Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:42 AM JST

PDB ID	:	7CEK
Title	:	Crystal structure of T2R-TTL-BML-284 complex
Authors	:	Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on	:	2020-06-23
Resolution	:	2.70 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:

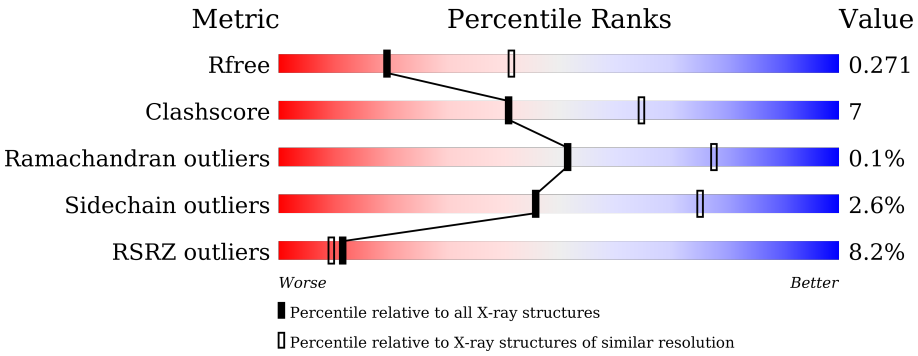
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	450	4% 84% 13%
1	C	450	% 81% 16%
2	B	445	4% 80% 15%
2	D	445	6% 79% 16% 5%
3	E	143	7% 66% 20% 14%
4	F	384	27% 69% 19% 9%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34902 atoms, of which 17075 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	S	0	2	0
			6768	2173	3334	583	655	23			
1	C	440	Total	C	H	N	O	S	0	6	0
			6839	2196	3373	587	660	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	3	0
			6593	2111	3234	574	647	27			
2	D	423	Total	C	H	N	O	S	0	1	0
			6520	2089	3195	564	644	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	2	0
			2061	631	1036	185	204	5			

There are 2 discrepancies between the modelled and reference sequences:

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

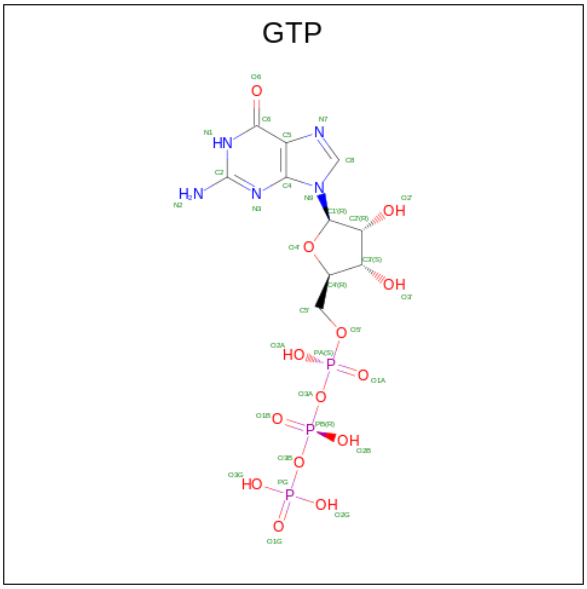
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	349	Total	C	H	N	O	S	0	0	0
			5650	1825	2801	488	522	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	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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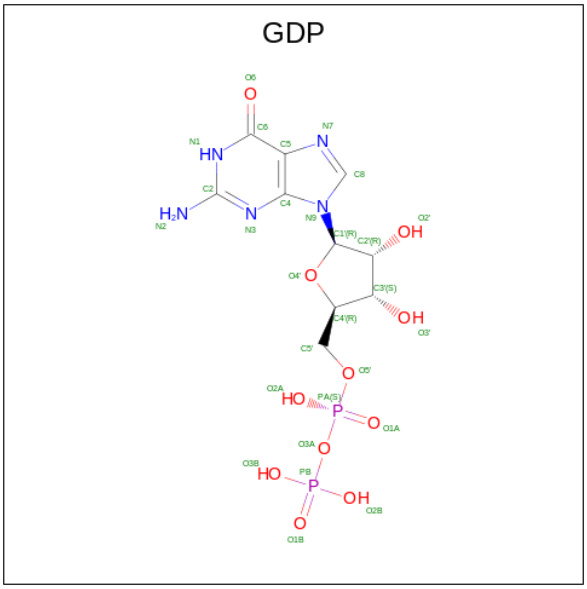
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

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

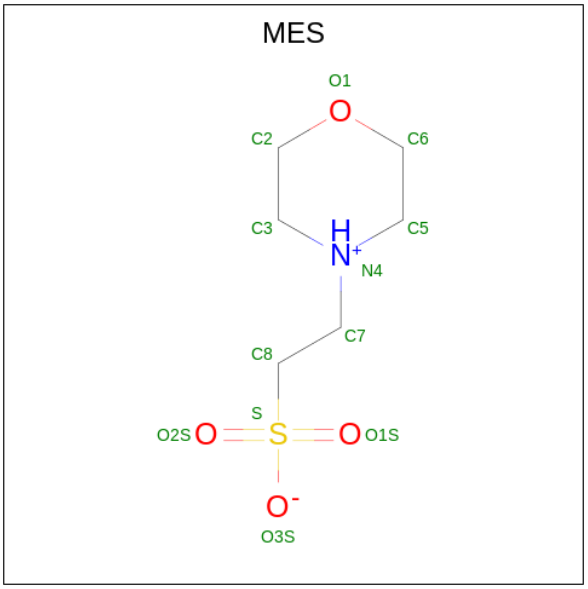
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	2	Total Ca 2 2	0	0
7	C	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0

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



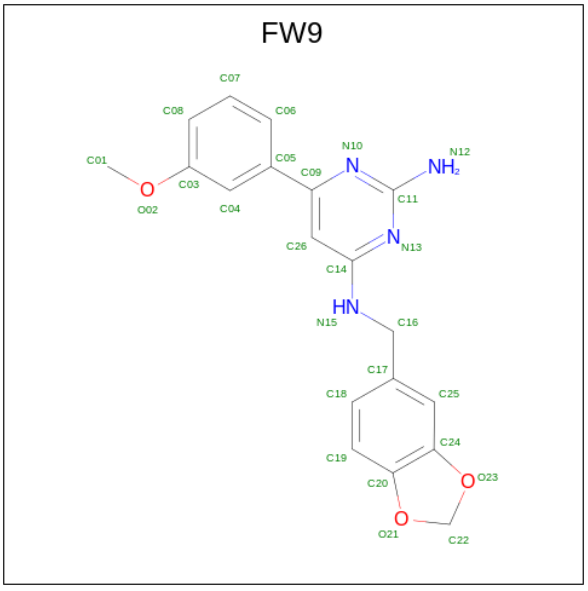
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C H N O P 38 10 10 5 11 2	0	0

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



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

- Molecule 10 is N4-(1,3-benzodioxol-5-ylmethyl)-6-(3-methoxyphenyl)pyrimidine-2,4-diamine (three-letter code: FW9) (formula: $C_{19}H_{18}N_4O_3$) (labeled as "Ligand of Interest" by depositor).

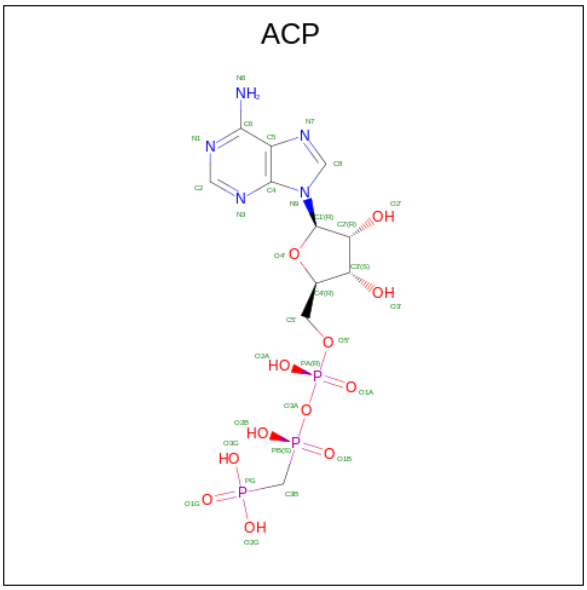


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			44	19	18	4	3		
10	D	1	Total	C	H	N	O	0	0
			44	19	18	4	3		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Cl	0	0
			1	1		

- Molecule 12 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
12	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	34	Total	O	0	0
			34	34		
13	B	25	Total	O	0	0
			25	25		
13	C	54	Total	O	0	0
			54	54		

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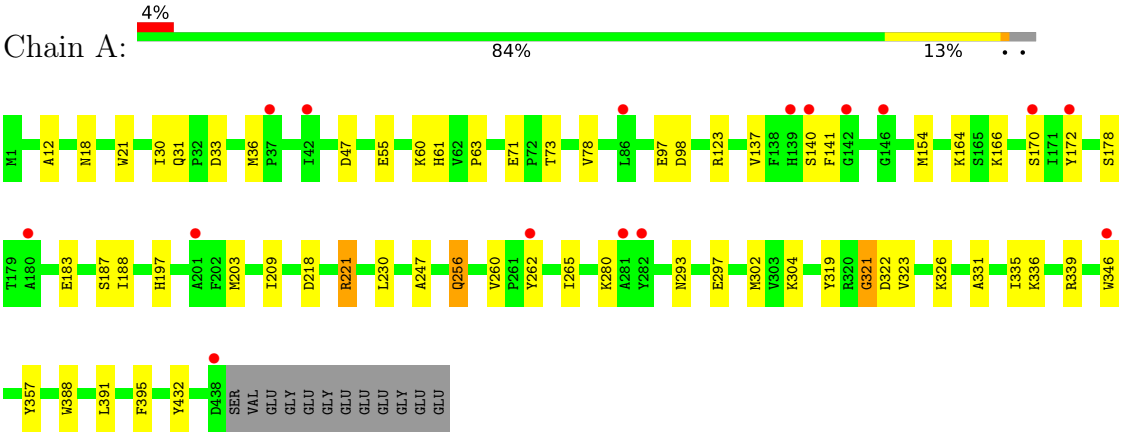
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	15	Total O 15 15	0	0
13	E	1	Total O 1 1	0	0
13	F	9	Total O 9 9	0	0

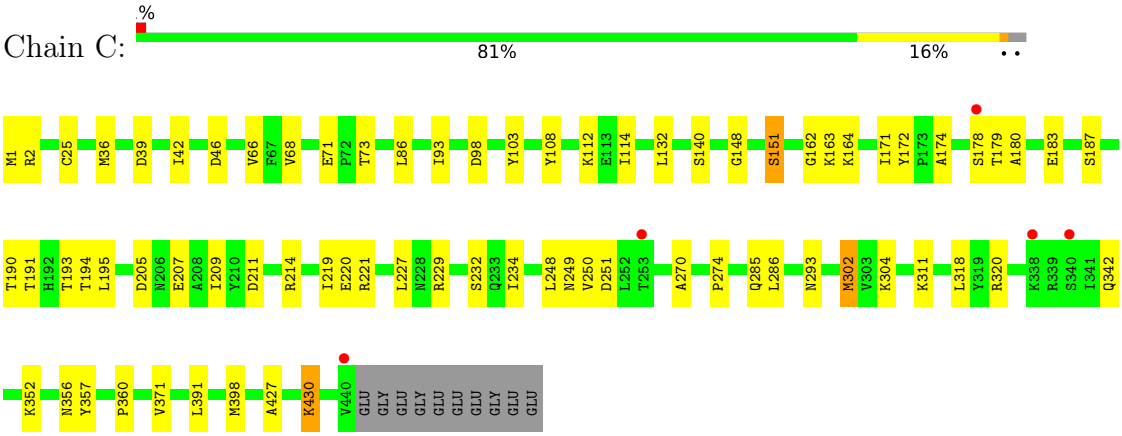
3 Residue-property plots (i)

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.

