Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:34 am BST

PDB ID	:	6NNG
Title	:	Tubulin-RB3_SLD-TTL in complex with compound DJ95
Authors	:	Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on	:	2019-01-15
Resolution	:	2.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

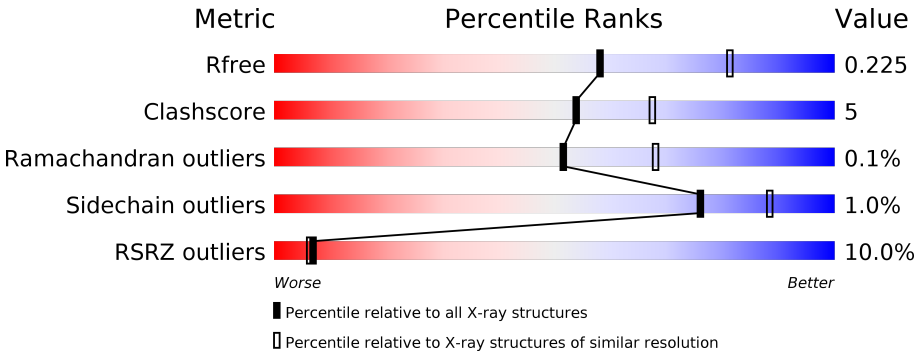
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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% 85% 12% ·
1	C	450	% 89% 9% ·
2	B	445	4% 81% 14% ·
2	D	445	14% 78% 16% 5%
3	E	143	12% 78% 7% 15%
4	F	384	26% 75% 13% 12%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17861 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	439	Total	C	N	O	S	0	0	0
			3412	2157	581	652	22			
1	C	440	Total	C	N	O	S	0	0	0
			3430	2171	583	655	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3343	2101	571	645	26			
2	D	421	Total	C	N	O	S	0	0	0
			3264	2052	552	635	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			984	607	179	193	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

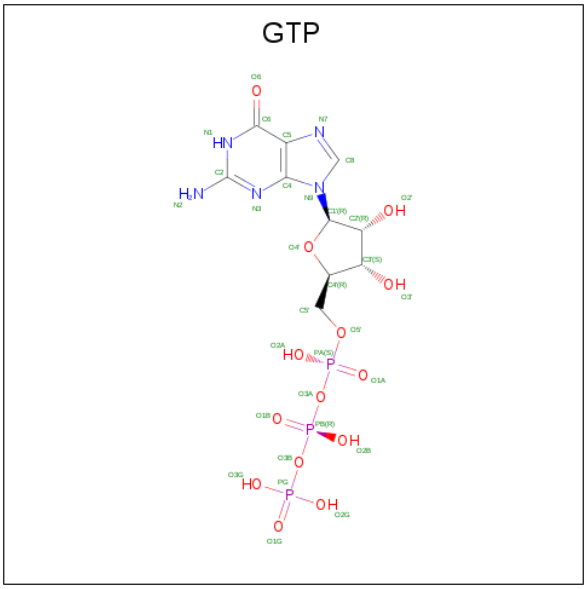
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	339	Total	C	N	O	S	0	0	0
			2643	1697	458	475	13			

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		
5	D	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	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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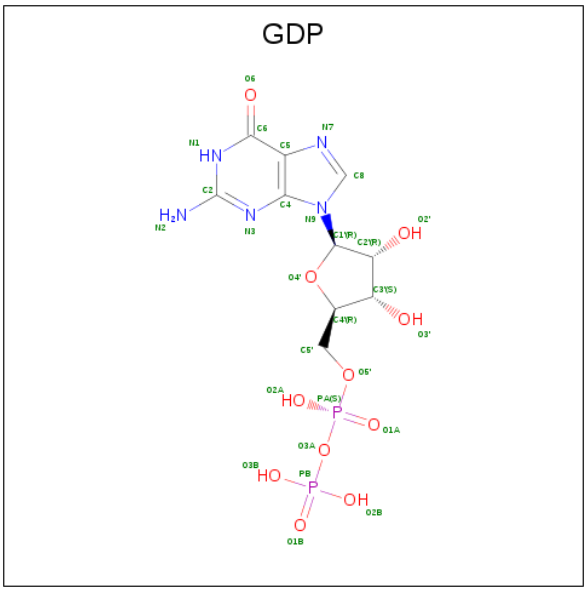
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

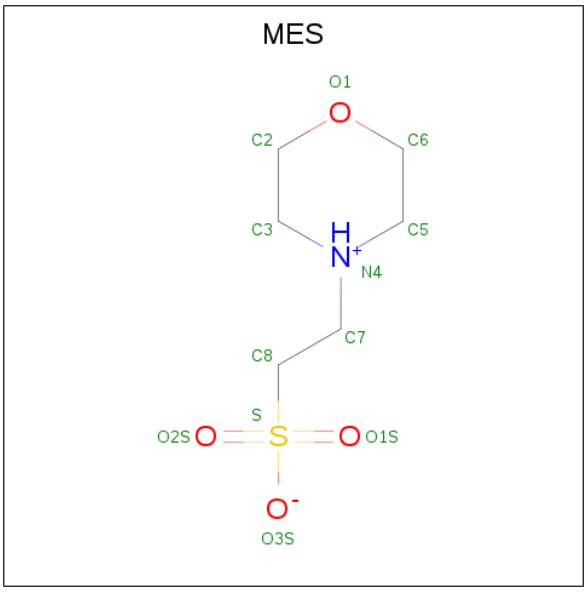
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



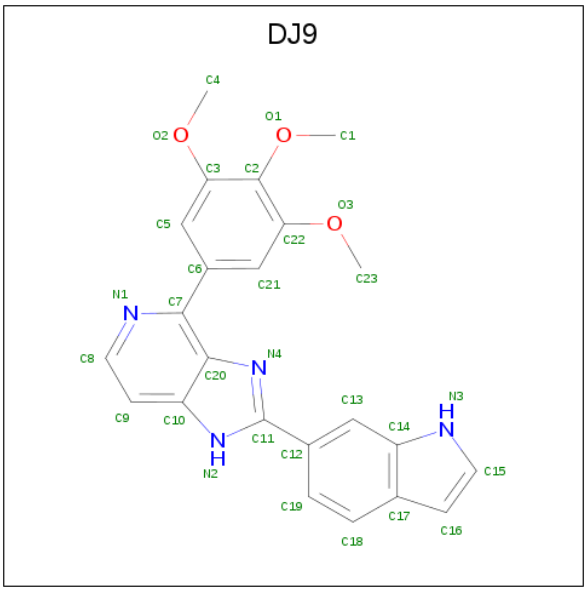
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0

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



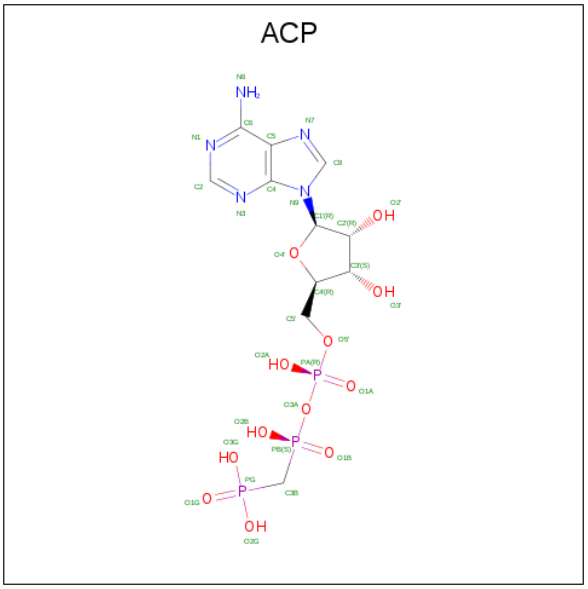
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 2-(1H-indol-6-yl)-4-(3,4,5-trimethoxyphenyl)-1H-imidazo[4,5-c]pyridine (three-letter code: DJ9) (formula: $C_{23}H_{20}N_4O_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			30	23	4	3		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

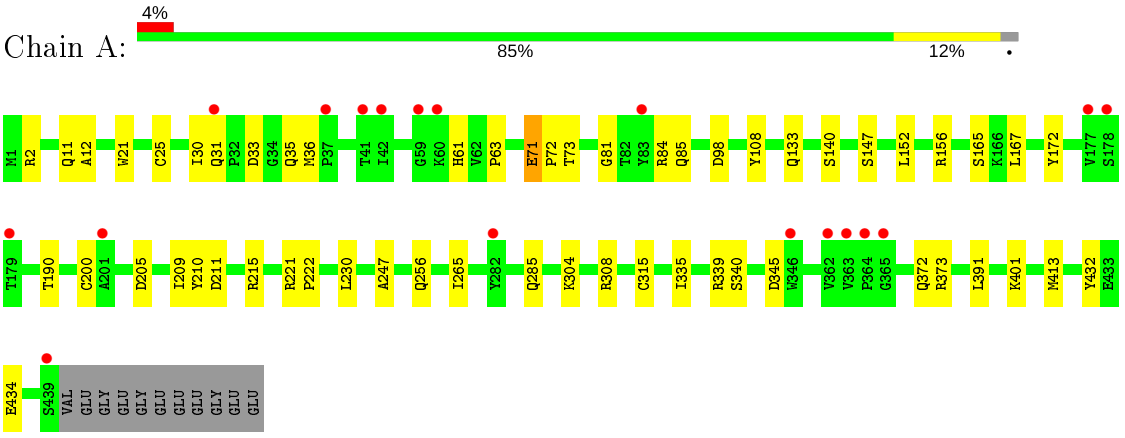
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	138	Total	O	0	0
			138	138		
12	B	119	Total	O	0	0
			119	119		
12	C	212	Total	O	0	0
			212	212		
12	D	41	Total	O	0	0
			41	41		
12	E	18	Total	O	0	0
			18	18		
12	F	42	Total	O	0	0
			42	42		

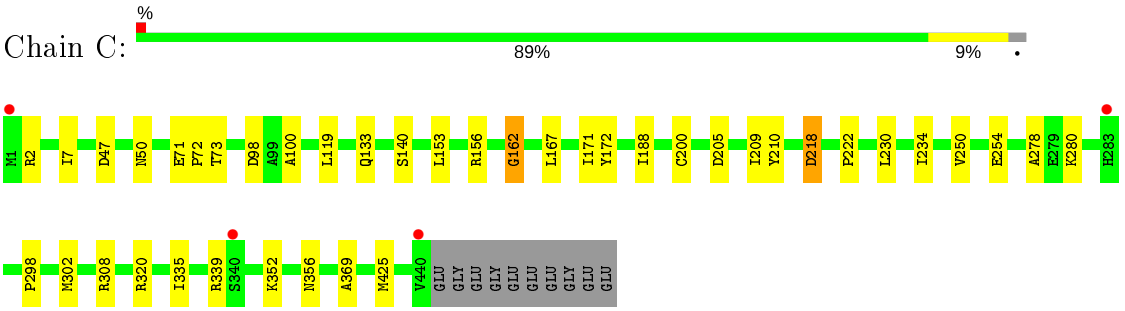
3 Residue-property plots (i)

