Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 02:19 pm GMT

PDB ID	:	5M7E
Title	:	Tubulin-BKM120 complex
Authors	:	Bohnacker, T.; Prota, A.E.; Steinmetz, M.O.; Wymann, M.P.
Deposited on	:	2016-10-27
Resolution	:	2.05 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 (i) 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 (i)) were used in the production of this report:

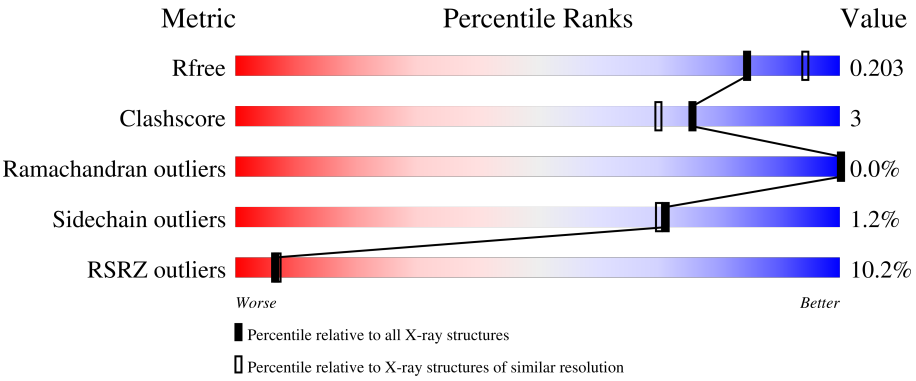
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.05 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.



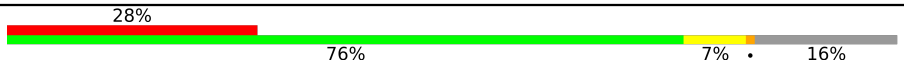
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	5% 89% 7% ·
1	C	451	2% 89% 8% ·
2	B	445	5% 88% 7% 5%
2	D	445	11% 86% 9% ·
3	E	143	10% 78% 8% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18092 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	436	Total	C	N	O	S	0	1	0
			3412	2160	580	649	23			
1	C	440	Total	C	N	O	S	0	4	0
			3449	2183	584	657	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	1	0
			3339	2099	571	643	26			
2	D	427	Total	C	N	O	S	0	0	0
			3349	2101	572	650	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	1	0
			1021	630	185	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	cloning artifact	UNP P63043
E	4	ALA	SER	cloning artifact	UNP P63043

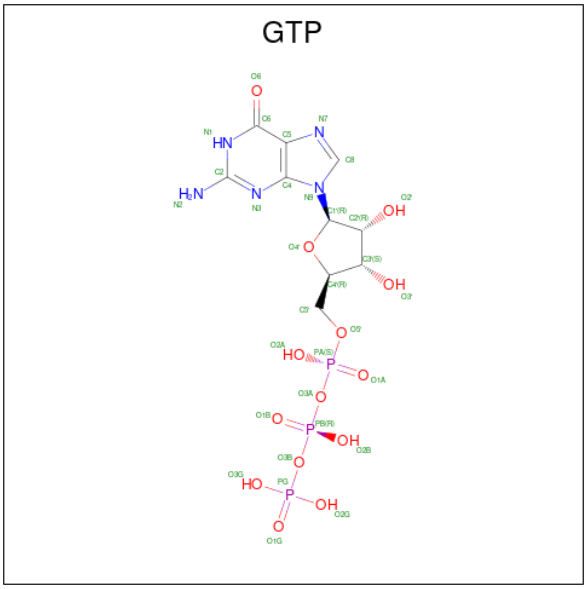
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	322	Total	C	N	O	S	0	0	0
			2623	1693	440	476	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		

Continued on next page...

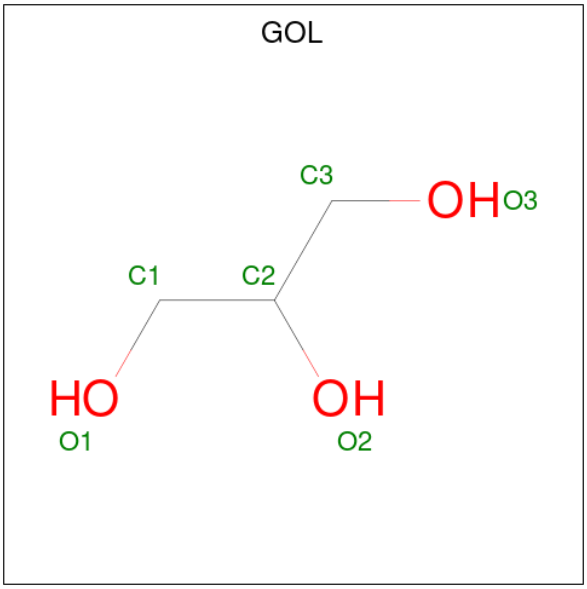
Continued from previous page...

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).

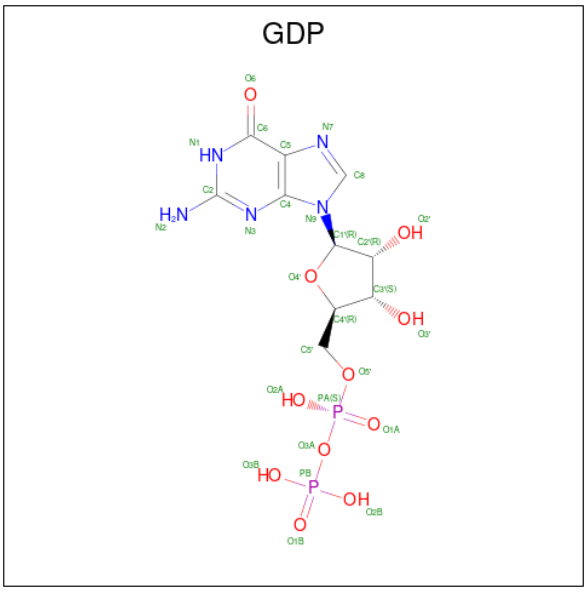
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



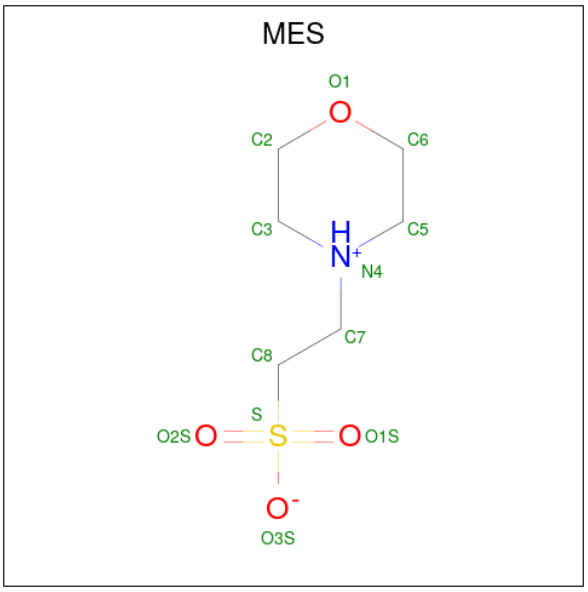
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0

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



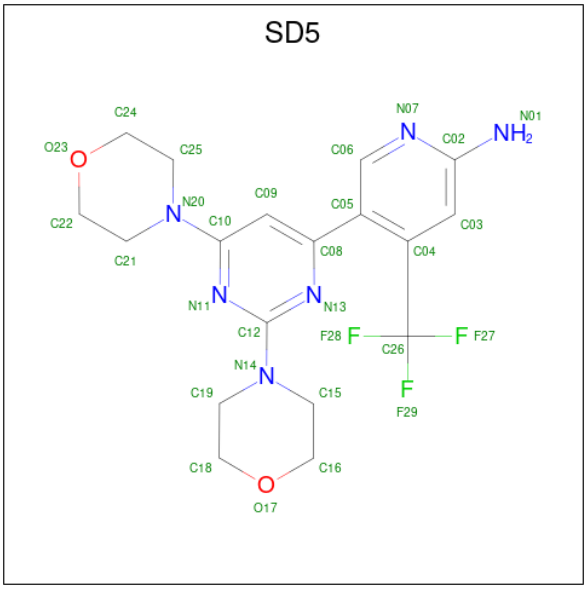
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



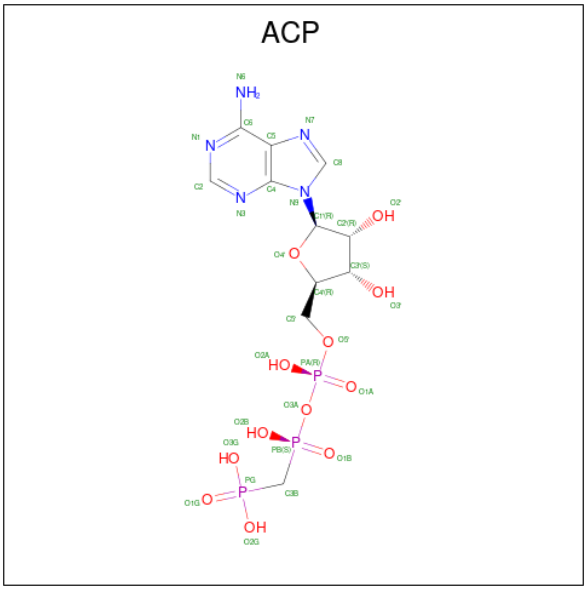
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 5-[2,6-di(morpholin-4-yl)pyrimidin-4-yl]-4-(trifluoromethyl)pyridin-2-amine (three-letter code: SD5) (formula: $C_{18}H_{21}F_3N_6O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	F	N	O	0	0
			29	18	3	6	2		

- 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	N	O	P	0	0
			31	11	5	12	3		

- Molecule 13 is water.