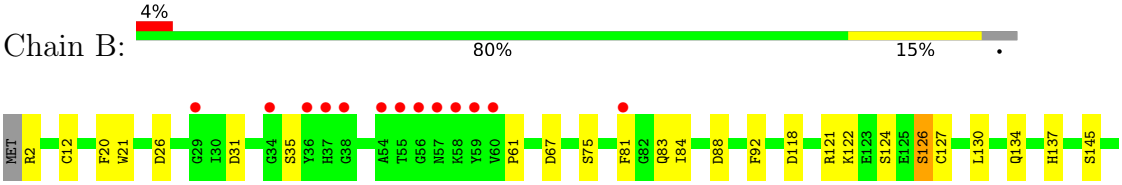
• Molecule 1: Tubulin alpha-1B chain

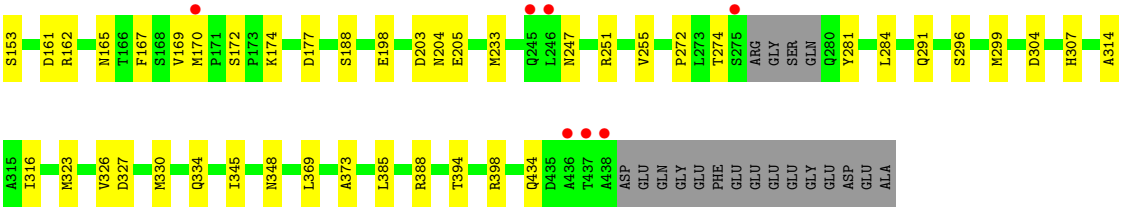


• Molecule 1: Tubulin alpha-1B chain



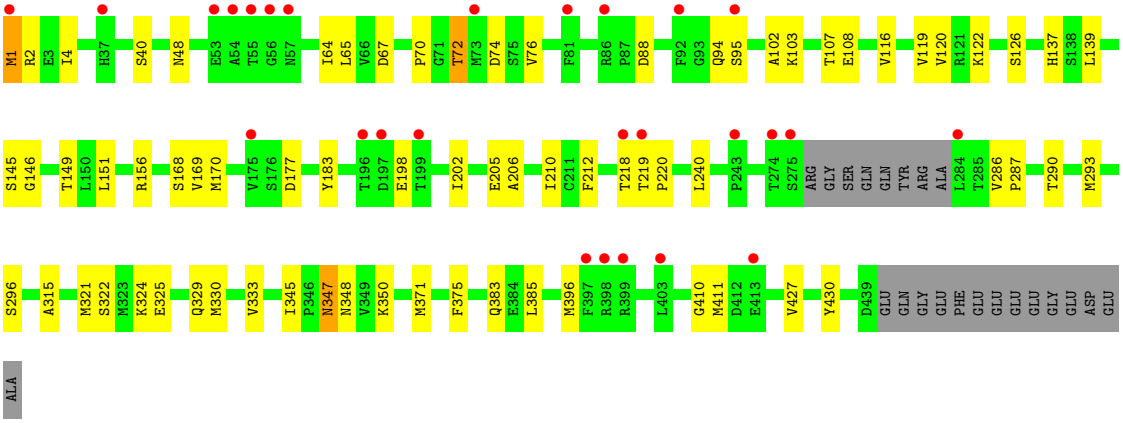
• Molecule 2: Tubulin beta chain





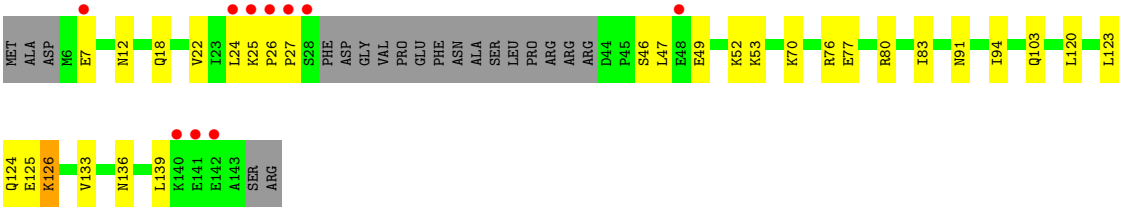
• Molecule 2: Tubulin beta chain

Chain D:



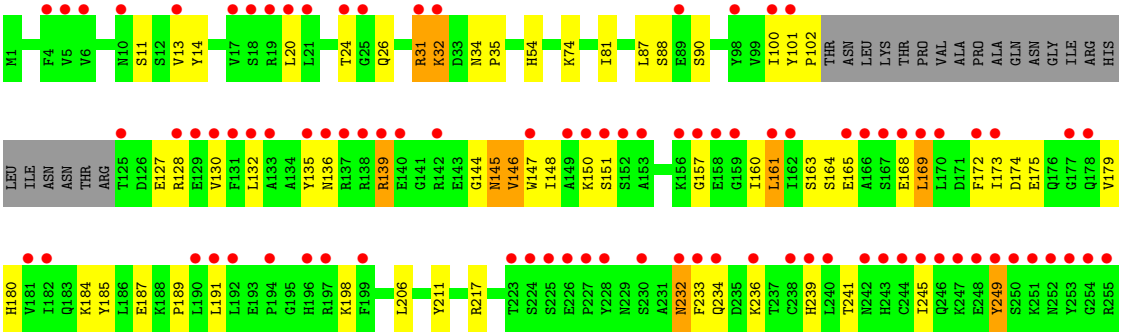
• Molecule 3: Stathmin-4

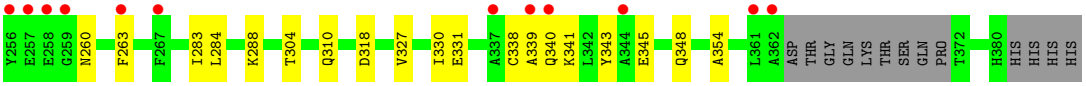
Chain E:



• Molecule 4: Tubulin tyrosine ligase

Chain F:




Y256
E257
E258
G259
N260
F263
F267
I283
L284
K288
T304
Q310
D318
V327
I330
E331
A337
C338
A339
Q340
K341
L342
Y343
A344
E345
Q348
A354
L361
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
PRO
T372
H380
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.57Å 158.08Å 181.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.70 48.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.26-2.70) 99.7 (48.26-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.228 , 0.271 0.228 , 0.271	Depositor DCC
R_{free} test set	1008 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	34902	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: CL, MG, FW9, CA, MES, GTP, ACP, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.34	0/3515	0.49	0/4772
1	C	0.38	2/3560 (0.1%)	0.49	0/4835
2	B	0.31	0/3442	0.46	0/4662
2	D	0.32	0/3401	0.48	0/4607
3	E	0.34	0/1036	0.43	0/1375
4	F	0.37	1/2914 (0.0%)	0.57	5/3936 (0.1%)
All	All	0.35	3/17868 (0.0%)	0.49	5/24187 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	F	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	GLN	CA-CB	-7.44	1.37	1.53
4	F	161	LEU	CG-CD2	7.10	1.78	1.51
1	C	342	GLN	CB-CG	-6.98	1.33	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	169	LEU	CD1-CG-CD2	10.04	140.63	110.50
4	F	161	LEU	CB-CG-CD1	8.05	124.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	161	LEU	CB-CG-CD2	-8.03	97.35	111.00
4	F	161	LEU	CD1-CG-CD2	6.03	128.59	110.50
4	F	169	LEU	CB-CG-CD2	-5.79	101.16	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	GLY	Peptide
4	F	145	ASN	Peptide