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

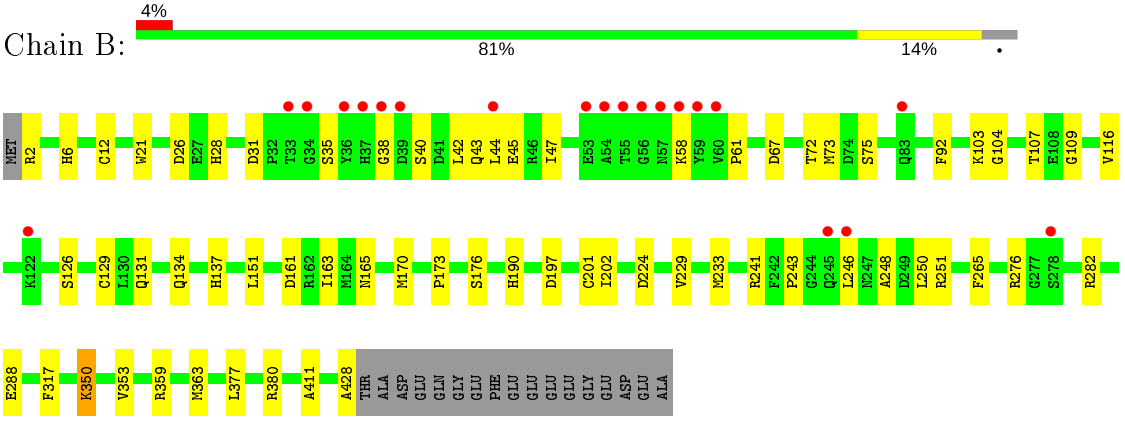
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

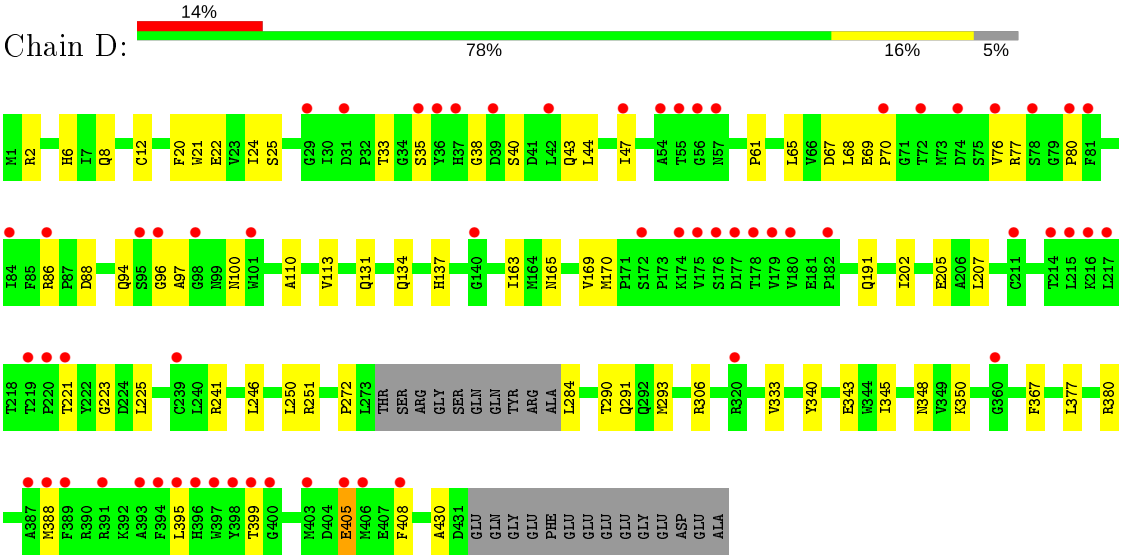


- Molecule 2: Tubulin beta-2B chain



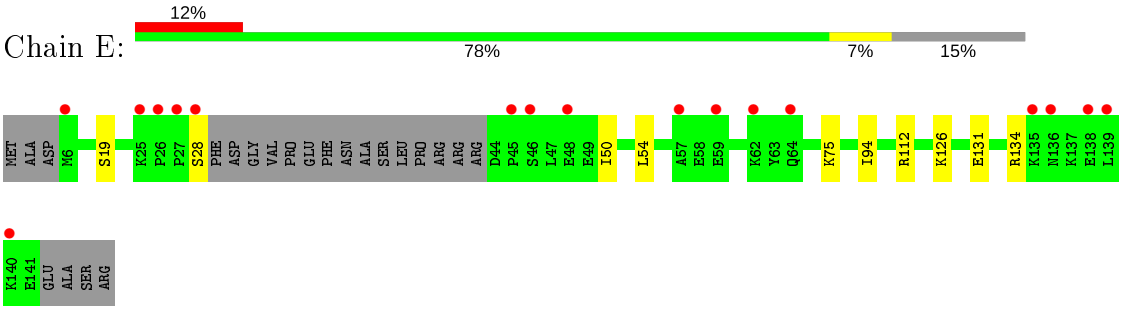
• Molecule 2: Tubulin beta-2B chain

Chain D:



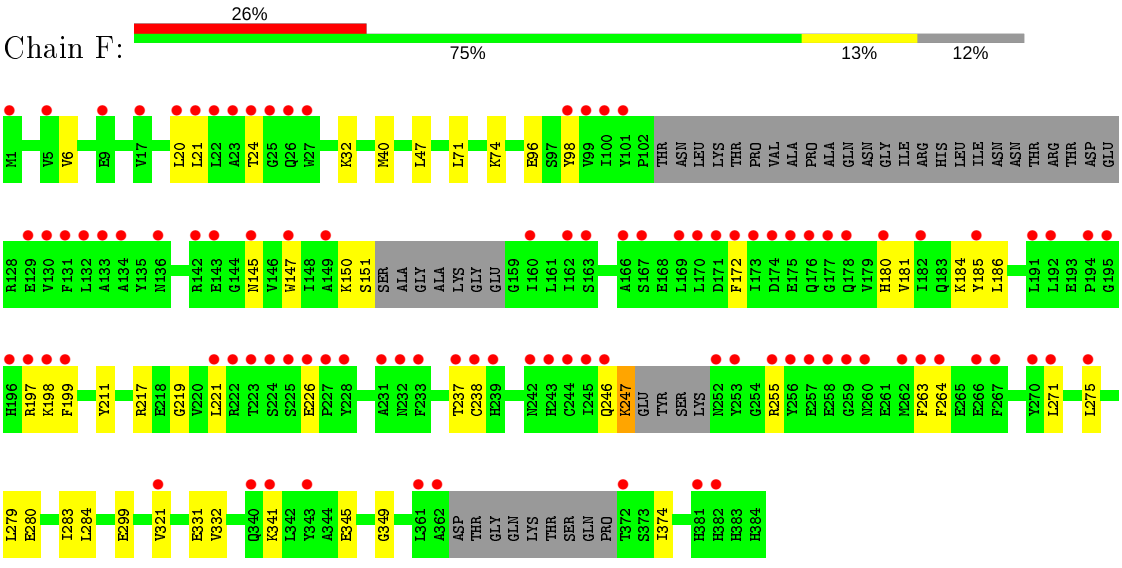
• Molecule 3: Stathmin-4

Chain E:



• Molecule 4: Tubulin Tyrosine Ligase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.42Å 157.98Å 182.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.40 48.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.25-2.40) 98.1 (48.25-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998: ???	Depositor
R, R_{free}	0.192 , 0.227 0.193 , 0.225	Depositor DCC
R_{free} test set	5845 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17861	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, DJ9, CA, GTP, ACP, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/3489	0.46	1/4739 (0.0%)
1	C	0.28	0/3508	0.48	2/4764 (0.0%)
2	B	0.25	0/3417	0.42	0/4629
2	D	0.30	1/3336 (0.0%)	0.46	0/4527
3	E	0.23	0/992	0.34	0/1319
4	F	0.27	0/2707	0.43	0/3671
All	All	0.27	1/17449 (0.0%)	0.45	3/23649 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	405	GLU	CB-CG	5.05	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	280	LYS	CB-CG-CD	-7.96	90.91	111.60
1	A	434	GLU	CA-CB-CG	5.49	125.47	113.40
1	C	218	ASP	CB-CG-OD1	-5.28	113.55	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3412	0	3309	37	0
1	C	3430	0	3335	24	0
2	B	3343	0	3212	39	0
2	D	3264	0	3099	45	0
3	E	984	0	988	9	0
4	F	2643	0	2490	32	0
5	A	32	0	12	2	0
5	C	32	0	12	1	0
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
9	B	24	0	24	2	0
10	B	30	0	0	1	0
11	F	31	0	13	1	0
12	A	138	0	0	2	0
12	B	119	0	0	1	0
12	C	212	0	0	0	0
12	D	41	0	0	0	0
12	E	18	0	0	1	0
12	F	42	0	0	0	0
All	All	17861	0	16518	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (180) 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:199:PHE:HB2	4:F:221:LEU:HD21	1.41	0.98
4:F:199:PHE:HB2	4:F:221:LEU:CD2	2.07	0.84
4:F:199:PHE:CB	4:F:221:LEU:HD21	2.20	0.72
1:A:372:GLN:HE21	1:A:373:ARG:HH12	1.38	0.70
4:F:271:LEU:HD23	4:F:275:LEU:HD12	1.79	0.64
2:B:173:PRO:HA	2:B:176:SER:HB2	1.82	0.61
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.81	0.61
3:E:75:LYS:NZ	12:E:201:HOH:O	2.25	0.61
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:THR:HG22	2:D:223:GLY:H	1.65	0.61
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.82	0.60
1:A:71:GLU:OE1	1:A:73:THR:N	2.32	0.60
2:B:38:GLY:HA3	2:B:43:GLN:HE22	1.65	0.60
2:B:170:MET:HG2	2:B:377:LEU:HD21	1.85	0.58
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.17	0.58
2:D:20:PHE:O	2:D:24:ILE:HG13	2.02	0.58
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.86	0.58
1:C:47:ASP:H	1:C:50:ASN:HD22	1.52	0.57
2:D:70:PRO:HG3	2:D:94:GLN:HA	1.86	0.57
2:D:65:LEU:HD22	2:D:76:VAL:HG11	1.86	0.57
2:B:246:LEU:HD22	2:B:350:LYS:HE2	1.86	0.56
2:B:26:ASP:CG	2:B:359:ARG:HE	2.08	0.56
4:F:199:PHE:CD2	4:F:221:LEU:HD21	2.41	0.56
2:B:161:ASP:O	2:B:251:ARG:NH2	2.39	0.56
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.41	0.56
2:D:246:LEU:HD21	2:D:350:LYS:HB3	1.88	0.56
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.87	0.55
4:F:263:PHE:CE1	4:F:341:LYS:HD3	2.42	0.54
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.89	0.54
2:D:38:GLY:HA3	2:D:43:GLN:HE22	1.72	0.54
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.90	0.54
2:B:42:LEU:HD13	2:B:243:PRO:HG2	1.89	0.53
2:D:97:ALA:HB3	5:D:501:GTP:O3G	2.09	0.53
1:A:308:ARG:HG2	1:A:340:SER:HB2	1.90	0.52
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.90	0.52
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.89	0.52
2:B:282:ARG:NH2	2:B:288:GLU:OE2	2.37	0.52
2:B:44:LEU:HA	2:B:47:ILE:HB	1.92	0.52
2:D:395:LEU:CD1	2:D:399:THR:HG23	2.40	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.92	0.51
4:F:32:LYS:HD3	4:F:32:LYS:N	2.26	0.51
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.92	0.51
2:D:205:GLU:HB3	2:D:380:ARG:HH12	1.75	0.51
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.92	0.51
2:D:6:HIS:HE2	2:D:8:GLN:HE21	1.56	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.50
4:F:71:LEU:HG	4:F:332:VAL:HG11	1.94	0.50
2:B:134:GLN:HA	2:B:165:ASN:O	2.11	0.50
1:A:211:ASP:OD1	1:A:304:LYS:NZ	2.30	0.50
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ASP:OD1	2:B:359:ARG:NE	2.44	0.49
1:A:33:ASP:HA	1:A:85:GLN:HG3	1.94	0.49
2:D:6:HIS:HE2	2:D:8:GLN:HG3	1.77	0.49
4:F:184:LYS:O	11:F:402:ACP:N6	2.45	0.49
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.94	0.49
2:B:224:ASP:OD2	2:B:276:ARG:NH2	2.42	0.49
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.94	0.49
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.94	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.48
4:F:199:PHE:CG	4:F:221:LEU:HD21	2.48	0.48
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.48	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.27	0.48
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.96	0.48
4:F:6:VAL:O	4:F:32:LYS:HG3	2.14	0.47
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.97	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.97	0.47
2:D:24:ILE:HG22	2:D:241:ARG:CZ	2.44	0.47
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.49	0.47
1:C:188:ILE:HD12	1:C:425:MET:HG3	1.96	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.97	0.47
2:D:191:GLN:HE22	3:E:126:LYS:NZ	2.14	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.46
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.79	0.46
1:A:165:SER:OG	1:A:256:GLN:NE2	2.48	0.46
2:D:33:THR:HG23	2:D:35:SER:H	1.80	0.46
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.50	0.46
4:F:145:ASN:CG	4:F:147:TRP:HE1	2.19	0.46
1:C:47:ASP:N	1:C:50:ASN:HD22	2.12	0.46
2:D:134:GLN:HA	2:D:165:ASN:O	2.15	0.46
2:B:72:THR:O	2:B:75:SER:OG	2.31	0.46
2:D:40:SER:H	2:D:43:GLN:NE2	2.13	0.46
1:A:98:ASP:HB2	5:A:501:GTP:O3G	2.16	0.46
2:D:44:LEU:HA	2:D:47:ILE:HB	1.98	0.46
1:A:31:GLN:HG2	1:A:35:GLN:O	2.16	0.46
1:A:31:GLN:NE2	1:A:35:GLN:HB2	2.30	0.46
2:B:246:LEU:HG	2:B:248:ALA:HB2	1.98	0.46
2:B:317:PHE:HB2	2:B:353:VAL:HG22	1.98	0.46
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.97	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:NE2	12:A:611:HOH:O	2.47	0.45
2:B:202:ILE:HD13	2:B:229:VAL:HG13	1.98	0.45
1:A:152:LEU:HD11	3:E:54:LEU:HD11	1.98	0.45
1:A:247:ALA:HB3	3:E:19:SER:OG	2.16	0.45
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.51	0.45
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.57	0.45
1:C:2:ARG:HB3	1:C:133:GLN:HB2	1.99	0.45
2:D:24:ILE:HD12	2:D:25:SER:N	2.31	0.45
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.99	0.45
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.99	0.45
4:F:217:ARG:NH2	4:F:345:GLU:OE1	2.50	0.45
2:B:2:ARG:HA	2:B:129:CYS:O	2.17	0.45
4:F:247:LYS:H	4:F:247:LYS:HD3	1.82	0.45
2:B:190:HIS:HD2	2:B:411:ALA:HA	1.81	0.44
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.44
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.51	0.44
2:B:73:MET:SD	2:B:92:PHE:HB3	2.58	0.44
2:D:2:ARG:CZ	2:D:131:GLN:HB3	2.47	0.44
2:B:40:SER:OG	2:B:42:LEU:HB2	2.18	0.44
4:F:151:SER:HA	4:F:180:HIS:CD2	2.53	0.44
4:F:40:MET:HE1	4:F:47:LEU:HG	1.99	0.44
2:B:380:ARG:NH1	12:B:612:HOH:O	2.44	0.44
3:E:50:ILE:O	3:E:54:LEU:HG	2.18	0.44
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.53	0.44
2:D:69:GLU:HG2	2:D:96:GLY:HA2	1.99	0.44
2:D:86:ARG:HE	2:D:88:ASP:HB2	1.82	0.43
1:A:372:GLN:HE21	1:A:373:ARG:NH1	2.13	0.43
2:B:2:ARG:CZ	2:B:131:GLN:HB3	2.49	0.43
1:A:85:GLN:HG2	1:A:85:GLN:H	1.66	0.43
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.53	0.43
1:A:11:GLN:HB3	5:A:501:GTP:O2A	2.18	0.43
2:B:31:ASP:OD2	2:B:35:SER:N	2.45	0.43
9:B:504:MES:H81	9:B:504:MES:H51	1.56	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.43
2:D:293:MET:CG	2:D:367:PHE:HB2	2.48	0.43
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.00	0.43
2:D:6:HIS:NE2	2:D:8:GLN:HG3	2.34	0.43
2:B:197:ASP:OD2	9:B:503:MES:H31	2.19	0.42
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.01	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.54	0.42
1:A:81:GLY:O	1:A:84:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:LYS:HB2	10:B:505:DJ9:C17	2.50	0.42
2:B:28:HIS:NE2	2:B:241:ARG:HB3	2.34	0.42
2:B:45:GLU:HB3	2:B:243:PRO:HG3	2.02	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
2:D:110:ALA:O	2:D:113:VAL:HG12	2.20	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.42
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.02	0.42
1:A:156:ARG:HA	1:A:156:ARG:HD2	1.89	0.42
1:A:2:ARG:O	1:A:133:GLN:NE2	2.50	0.42
2:D:12:CYS:SG	2:D:169:VAL:HG21	2.59	0.42
4:F:150:LYS:CB	4:F:181:VAL:H	2.33	0.42
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.42
2:D:293:MET:HG3	2:D:367:PHE:HB2	2.01	0.41
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.55	0.41
4:F:237:THR:O	4:F:246:GLN:NE2	2.53	0.41
2:B:233:MET:HE2	2:B:233:MET:HB3	1.89	0.41
2:B:276:ARG:HB3	2:B:276:ARG:HE	1.57	0.41
2:D:405:GLU:O	2:D:408:PHE:HB2	2.20	0.41
3:E:131:GLU:HG2	3:E:134:ARG:NH2	2.34	0.41
4:F:74:LYS:NZ	4:F:331:GLU:OE2	2.45	0.41
2:D:207:LEU:HB3	2:D:225:LEU:HD22	2.02	0.41
2:D:290:THR:HG22	2:D:333:VAL:HG21	2.02	0.41
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.44	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.56	0.41
2:D:291:GLN:O	2:D:291:GLN:HG2	2.20	0.41
1:A:215:ARG:NH2	12:A:619:HOH:O	2.53	0.41
1:A:25:CYS:HB3	1:A:30:ILE:O	2.21	0.41
1:A:401:LYS:HE3	2:B:428:ALA:HB1	2.02	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.41
2:D:67:ASP:OD2	2:D:68:LEU:N	2.54	0.41
4:F:184:LYS:HD2	4:F:185:TYR:N	2.36	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.55	0.41
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.03	0.41
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.20	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
1:A:345:ASP:HB3	3:E:28:SER:HB2	2.02	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.40
2:D:395:LEU:HD13	2:D:399:THR:HG23	2.04	0.40
2:B:103:LYS:HA	2:B:107:THR:OG1	2.22	0.40
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.36	0.40
2:D:22:GLU:OE1	2:D:80:PRO:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.40
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.03	0.40
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.56	0.40
2:B:104:GLY:O	2:B:109:GLY:HA3	2.21	0.40
1:C:100:ALA:HB1	2:D:251:ARG:HG2	2.03	0.40
2:D:388:MET:HB3	2:D:388:MET:HE2	1.80	0.40
4:F:199:PHE:CZ	4:F:321:VAL:HG22	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/450 (97%)	429 (98%)	8 (2%)	0	100	100
1	C	438/450 (97%)	431 (98%)	6 (1%)	1 (0%)	47	62
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	417/445 (94%)	411 (99%)	6 (1%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	329/384 (86%)	314 (95%)	14 (4%)	1 (0%)	41	55
All	All	2163/2317 (93%)	2119 (98%)	42 (2%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLY
4	F	186	LEU