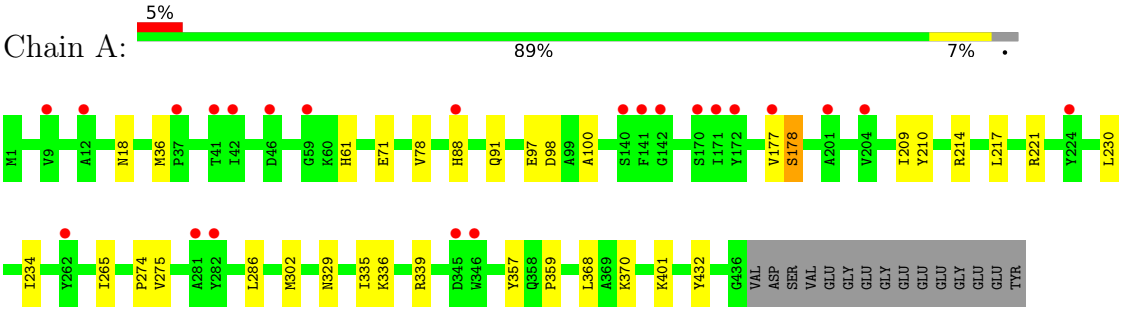
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	137	Total O 137 137	0	0
13	B	130	Total O 130 130	0	0
13	C	232	Total O 232 232	0	0
13	D	100	Total O 100 100	0	0
13	E	25	Total O 25 25	0	0
13	F	57	Total O 57 57	0	0

3 Residue-property plots (i)

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

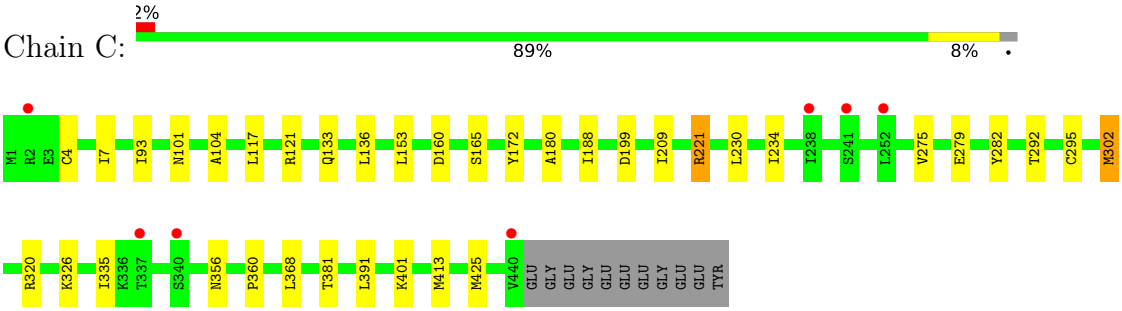
• Molecule 1: Tubulin alpha-1B chain

Chain A:



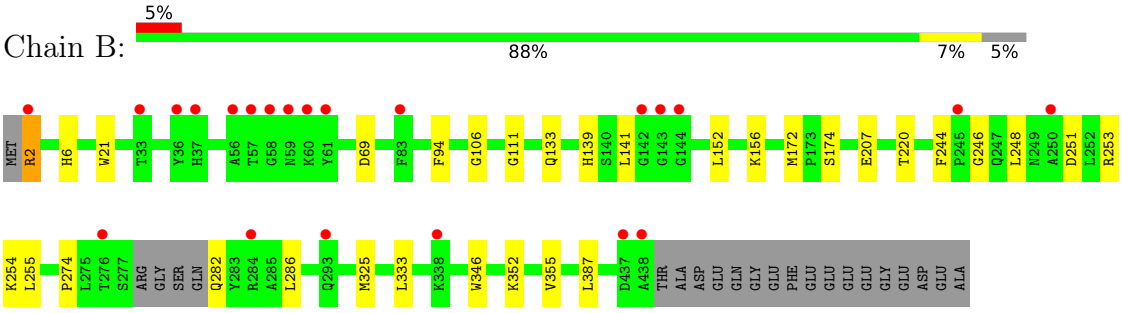
• Molecule 1: Tubulin alpha-1B chain

Chain C:



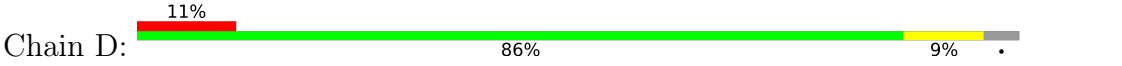
• Molecule 2: Tubulin beta-2B chain

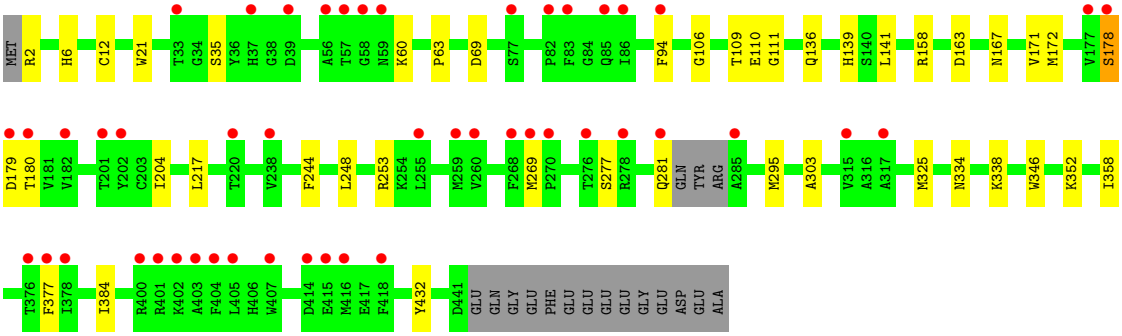
Chain B:



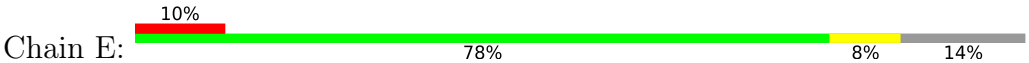
• Molecule 2: Tubulin beta-2B chain

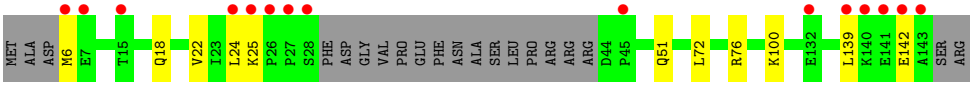
Chain D:



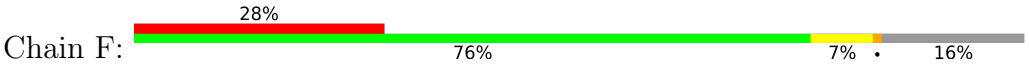


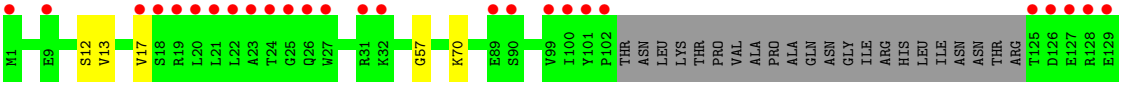
• Molecule 3: Stathmin-4

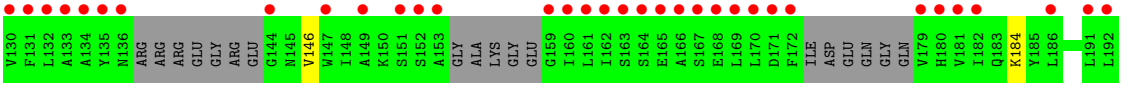


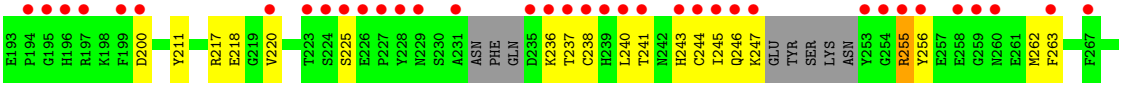


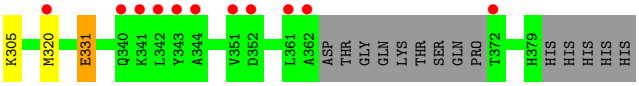
• Molecule 4: Tubulin-Tyrosine Ligase











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.59Å 157.99Å 179.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.93 – 2.05 49.38 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.93-2.05) 99.8 (49.38-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.173 , 0.203 0.173 , 0.203	Depositor DCC
R_{free} test set	9356 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18092	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: MES, SD5, GDP, MG, GTP, ACP, GOL, 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	0.39	0/3493	0.53	0/4741
1	C	0.48	1/3539 (0.0%)	0.58	0/4805
2	B	0.41	0/3416	0.54	0/4626
2	D	0.35	0/3422	0.52	0/4635
3	E	0.39	0/1033	0.45	0/1371
4	F	0.34	0/2680	0.48	0/3619
All	All	0.40	1/17583 (0.0%)	0.53	0/23797

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
2	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-6.45	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	178	SER	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	3412	0	3327	22	0
1	C	3449	0	3368	23	0
2	B	3339	0	3221	22	0
2	D	3349	0	3223	24	0
3	E	1021	0	1036	7	0
4	F	2623	0	2605	16	0
5	A	32	0	12	0	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
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
8	F	12	0	16	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	12	2	0
11	B	29	0	21	1	0
12	F	31	0	14	5	0
13	A	137	0	0	0	0
13	B	130	0	0	1	1
13	C	232	0	0	4	1
13	D	100	0	0	2	0
13	E	25	0	0	0	0
13	F	57	0	0	1	0
All	All	18092	0	16899	105	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 3.