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	3434	3334	3345	33	0
1	C	3466	3373	3386	47	1
2	B	3359	3234	3244	41	0
2	D	3325	3195	3206	49	0
3	E	1025	1036	1039	21	1
4	F	2849	2801	2816	69	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	10	12	3	0
9	B	12	12	12	0	0
10	B	26	18	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	26	18	0	0	0
11	D	1	0	0	0	0
12	F	31	14	14	2	0
13	A	34	0	0	0	0
13	B	25	0	0	2	0
13	C	54	0	0	0	0
13	D	15	0	0	3	0
13	E	1	0	0	1	0
13	F	9	0	0	0	0
All	All	17827	17075	17110	247	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (247) 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)
4:F:161:LEU:CG	4:F:161:LEU:CD2	1.78	1.58
4:F:161:LEU:HD22	4:F:172:PHE:CD1	1.95	1.01
3:E:125:GLU:OE2	13:E:301:HOH:O	1.83	0.97
4:F:169:LEU:N	4:F:169:LEU:HD23	1.81	0.92
4:F:161:LEU:CD2	4:F:161:LEU:CB	2.47	0.92
1:A:178:SER:OG	1:A:183:GLU:OE2	1.96	0.81
4:F:146:VAL:HG12	4:F:185:TYR:HB3	1.64	0.79
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.15	0.79
2:B:198:GLU:OE1	13:B:601:HOH:O	2.01	0.79
2:D:383:GLN:HB2	2:D:427:VAL:HG23	1.64	0.78
4:F:168:GLU:C	4:F:169:LEU:HD23	2.04	0.78
2:D:347:ASN:O	2:D:350:LYS:NZ	2.19	0.76
2:D:430:TYR:OH	13:D:601:HOH:O	2.03	0.75
4:F:146:VAL:CG1	4:F:185:TYR:HB3	2.18	0.73
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.09	0.70
2:B:81:PHE:O	2:B:84:ILE:HG22	1.93	0.68
2:D:198:GLU:OE2	13:D:602:HOH:O	2.11	0.68
3:E:46:SER:HG	3:E:49:GLU:H	1.41	0.68
4:F:217:ARG:NH2	4:F:345:GLU:OE2	2.25	0.68
4:F:283:ILE:HG23	4:F:327:VAL:HG21	1.76	0.68
2:D:183:TYR:OH	2:D:396:MET:O	2.13	0.67
2:D:2:ARG:NH1	13:D:603:HOH:O	2.27	0.66
2:D:67:ASP:OD2	2:D:72:THR:HG21	1.95	0.66
4:F:88:SER:OG	4:F:90:SER:OG	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HG3	2:B:385:LEU:HD11	1.78	0.66
2:D:145:SER:O	2:D:149:THR:HG23	1.97	0.65
2:D:218:THR:O	2:D:219:THR:HB	1.95	0.65
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.80	0.64
4:F:144:GLY:HA3	4:F:187:GLU:OE2	1.98	0.64
4:F:161:LEU:CD2	4:F:172:PHE:CD1	2.79	0.63
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.99	0.63
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.80	0.63
2:B:126:SER:OG	2:B:126:SER:O	2.15	0.62
1:C:36:MET:HE2	1:C:39:ASP:HB2	1.83	0.61
1:C:270:ALA:O	1:C:302:MET:SD	2.58	0.61
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.82	0.61
2:D:116:VAL:O	2:D:119:VAL:HG12	1.99	0.61
4:F:146:VAL:HG21	4:F:187:GLU:CD	2.19	0.61
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.83	0.60
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.83	0.60
1:C:302:MET:SD	1:C:302:MET:N	2.75	0.60
2:D:107:THR:OG1	2:D:108:GLU:N	2.33	0.60
4:F:136:ASN:HA	4:F:139:ARG:HB3	1.83	0.60
2:B:204:ASN:ND2	8:B:501:GDP:O2'	2.35	0.60
2:B:83:GLN:H	2:B:83:GLN:NE2	1.98	0.59
3:E:136:ASN:HA	3:E:139:LEU:HD23	1.84	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.04	0.58
1:C:132:LEU:O	1:C:164:LYS:NZ	2.36	0.58
4:F:161:LEU:HD21	4:F:172:PHE:HB3	1.85	0.57
2:B:177:ASP:O	1:C:352:LYS:NZ	2.28	0.57
4:F:241:THR:OG1	12:F:402:ACP:O3'	2.22	0.57
2:D:218:THR:O	2:D:219:THR:CB	2.52	0.56
1:A:321:GLY:O	1:A:357:TYR:HA	2.05	0.56
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.36	0.56
4:F:146:VAL:HG11	4:F:187:GLU:HG2	1.87	0.56
1:C:179:THR:CG2	2:D:350:LYS:HD2	2.37	0.55
2:B:12:CYS:SG	2:B:169:VAL:HG21	2.47	0.55
1:C:360:PRO:HG2	1:C:371:VAL:HG23	1.89	0.55
4:F:151:SER:OG	4:F:180:HIS:ND1	2.40	0.54
2:B:274:THR:HG21	2:B:369:LEU:HD11	1.89	0.54
4:F:163:SER:HB3	4:F:169:LEU:HG	1.89	0.53
2:D:169:VAL:HA	2:D:202:ILE:O	2.09	0.53
1:C:190:THR:O	1:C:194:THR:HG23	2.09	0.53
1:C:179:THR:HG23	2:D:350:LYS:HD2	1.91	0.53
2:D:146:GLY:O	2:D:149:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:N	2:D:48:ASN:OD1	2.41	0.52
3:E:126:LYS:NZ	3:E:126:LYS:HB3	2.23	0.52
4:F:318:ASP:HB3	4:F:330:ILE:HD11	1.92	0.52
8:B:501:GDP:H8	8:B:501:GDP:H5"	1.74	0.51
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.26	0.51
4:F:304:THR:O	4:F:310:GLN:NE2	2.43	0.51
2:D:385:LEU:HD23	2:D:385:LEU:C	2.31	0.51
4:F:150:LYS:HE3	12:F:402:ACP:H8	1.93	0.51
1:C:174:ALA:O	1:C:178:SER:HB3	2.10	0.51
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.93	0.51
2:B:291:GLN:O	2:B:291:GLN:NE2	2.43	0.51
1:A:336:LYS:HD2	3:E:24:LEU:HD23	1.91	0.51
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.93	0.51
4:F:161:LEU:CD2	4:F:161:LEU:HB3	2.39	0.51
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.37	0.50
3:E:53:LYS:HE2	3:E:53:LYS:N	2.27	0.50
4:F:20:LEU:HD21	4:F:348:GLN:OE1	2.11	0.50
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.95	0.49
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.46	0.49
3:E:25:LYS:HG2	3:E:26:PRO:CD	2.43	0.49
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.48	0.49
2:B:272:PRO:HB3	2:B:284:LEU:HD22	1.95	0.49
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.94	0.49
4:F:151:SER:OG	4:F:180:HIS:CG	2.66	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.49
2:D:321:MET:HB3	2:D:371:MET:HE2	1.95	0.49
2:D:329:GLN:O	2:D:333:VAL:HG23	2.13	0.48
4:F:169:LEU:O	4:F:173:ILE:HG13	2.13	0.48
4:F:232:ASN:HD21	4:F:234:GLN:HB3	1.79	0.48
2:B:307:HIS:O	2:B:434:GLN:NE2	2.46	0.48
2:D:102:ALA:HB2	2:D:411:MET:CE	2.44	0.48
2:D:218:THR:HG23	2:D:219:THR:OG1	2.13	0.48
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.94	0.48
2:B:161:ASP:O	2:B:251:ARG:NH2	2.46	0.48
3:E:47:LEU:HD23	3:E:47:LEU:O	2.14	0.48
4:F:31:ARG:HE	4:F:32:LYS:HD2	1.79	0.48
4:F:151:SER:OG	4:F:180:HIS:CE1	2.67	0.48
4:F:161:LEU:HD22	4:F:172:PHE:CG	2.43	0.48
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.42	0.48
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.95	0.48
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ASP:OD1	2:B:121:ARG:NH2	2.47	0.48
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.48
2:D:322:SER:HB3	2:D:325:GLU:CB	2.44	0.48
2:B:174:LYS:HD3	2:B:205:GLU:HG3	1.96	0.47
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.95	0.47
1:C:42:ILE:HD12	1:C:42:ILE:H	1.79	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.95	0.47
4:F:161:LEU:HD22	4:F:172:PHE:CE1	2.42	0.47
4:F:232:ASN:ND2	4:F:234:GLN:HB3	2.29	0.47
2:D:322:SER:HB3	2:D:325:GLU:HB3	1.96	0.47
2:B:296:SER:HA	2:B:299:MET:HG2	1.97	0.47
1:C:46:ASP:OD1	1:C:46:ASP:N	2.44	0.47
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.41	0.47
2:D:65:LEU:N	2:D:65:LEU:HD12	2.30	0.47
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.96	0.47
4:F:338:CYS:SG	4:F:339:ALA:N	2.88	0.47
2:B:83:GLN:H	2:B:83:GLN:CD	2.18	0.47
2:B:134:GLN:HA	2:B:165:ASN:O	2.15	0.47
4:F:169:LEU:O	4:F:173:ILE:N	2.47	0.46
1:C:229:ARG:O	1:C:232:SER:OG	2.29	0.46
2:D:145:SER:OG	2:D:146:GLY:N	2.48	0.46
1:A:304:LYS:HB2	4:F:54:HIS:HE1	1.80	0.46
4:F:135:TYR:OH	4:F:165:GLU:HA	2.15	0.46
2:D:410:GLY:C	3:E:133:VAL:HG13	2.36	0.46
4:F:184:LYS:NZ	4:F:185:TYR:O	2.48	0.46
4:F:102:PRO:HB3	4:F:174:ASP:HA	1.97	0.46
2:B:326:VAL:HG23	2:B:327:ASP:N	2.30	0.46
1:C:1:MET:HG2	1:C:2:ARG:H	1.80	0.46
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.15	0.46
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.98	0.46
2:D:70:PRO:HD3	2:D:94:GLN:O	2.15	0.46
4:F:161:LEU:CD2	4:F:172:PHE:CG	2.99	0.46
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.98	0.45
1:A:331:ALA:O	1:A:335:ILE:HG12	2.16	0.45
2:B:31:ASP:OD1	2:B:35:SER:N	2.47	0.45
2:B:124:SER:O	2:B:127:CYS:HB2	2.16	0.45
2:D:4:ILE:HD11	2:D:240:LEU:HD13	1.99	0.45
2:D:103:LYS:HA	2:D:107:THR:OG1	2.17	0.45
1:A:137:VAL:HG21	1:A:154:MET:SD	2.57	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.45
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	1.99	0.45
2:D:293:MET:CG	2:D:375:PHE:HB2	2.47	0.45
4:F:284:LEU:O	4:F:288:LYS:HG3	2.17	0.45
4:F:127:GLU:HB3	4:F:130:VAL:CG2	2.47	0.45
4:F:146:VAL:HG21	4:F:187:GLU:CG	2.47	0.45
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.99	0.45
1:C:214:ARG:HG2	1:C:219:ILE:O	2.17	0.45
2:D:64:ILE:CD1	2:D:120:VAL:HG22	2.46	0.45
4:F:245:ILE:O	4:F:249:TYR:HB2	2.16	0.45
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.52	0.45
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.99	0.44
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.52	0.44
1:A:36:MET:HB2	1:A:61:HIS:ND1	2.32	0.44
4:F:13:VAL:HG13	4:F:14:TYR:H	1.82	0.44
4:F:245:ILE:O	4:F:245:ILE:HG22	2.17	0.44
1:C:427:ALA:O	1:C:430:LYS:HG3	2.18	0.44
1:A:188:ILE:HG13	1:A:395:PHE:CD2	2.53	0.44
2:B:345:ILE:HG22	2:B:348:ASN:HB3	1.99	0.44
4:F:148:ILE:HG22	4:F:185:TYR:HB2	1.99	0.44
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.53	0.44
1:C:220:GLU:HB2	2:D:324:LYS:HD2	1.99	0.44
4:F:179:VAL:C	4:F:180:HIS:HD1	2.21	0.44
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.83	0.44
2:D:139:LEU:HD11	2:D:168:SER:HB3	2.00	0.44
4:F:172:PHE:HA	4:F:175:GLU:HB2	1.99	0.44
2:B:330:MET:O	2:B:334:GLN:HG3	2.18	0.44
1:C:151[B]:SER:HB3	1:C:193:THR:CG2	2.47	0.44
3:E:123:LEU:HD23	3:E:126:LYS:HD3	1.99	0.43
1:A:55:GLU:HA	1:A:60:LYS:O	2.18	0.43
1:C:108:TYR:O	1:C:112:LYS:HB2	2.18	0.43
4:F:146:VAL:HB	4:F:184:LYS:HZ1	1.83	0.43
4:F:172:PHE:CD1	4:F:172:PHE:O	2.71	0.43
2:B:67:ASP:O	2:B:92:PHE:HA	2.19	0.43
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.33	0.43
1:C:25:CYS:SG	1:C:86:LEU:HD21	2.59	0.43
1:C:179:THR:HA	2:D:350:LYS:HD2	2.00	0.43
4:F:234:GLN:O	4:F:236:LYS:NZ	2.49	0.43
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.53	0.43
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.99	0.43
1:A:203:MET:HE1	1:A:388:TRP:CH2	2.54	0.43
2:D:102:ALA:HB2	2:D:411:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:101:TYR:HE1	4:F:179:VAL:HG21	1.83	0.42
1:A:30:ILE:HG12	1:A:36:MET:SD	2.59	0.42
2:B:172:SER:N	13:B:607:HOH:O	2.49	0.42
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.46	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
1:C:318:LEU:HD12	1:C:318:LEU:N	2.34	0.42
2:B:153:SER:HB3	3:E:76:ARG:HH22	1.83	0.42
2:B:251:ARG:O	2:B:255:VAL:HG23	2.19	0.42
2:D:88:ASP:OD1	2:D:88:ASP:N	2.41	0.42
3:E:120:LEU:O	3:E:124:GLN:HG3	2.19	0.42
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.18	0.42
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.20	0.42
2:D:126:SER:O	2:D:126:SER:OG	2.37	0.42
2:B:145:SER:OG	2:B:188:SER:OG	2.35	0.42
2:B:167:PHE:CE1	2:B:233:MET:HG2	2.54	0.42
1:C:234:ILE:HD12	1:C:234:ILE:H	1.85	0.42
1:A:97:GLU:HB3	2:B:2:ARG:NH1	2.34	0.42
1:C:249:ASN:CG	1:C:356:ASN:HD21	2.17	0.42
2:D:290:THR:HG22	2:D:333:VAL:HG21	2.00	0.42
3:E:139:LEU:HD12	3:E:139:LEU:C	2.40	0.42
4:F:189:PRO:HG2	4:F:191:LEU:HD21	2.02	0.42
4:F:236:LYS:HD3	4:F:236:LYS:HA	1.81	0.42
2:D:139:LEU:HD12	2:D:170:MET:SD	2.59	0.42
2:D:206:ALA:O	2:D:210:ILE:HG13	2.19	0.42
2:B:203:ASP:OD2	2:B:388:ARG:NH1	2.47	0.42
2:D:321:MET:HB3	2:D:371:MET:CE	2.49	0.42
4:F:164:SER:HG	4:F:233:PHE:HE1	1.67	0.41
1:A:221:ARG:NH1	2:B:327:ASP:OD2	2.54	0.41
2:D:293:MET:HE1	2:D:315:ALA:HB1	2.02	0.41
2:B:394:THR:O	2:B:398:ARG:HG2	2.21	0.41
2:D:290:THR:HG23	2:D:330:MET:SD	2.60	0.41
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.85	0.41
2:B:314:ALA:HB1	10:B:506:FW9:C16	2.50	0.41
3:E:26:PRO:HB2	3:E:27:PRO:HD2	2.03	0.41
3:E:52:LYS:HB3	3:E:53:LYS:HE2	2.02	0.41
2:B:323:MET:HA	2:B:326:VAL:HG22	2.02	0.41
4:F:157:GLY:C	4:F:160:ILE:HD11	2.41	0.41
1:A:172:TYR:CZ	1:A:391:LEU:HD13	2.56	0.41
2:B:316:ILE:O	2:B:373:ALA:HA	2.20	0.41
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.55	0.41
2:D:94:GLN:HG2	2:D:95:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.03	0.41
1:C:191:THR:O	1:C:195:LEU:HB2	2.21	0.41
3:E:7:GLU:O	3:E:22:VAL:HG23	2.21	0.41
4:F:145:ASN:O	4:F:147:TRP:HD1	2.03	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.41
1:A:187:SER:HB2	1:A:391:LEU:HD21	2.03	0.41
1:A:293:ASN:OD1	1:A:335:ILE:HD12	2.20	0.41
4:F:24:THR:HG22	4:F:26:GLN:HG3	2.02	0.41
4:F:198:LYS:HE2	4:F:239:HIS:O	2.20	0.41
1:A:262:TYR:CE1	1:A:346:TRP:CZ2	3.09	0.41
1:C:286:LEU:N	1:C:286:LEU:HD12	2.36	0.41
1:A:256:GLN:OE1	1:A:260:VAL:O	2.39	0.40
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.86	0.40
2:B:130:LEU:O	2:B:162[A]:ARG:NH1	2.52	0.40
2:B:20:PHE:CD1	2:B:233:MET:HB3	2.56	0.40
2:D:293:MET:CE	2:D:315:ALA:HB1	2.51	0.40
1:A:247:ALA:HB2	3:E:12[A]:ASN:OD1	2.22	0.40
1:C:270:ALA:C	1:C:302:MET:SD	3.00	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)
1:C:285:GLN:NE2	3:E:91:ASN:OD1[4_455]	2.09	0.11