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	366/378 (97%)	363 (99%)	3 (1%)	81 91
1	C	369/378 (98%)	367 (100%)	2 (0%)	88 95
2	B	364/383 (95%)	359 (99%)	5 (1%)	67 82
2	D	352/383 (92%)	349 (99%)	3 (1%)	78 90
3	E	105/127 (83%)	104 (99%)	1 (1%)	76 88
4	F	269/342 (79%)	265 (98%)	4 (2%)	65 80
All	All	1825/1991 (92%)	1807 (99%)	18 (1%)	76 88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	315	CYS
2	B	58	LYS
2	B	126	SER
2	B	137	HIS
2	B	350	LYS
2	B	363	MET
1	C	218	ASP
1	C	302	MET
2	D	77	ARG
2	D	100	ASN
2	D	137	HIS
3	E	112	ARG
4	F	172	PHE
4	F	197	ARG
4	F	247	LYS
4	F	255	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	256	GLN
1	A	283	HIS
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	356	ASN
1	A	372	GLN
2	B	11	GLN
2	B	15	GLN
2	B	43	GLN
2	B	52	ASN
2	B	247	ASN
2	B	426	GLN
1	C	50	ASN
1	C	309	HIS
2	D	8	GLN
2	D	43	GLN
2	D	100	ASN
3	E	90	ASN
3	E	92	ASN
3	E	136	ASN
4	F	180	HIS
4	F	260	ASN
4	F	310	GLN
4	F	340	GLN
4	F	382	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	MES	B	504	-	12,12,12	2.27	1 (8%)	14,16,16	2.02	6 (42%)
8	GDP	B	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.96	7 (22%)
5	GTP	C	501	6	26,34,34	4.50	15 (57%)	33,54,54	1.80	8 (24%)
5	GTP	A	501	6	26,34,34	4.51	15 (57%)	33,54,54	1.86	8 (24%)
10	DJ9	B	505	2	30,34,34	1.80	6 (20%)	36,49,49	1.59	9 (25%)
11	ACP	F	402	6	27,33,33	4.70	10 (37%)	32,52,52	2.36	5 (15%)
9	MES	B	503	-	12,12,12	2.25	1 (8%)	14,16,16	2.28	8 (57%)
5	GTP	D	501	-	26,34,34	4.54	15 (57%)	33,54,54	1.84	8 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
10	DJ9	B	505	2	-	0/14/14/14	0/5/5/5
11	ACP	F	402	6	-	8/15/38/38	0/3/3/3
9	MES	B	503	-	-	2/6/14/14	0/1/1/1
5	GTP	D	501	-	-	6/18/38/38	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O4'-C1'	15.29	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	C2'-C1'	-14.99	1.31	1.53
5	D	501	GTP	C2'-C3'	-10.68	1.24	1.53
5	C	501	GTP	C2'-C3'	-10.57	1.24	1.53
5	A	501	GTP	C2'-C3'	-10.44	1.24	1.53
5	D	501	GTP	C4-N3	8.89	1.49	1.35
5	A	501	GTP	C4-N3	8.78	1.49	1.35
5	C	501	GTP	C2'-C1'	8.70	1.67	1.53
5	C	501	GTP	C4-N3	8.68	1.49	1.35
5	D	501	GTP	C2'-C1'	8.64	1.66	1.53
5	A	501	GTP	C2'-C1'	8.47	1.66	1.53
9	B	504	MES	C8-S	-7.60	1.66	1.77
9	B	503	MES	C8-S	-7.50	1.66	1.77
5	A	501	GTP	O4'-C1'	-7.44	1.30	1.41
5	D	501	GTP	C6-C5	7.23	1.53	1.41
5	C	501	GTP	C6-C5	7.21	1.53	1.41
5	A	501	GTP	C6-C5	7.10	1.53	1.41
5	D	501	GTP	O4'-C1'	-7.04	1.31	1.41
5	C	501	GTP	O4'-C1'	-6.91	1.31	1.41
10	B	505	DJ9	C6-C7	-6.84	1.39	1.49
11	F	402	ACP	PB-O3A	6.29	1.65	1.58
11	F	402	ACP	O4'-C4'	-6.29	1.30	1.45
5	C	501	GTP	C6-N1	6.05	1.43	1.33
5	A	501	GTP	C6-N1	6.04	1.43	1.33
5	D	501	GTP	C6-N1	6.01	1.43	1.33
5	D	501	GTP	C2-N2	5.89	1.45	1.33
5	A	501	GTP	C2-N2	5.76	1.45	1.33
5	C	501	GTP	C2-N2	5.73	1.45	1.33
5	A	501	GTP	C2-N1	5.07	1.44	1.35
5	C	501	GTP	C2-N1	5.05	1.44	1.35
5	D	501	GTP	C2-N1	5.05	1.44	1.35
8	B	501	GDP	C6-C5	4.23	1.48	1.41
5	C	501	GTP	C5'-C4'	-4.14	1.38	1.51
5	D	501	GTP	C5'-C4'	-4.06	1.38	1.51
5	A	501	GTP	C5'-C4'	-3.86	1.39	1.51
10	B	505	DJ9	C12-C11	-3.75	1.38	1.48
5	A	501	GTP	C3'-C4'	3.32	1.61	1.53
5	A	501	GTP	O3'-C3'	3.27	1.50	1.43
5	C	501	GTP	O3'-C3'	3.18	1.50	1.43
11	F	402	ACP	C6-N6	3.16	1.45	1.34
5	D	501	GTP	O3'-C3'	3.15	1.50	1.43
5	D	501	GTP	C3'-C4'	3.12	1.61	1.53
5	C	501	GTP	C3'-C4'	2.95	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O3'-C3'	-2.95	1.36	1.43
11	F	402	ACP	O2'-C2'	2.84	1.49	1.43
5	C	501	GTP	O4'-C4'	2.75	1.51	1.45
5	D	501	GTP	O4'-C4'	2.69	1.51	1.45
11	F	402	ACP	C5-C4	-2.63	1.34	1.40
5	D	501	GTP	C2-N3	2.57	1.46	1.34
5	A	501	GTP	O4'-C4'	2.56	1.50	1.45
5	A	501	GTP	C2-N3	2.54	1.46	1.34
5	C	501	GTP	C2-N3	2.54	1.46	1.34
10	B	505	DJ9	C11-N4	-2.45	1.32	1.35
8	B	501	GDP	C5-C4	2.35	1.47	1.40
5	A	501	GTP	O6-C6	-2.34	1.18	1.24
10	B	505	DJ9	C11-N2	-2.33	1.32	1.35
5	C	501	GTP	O6-C6	-2.33	1.18	1.24
5	D	501	GTP	O6-C6	-2.28	1.18	1.24
10	B	505	DJ9	O2-C3	2.23	1.40	1.37
5	A	501	GTP	O2'-C2'	2.19	1.48	1.43
10	B	505	DJ9	O3-C22	2.16	1.40	1.37
5	D	501	GTP	O2'-C2'	2.15	1.48	1.43
11	F	402	ACP	C2-N3	2.15	1.35	1.32
5	C	501	GTP	O2'-C2'	2.12	1.48	1.43
11	F	402	ACP	PB-O2B	-2.05	1.51	1.56

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	402	ACP	C5-C6-N6	8.59	133.41	120.35
11	F	402	ACP	N6-C6-N1	-5.72	106.70	118.57
11	F	402	ACP	N3-C2-N1	-5.65	119.85	128.68
5	C	501	GTP	N3-C2-N1	-5.41	120.00	127.22
5	D	501	GTP	N3-C2-N1	-5.39	120.03	127.22
5	A	501	GTP	N3-C2-N1	-5.32	120.12	127.22
9	B	503	MES	C5-N4-C3	4.92	119.91	108.83
8	B	501	GDP	C2-N3-C4	4.82	120.86	115.36
8	B	501	GDP	C6-C5-C4	-4.26	116.73	120.80
5	C	501	GTP	C2-N3-C4	4.16	120.11	115.36
5	D	501	GTP	C2-N3-C4	4.11	120.06	115.36
8	B	501	GDP	C6-N1-C2	4.05	122.37	115.93
11	F	402	ACP	C3'-C2'-C1'	3.95	106.92	100.98
9	B	504	MES	C5-N4-C3	3.93	117.69	108.83
8	B	501	GDP	C5-C6-N1	-3.89	118.11	123.43
5	A	501	GTP	C2-N3-C4	3.88	119.79	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	GTP	C1'-N9-C4	-3.79	119.98	126.64
10	B	505	DJ9	C8-N1-C7	3.71	120.67	117.99
5	C	501	GTP	C1'-N9-C4	-3.67	120.19	126.64
5	D	501	GTP	C1'-N9-C4	-3.52	120.45	126.64
8	B	501	GDP	N3-C2-N1	-3.36	122.74	127.22
10	B	505	DJ9	C6-C7-N1	3.34	120.36	115.32
9	B	504	MES	C6-C5-N4	-3.28	105.13	110.10
5	A	501	GTP	C3'-C2'-C1'	3.20	105.79	100.98
5	D	501	GTP	PB-O3B-PG	-3.12	122.13	132.83
10	B	505	DJ9	O3-C22-C2	2.97	120.38	115.16
9	B	503	MES	C7-N4-C5	2.91	118.68	111.23
8	B	501	GDP	PA-O3A-PB	-2.89	122.90	132.83
5	D	501	GTP	C3'-C2'-C1'	2.84	105.26	100.98
5	D	501	GTP	PA-O3A-PB	-2.81	123.20	132.83
8	B	501	GDP	C4-C5-N7	-2.79	106.49	109.40
5	C	501	GTP	C3'-C2'-C1'	2.72	105.08	100.98
9	B	503	MES	C7-N4-C3	2.69	118.12	111.23
10	B	505	DJ9	O2-C3-C2	2.68	119.88	115.16
5	C	501	GTP	C5-C6-N1	-2.61	119.86	123.43
5	A	501	GTP	C5-C6-N1	-2.61	119.86	123.43
5	A	501	GTP	PB-O3B-PG	-2.59	123.93	132.83
9	B	504	MES	O3S-S-C8	2.57	109.93	105.77
5	D	501	GTP	C5-C6-N1	-2.52	119.98	123.43
11	F	402	ACP	PA-O3A-PB	-2.48	124.71	132.56
9	B	503	MES	O3S-S-C8	2.46	109.74	105.77
9	B	503	MES	C2-C3-N4	-2.44	106.41	110.10
5	C	501	GTP	PB-O3B-PG	-2.41	124.57	132.83
5	A	501	GTP	C6-N1-C2	2.40	119.74	115.93
5	C	501	GTP	C6-N1-C2	2.39	119.73	115.93
9	B	503	MES	O1S-S-C8	2.37	109.77	106.92
5	D	501	GTP	C6-N1-C2	2.37	119.69	115.93
10	B	505	DJ9	O3-C22-C21	-2.34	120.09	124.12
9	B	504	MES	O2S-S-C8	2.29	109.67	106.92
9	B	504	MES	C7-N4-C5	2.21	116.88	111.23
9	B	504	MES	C7-N4-C3	2.15	116.74	111.23
5	A	501	GTP	PA-O3A-PB	-2.13	125.53	132.83
9	B	503	MES	C6-C5-N4	-2.13	106.88	110.10
10	B	505	DJ9	C11-N2-C10	2.11	107.97	103.78
10	B	505	DJ9	C12-C13-C14	-2.09	119.61	121.44
9	B	503	MES	O2S-S-C8	2.08	109.42	106.92
5	C	501	GTP	PA-O3A-PB	-2.01	125.92	132.83
10	B	505	DJ9	C12-C11-N2	2.01	126.20	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	505	DJ9	C23-O3-C22	-2.00	114.50	117.53

There are no chirality outliers.