All (105) 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:146:VAL:O	4:F:184:LYS:NZ	2.15	0.80
1:A:221:ARG:HD3	2:B:325:MET:HG3	1.66	0.76
1:C:279:GLU:O	13:C:601:HOH:O	2.09	0.69
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.38	0.64
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.63
12:F:402:ACP:O2G	12:F:402:ACP:O2B	2.17	0.62
2:B:253[A]:ARG:NH1	10:B:504:MES:O1S	2.31	0.62
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.35	0.60
12:F:402:ACP:O2B	12:F:402:ACP:O1A	2.19	0.60
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.84	0.59
4:F:237:THR:O	4:F:246:GLN:NE2	2.33	0.59
2:D:432:TYR:OH	13:D:601:HOH:O	2.16	0.58
2:B:2:ARG:HD2	2:B:133:GLN:HG2	1.86	0.57
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.85	0.57
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.39	0.57
4:F:243:HIS:HE1	4:F:247:LYS:HD2	1.70	0.55
3:E:139:LEU:O	3:E:142:GLU:HG2	2.06	0.55
2:B:244:PHE:O	2:B:246:GLY:N	2.39	0.55
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.42	0.54
2:B:325:MET:SD	2:B:355:VAL:HG21	2.48	0.54
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.90	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.53
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.90	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.21	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.10	0.52
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.45	0.52
1:C:133:GLN:NE2	13:C:606:HOH:O	2.41	0.52
4:F:331:GLU:OE2	12:F:402:ACP:O1G	2.29	0.51
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.75	0.51
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.91	0.51
4:F:241:THR:OG1	12:F:402:ACP:O3'	2.27	0.51
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.94	0.50
2:B:282:GLN:N	13:B:608:HOH:O	2.44	0.49
2:B:69:ASP:O	2:B:94:PHE:HA	2.12	0.49
2:D:178:SER:OG	2:D:179:ASP:O	2.29	0.49
2:B:333:LEU:HD21	4:F:57:GLY:HA3	1.95	0.48
2:D:35:SER:OG	2:D:60:LYS:HE2	2.14	0.48
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.48
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.95	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.54	0.47
2:B:253[A]:ARG:NH2	10:B:504:MES:O1S	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:HA	2:B:2:ARG:NH2	2.29	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.47
4:F:243:HIS:CE1	4:F:247:LYS:HD2	2.48	0.47
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.47	0.47
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.14	0.47
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.96	0.46
1:A:329:ASN:OD1	3:E:22:VAL:HG21	2.15	0.46
1:C:101:ASN:ND2	1:C:180:ALA:HB2	2.31	0.46
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.98	0.46
2:B:251:ASP:O	2:B:255:LEU:HG	2.15	0.46
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.98	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.15	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.46
1:C:221:ARG:HG3	2:D:325:MET:HB3	1.98	0.46
2:B:352:LYS:HD3	11:B:505:SD5:H25	1.99	0.45
1:A:88:HIS:N	1:A:91:GLN:OE1	2.35	0.45
2:D:281:GLN:NE2	13:D:602:HOH:O	2.29	0.45
4:F:70:LYS:NZ	13:F:501:HOH:O	2.38	0.45
4:F:13:VAL:O	4:F:17:VAL:HG23	2.16	0.45
2:D:141:LEU:HD12	2:D:172:MET:SD	2.56	0.45
2:D:69:ASP:O	2:D:94:PHE:HA	2.17	0.45
4:F:255:ARG:HG2	4:F:256:TYR:CE2	2.52	0.45
2:D:163:ASP:O	2:D:253:ARG:NH2	2.48	0.45
2:B:152:LEU:HD11	2:B:156:LYS:HZ1	1.82	0.44
4:F:331:GLU:OE2	12:F:402:ACP:O2B	2.36	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.53	0.44
1:A:221:ARG:CD	2:B:325:MET:HG3	2.42	0.44
1:A:359:PRO:HB2	1:A:370:LYS:HE2	1.99	0.44
2:D:179:ASP:HB3	2:D:180:THR:HA	2.00	0.43
3:E:24:LEU:O	3:E:25:LYS:HG3	2.18	0.43
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.00	0.43
4:F:236:LYS:HB3	4:F:240:LEU:HD12	2.00	0.43
1:A:177:VAL:O	1:A:177:VAL:HG23	2.19	0.43
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.01	0.43
2:D:217:LEU:HA	2:D:277:SER:HB3	2.00	0.43
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.42
1:A:234:ILE:HD13	1:A:302:MET:SD	2.59	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.20	0.42
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.01	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HA	1:C:356:ASN:O	2.20	0.42
2:D:334:ASN:HD21	2:D:338:LYS:NZ	2.18	0.42
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.54	0.42
1:C:104:ALA:HB2	1:C:413:MET:SD	2.60	0.42
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.02	0.42
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.50	0.42
3:E:100:LYS:HB3	3:E:100:LYS:HE2	1.84	0.41
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.41
1:C:320:ARG:HG3	1:C:360:PRO:HG3	2.02	0.41
3:E:72:LEU:O	3:E:76:ARG:HG2	2.20	0.41
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.55	0.41
2:D:109:THR:OG1	2:D:110:GLU:N	2.52	0.41
1:C:234:ILE:HD13	1:C:302:MET:SD	2.61	0.41
1:C:160:ASP:OD2	13:C:602:HOH:O	2.21	0.41
2:B:174:SER:CB	2:B:207:GLU:HB2	2.51	0.41
1:C:282:TYR:HB3	13:C:601:HOH:O	2.21	0.41
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.56	0.41
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.56	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.41
4:F:244:CYS:SG	4:F:245:ILE:N	2.94	0.40
1:C:326:LYS:HB3	1:C:326:LYS:HE3	1.88	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)
13:B:642:HOH:O	13:C:601:HOH:O[4_555]	1.97	0.23

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	435/451 (96%)	429 (99%)	5 (1%)	1 (0%)	47 39
1	C	442/451 (98%)	433 (98%)	9 (2%)	0	100 100
2	B	420/445 (94%)	415 (99%)	5 (1%)	0	100 100
2	D	423/445 (95%)	418 (99%)	5 (1%)	0	100 100
3	E	120/143 (84%)	120 (100%)	0	0	100 100
4	F	306/384 (80%)	302 (99%)	4 (1%)	0	100 100
All	All	2146/2319 (92%)	2117 (99%)	28 (1%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER

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	368/379 (97%)	367 (100%)	1 (0%)	92 93
1	C	375/379 (99%)	372 (99%)	3 (1%)	81 82
2	B	367/383 (96%)	363 (99%)	4 (1%)	73 73
2	D	368/383 (96%)	364 (99%)	4 (1%)	73 73
3	E	111/127 (87%)	109 (98%)	2 (2%)	59 55
4	F	289/342 (84%)	280 (97%)	9 (3%)	40 33
All	All	1878/1993 (94%)	1855 (99%)	23 (1%)	71 70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	SER
2	B	2	ARG
2	B	139	HIS
2	B	220	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	248	LEU
1	C	221	ARG
1	C	302	MET
1	C	381	THR
2	D	2	ARG
2	D	139	HIS
2	D	158	ARG
2	D	384	ILE
3	E	6	MET
3	E	51	GLN
4	F	12	SER
4	F	211	TYR
4	F	225	SER
4	F	238	CYS
4	F	255	ARG
4	F	262	MET
4	F	305	LYS
4	F	320	MET
4	F	331	GLU

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

Mol	Chain	Res	Type
2	D	334	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 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.14	1 (3%)	32,54,54	1.24	4 (12%)
9	GDP	D	501	6	24,30,30	0.92	1 (4%)	30,47,47	1.23	4 (13%)
5	GTP	C	501	6	26,34,34	1.18	1 (3%)	32,54,54	1.26	3 (9%)
10	MES	B	504	-	12,12,12	2.05	1 (8%)	14,16,16	2.07	3 (21%)
12	ACP	F	402	6	27,33,33	1.72	6 (22%)	32,52,52	1.53	5 (15%)
8	GOL	F	404	-	5,5,5	0.36	0	5,5,5	0.19	0
8	GOL	F	403	-	5,5,5	0.35	0	5,5,5	0.32	0
11	SD5	B	505	-	32,32,32	1.40	4 (12%)	42,46,46	1.59	9 (21%)
9	GDP	B	501	6	24,30,30	1.05	2 (8%)	30,47,47	1.24	3 (10%)
8	GOL	A	504	-	5,5,5	0.31	0	5,5,5	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
12	ACP	F	402	6	-	8/15/38/38	0/3/3/3
8	GOL	F	404	-	-	2/4/4/4	-
8	GOL	F	403	-	-	2/4/4/4	-
11	SD5	B	505	-	-	0/18/34/34	0/4/4/4
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
8	GOL	A	504	-	-	4/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-6.80	1.67	1.77
12	F	402	ACP	PG-O1G	5.58	1.61	1.50
5	C	501	GTP	C5-C6	-4.26	1.38	1.47
11	B	505	SD5	C26-C04	-4.09	1.41	1.50
5	A	501	GTP	C5-C6	-3.59	1.40	1.47
11	B	505	SD5	F29-C26	-3.48	1.20	1.32
11	B	505	SD5	C05-C08	-3.45	1.39	1.48
12	F	402	ACP	PG-O2G	-2.89	1.48	1.54
12	F	402	ACP	PG-O3G	2.87	1.61	1.54
12	F	402	ACP	C5-C4	2.48	1.47	1.40
9	B	501	GDP	O4'-C1'	2.47	1.44	1.41
9	B	501	GDP	C6-N1	-2.45	1.34	1.37
12	F	402	ACP	PB-O3A	2.27	1.60	1.58
9	D	501	GDP	C6-N1	-2.25	1.34	1.37
11	B	505	SD5	C06-N07	2.07	1.38	1.34
12	F	402	ACP	PB-O2B	2.04	1.61	1.56