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	438/450 (97%)	421 (96%)	17 (4%)	0	100	100
1	C	444/450 (99%)	428 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
2	D	420/445 (94%)	399 (95%)	19 (4%)	2 (0%)	29	54
3	E	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
4	F	343/384 (89%)	326 (95%)	16 (5%)	1 (0%)	41	66
All	All	2190/2317 (94%)	2095 (96%)	92 (4%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	72	THR
4	F	146	VAL
2	D	220	PRO

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	371/378 (98%)	362 (98%)	9 (2%)	49	77
1	C	377/378 (100%)	367 (97%)	10 (3%)	44	74
2	B	370/383 (97%)	362 (98%)	8 (2%)	52	79
2	D	367/383 (96%)	355 (97%)	12 (3%)	38	67
3	E	112/127 (88%)	108 (96%)	4 (4%)	35	64
4	F	311/342 (91%)	303 (97%)	8 (3%)	46	75
All	All	1908/1991 (96%)	1857 (97%)	51 (3%)	46	74

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	164	LYS
1	A	218	ASP
1	A	221	ARG

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	280	LYS
1	A	302	MET
1	A	322	ASP
1	A	326	LYS
2	B	26	ASP
2	B	75	SER
2	B	88	ASP
2	B	122	LYS
2	B	126	SER
2	B	137	HIS
2	B	247	ASN
2	B	281	TYR
1	C	151[A]	SER
1	C	151[B]	SER
1	C	163	LYS
1	C	221	ARG
1	C	251	ASP
1	C	293	ASN
1	C	302	MET
1	C	311	LYS
1	C	398	MET
1	C	430	LYS
2	D	1	MET
2	D	40	SER
2	D	74	ASP
2	D	122	LYS
2	D	137	HIS
2	D	151	LEU
2	D	156	ARG
2	D	177	ASP
2	D	205	GLU
2	D	212	PHE
2	D	296	SER
2	D	347	ASN
3	E	70	LYS
3	E	77	GLU
3	E	103	GLN
3	E	126	LYS
4	F	11	SER
4	F	31	ARG
4	F	32	LYS

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Mol	Chain	Res	Type
4	F	139	ARG
4	F	211	TYR
4	F	232	ASN
4	F	249	TYR
4	F	260	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	91	GLN
1	A	107	HIS
1	A	128	GLN
1	A	197	HIS
1	A	256	GLN
1	A	329	ASN
2	B	83	GLN
2	B	334	GLN
1	C	61	HIS
1	C	197	HIS
1	C	342	GLN
2	D	105	HIS
4	F	232	ASN
4	F	252	ASN
4	F	260	ASN

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 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	D	504	6	26,34,34	1.16	2 (7%)	32,54,54	1.58	6 (18%)
5	GTP	C	501	6	26,34,34	1.08	2 (7%)	32,54,54	1.53	5 (15%)
9	MES	B	503	-	12,12,12	2.10	1 (8%)	14,16,16	1.78	3 (21%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.59	5 (15%)
10	FW9	D	503	-	29,29,29	1.40	4 (13%)	39,40,40	1.11	4 (10%)
8	GDP	B	501	6	24,30,30	1.03	2 (8%)	30,47,47	1.47	7 (23%)
10	FW9	B	506	-	29,29,29	1.30	3 (10%)	39,40,40	0.96	2 (5%)
12	ACP	F	402	6	27,33,33	2.67	7 (25%)	32,52,52	1.69	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	504	6	-	5/18/38/38	0/3/3/3
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
10	FW9	D	503	-	-	2/11/17/17	0/4/4/4
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
10	FW9	B	506	-	-	0/11/17/17	0/4/4/4
12	ACP	F	402	6	-	6/15/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	O4'-C1'	8.41	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-6.86	1.67	1.77
12	F	402	ACP	PB-O3A	6.62	1.65	1.58
5	D	504	GTP	C5-C6	-3.92	1.39	1.47
10	D	503	FW9	C14-N15	3.89	1.42	1.36
5	C	501	GTP	C5-C6	-3.82	1.39	1.47
5	A	501	GTP	C5-C6	-3.70	1.39	1.47
10	B	506	FW9	C14-N15	3.66	1.41	1.36
12	F	402	ACP	C2'-C1'	-3.44	1.48	1.53
12	F	402	ACP	O4'-C4'	3.21	1.52	1.45
12	F	402	ACP	C6-N6	3.19	1.45	1.34
8	B	501	GDP	C6-N1	-2.69	1.33	1.37
12	F	402	ACP	C4-N3	-2.55	1.32	1.35
12	F	402	ACP	C2'-C3'	-2.54	1.46	1.53
10	B	506	FW9	C11-N12	2.51	1.38	1.33
10	D	503	FW9	C11-N10	2.38	1.39	1.35
5	D	504	GTP	C2-N3	2.37	1.38	1.33
10	D	503	FW9	C11-N13	2.32	1.39	1.35
10	D	503	FW9	C11-N12	2.32	1.38	1.33
10	B	506	FW9	C11-N10	2.28	1.39	1.35
5	C	501	GTP	C2-N3	2.20	1.38	1.33
8	B	501	GDP	O4'-C1'	2.18	1.44	1.41
5	A	501	GTP	C2-N3	2.06	1.38	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	402	ACP	C3'-C2'-C1'	4.84	108.27	100.98
9	B	503	MES	C5-N4-C3	4.80	119.62	108.83
12	F	402	ACP	N3-C2-N1	-4.09	122.29	128.68
5	C	501	GTP	PB-O3B-PG	-3.72	120.05	132.83
12	F	402	ACP	C4-C5-N7	-3.57	105.68	109.40
5	D	504	GTP	PB-O3B-PG	-3.54	120.69	132.83
5	A	501	GTP	PA-O3A-PB	-3.36	121.31	132.83
5	D	504	GTP	C8-N7-C5	3.31	109.30	102.99
5	A	501	GTP	C5-C6-N1	3.26	119.72	113.95
5	D	504	GTP	C5-C6-N1	3.15	119.52	113.95
5	C	501	GTP	C5-C6-N1	3.05	119.34	113.95
5	A	501	GTP	C8-N7-C5	2.98	108.68	102.99
8	B	501	GDP	C2'-C3'-C4'	2.94	108.35	102.64
5	A	501	GTP	PB-O3B-PG	-2.90	122.86	132.83
5	C	501	GTP	C8-N7-C5	2.84	108.39	102.99
5	D	504	GTP	C2-N1-C6	-2.82	119.91	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	402	ACP	PB-O3A-PA	-2.81	123.66	132.56
5	C	501	GTP	PA-O3A-PB	-2.81	123.20	132.83
5	A	501	GTP	C2-N1-C6	-2.79	119.96	125.10
5	D	504	GTP	PA-O3A-PB	-2.71	123.53	132.83
8	B	501	GDP	C5-C6-N1	2.68	118.68	113.95
5	C	501	GTP	C2-N1-C6	-2.61	120.30	125.10
8	B	501	GDP	C8-N7-C5	2.56	107.87	102.99
5	D	504	GTP	C3'-C2'-C1'	2.56	104.83	100.98
8	B	501	GDP	PA-O3A-PB	-2.45	124.41	132.83
12	F	402	ACP	C2'-C3'-C4'	2.34	107.19	102.64
9	B	503	MES	O3S-S-C8	2.33	109.54	105.77
8	B	501	GDP	O4'-C4'-C5'	-2.32	101.76	109.37
8	B	501	GDP	O4'-C1'-C2'	2.27	110.25	106.93
10	B	506	FW9	C18-C19-C20	-2.22	115.82	120.06
10	D	503	FW9	C22-O21-C20	-2.19	102.49	105.34
9	B	503	MES	O2S-S-C8	2.17	109.53	106.92
10	D	503	FW9	C18-C19-C20	-2.16	115.94	120.06
12	F	402	ACP	O2A-PA-O1A	-2.14	101.65	112.24
10	D	503	FW9	C09-N10-C11	-2.09	115.14	116.34
10	D	503	FW9	N15-C14-N13	2.09	119.95	116.43
8	B	501	GDP	C5'-C4'-C3'	2.03	122.80	115.18
10	B	506	FW9	C19-C18-C17	2.01	123.79	121.03
12	F	402	ACP	C1'-N9-C4	-2.01	123.12	126.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	504	GTP	PB-O3B-PG-O3G
8	B	501	GDP	PA-O3A-PB-O3B
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	O4'-C4'-C5'-O5'
10	D	503	FW9	C04-C03-O02-C01
10	D	503	FW9	C08-C03-O02-C01

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Mol	Chain	Res	Type	Atoms
12	F	402	ACP	C3'-C4'-C5'-O5'
9	B	503	MES	C8-C7-N4-C3
5	D	504	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
12	F	402	ACP	C5'-O5'-PA-O2A
12	F	402	ACP	PG-C3B-PB-O2B
5	D	504	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PA-O3A-PB-O2B
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	504	GTP	PB-O3A-PA-O1A
5	D	504	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G

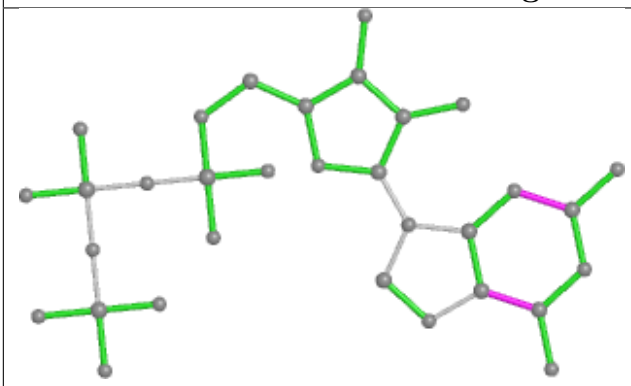
There are no ring outliers.

3 monomers are involved in 6 short contacts:

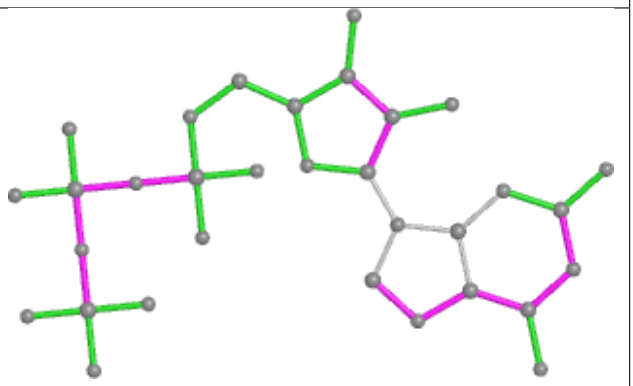
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	3	0
10	B	506	FW9	1	0
12	F	402	ACP	2	0

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

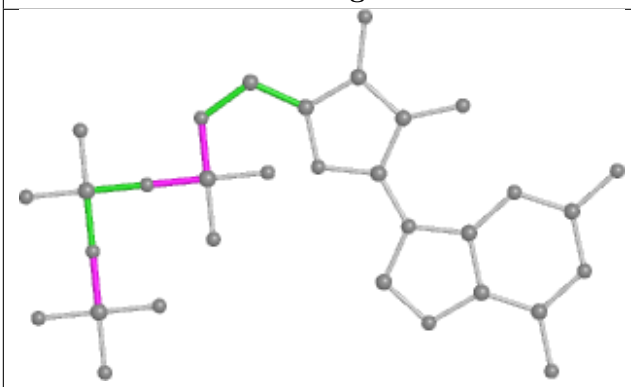
Ligand GTP D 504



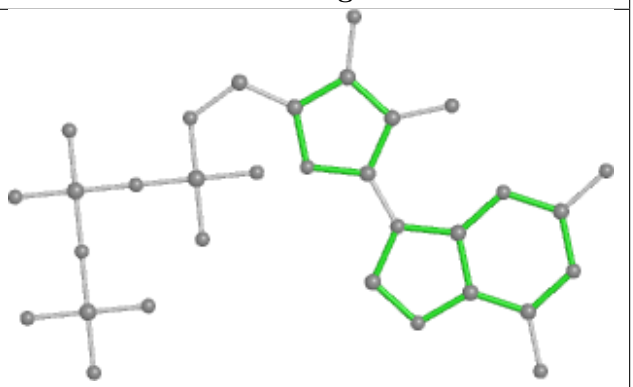
Bond lengths



Bond angles

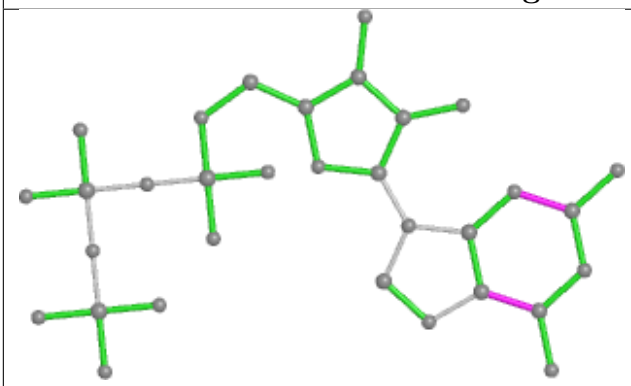


Torsions



Rings

Ligand GTP C 501



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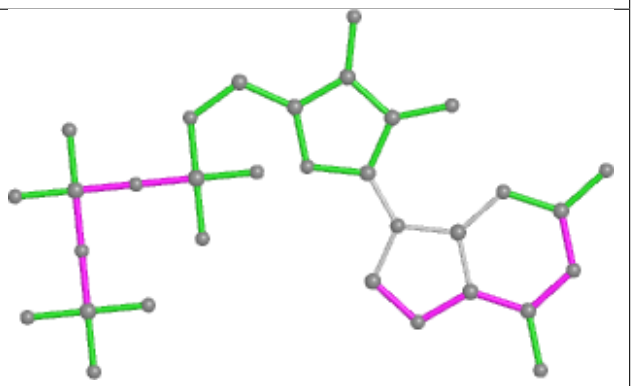