All (30) torsion outliers are listed below:

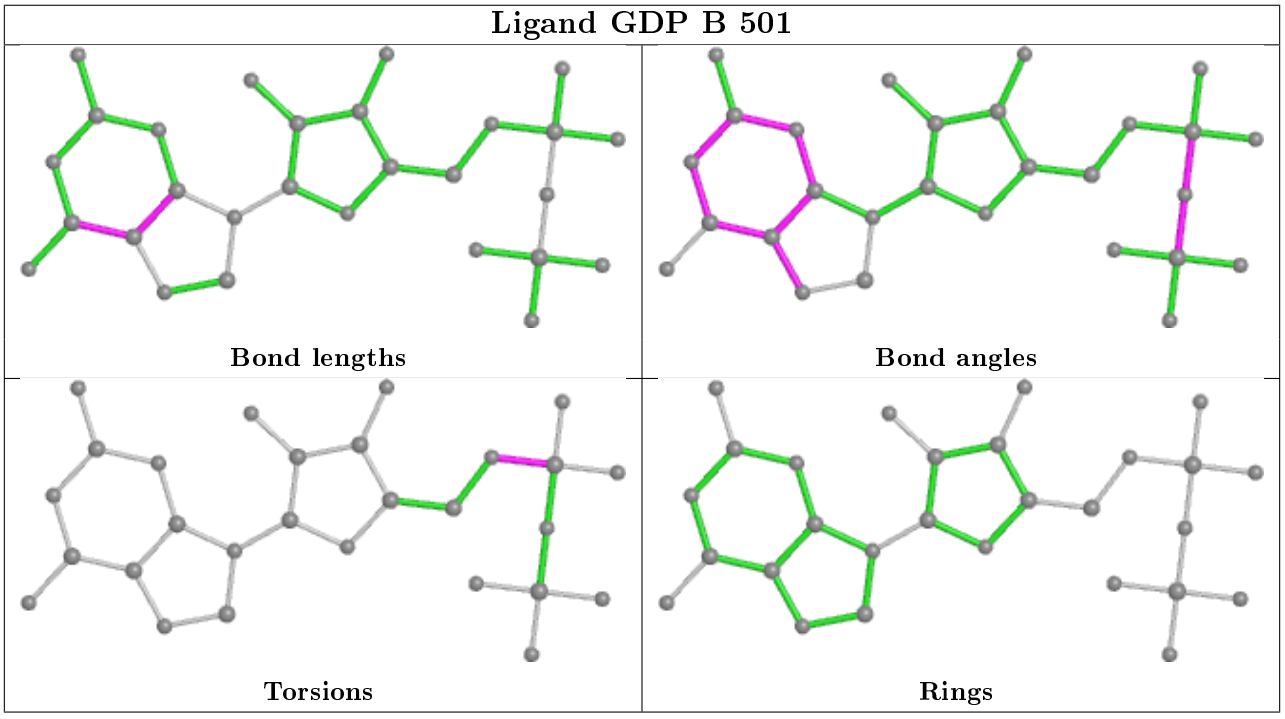
Mol	Chain	Res	Type	Atoms
9	B	504	MES	C7-C8-S-O1S
11	F	402	ACP	PB-C3B-PG-O1G
11	F	402	ACP	PB-C3B-PG-O2G
11	F	402	ACP	PB-C3B-PG-O3G
11	F	402	ACP	C5'-O5'-PA-O1A
11	F	402	ACP	C5'-O5'-PA-O2A
11	F	402	ACP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
9	B	503	MES	N4-C7-C8-S
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O3S
9	B	503	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	C4'-C5'-O5'-PA
11	F	402	ACP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	PB-O3B-PG-O3G
11	F	402	ACP	PB-O3A-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	PB-O3B-PG-O1G

There are no ring outliers.

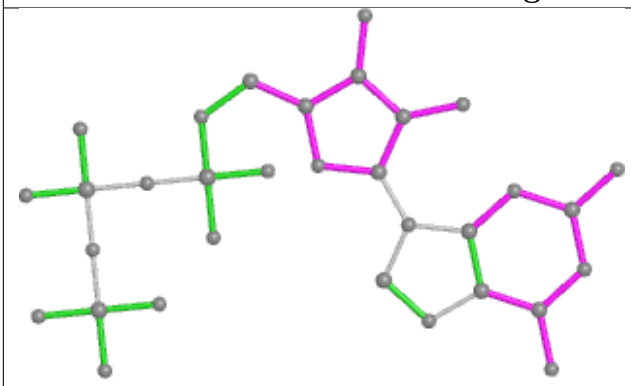
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	MES	1	0
8	B	501	GDP	1	0
5	C	501	GTP	1	0
5	A	501	GTP	2	0
10	B	505	DJ9	1	0
11	F	402	ACP	1	0
9	B	503	MES	1	0
5	D	501	GTP	1	0

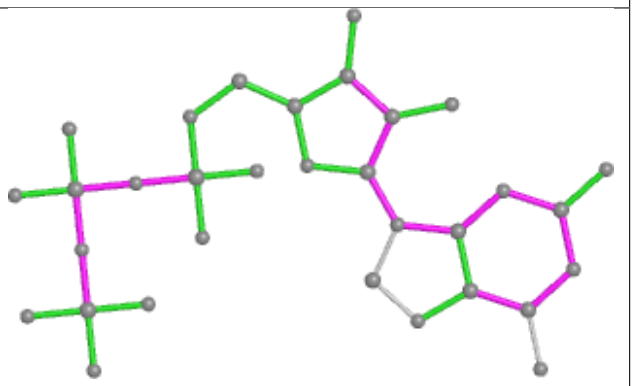
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



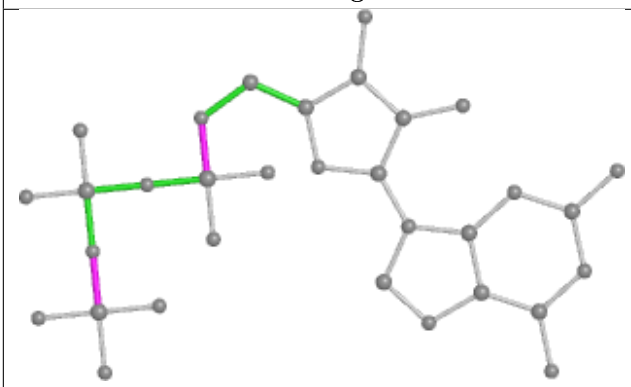
Ligand GTP C 501



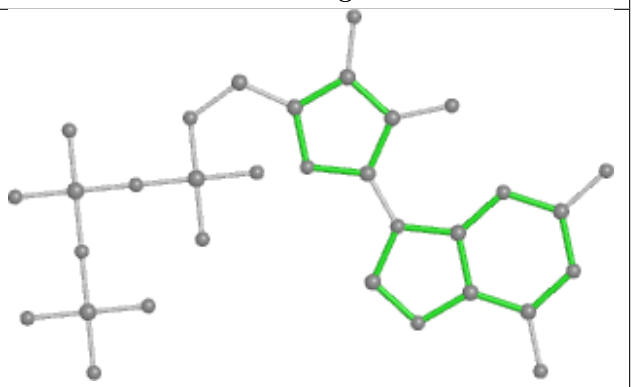
Bond lengths



Bond angles

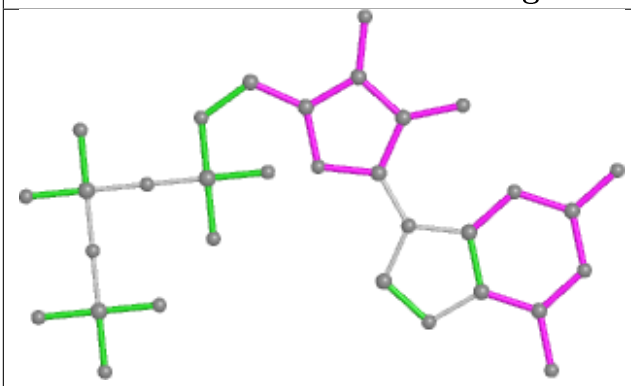


Torsions

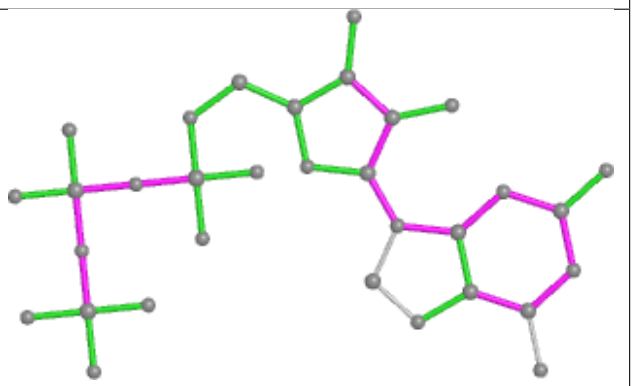


Rings

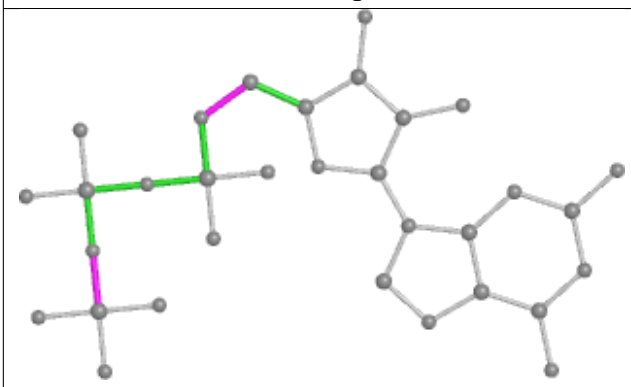
Ligand GTP A 501



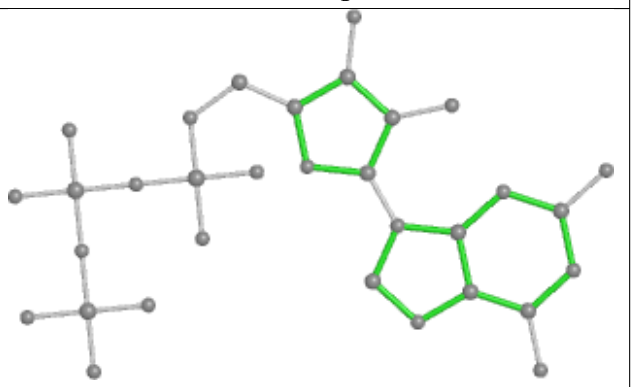
Bond lengths



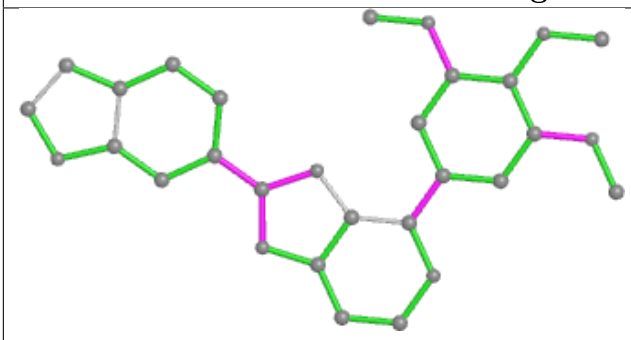
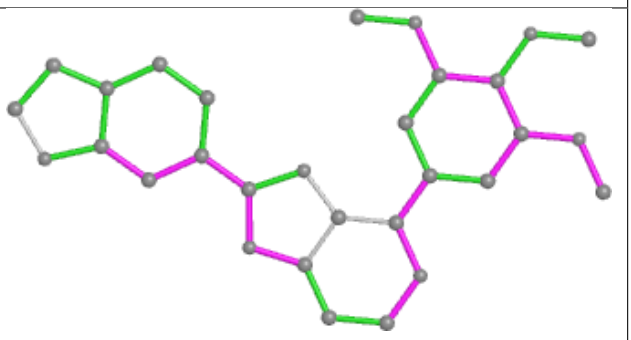
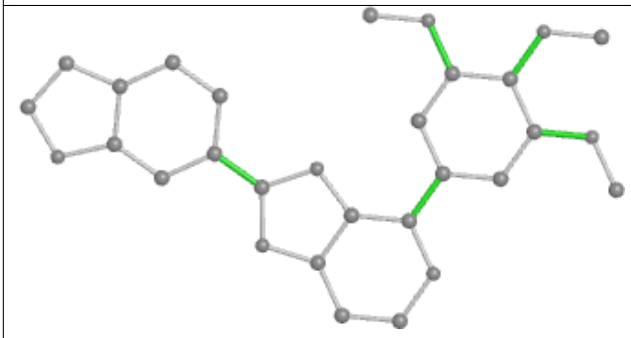
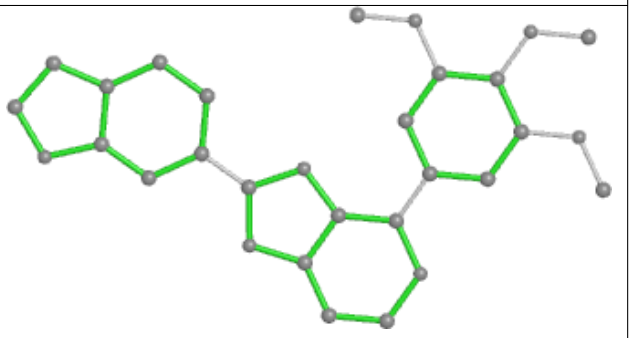
Bond angles