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	MES	C5-N4-C3	5.40	120.98	108.83
12	F	402	ACP	PB-O3A-PA	-4.97	116.80	132.56
10	B	504	MES	O2S-S-C8	4.18	111.95	106.92
11	B	505	SD5	N13-C12-N11	-3.78	120.07	126.31
11	B	505	SD5	C19-N14-C15	3.54	119.34	111.52
11	B	505	SD5	C12-N11-C10	3.46	121.36	115.03
5	C	501	GTP	C8-N7-C5	3.13	108.95	102.99
12	F	402	ACP	N3-C2-N1	-3.05	123.91	128.68
9	B	501	GDP	O6-C6-C5	-3.03	118.46	124.37
9	B	501	GDP	C5-C6-N1	2.98	119.22	113.95
11	B	505	SD5	F29-C26-C04	-2.89	107.67	112.70
12	F	402	ACP	C3'-C2'-C1'	2.89	105.32	100.98
10	B	504	MES	C7-N4-C3	2.80	118.41	111.23
11	B	505	SD5	C06-C05-C08	-2.79	116.43	121.16
5	A	501	GTP	C8-N7-C5	2.74	108.22	102.99
11	B	505	SD5	C09-C08-N13	-2.73	119.10	122.35
9	D	501	GDP	PA-O3A-PB	-2.64	123.75	132.83
5	A	501	GTP	C5-C6-N1	2.62	118.58	113.95
12	F	402	ACP	C4-C5-N7	-2.53	106.76	109.40
5	C	501	GTP	C5-C6-N1	2.53	118.42	113.95
11	B	505	SD5	N13-C12-N14	2.50	120.19	117.11
12	F	402	ACP	O3G-PG-C3B	2.50	112.45	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	501	GDP	C5-C6-N1	2.49	118.35	113.95
11	B	505	SD5	C25-N20-C21	2.44	116.91	111.52
5	A	501	GTP	PB-O3B-PG	-2.42	124.53	132.83
9	D	501	GDP	C8-N7-C5	2.26	107.29	102.99
9	B	501	GDP	PA-O3A-PB	-2.25	125.11	132.83
11	B	505	SD5	N11-C12-N14	2.11	119.71	117.11
9	D	501	GDP	O6-C6-C5	-2.09	120.30	124.37
5	C	501	GTP	N1-C2-N3	-2.06	119.48	123.32
5	A	501	GTP	PA-O3A-PB	-2.02	125.90	132.83

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O1A
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O3A
12	F	402	ACP	O4'-C4'-C5'-O5'
8	F	404	GOL	O1-C1-C2-C3
8	A	504	GOL	O1-C1-C2-O2
8	F	404	GOL	O1-C1-C2-O2
8	A	504	GOL	C1-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O1G
8	F	403	GOL	O1-C1-C2-O2
9	D	501	GDP	C5'-O5'-PA-O3A
8	F	403	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O2A
12	F	402	ACP	PG-C3B-PB-O2B
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
12	F	402	ACP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	A	504	GOL	O2-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C3

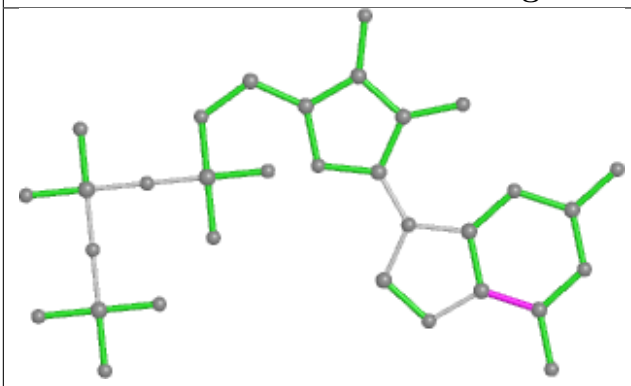
There are no ring outliers.

4 monomers are involved in 9 short contacts:

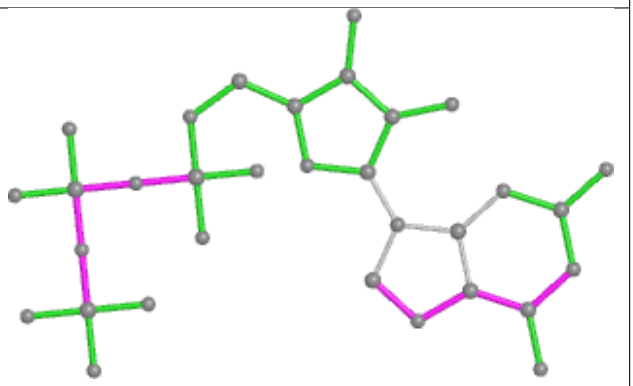
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
10	B	504	MES	2	0
12	F	402	ACP	5	0
11	B	505	SD5	1	0