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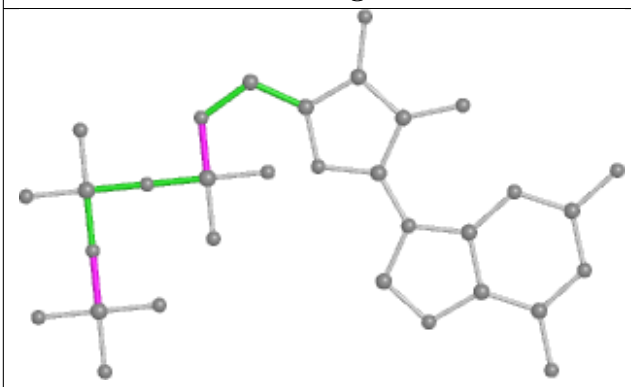

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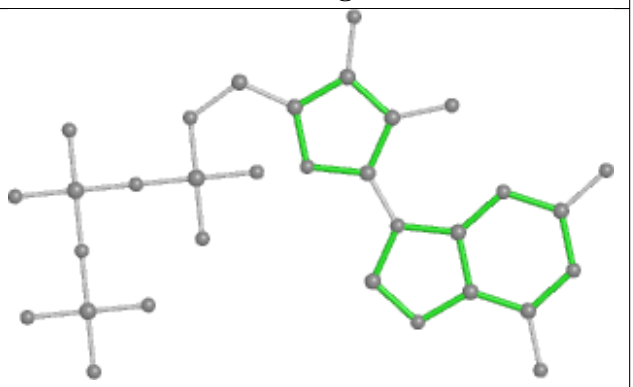
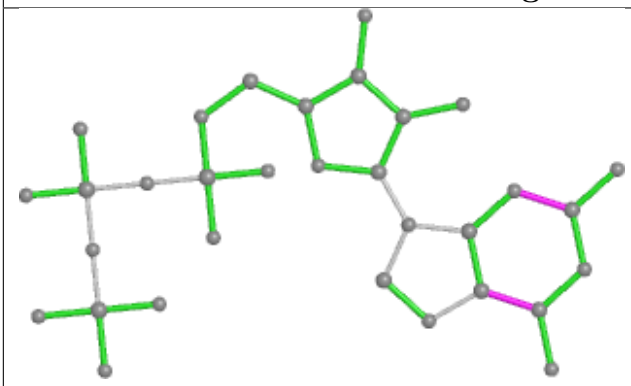


Rings

Ligand GTP A 501



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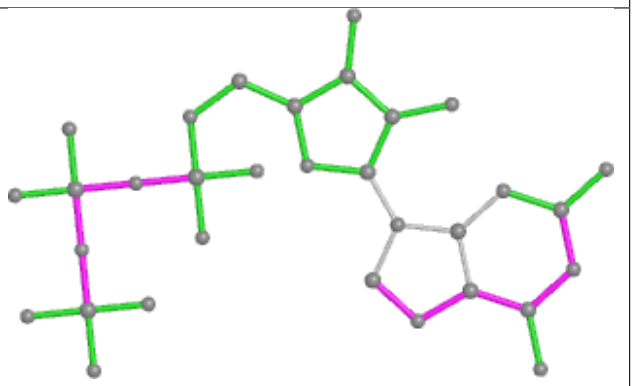

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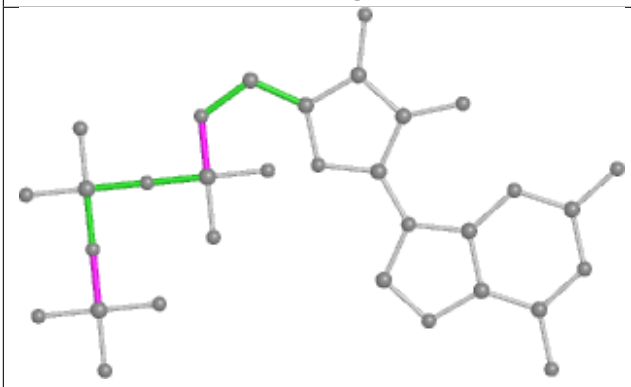

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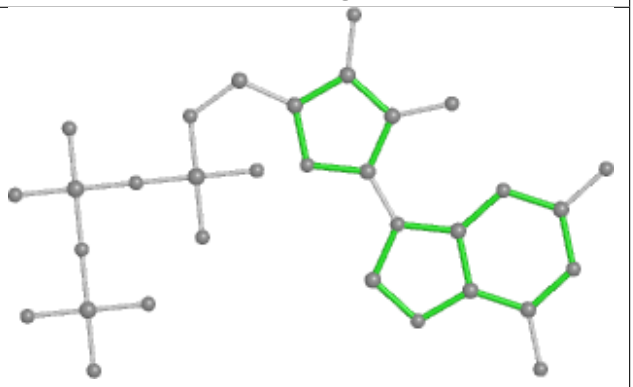
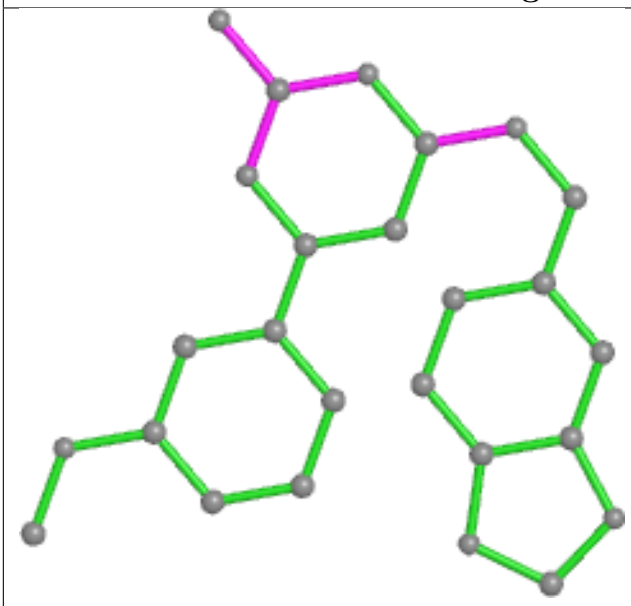


Rings

Ligand FW9 D 503



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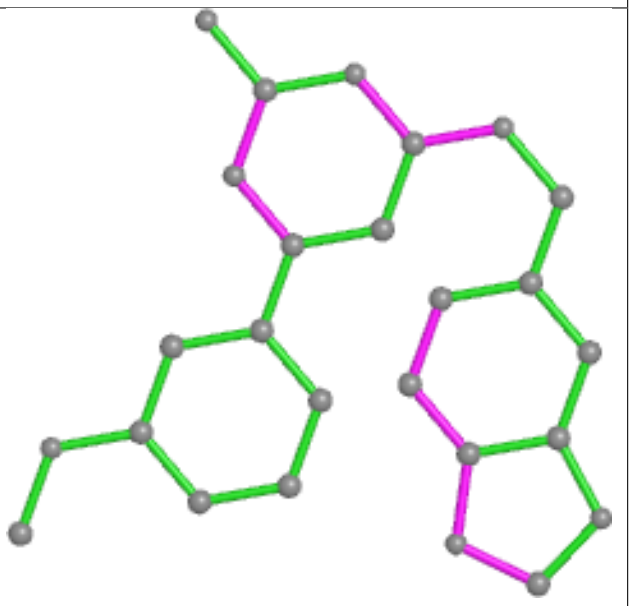

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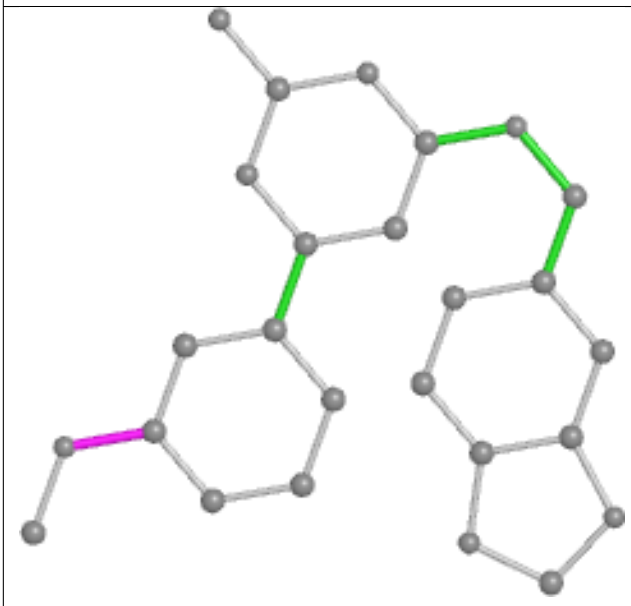

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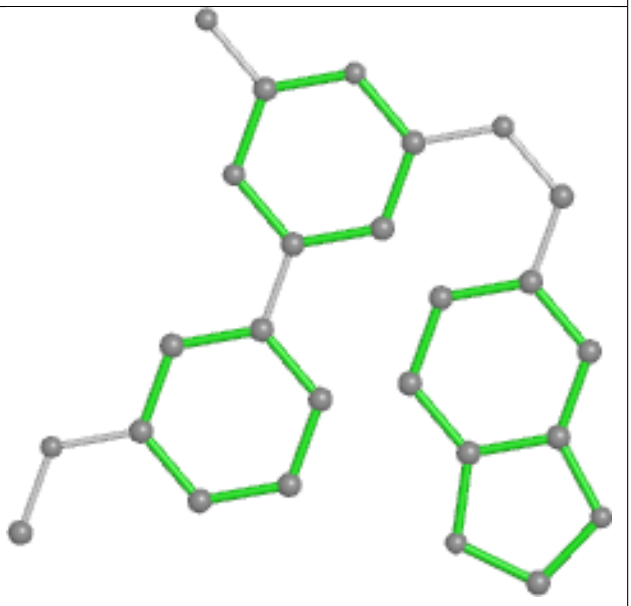
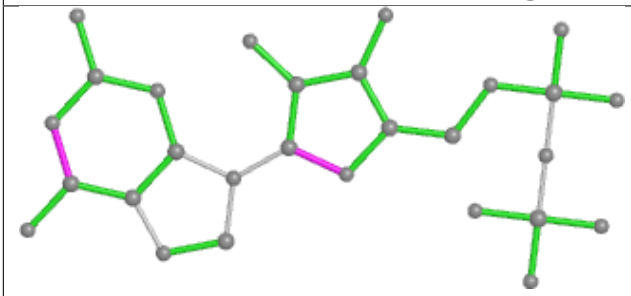


Rings

Ligand GDP B 501



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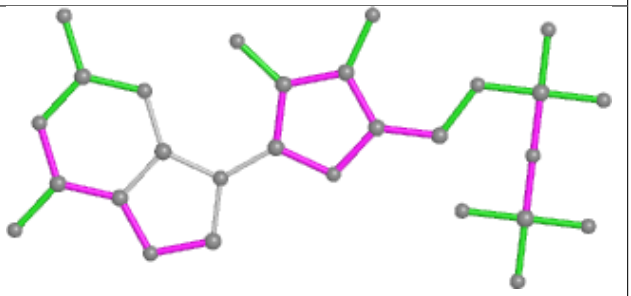

