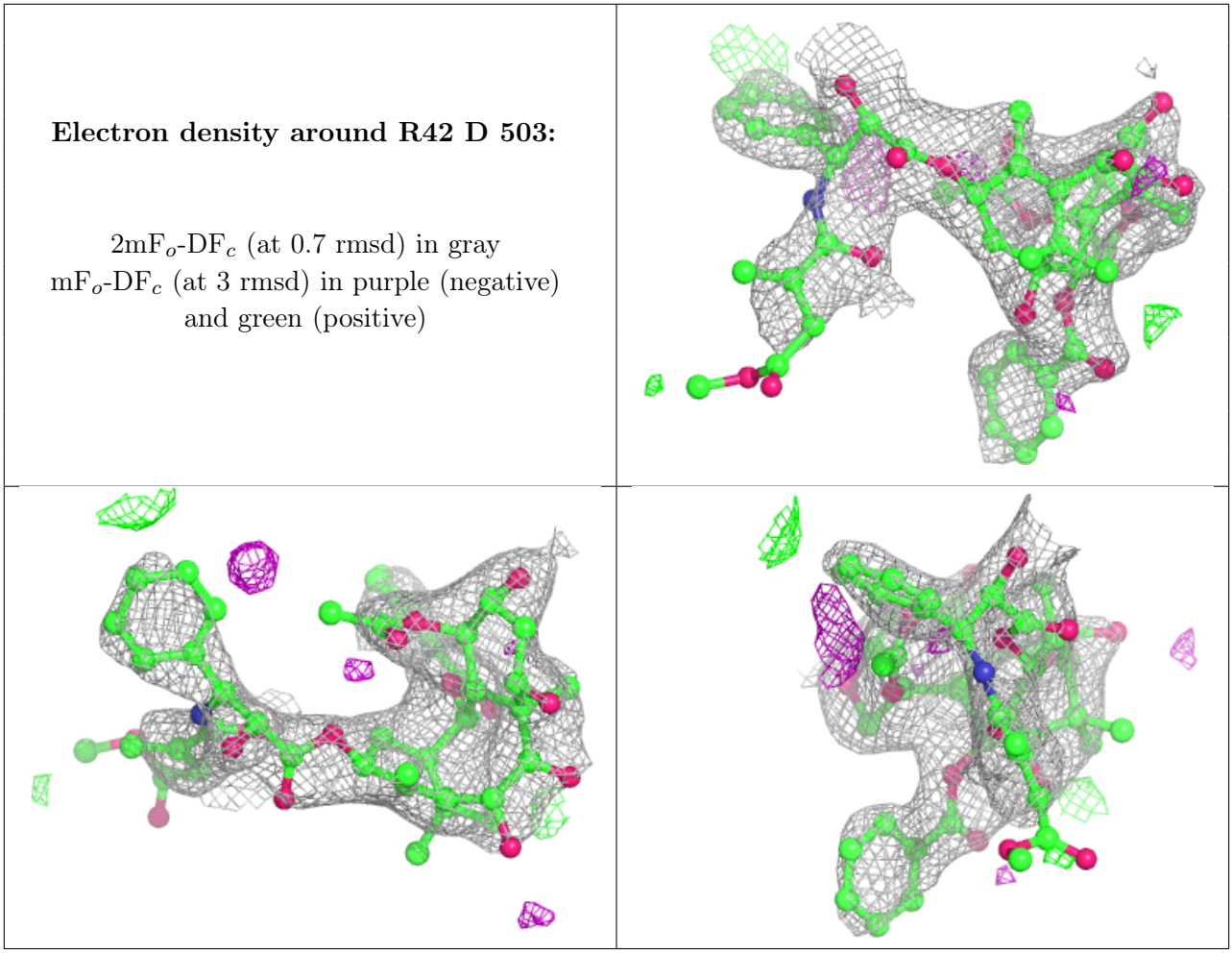






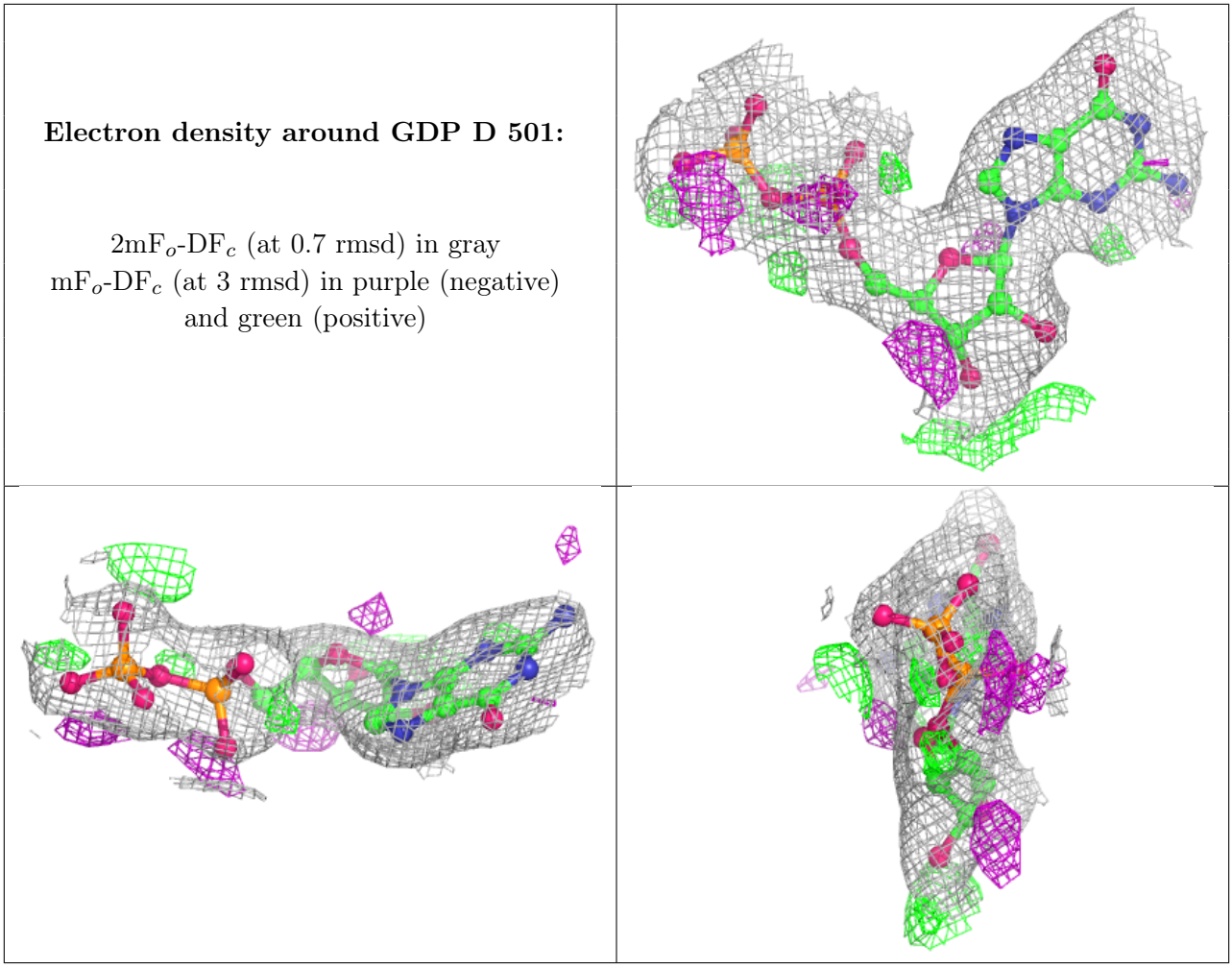
Electron density around R42 D 503:

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



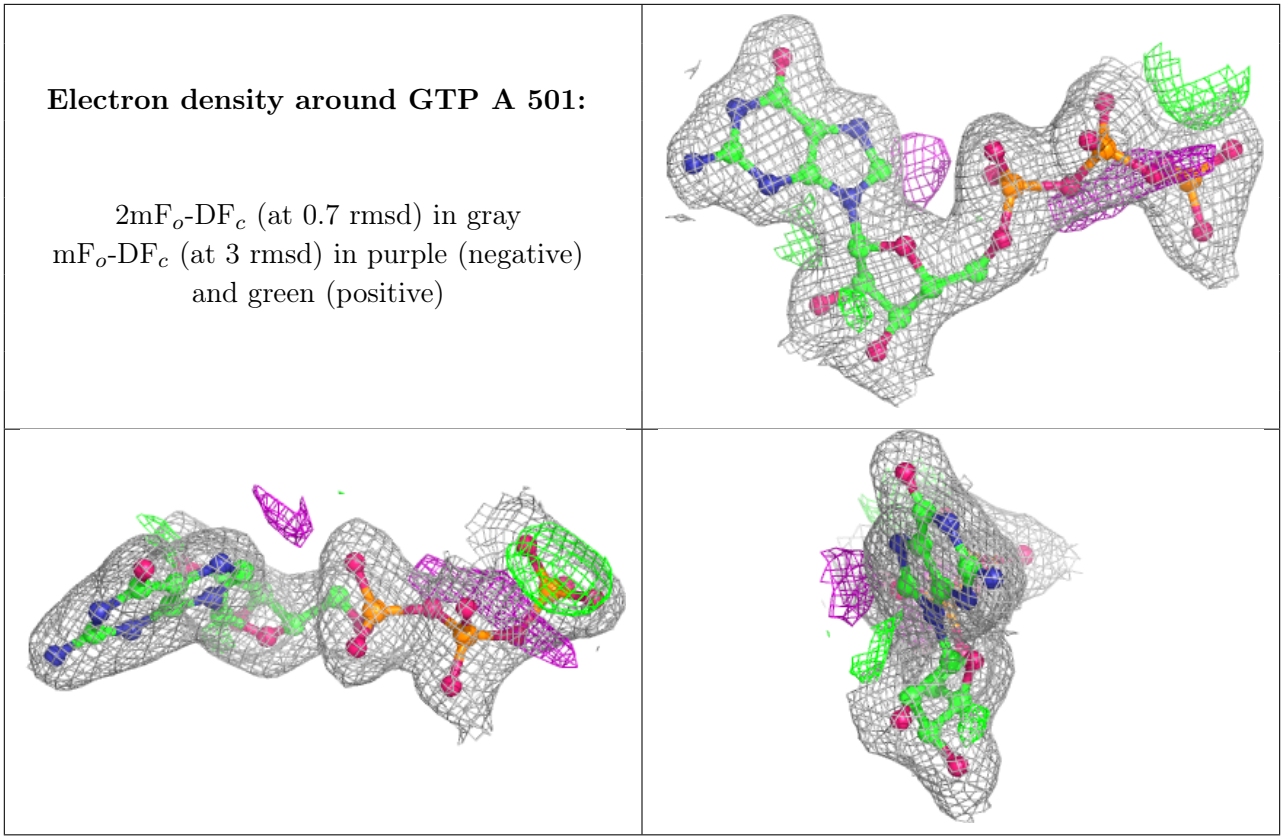
Electron density around GDP D 501:

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



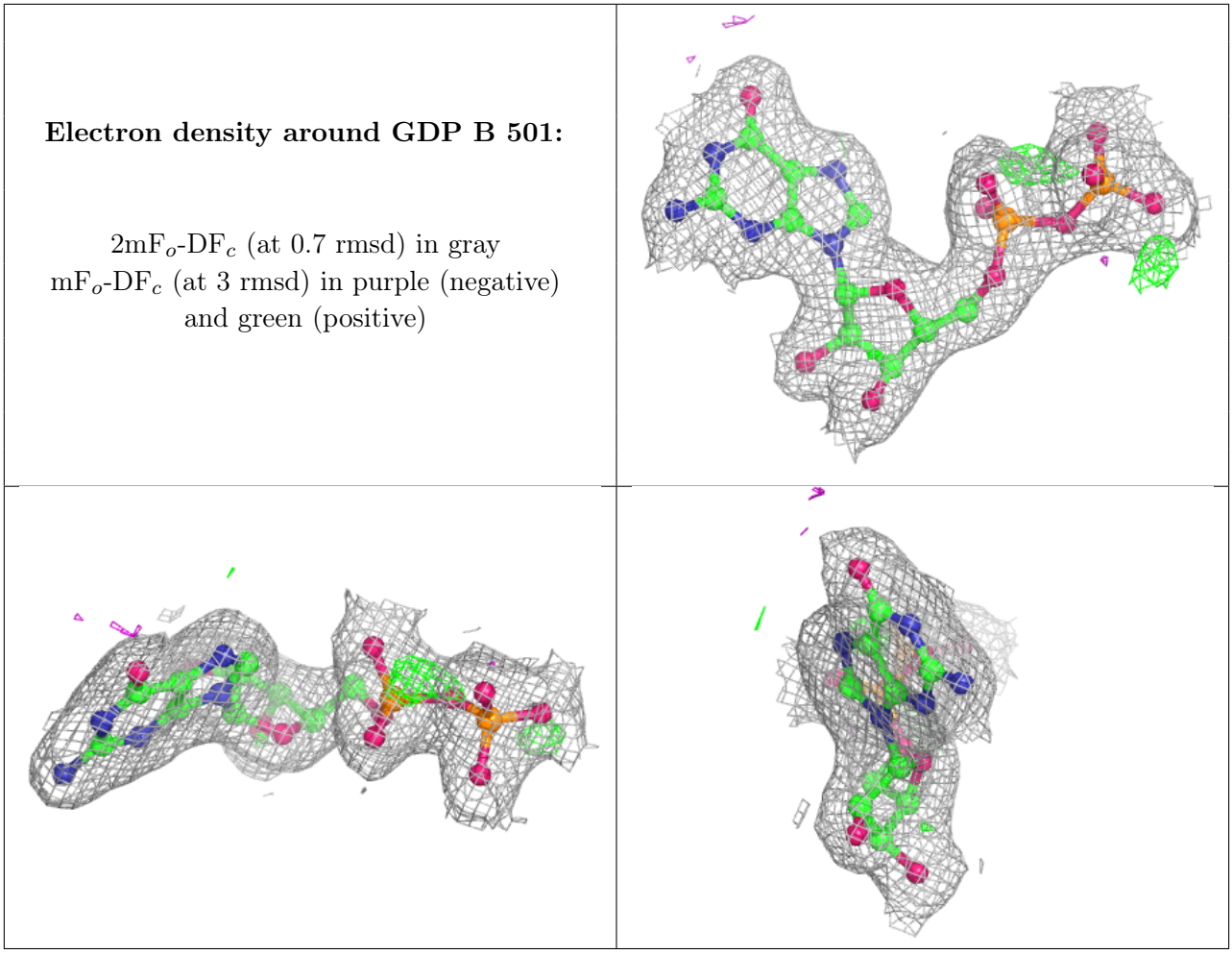
Electron density around GTP A 501:

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



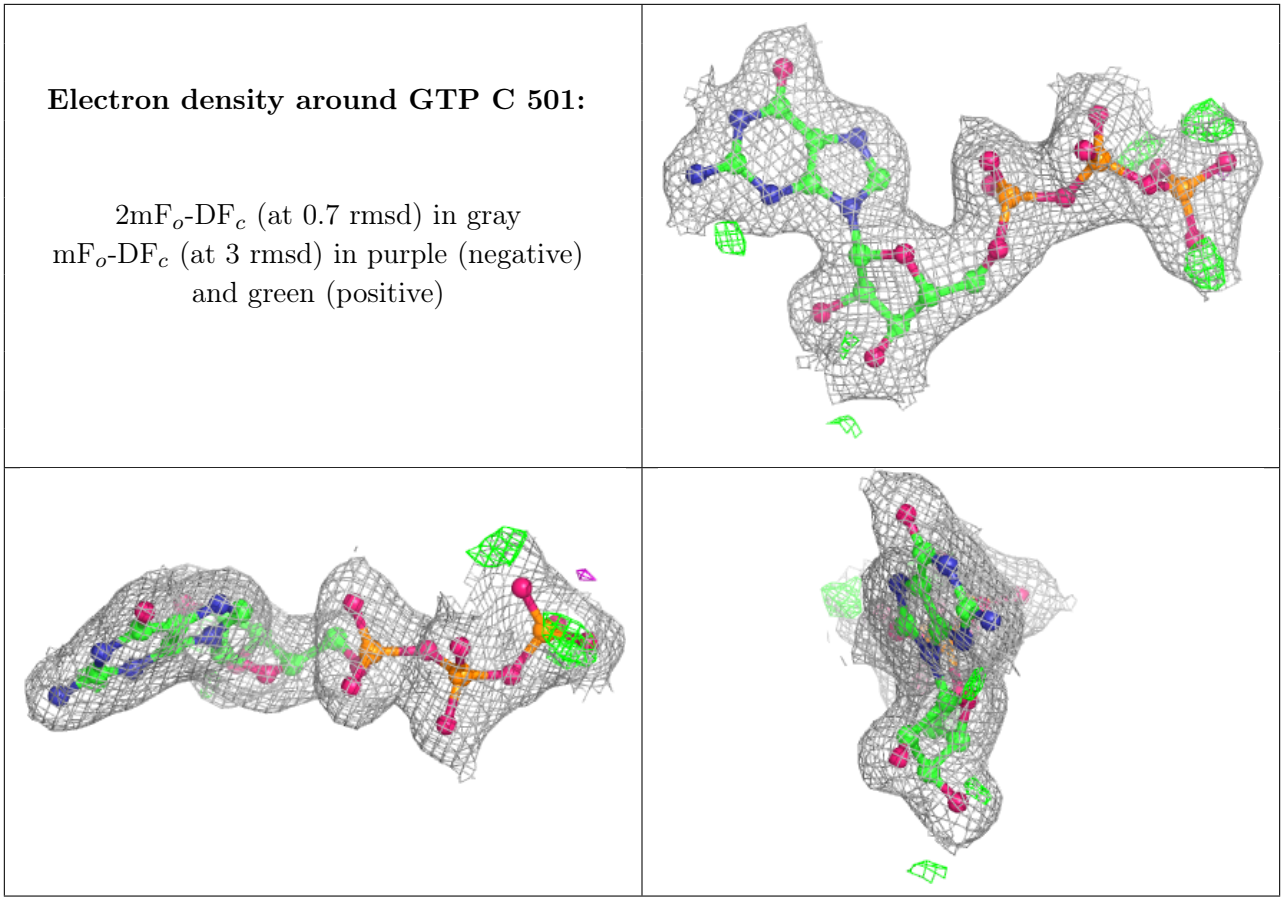
Electron density around GDP B 501:

$2mF_o$-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 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

There are no such residues in this entry.