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

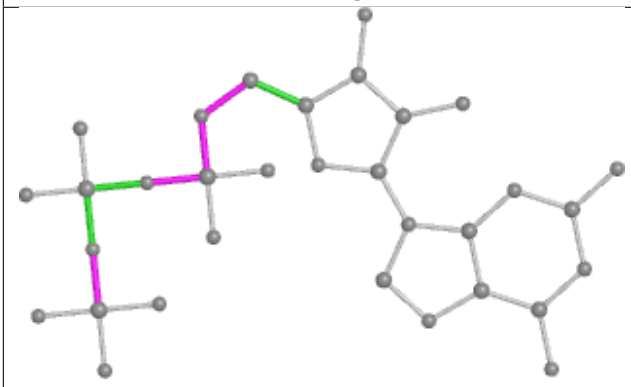
Ligand GTP A 501



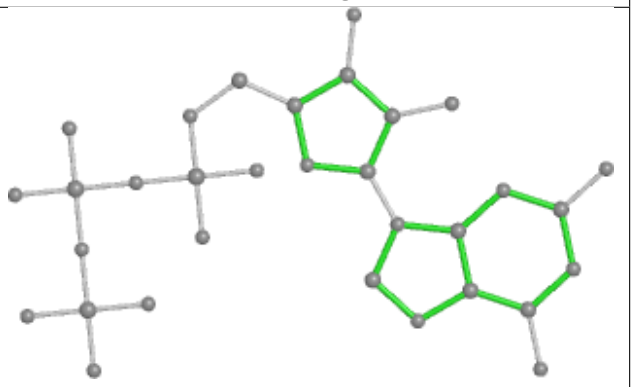
Bond lengths



Bond angles

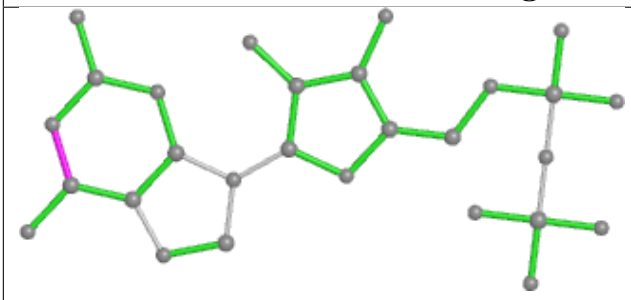


Torsions

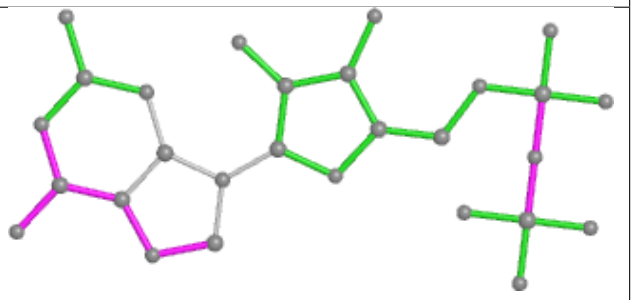


Rings

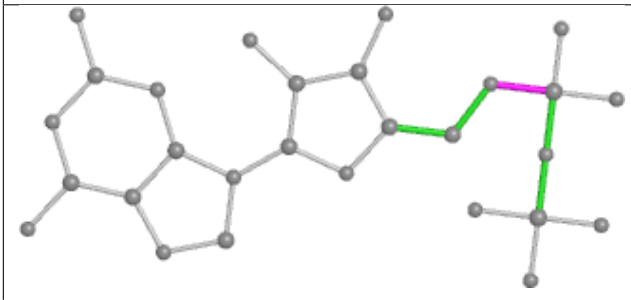
Ligand GDP D 501



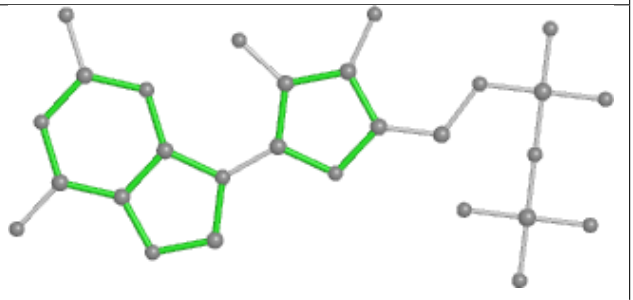
Bond lengths



Bond angles

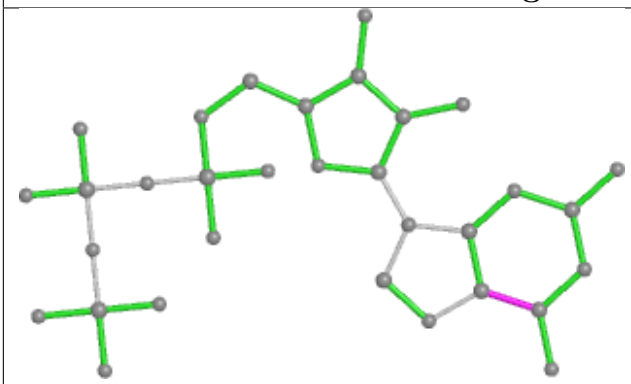


Torsions

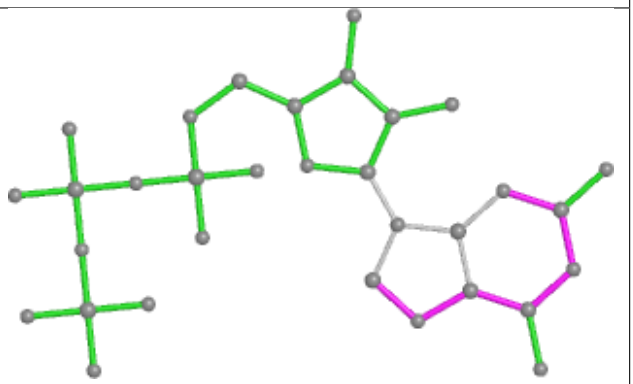


Rings

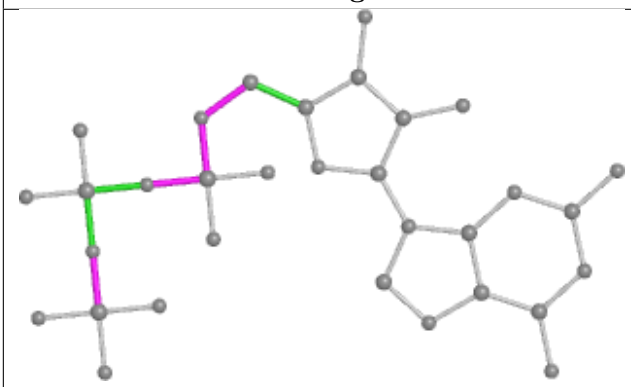
Ligand GTP C 501



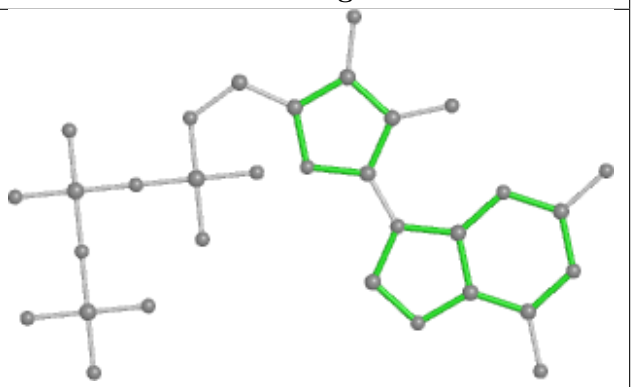
Bond lengths



Bond angles

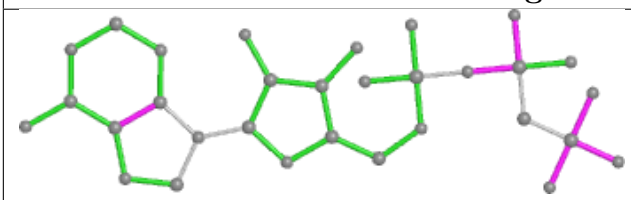


Torsions

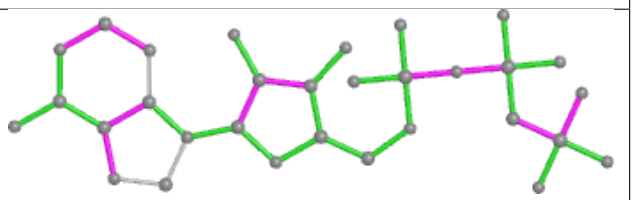


Rings

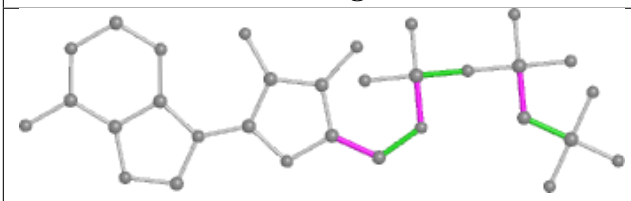
Ligand ACP F 402



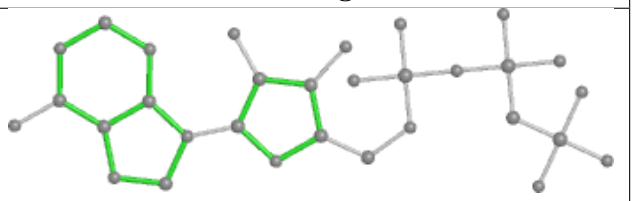
Bond lengths



Bond angles

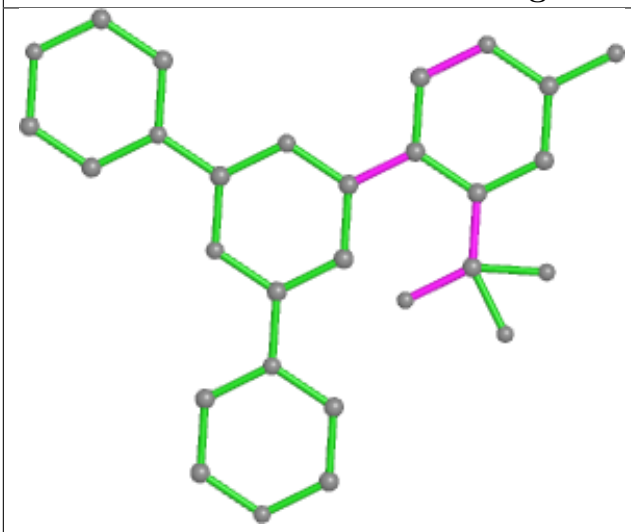


Torsions

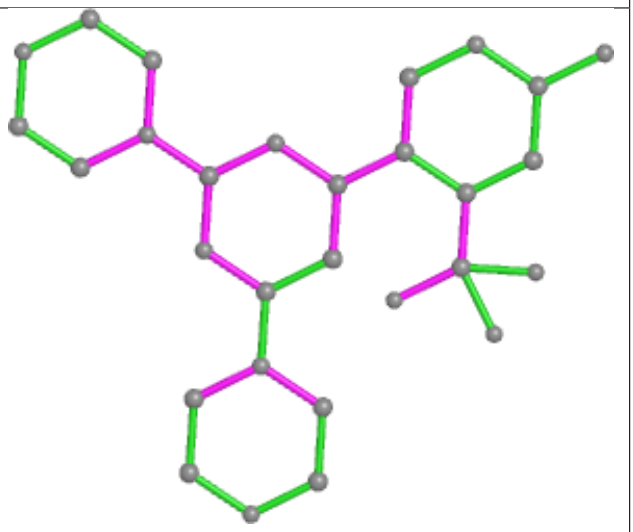


Rings

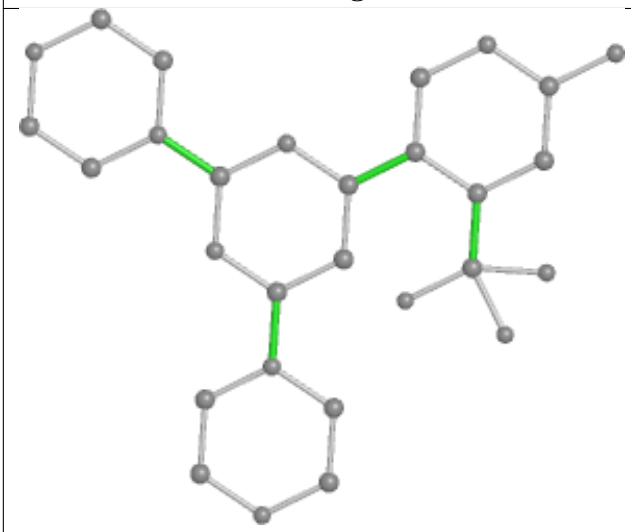
Ligand SD5 B 505



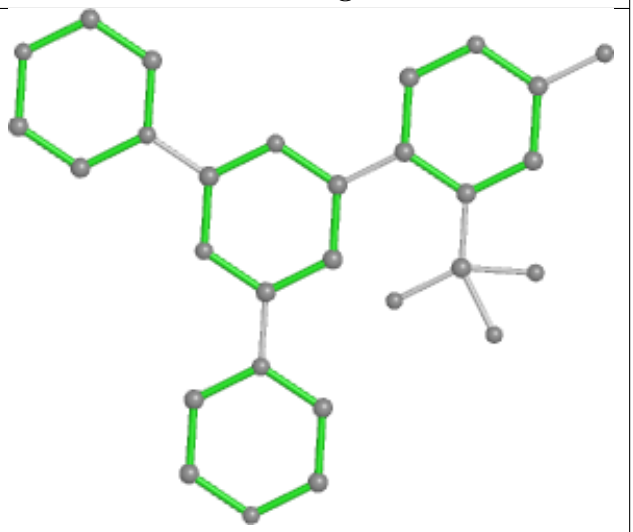
Bond lengths



Bond angles

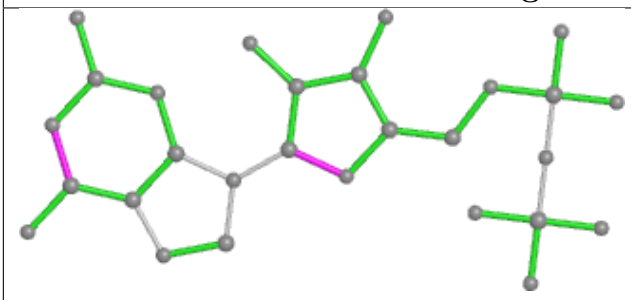


Torsions

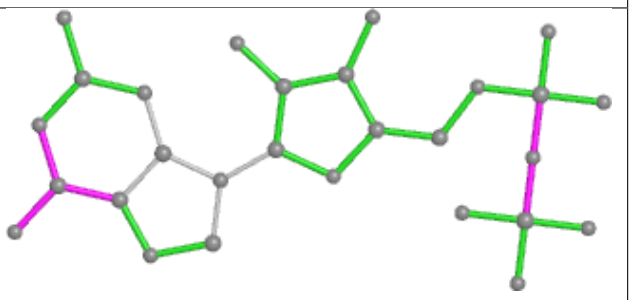


Rings

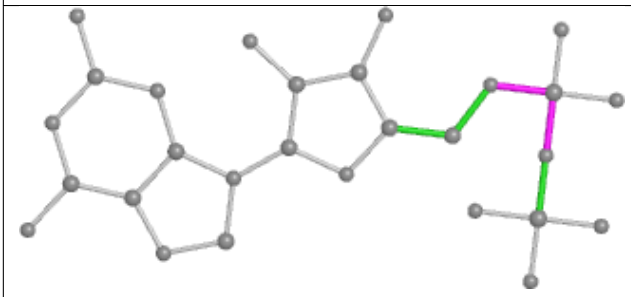
Ligand GDP B 501



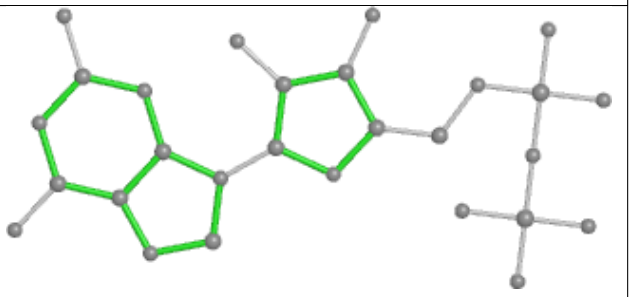
Bond lengths



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	436/451 (96%)	0.43	23 (5%) 26 28	32, 53, 85, 97	0
1	C	440/451 (97%)	0.17	7 (1%) 72 74	28, 41, 67, 90	0
2	B	423/445 (95%)	0.34	22 (5%) 27 29	30, 50, 85, 115	2 (0%)
2	D	427/445 (95%)	0.64	48 (11%) 5 5	33, 58, 89, 110	4 (0%)
3	E	123/143 (86%)	0.57	15 (12%) 4 3	37, 63, 103, 116	0
4	F	322/384 (83%)	1.35	107 (33%) 0 0	39, 72, 115, 138	0
All	All	2171/2319 (93%)	0.54	222 (10%) 6 7	28, 54, 93, 138	6 (0%)