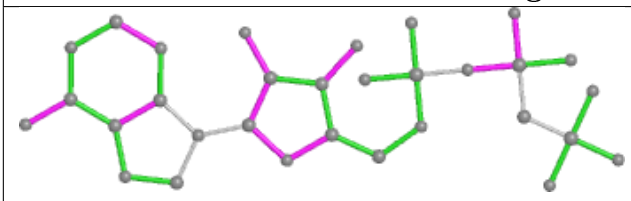
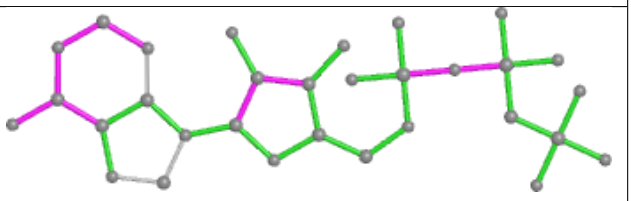
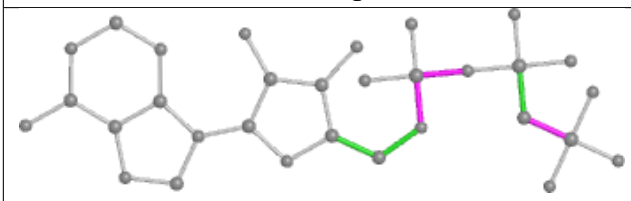
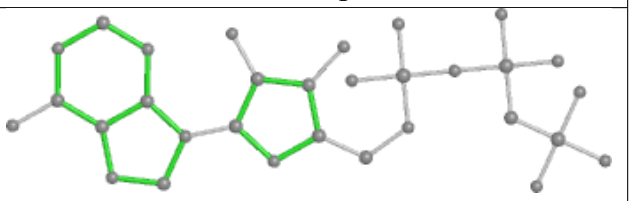


Torsions

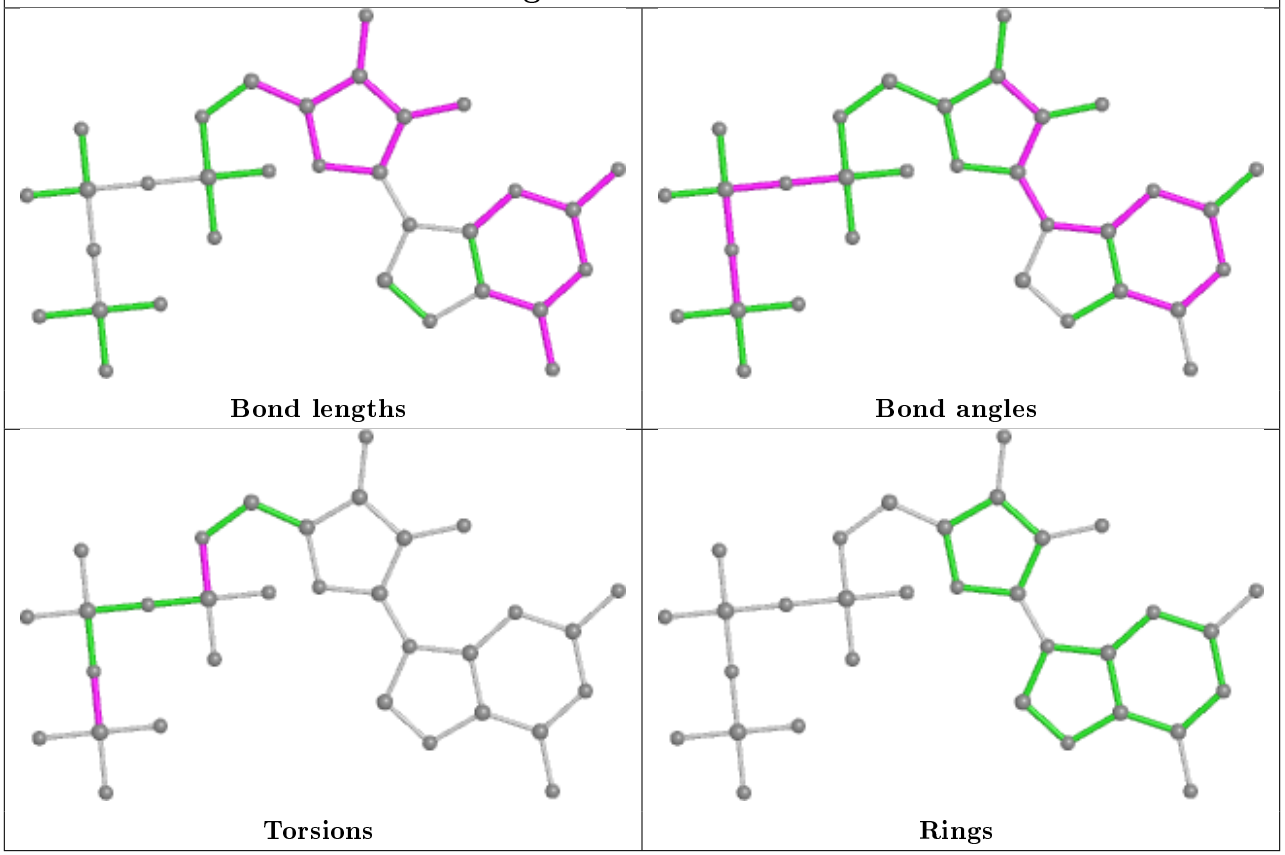


Rings

Ligand DJ9 B 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACP F 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP D 501



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	439/450 (97%)	0.28	18 (4%) 37 36	25, 43, 71, 95	0
1	C	440/450 (97%)	0.08	4 (0%) 84 82	20, 33, 57, 79	0
2	B	427/445 (95%)	0.25	20 (4%) 31 30	20, 41, 78, 118	0
2	D	421/445 (94%)	0.73	62 (14%) 2 2	31, 58, 89, 112	0
3	E	121/143 (84%)	0.67	17 (14%) 2 2	30, 57, 88, 109	0
4	F	339/384 (88%)	1.22	98 (28%) 0 0	29, 66, 112, 133	0
All	All	2187/2317 (94%)	0.49	219 (10%) 7 6	20, 47, 91, 133	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	54	ALA	8.1
4	F	173	ILE	7.7
2	B	55	THR	7.4
2	D	405	GLU	7.2
2	D	55	THR	6.7
2	B	57	ASN	6.6
4	F	166	ALA	6.5
4	F	259	GLY	6.4
4	F	199	PHE	6.1
4	F	170	LEU	6.1
4	F	101	TYR	6.0
2	D	95	SER	6.0
4	F	132	LEU	5.9
2	D	397	TRP	5.8
4	F	136	ASN	5.7
2	D	394	PHE	5.6
4	F	244	CYS	5.5
4	F	225	SER	5.5
4	F	256	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	5.3
4	F	194	PRO	5.2
4	F	169	LEU	5.1
2	B	36	TYR	4.9
4	F	253	TYR	4.9
4	F	129	GLU	4.8
4	F	133	ALA	4.6
3	E	139	LEU	4.5
4	F	255	ARG	4.5
2	B	56	GLY	4.5
4	F	134	ALA	4.4
2	D	393	ALA	4.4
3	E	48	GLU	4.3
4	F	172	PHE	4.3
4	F	176	GLN	4.3
4	F	233	PHE	4.2
2	B	58	LYS	4.2
3	E	57	ALA	4.2
3	E	46	SER	4.1
4	F	167	SER	4.1
2	D	37	HIS	4.1
4	F	362	ALA	4.1
2	B	59	TYR	4.1
2	D	80	PRO	4.1
4	F	100	ILE	4.1
2	D	391	ARG	4.0
1	A	42	ILE	4.0
2	D	216	LYS	4.0
2	D	387	ALA	4.0
2	D	39	ASP	4.0
2	D	389	PHE	3.9
2	D	177	ASP	3.9
4	F	227	PRO	3.9
4	F	22	LEU	3.9
2	D	175	VAL	3.8
4	F	147	TRP	3.8
4	F	178	GLN	3.7
2	D	395	LEU	3.7
2	D	178	THR	3.6
2	D	398	TYR	3.6
2	D	400	GLY	3.6
1	A	178	SER	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	21	LEU	3.5
2	D	98	GLY	3.5
4	F	143	GLU	3.5
2	D	220	PRO	3.4
4	F	223	THR	3.4
4	F	17	VAL	3.4
4	F	195	GLY	3.4
4	F	1	MET	3.4
2	D	72	THR	3.4
1	A	179	THR	3.3
4	F	372	THR	3.3
4	F	9	GLU	3.3
3	E	28	SER	3.3
4	F	191	LEU	3.2
2	D	54	ALA	3.2
4	F	263	PHE	3.2
2	D	399	THR	3.2
4	F	192	LEU	3.2
4	F	258	GLU	3.1
2	B	33	THR	3.1
2	B	245	GLN	3.1
2	D	176	SER	3.1
1	C	1	MET	3.1
3	E	27	PRO	3.1
2	D	320	ARG	3.1
1	C	440	VAL	3.0
2	D	140	GLY	3.0
4	F	25	GLY	3.0
2	D	219	THR	3.0
4	F	243	HIS	3.0
2	D	74	ASP	3.0
2	D	76	VAL	3.0
4	F	270	TYR	2.9
4	F	246	GLN	2.9
2	B	39	ASP	2.9
4	F	197	ARG	2.9
4	F	171	ASP	2.9
4	F	24	THR	2.9
1	A	31	GLN	2.9
2	D	78	SER	2.9
3	E	136	ASN	2.9
1	A	177	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	27	TRP	2.9
2	D	396	HIS	2.9
1	A	41	THR	2.8
2	D	214	THR	2.8
2	D	56	GLY	2.8
2	B	37	HIS	2.8
4	F	20	LEU	2.8
4	F	177	GLY	2.8
3	E	25	LYS	2.8
2	B	44	LEU	2.8
2	D	215	LEU	2.8
4	F	131	PHE	2.8
4	F	252	ASN	2.7
4	F	275	LEU	2.7
3	E	6	MET	2.7
2	D	221	THR	2.7
4	F	260	ASN	2.7
4	F	196	HIS	2.7
4	F	149	ALA	2.6
2	D	217	LEU	2.6
4	F	242	ASN	2.6
1	A	201	ALA	2.6
4	F	224	SER	2.6
4	F	238	CYS	2.6
2	D	35	SER	2.6
1	A	362	VAL	2.6
2	D	70	PRO	2.6
2	D	403	MET	2.6
2	D	360	GLY	2.6
4	F	174	ASP	2.6
4	F	5	VAL	2.6
3	E	138	GLU	2.6
4	F	381	HIS	2.5
3	E	59	GLU	2.5
2	D	180	VAL	2.5
4	F	142	ARG	2.5
2	B	246	LEU	2.5
2	D	179	VAL	2.5
4	F	160	ILE	2.5
2	B	53	GLU	2.5
2	D	29	GLY	2.5
1	A	439	SER	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	163	SER	2.4
2	D	408	PHE	2.4
4	F	23	ALA	2.4
4	F	267	PHE	2.4
4	F	257	GLU	2.4
4	F	226	GLU	2.4
2	D	81	PHE	2.4
4	F	239	HIS	2.4
1	A	282	TYR	2.4
4	F	340	GLN	2.4
2	D	211	CYS	2.4
4	F	264	PHE	2.4
4	F	99	VAL	2.4
4	F	180	HIS	2.3
4	F	228	TYR	2.3
2	D	239	CYS	2.3
4	F	266	GLU	2.3
1	A	364	PRO	2.3
4	F	98	TYR	2.3
2	D	42	LEU	2.3
4	F	321	VAL	2.3
1	C	283	HIS	2.3
4	F	221	LEU	2.3
4	F	237	THR	2.3
4	F	222	ARG	2.3
4	F	271	LEU	2.3
4	F	130	VAL	2.3
3	E	62	LYS	2.3
4	F	382	HIS	2.3
3	E	26	PRO	2.3
1	A	59	GLY	2.2
2	D	57	ASN	2.2
2	D	174	LYS	2.2
3	E	140	LYS	2.2
2	D	172	SER	2.2
4	F	162	ILE	2.2
1	A	363	VAL	2.2
4	F	361	LEU	2.2
1	A	83	TYR	2.2
2	B	278	SER	2.2
2	B	34	GLY	2.2
2	D	31	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	83	GLN	2.2
2	D	84	ILE	2.2
2	D	406	MET	2.2
4	F	145	ASN	2.1
4	F	341	LYS	2.1
2	D	47	ILE	2.1
2	B	122	LYS	2.1
1	C	340	SER	2.1
3	E	45	PRO	2.1
2	B	38	GLY	2.1
1	A	346	TRP	2.1
2	D	101	TRP	2.1
2	B	60	VAL	2.1
2	D	182	PRO	2.1
4	F	262	MET	2.1
4	F	185	TYR	2.1
4	F	198	LYS	2.1
4	F	175	GLU	2.1
2	D	36	TYR	2.1
3	E	135	LYS	2.1
4	F	232	ASN	2.1
1	A	60	LYS	2.1
4	F	343	TYR	2.1
2	D	388	MET	2.0
1	A	365	GLY	2.0
2	D	96	GLY	2.0
1	A	37	PRO	2.0
4	F	26	GLN	2.0
4	F	245	ILE	2.0
4	F	182	ILE	2.0
3	E	64	GLN	2.0
2	D	86	ARG	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 carbohydrates in this entry.