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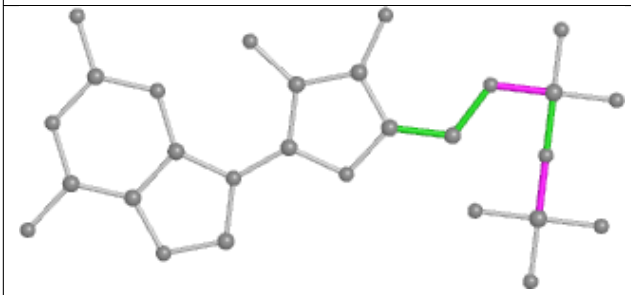

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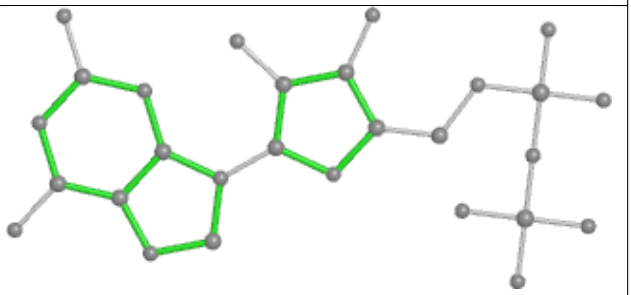
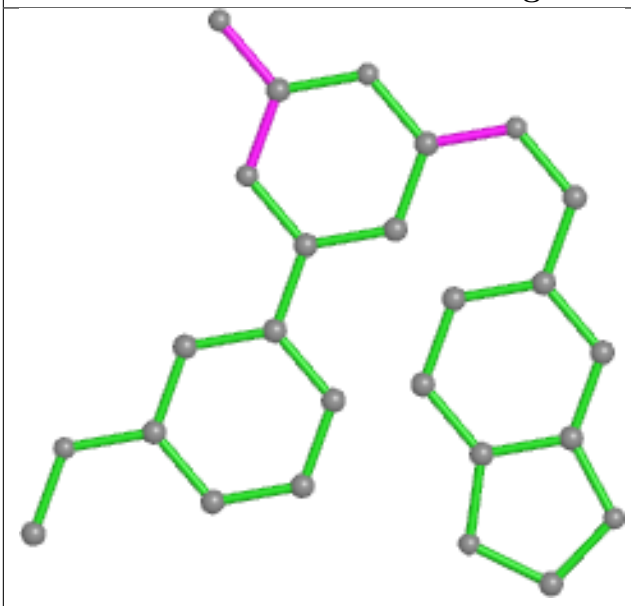
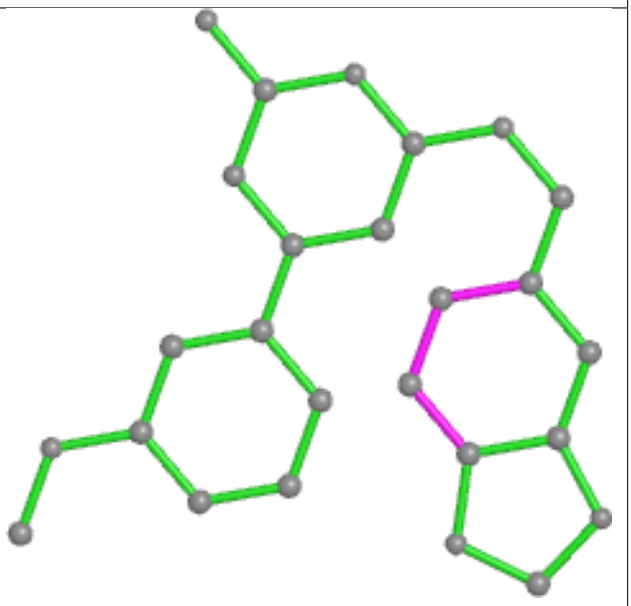


Rings

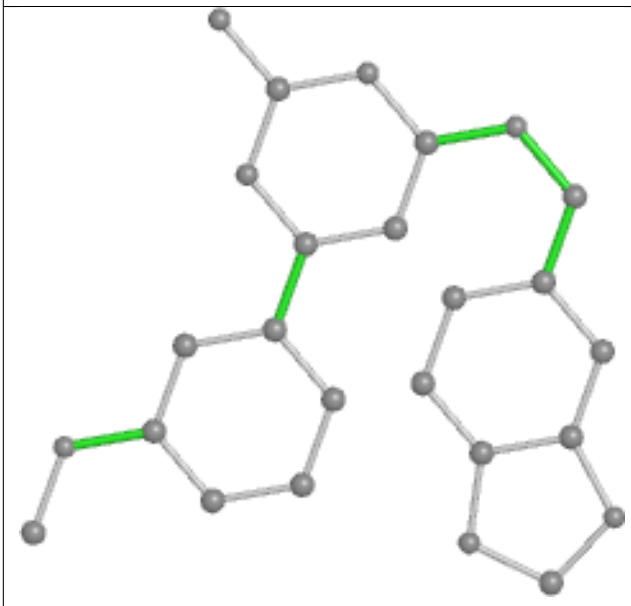
Ligand FW9 B 506



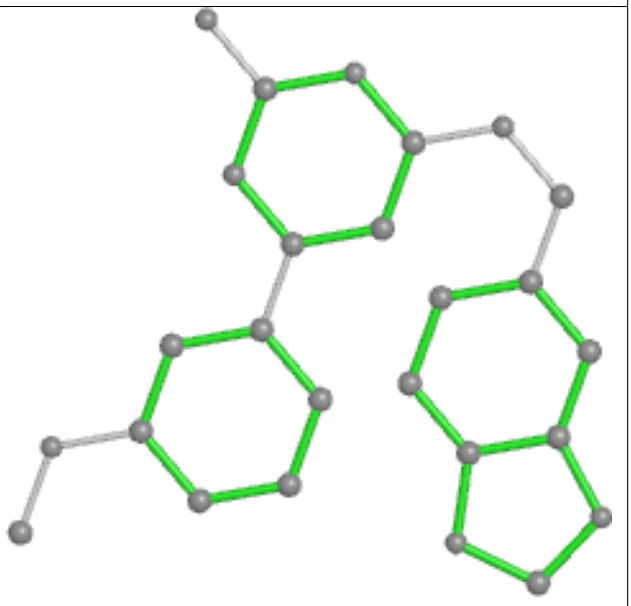
Bond lengths



Bond angles

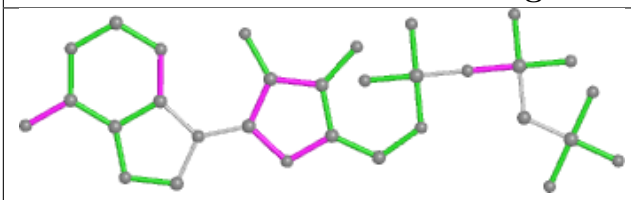


Torsions

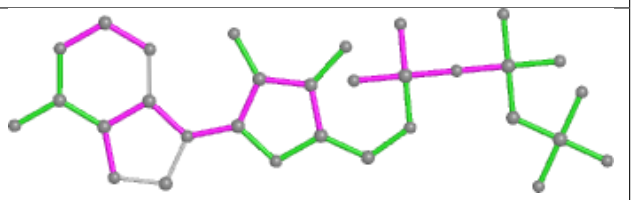


Rings

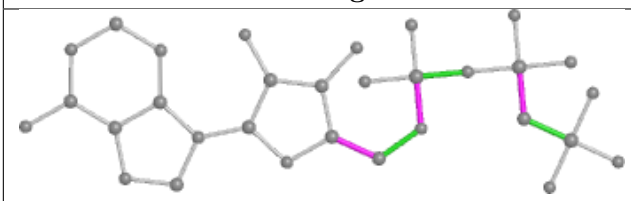
Ligand ACP F 402



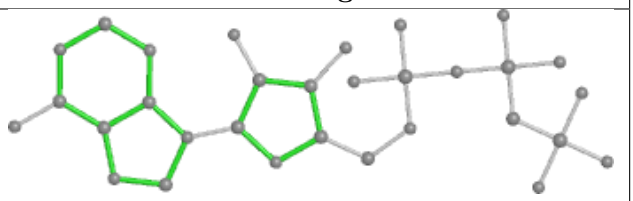
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	438/450 (97%)	0.43	16 (3%) 41 41	47, 61, 78, 109	0
1	C	440/450 (97%)	0.25	5 (1%) 80 82	38, 52, 69, 78	0
2	B	425/445 (95%)	0.47	20 (4%) 31 30	43, 61, 84, 99	0
2	D	423/445 (95%)	0.57	27 (6%) 19 18	51, 72, 89, 98	0
3	E	123/143 (86%)	0.55	10 (8%) 12 10	53, 69, 93, 109	0
4	F	349/384 (90%)	1.24	103 (29%) 0 0	58, 82, 130, 139	0
All	All	2198/2317 (94%)	0.56	181 (8%) 11 9	38, 65, 103, 139	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	9.5
4	F	173	ILE	7.3
2	D	275	SER	7.2
4	F	169	LEU	6.9
4	F	249	TYR	6.6
4	F	132	LEU	6.5
4	F	159	GLY	5.6
4	F	253	TYR	5.6
4	F	157	GLY	5.4
4	F	170	LEU	5.3
2	B	437	THR	5.3
4	F	233	PHE	5.2
2	B	438	ALA	5.0
1	A	282	TYR	4.9
4	F	182	ILE	4.8
4	F	251	LYS	4.8
1	A	281	ALA	4.6
4	F	151	SER	4.6
2	D	55	THR	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	55	THR	4.4
3	E	27	PRO	4.4
2	D	1	MET	4.4
4	F	17	VAL	4.3
4	F	177	GLY	4.3
2	B	57	ASN	4.3
4	F	255	ARG	4.2
4	F	240	LEU	3.9
4	F	234	GLN	3.9
4	F	250	SER	3.9
2	B	59	TYR	3.8
1	A	438	ASP	3.8
4	F	129	GLU	3.8
2	B	245	GLN	3.8
4	F	136	ASN	3.8
4	F	13	VAL	3.7
4	F	223	THR	3.7
3	E	26	PRO	3.6
2	D	92	PHE	3.6
2	B	436	ALA	3.6
4	F	128	ARG	3.6
4	F	181	VAL	3.6
4	F	242	ASN	3.6
1	A	262	TYR	3.6
4	F	101	TYR	3.5
2	B	56	GLY	3.5
4	F	245	ILE	3.5
4	F	239	HIS	3.5
4	F	254	GLY	3.5
4	F	199	PHE	3.4
2	B	36	TYR	3.4
3	E	28	SER	3.4
4	F	256	TYR	3.4
4	F	137	ARG	3.4
2	D	399	ARG	3.3
4	F	252	ASN	3.3
4	F	243	HIS	3.3
4	F	190	LEU	3.2
1	C	178	SER	3.2
4	F	236	LYS	3.2
4	F	21	LEU	3.2
4	F	152	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	54	ALA	3.2
4	F	362	ALA	3.2
4	F	361	LEU	3.2
4	F	162	ILE	3.1
4	F	5	VAL	3.1
4	F	194	PRO	3.1
4	F	246	GLN	3.1
4	F	153	ALA	3.1
4	F	238	CYS	3.1
4	F	150	LYS	3.1
2	D	243	PRO	3.1
4	F	257	GLU	3.0
4	F	248	GLU	3.0
4	F	138	ARG	2.9
4	F	125	THR	2.9
4	F	247	LYS	2.9
4	F	226	GLU	2.9
2	D	95	SER	2.9
2	D	398	ARG	2.9
2	D	37	HIS	2.8
1	C	340	SER	2.8
4	F	142	ARG	2.8
2	D	56	GLY	2.8
2	D	219	THR	2.8
4	F	166	ALA	2.8
4	F	100	ILE	2.8
4	F	156	LYS	2.8
1	C	440	VAL	2.7
4	F	139	ARG	2.7
4	F	258	GLU	2.7
4	F	259	GLY	2.7
4	F	131	PHE	2.7
2	B	275	SER	2.7
4	F	19	ARG	2.7
4	F	344	ALA	2.6
4	F	130	VAL	2.6
2	D	274	THR	2.6
2	D	284	LEU	2.6
4	F	165	GLU	2.6
4	F	263	PHE	2.6
2	D	218	THR	2.6
4	F	196	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	403	LEU	2.6
4	F	32	LYS	2.5
4	F	18	SER	2.5
4	F	225	SER	2.5
4	F	227	PRO	2.5
3	E	48	GLU	2.5
4	F	168	GLU	2.5
4	F	232	ASN	2.5
4	F	20	LEU	2.5
4	F	228	TYR	2.5
1	C	253	THR	2.5
4	F	98	TYR	2.5
4	F	197	ARG	2.5
2	B	60	VAL	2.4
4	F	339	ALA	2.4
4	F	244	CYS	2.4
4	F	178	GLN	2.4
1	A	139	HIS	2.4
1	A	140	SER	2.4
4	F	172	PHE	2.4
4	F	140	GLU	2.4
2	D	53	GLU	2.3
3	E	25	LYS	2.3
2	B	37	HIS	2.3
3	E	24	LEU	2.3
4	F	133	ALA	2.3
4	F	230	SER	2.3
4	F	340	GLN	2.3
4	F	89	GLU	2.3
1	C	338	LYS	2.3
2	D	57	ASN	2.3
2	B	81	PHE	2.3
1	A	146	GLY	2.3
4	F	147	TRP	2.3
2	B	246	LEU	2.3
2	D	54	ALA	2.3
4	F	24	THR	2.3
4	F	10	ASN	2.2
2	D	413	GLU	2.2
1	A	172	TYR	2.2
2	D	197	ASP	2.2
1	A	142	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	2.2
1	A	37	PRO	2.2
3	E	141	GLU	2.2
2	D	81	PHE	2.2
1	A	86	LEU	2.2
4	F	192	LEU	2.2
4	F	149	ALA	2.2
4	F	135	TYR	2.2
4	F	6	VAL	2.2
2	B	170	MET	2.2
2	D	199	THR	2.1
3	E	140	LYS	2.1
2	D	397	PHE	2.1
2	B	29	GLY	2.1
4	F	25	GLY	2.1
1	A	201	ALA	2.1
4	F	337	ALA	2.1
2	D	73	MET	2.1
1	A	42	ILE	2.1
2	B	38	GLY	2.1
4	F	31	ARG	2.1
3	E	142	GLU	2.1
2	D	196	THR	2.1
4	F	158	GLU	2.1
1	A	170	SER	2.1
3	E	7	GLU	2.1
4	F	191	LEU	2.0
2	D	86	ARG	2.0
2	B	58	LYS	2.0
4	F	4	PHE	2.0
1	A	346	TRP	2.0
4	F	267	PHE	2.0
1	A	180	ALA	2.0
2	B	34	GLY	2.0
4	F	167	SER	2.0
4	F	224	SER	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)