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	9.4
4	F	182	ILE	7.7
4	F	161	LEU	7.0
4	F	372	THR	6.8
4	F	179	VAL	6.6
4	F	231	ALA	6.2
2	B	59	ASN	6.0
1	A	282	TYR	6.0
2	D	57	THR	5.9
4	F	20	LEU	5.8
4	F	130	VAL	5.8
4	F	172	PHE	5.6
2	B	58	GLY	5.5
4	F	100	ILE	5.5
4	F	133	ALA	5.5
4	F	244	CYS	5.5
4	F	240	LEU	5.4
4	F	169	LEU	5.4
4	F	362	ALA	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	5.3
4	F	253	TYR	5.3
2	B	438	ALA	5.3
3	E	6	MET	5.3
2	D	407	TRP	5.1
4	F	99	VAL	5.1
4	F	256	TYR	5.1
2	D	82	PRO	5.1
3	E	27	PRO	5.0
2	B	57	THR	5.0
4	F	22	LEU	5.0
2	B	245	PRO	5.0
4	F	170	LEU	4.7
4	F	226	GLU	4.6
4	F	101	TYR	4.6
3	E	139	LEU	4.6
4	F	134	ALA	4.5
2	D	180	THR	4.5
4	F	227	PRO	4.5
1	A	46	ASP	4.5
1	C	340	SER	4.4
4	F	162	ILE	4.4
2	D	400	ARG	4.4
4	F	135	TYR	4.2
4	F	259	GLY	4.2
4	F	237	THR	4.1
2	D	179	ASP	4.0
1	A	281	ALA	3.9
4	F	165	GLU	3.9
4	F	239	HIS	3.9
1	C	440	VAL	3.9
2	D	37	HIS	3.9
3	E	25	LYS	3.8
4	F	1	MET	3.8
3	E	141	GLU	3.8
4	F	194	PRO	3.8
4	F	129	GLU	3.8
1	A	171	ILE	3.8
4	F	361	LEU	3.7
4	F	245	ILE	3.7
2	D	58	GLY	3.7
4	F	241	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	41	THR	3.7
2	B	276	THR	3.7
3	E	142	GLU	3.6
2	D	77	SER	3.6
4	F	166	ALA	3.6
1	A	42	ILE	3.6
2	D	401	ARG	3.6
2	D	404	PHE	3.6
3	E	26	PRO	3.6
2	B	284	ARG	3.6
2	D	317	ALA	3.5
4	F	149	ALA	3.5
4	F	258	GLU	3.5
4	F	199	PHE	3.5
4	F	236	LYS	3.5
4	F	152	SER	3.5
4	F	243	HIS	3.5
4	F	167	SER	3.4
4	F	263	PHE	3.4
2	D	59	ASN	3.4
4	F	225	SER	3.4
2	B	437	ASP	3.3
2	B	37	HIS	3.3
4	F	197	ARG	3.3
4	F	255	ARG	3.3
4	F	247	LYS	3.3
3	E	143	ALA	3.3
4	F	192	LEU	3.3
2	D	268	PHE	3.3
4	F	246	GLN	3.3
2	D	405	LEU	3.3
2	B	33	THR	3.2
4	F	238	CYS	3.2
4	F	159	GLY	3.2
4	F	181	VAL	3.2
2	B	56	ALA	3.2
4	F	229	ASN	3.2
2	D	238	VAL	3.1
4	F	144	GLY	3.1
2	D	39	ASP	3.1
4	F	27	TRP	3.1
4	F	25	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	90	SER	3.1
4	F	163	SER	3.1
4	F	17	VAL	3.1
2	D	220	THR	3.0
1	A	262	TYR	3.0
4	F	160	ILE	3.0
2	D	83	PHE	3.0
4	F	200	ASP	3.0
2	D	86	ILE	2.9
1	A	88	HIS	2.9
4	F	228	TYR	2.9
4	F	344	ALA	2.9
4	F	21	LEU	2.9
4	F	31	ARG	2.9
2	D	202	TYR	2.9
4	F	235	ASP	2.9
3	E	24	LEU	2.9
2	D	378	ILE	2.9
4	F	195	GLY	2.9
4	F	24	THR	2.9
2	D	315	VAL	2.8
4	F	126	ASP	2.8
3	E	28	SER	2.8
2	D	402	LYS	2.8
4	F	128	ARG	2.8
4	F	23	ALA	2.8
4	F	102	PRO	2.8
2	D	415	GLU	2.8
2	B	250	ALA	2.8
1	A	346	TRP	2.8
2	D	269	MET	2.8
4	F	89	GLU	2.8
4	F	224	SER	2.8
2	D	260	VAL	2.7
4	F	341	LYS	2.7
4	F	32	LYS	2.7
1	C	252	LEU	2.7
1	C	337	THR	2.7
2	D	376	THR	2.7
4	F	171	ASP	2.7
2	D	94	PHE	2.7
3	E	140	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	351	VAL	2.6
2	B	83	PHE	2.6
2	D	416	MET	2.6
4	F	191	LEU	2.6
2	D	403	ALA	2.6
4	F	342	LEU	2.6
4	F	127	GLU	2.6
4	F	153	ALA	2.6
2	D	56	ALA	2.6
4	F	26	GLN	2.6
4	F	186	LEU	2.6
4	F	352	ASP	2.5
4	F	320	MET	2.5
2	D	182	VAL	2.5
2	D	285	ALA	2.5
2	D	418	PHE	2.5
4	F	180	HIS	2.5
4	F	19	ARG	2.5
2	D	414	ASP	2.5
4	F	254	GLY	2.5
3	E	132	GLU	2.5
1	C	2	ARG	2.5
4	F	196	HIS	2.5
2	D	201	THR	2.4
4	F	220	VAL	2.4
4	F	136	ASN	2.4
4	F	125	THR	2.4
4	F	18	SER	2.4
3	E	45	PRO	2.4
2	D	33	THR	2.4
4	F	168	GLU	2.4
3	E	7	GLU	2.4
1	A	9	VAL	2.4
2	B	36	TYR	2.4
1	C	241	SER	2.4
2	B	60	LYS	2.4
2	D	259	MET	2.4
4	F	147	TRP	2.4
4	F	343	TYR	2.4
4	F	260	ASN	2.3
2	D	177	VAL	2.3
2	D	276	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	223	THR	2.3
2	D	281	GLN	2.3
4	F	164	SER	2.3
1	A	177	VAL	2.3
1	C	238	ILE	2.3
1	A	37	PRO	2.2
2	D	85	GLN	2.2
1	A	201	ALA	2.2
2	D	270	PRO	2.2
1	A	59	GLY	2.2
1	A	345	ASP	2.2
4	F	267	PHE	2.2
1	A	142	GLY	2.2
2	D	278	ARG	2.2
2	B	2	ARG	2.1
2	B	293	GLN	2.1
2	D	255	LEU	2.1
1	A	172	TYR	2.1
1	A	170	SER	2.1
3	E	15	THR	2.1
4	F	9	GLU	2.1
1	A	140	SER	2.1
1	A	141	PHE	2.1
2	D	178	SER	2.1
2	B	61	TYR	2.1
4	F	151	SER	2.1
1	A	12	ALA	2.1
2	D	377	PHE	2.1
1	A	204	VAL	2.0
2	B	142	GLY	2.0
4	F	340	GLN	2.0
2	B	144	GLY	2.0
1	A	224	TYR	2.0
2	B	338	LYS	2.0
2	B	143	GLY	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)