6.4 Ligands (i)

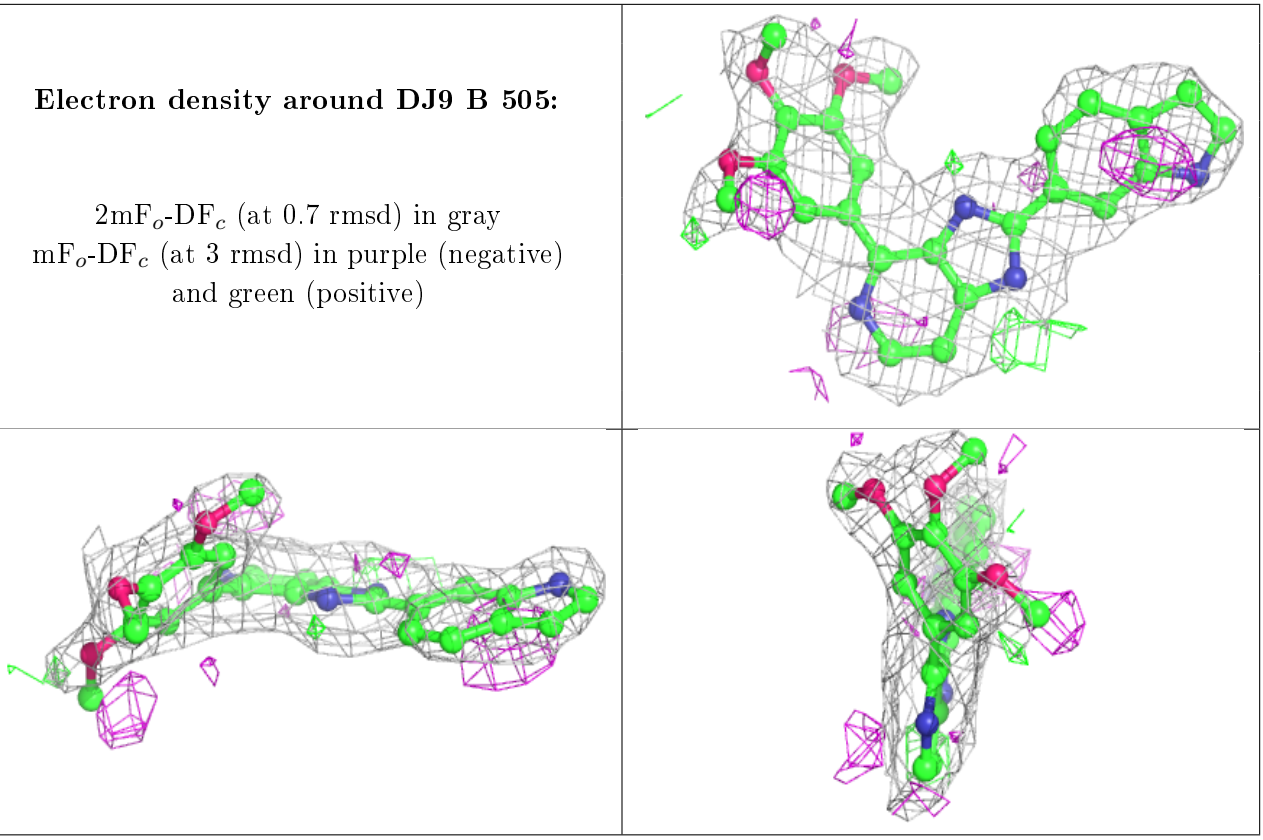
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.82	0.06	68,68,68,68	0
9	MES	B	503	12/12	0.83	0.22	64,85,106,110	0
10	DJ9	B	505	30/30	0.85	0.22	51,61,68,74	0
9	MES	B	504	12/12	0.89	0.23	61,67,89,92	0
11	ACP	F	402	31/31	0.90	0.17	63,86,116,117	0
6	MG	C	502	1/1	0.96	0.13	26,26,26,26	0
7	CA	A	503	1/1	0.96	0.04	61,61,61,61	0
7	CA	C	503	1/1	0.97	0.05	46,46,46,46	0
5	GTP	A	501	32/32	0.97	0.21	25,32,37,41	0
5	GTP	D	501	32/32	0.97	0.12	49,58,64,68	0
8	GDP	B	501	28/28	0.98	0.18	21,30,35,41	0
5	GTP	C	501	32/32	0.98	0.17	25,27,31,32	0
6	MG	B	502	1/1	0.98	0.18	33,33,33,33	0
6	MG	A	502	1/1	0.99	0.17	26,26,26,26	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.

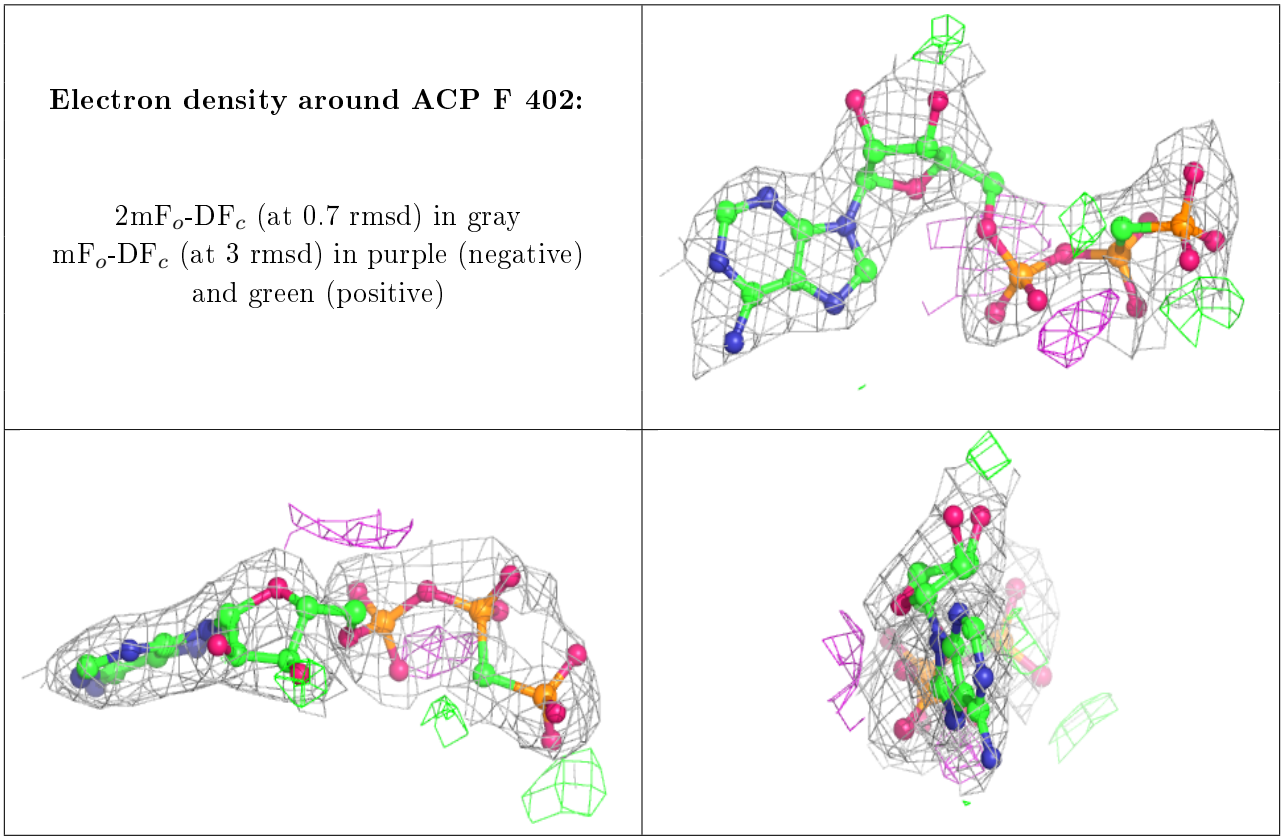
Electron density around DJ9 B 505:

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



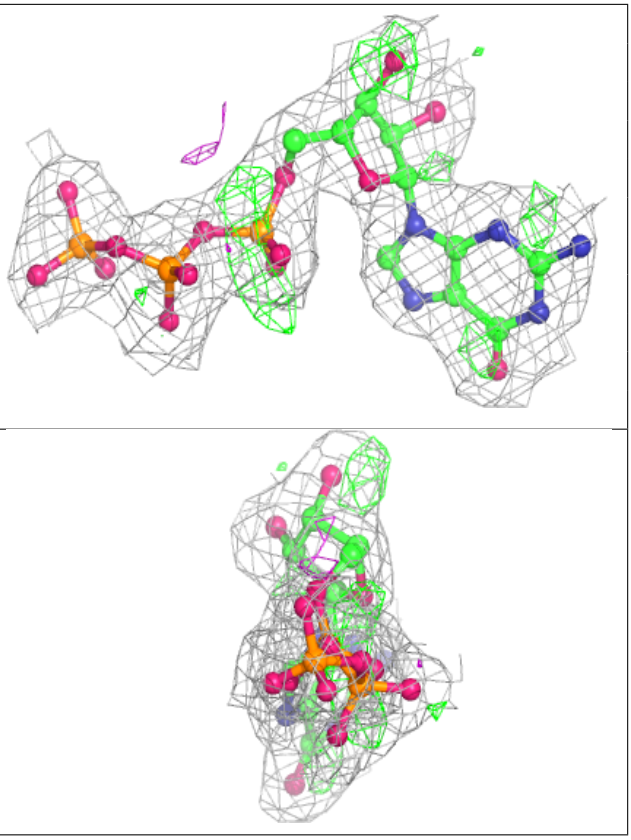
Electron density around ACP F 402:

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



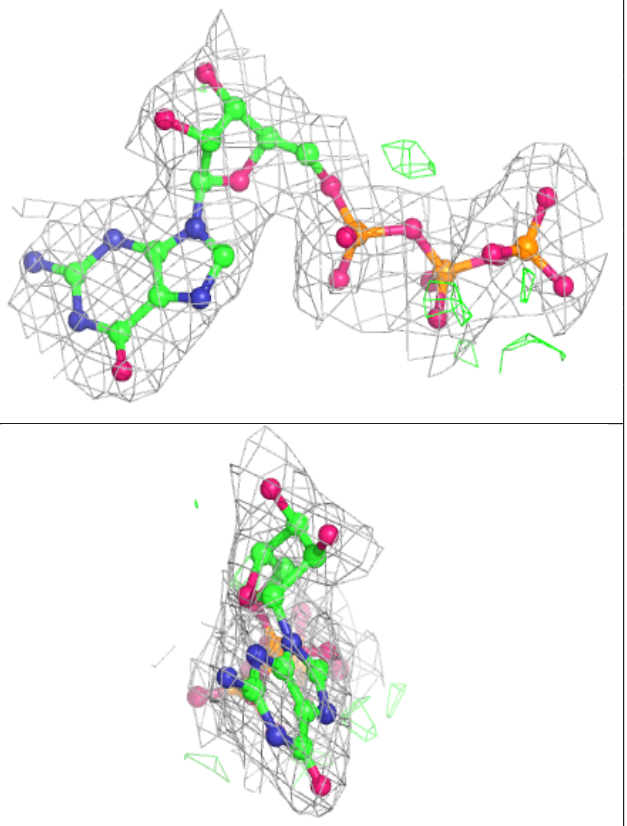
Electron density around GTP A 501:

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



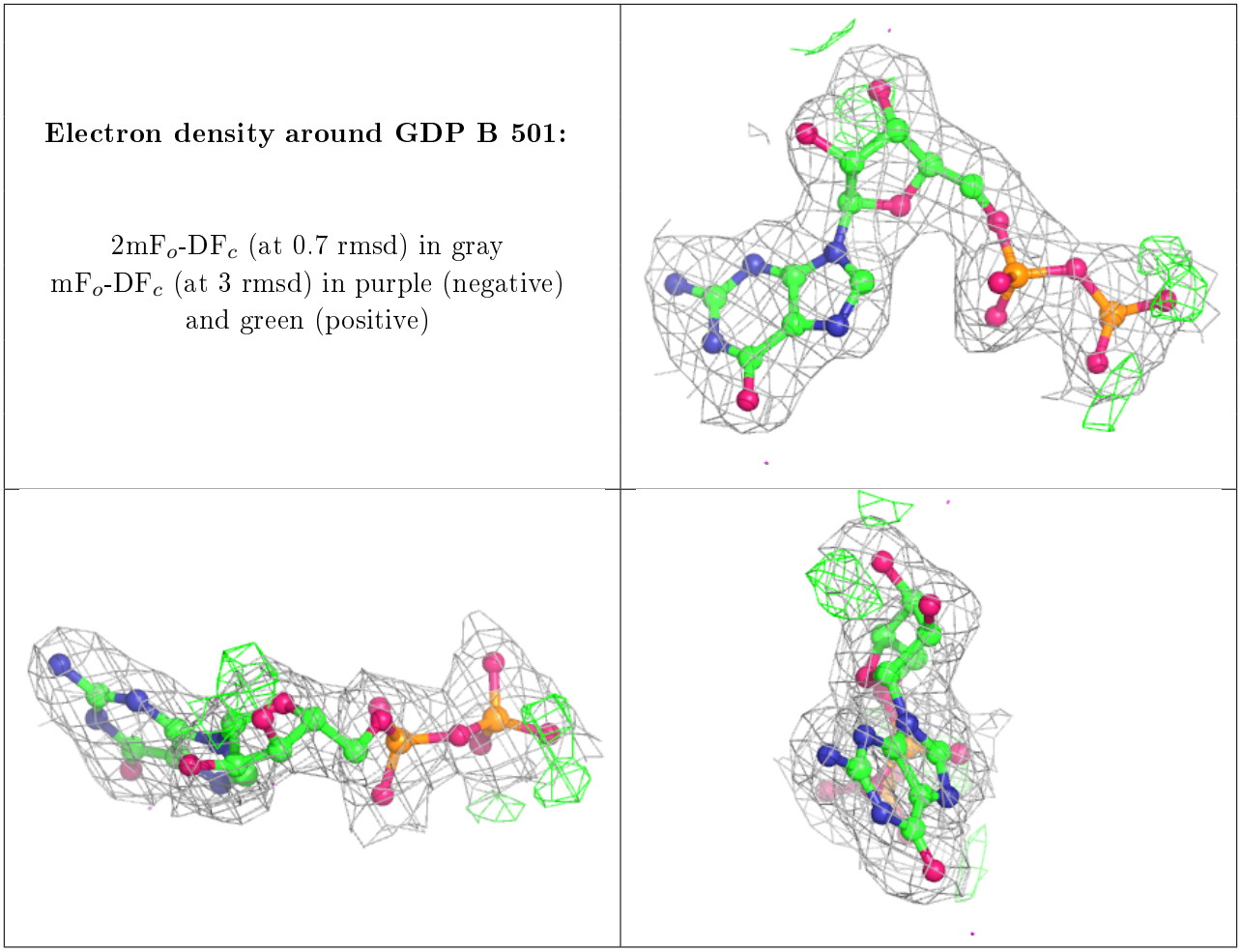
Electron density around GTP D 501:

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



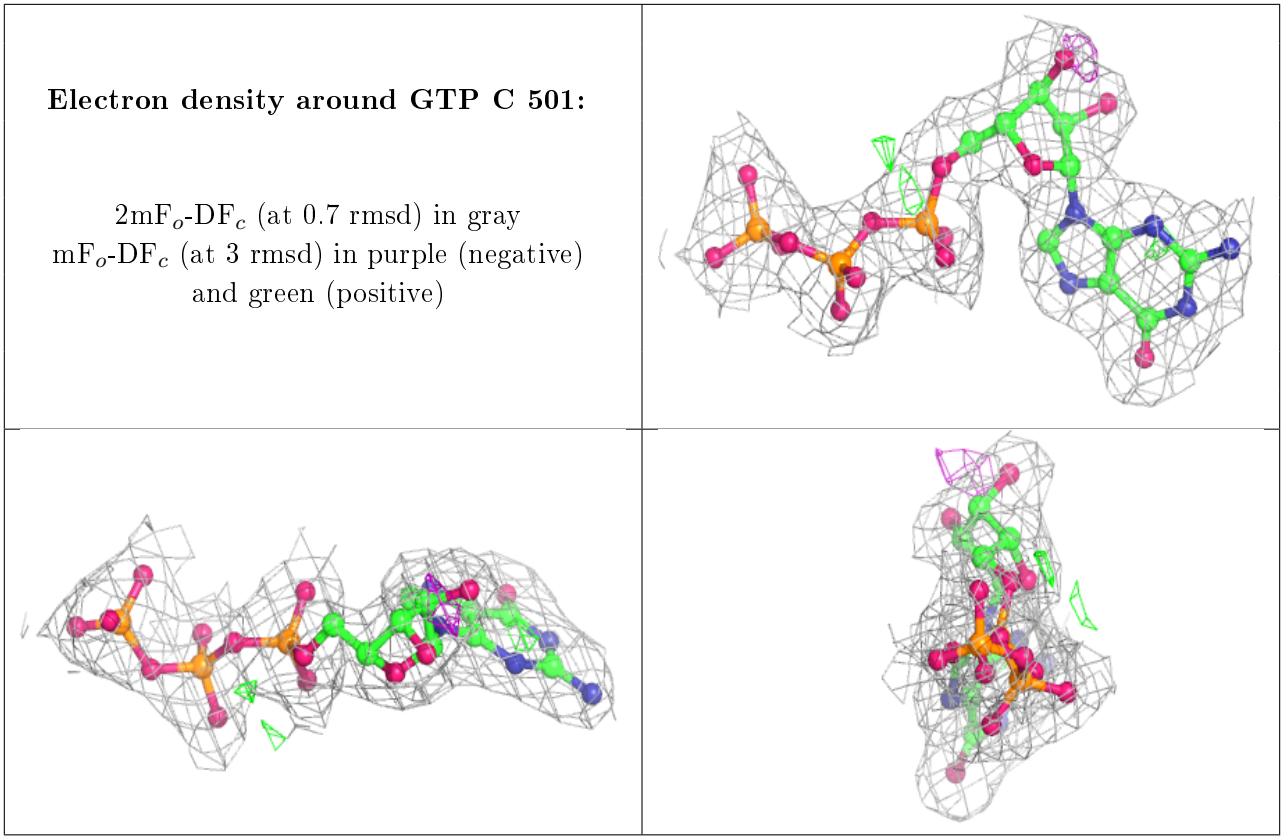
Electron density around GDP B 501:

$2mF_o$-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.