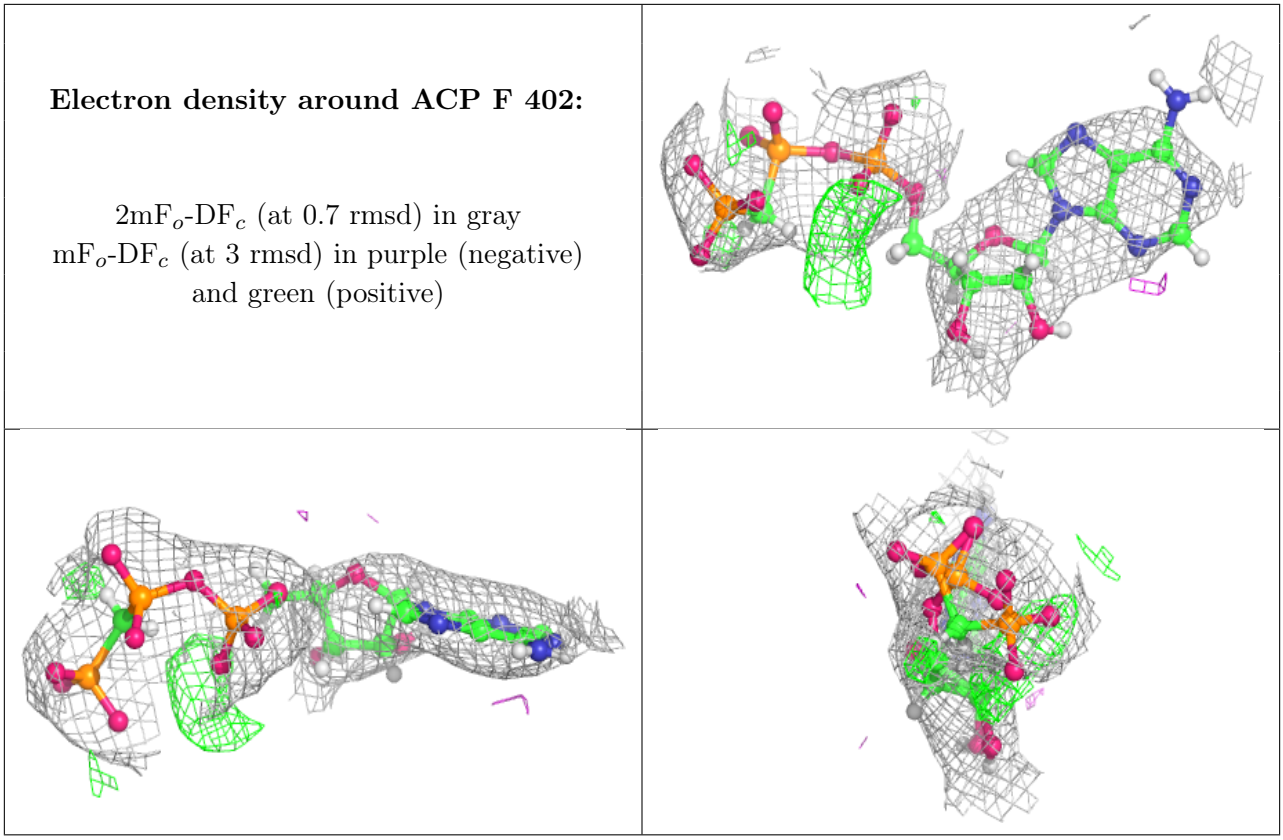
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	D	502	1/1	0.68	0.10	98,98,98,98	0
7	CA	B	504	1/1	0.82	0.08	97,97,97,97	0
12	ACP	F	402	31/31	0.83	0.20	99,108,133,133	0
7	CA	E	201	1/1	0.85	0.12	95,95,95,95	0
7	CA	B	505	1/1	0.87	0.09	88,88,88,88	0
11	CL	D	505	1/1	0.89	1.25	118,118,118,118	0
6	MG	F	401	1/1	0.89	0.16	106,106,106,106	0
10	FW9	B	506	26/26	0.90	0.26	55,67,81,89	0
6	MG	D	501	1/1	0.91	0.08	79,79,79,79	0
10	FW9	D	503	26/26	0.91	0.25	58,66,80,82	0
5	GTP	D	504	32/32	0.94	0.16	66,73,86,94	0
8	GDP	B	501	28/28	0.95	0.27	46,55,66,77	0
9	MES	B	503	12/12	0.95	0.14	55,67,75,76	0
7	CA	A	503	1/1	0.95	0.07	79,79,79,79	0
5	GTP	A	501	32/32	0.97	0.28	47,55,67,73	0
5	GTP	C	501	32/32	0.98	0.22	38,49,61,71	0
7	CA	C	503	1/1	0.98	0.11	66,66,66,66	0
6	MG	A	502	1/1	0.98	0.26	53,53,53,53	0
6	MG	B	502	1/1	0.98	0.27	55,55,55,55	0
6	MG	C	502	1/1	0.98	0.25	44,44,44,44	0

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

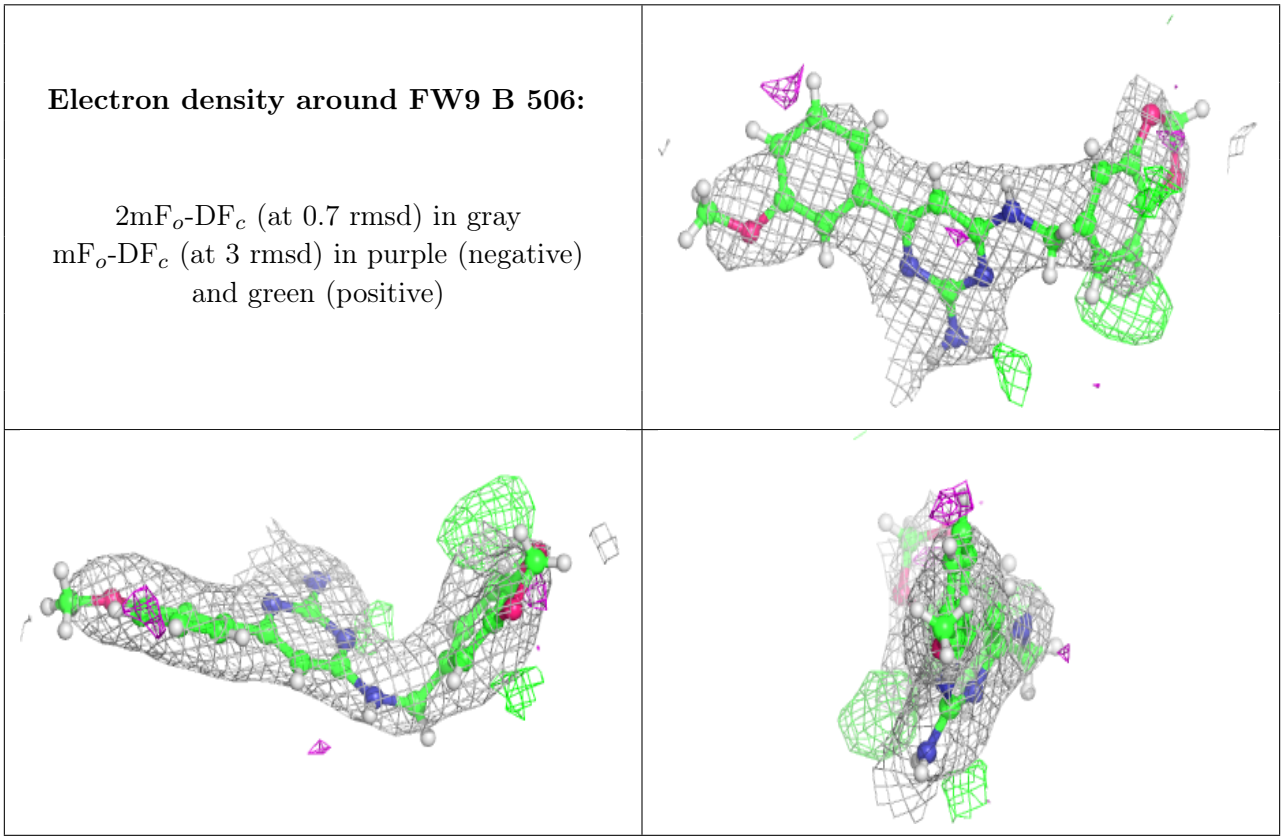
Electron density around ACP F 402:

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



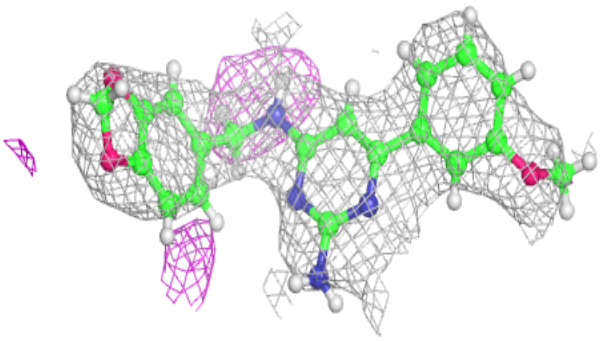
Electron density around FW9 B 506:

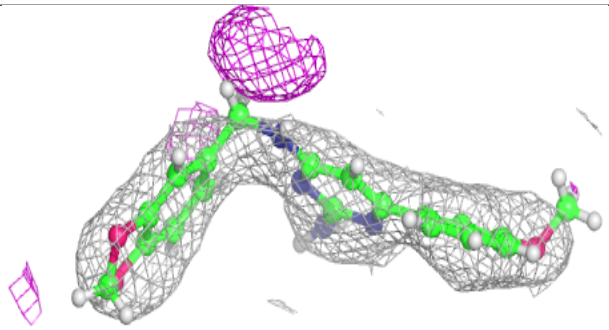
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

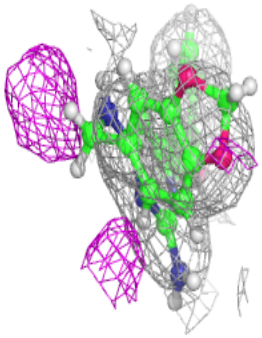


Electron density around FW9 D 503:

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

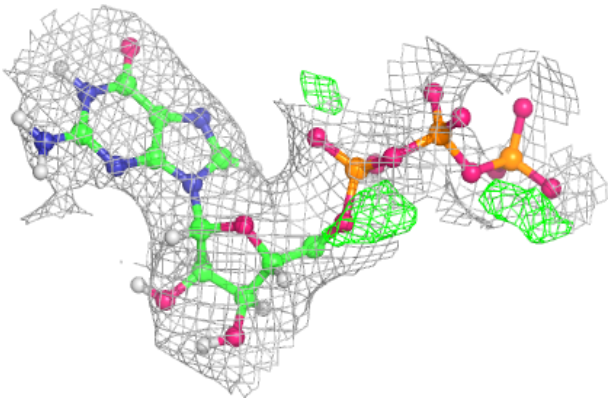


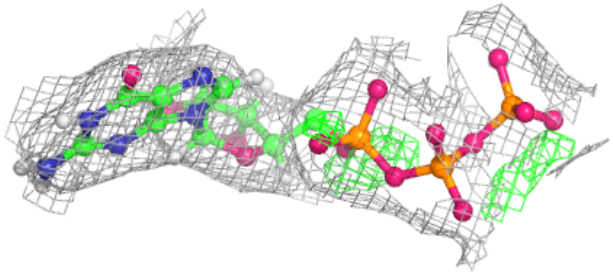


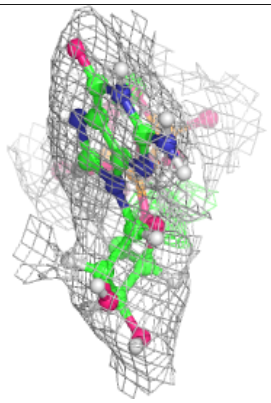


Electron density around GTP D 504:

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

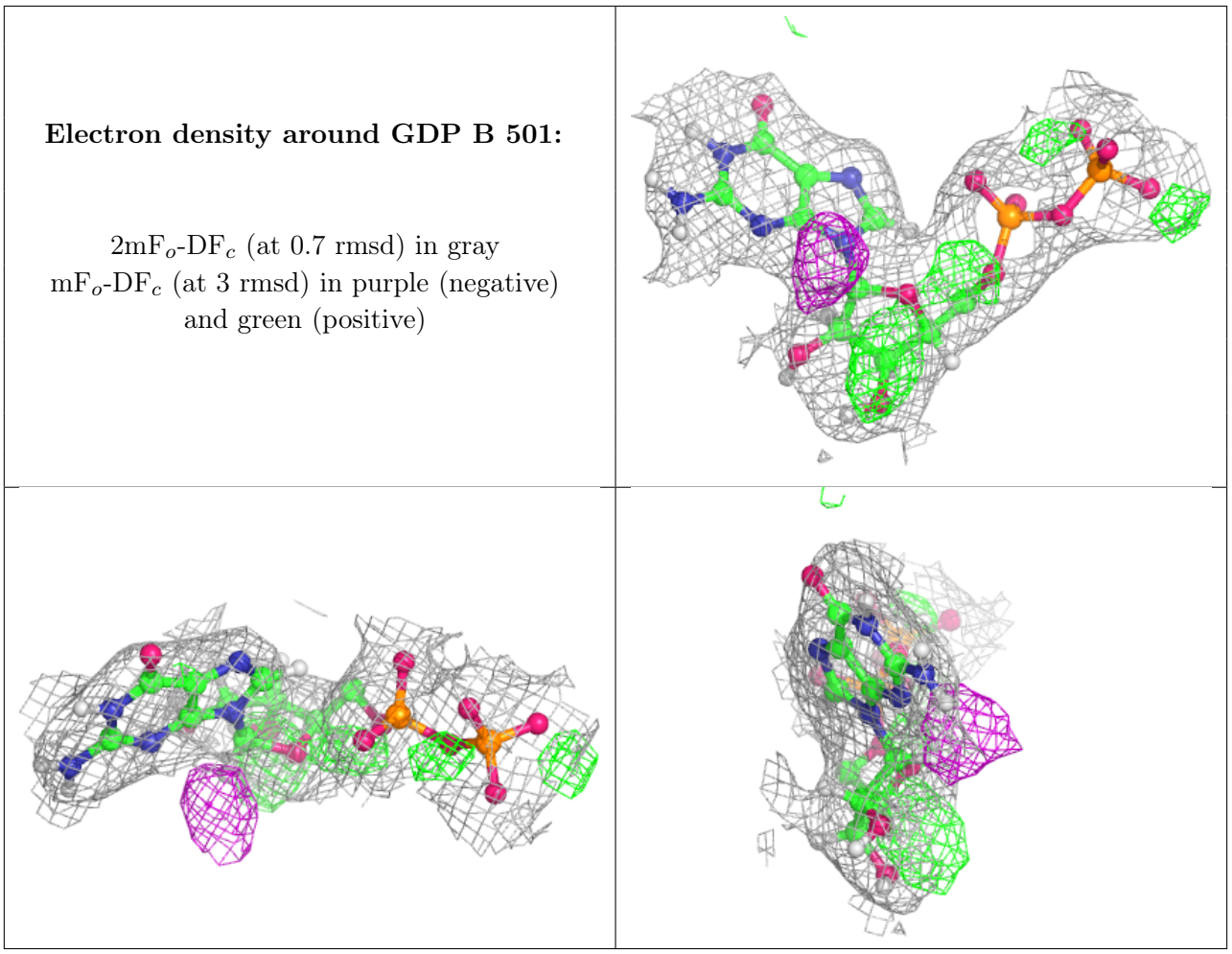






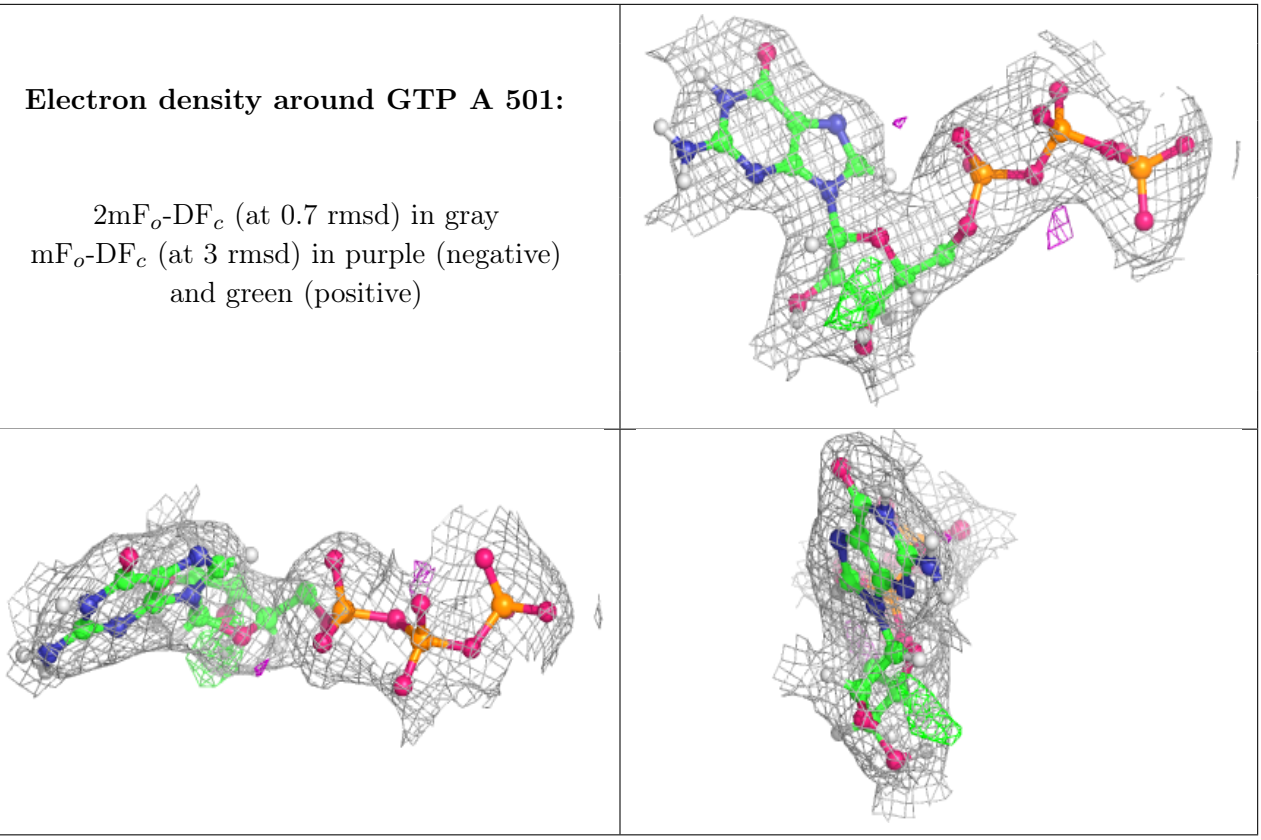
Electron density around GDP B 501:

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



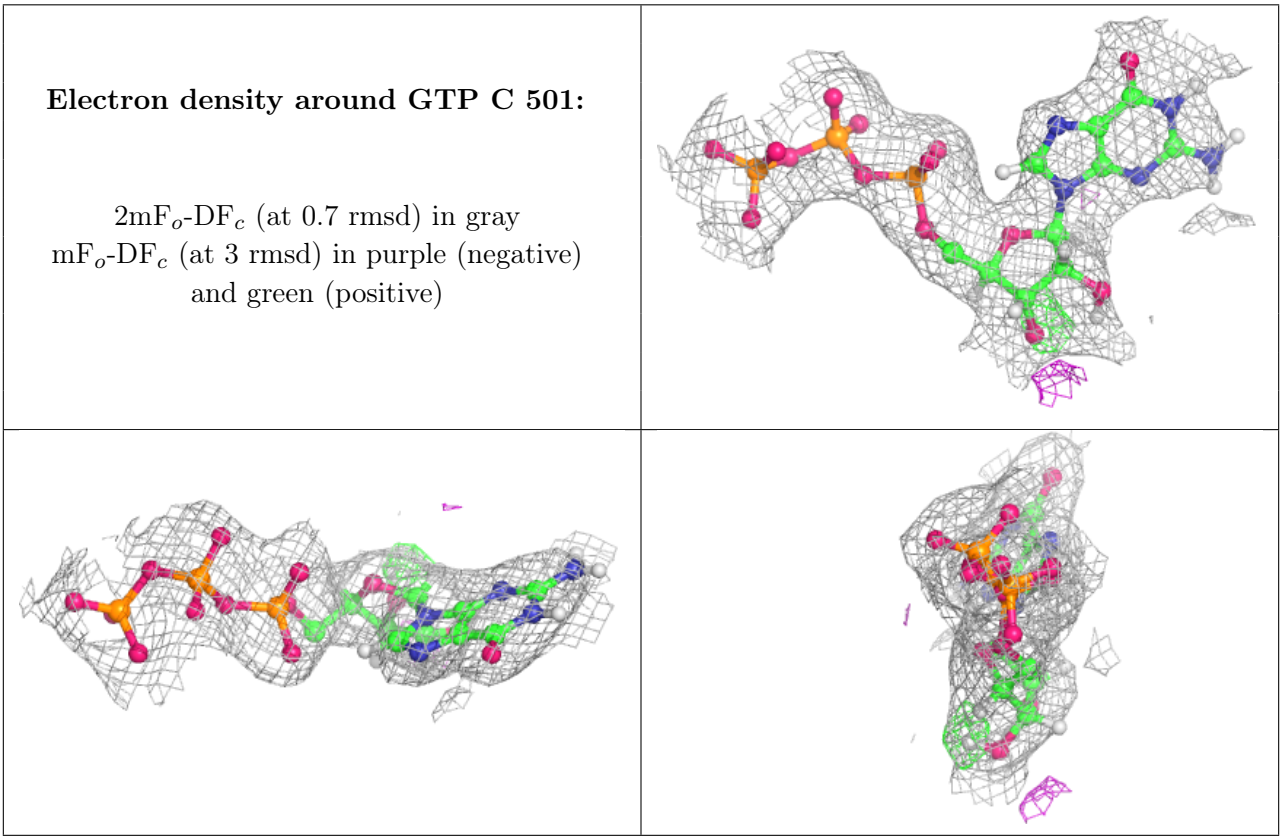
Electron density around GTP A 501:

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



Electron density around GTP C 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.