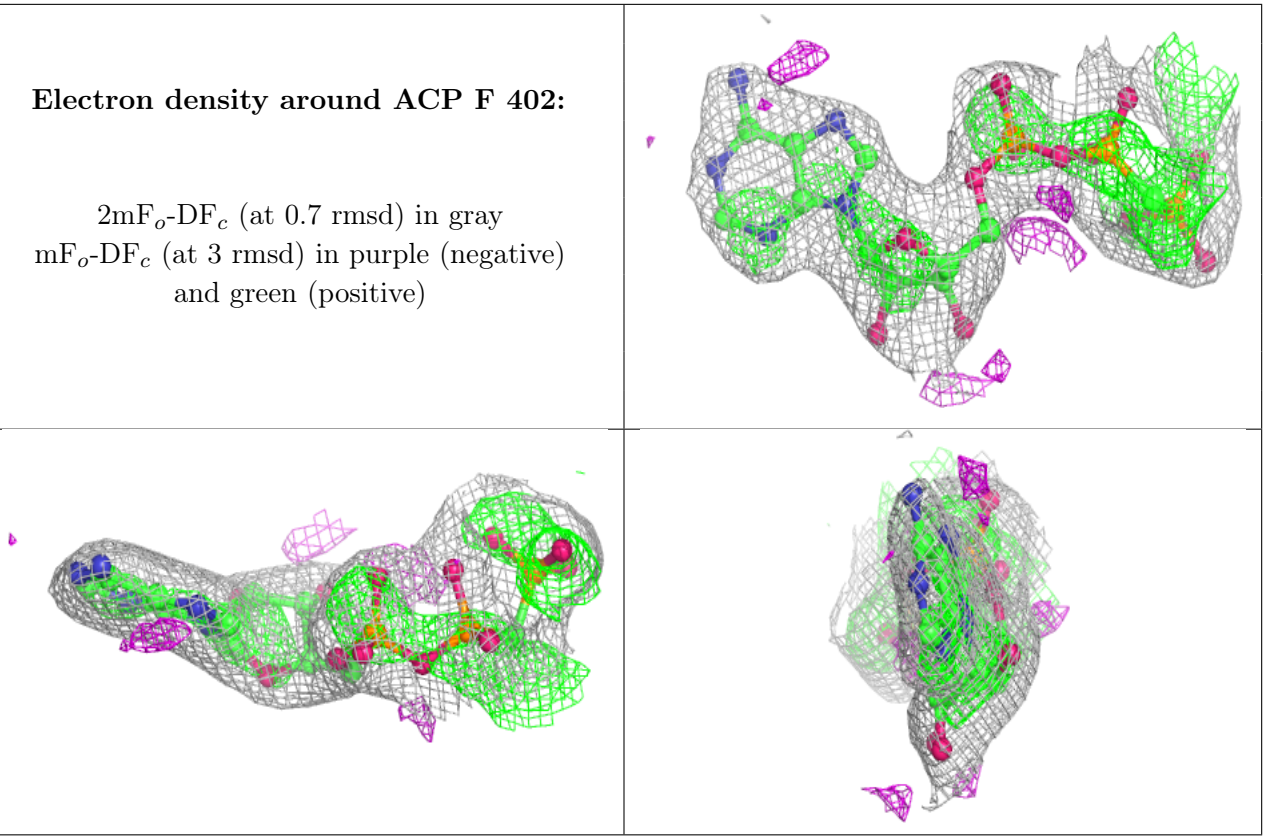
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	MG	F	401	1/1	0.56	0.31	118,118,118,118	0
8	GOL	F	403	6/6	0.80	0.23	105,109,111,113	0
8	GOL	F	404	6/6	0.82	0.29	110,116,117,118	0
12	ACP	F	402	31/31	0.86	0.19	121,133,175,180	0
8	GOL	A	504	6/6	0.87	0.16	68,78,84,87	0
7	CA	B	503	1/1	0.88	0.21	114,114,114,114	0
6	MG	D	502	1/1	0.90	0.07	50,50,50,50	0
11	SD5	B	505	29/29	0.93	0.14	39,54,72,77	0
10	MES	B	504	12/12	0.94	0.12	50,58,77,82	0
7	CA	A	503	1/1	0.95	0.06	73,73,73,73	0
6	MG	A	502	1/1	0.96	0.17	36,36,36,36	0
9	GDP	D	501	28/28	0.97	0.11	40,52,59,61	0
6	MG	B	502	1/1	0.98	0.24	31,31,31,31	0
7	CA	C	503	1/1	0.98	0.03	53,53,53,53	0
5	GTP	A	501	32/32	0.98	0.19	30,34,38,41	0
6	MG	C	502	1/1	0.99	0.18	36,36,36,36	0
9	GDP	B	501	28/28	0.99	0.17	27,34,37,41	0
5	GTP	C	501	32/32	0.99	0.15	24,30,34,35	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.

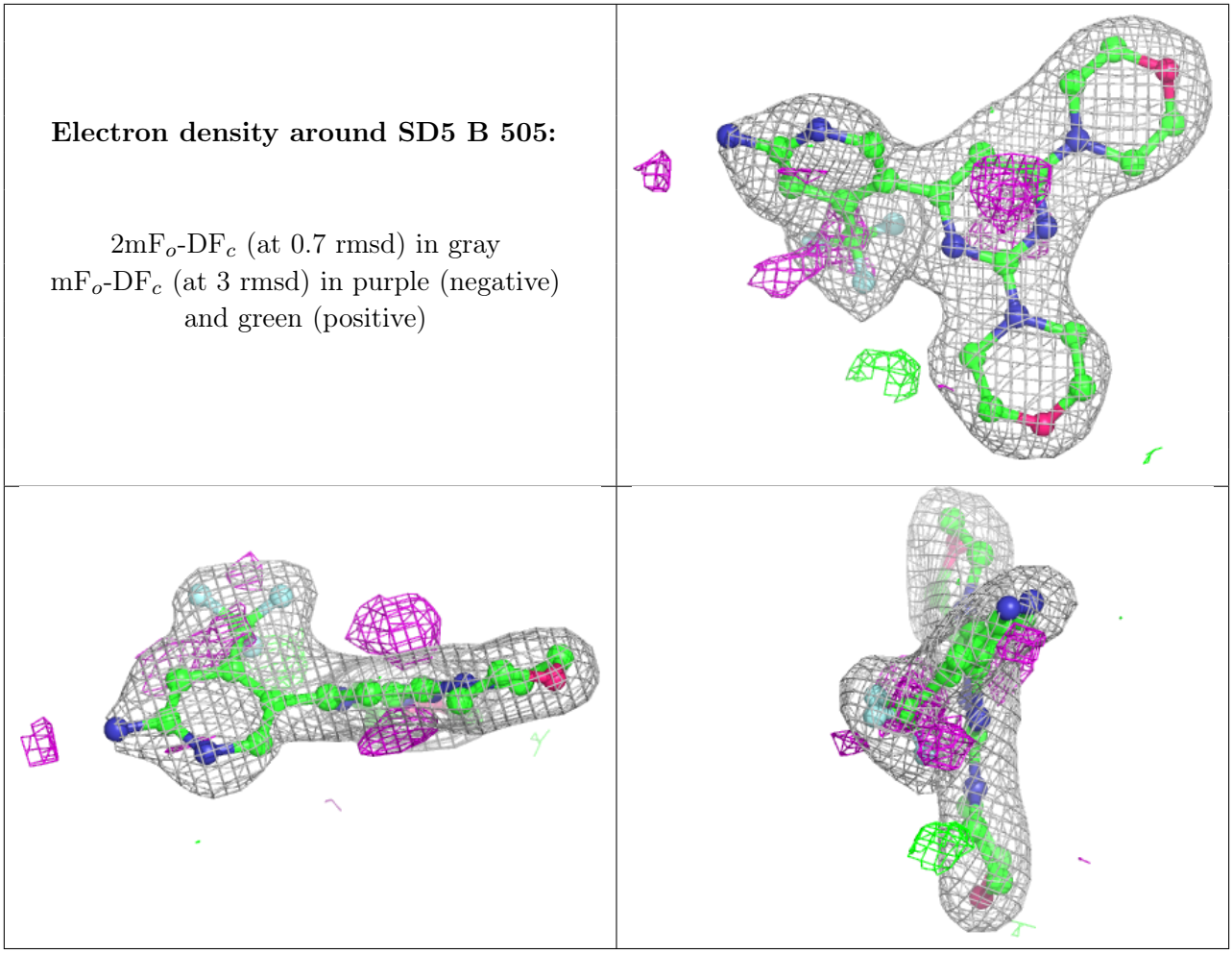
Electron density around ACP F 402:

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



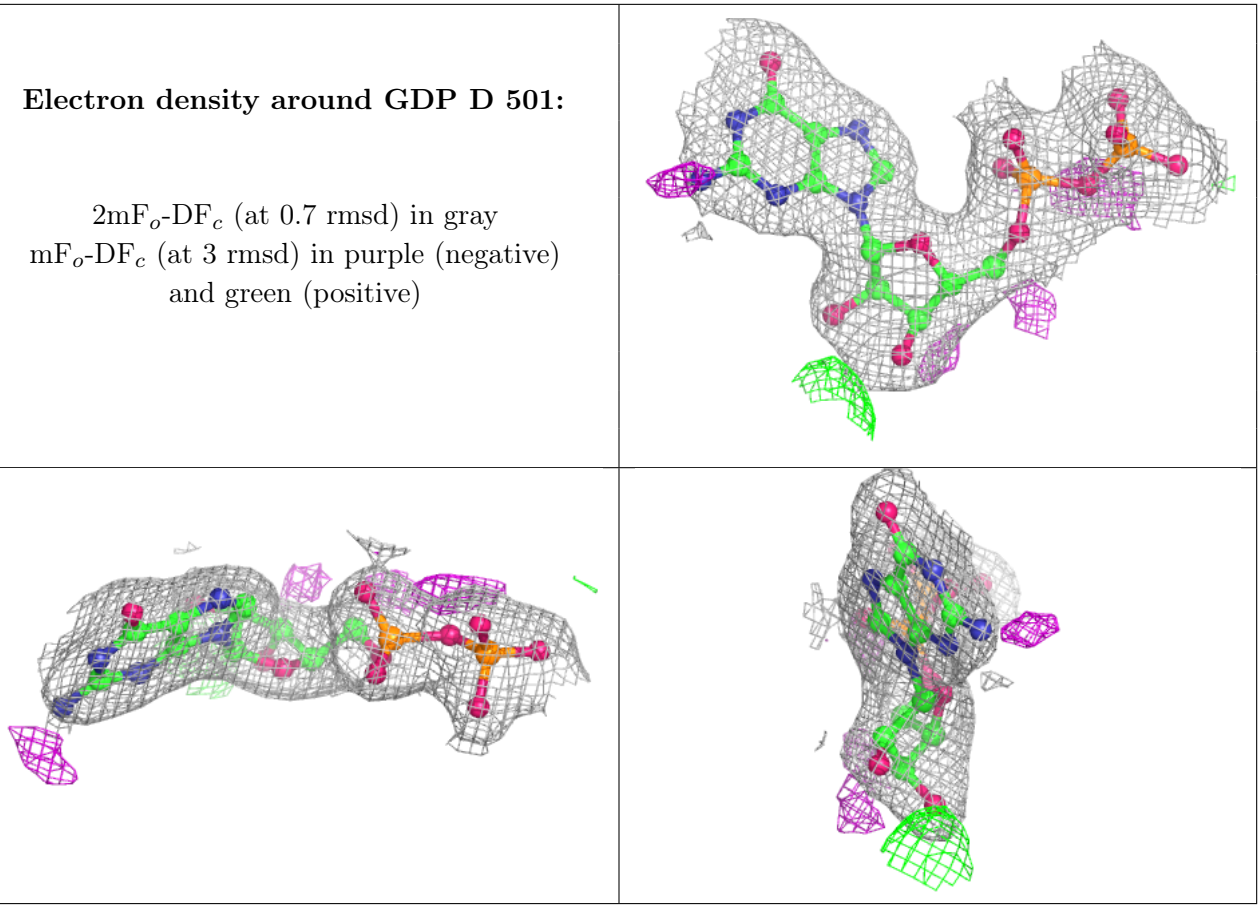
Electron density around SD5 B 505:

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



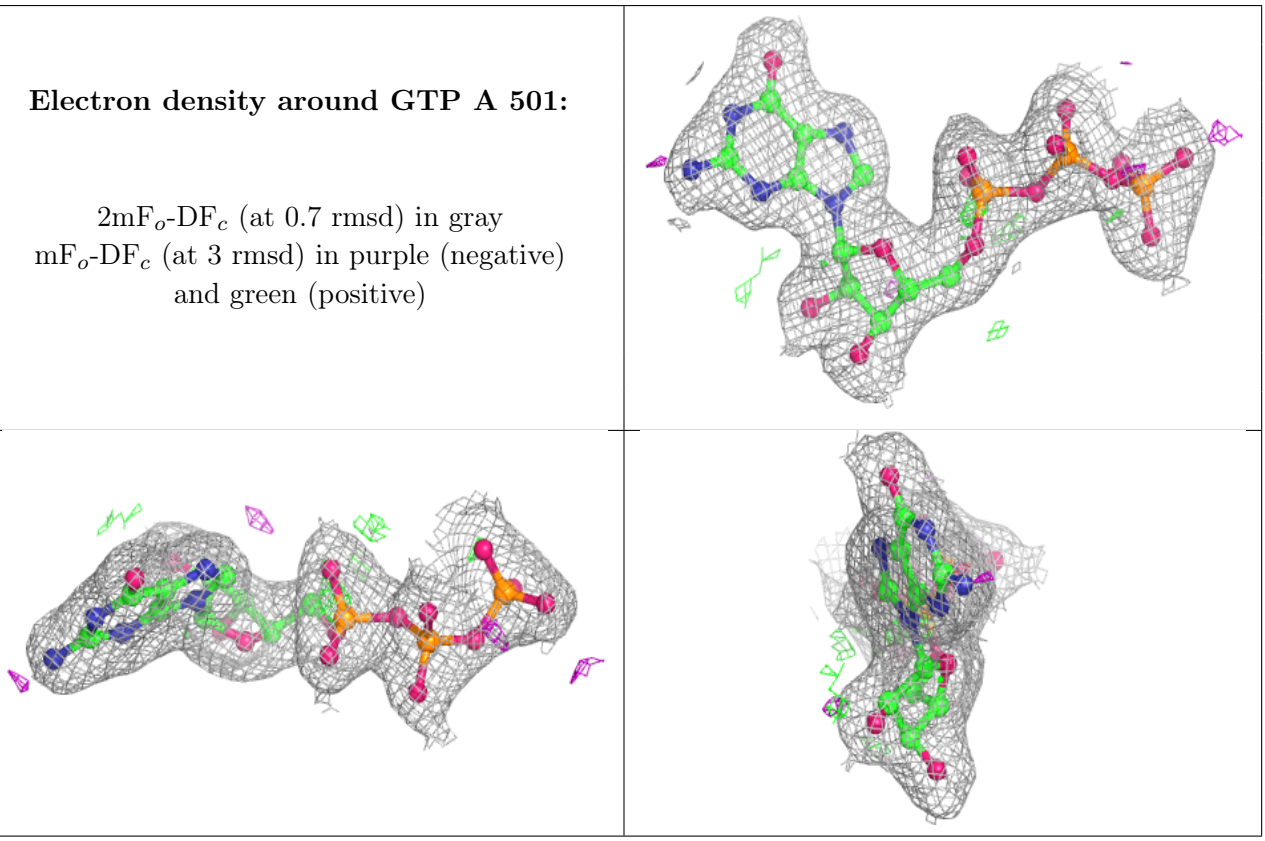
Electron density around GDP D 501:

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



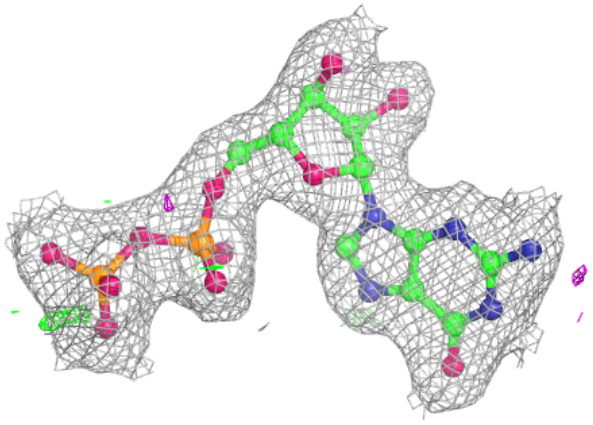
Electron density around GTP A 501:

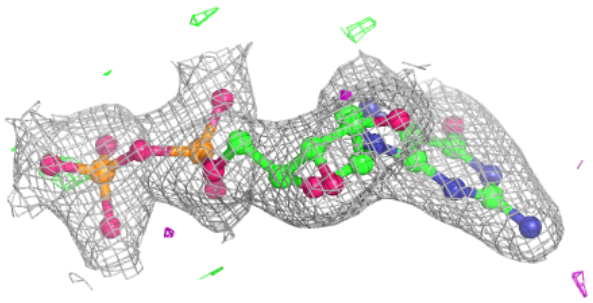
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

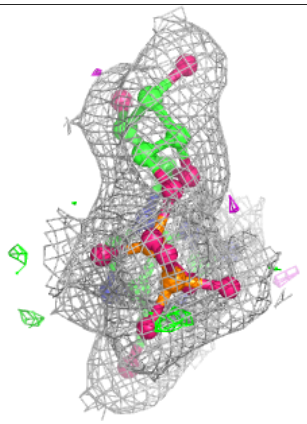


Electron density around GDP B 501:

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

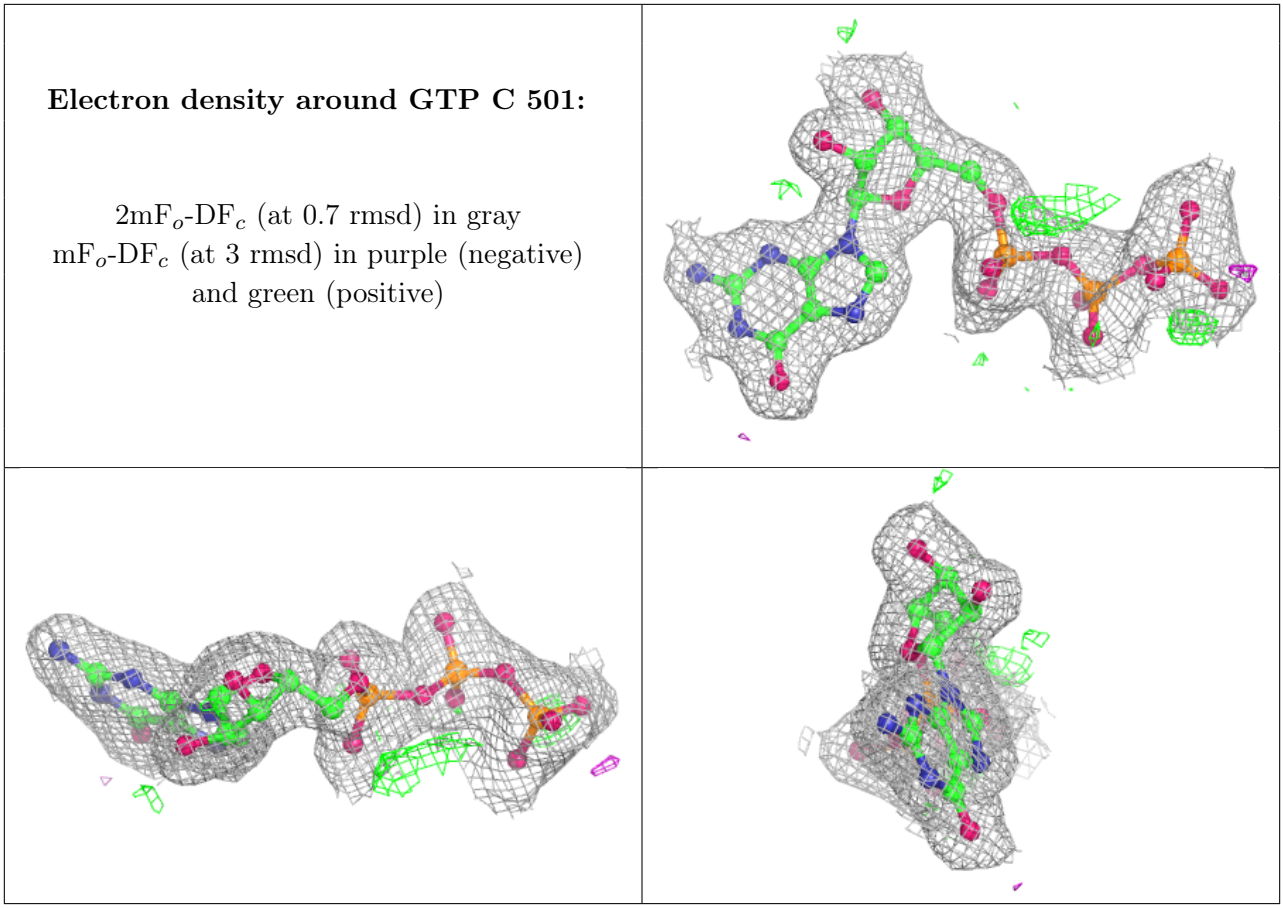






Electron density around GTP C 501:

$2mF_o$-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.