Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 07:04 am GMT

PDB ID	:	6GF3
Title	:	Tubulin-Jerantinine B acetate complex
Authors	:	Smedley, C.J.; Stanley, P.A.; Qazzaz, M.E.; Prota, A.E.; Olieric, N.; Collins, H.; Eastman, H.; Barrow, A.S.; Lim, K.-H.; Kam, T.-S.; Smith, B.J.; Duivenvoorden, H.M.; Parker, B.S.; Bradshaw, T.D.; Steinmetz, M.O.; Moses, J.E.
Deposited on	:	2018-04-29
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

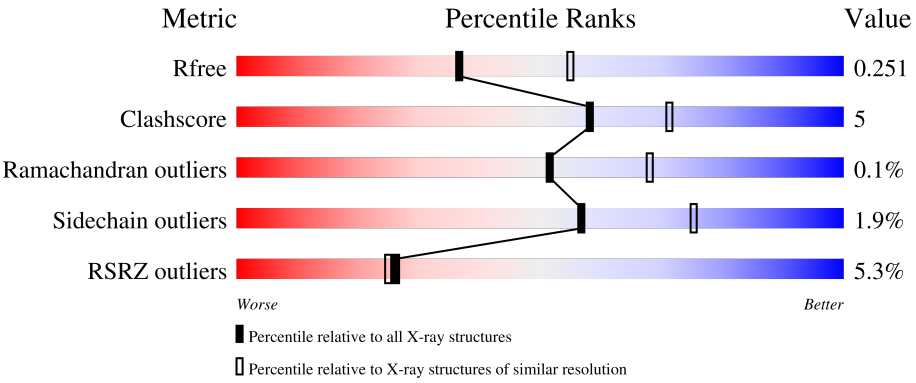
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.40 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.



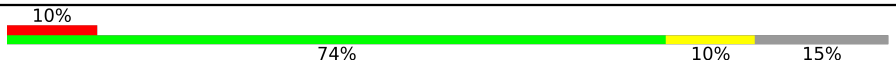
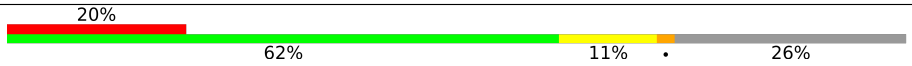
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	84% 12% •
1	C	451	87% 10% •
2	B	445	2% 81% 14% 5%
3	D	445	2% 82% 12% • 5%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 17309 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	437	Total	C	N	O	S	0	6	0
			3445	2188	583	652	22			
1	C	440	Total	C	N	O	S	0	8	0
			3474	2198	588	664	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	6	0
			3344	2103	569	645	27			

- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	421	Total	C	N	O	S	0	2	0
			3316	2085	562	641	28			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	247	ASN	GLN	conflict	UNP Q6B856

- Molecule 4 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	121	Total	C	N	O	S	0	1	0
			1006	621	182	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043

Continued on next page...

Continued from previous page...

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

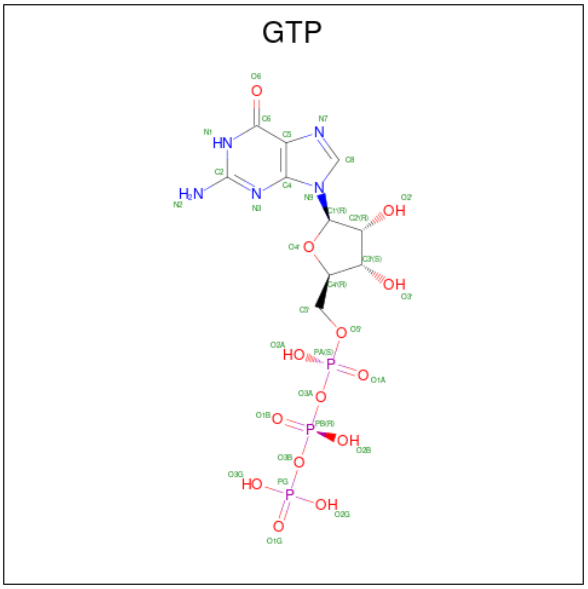
- Molecule 5 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	284	Total	C	N	O	S	0	4	0
			2354	1530	392	420	12			

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 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
6	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

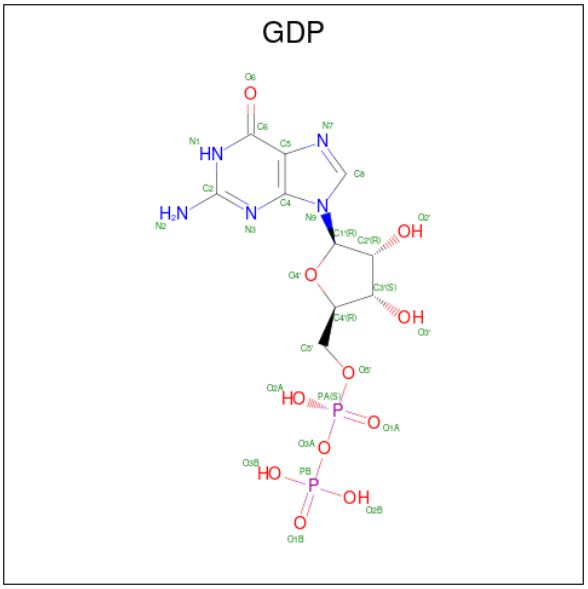
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

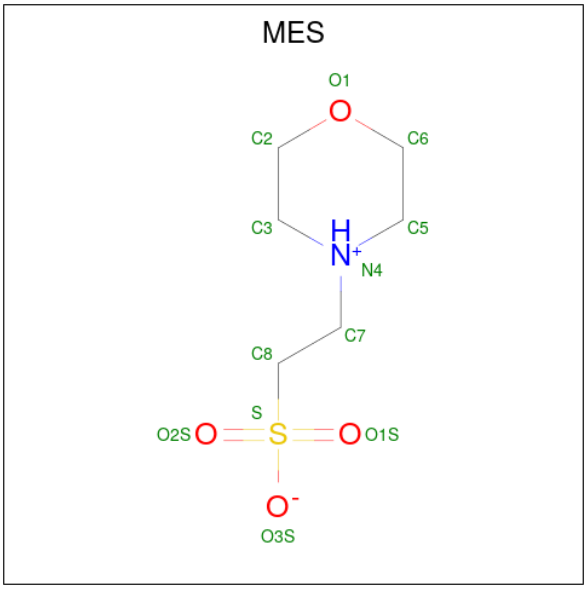
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

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



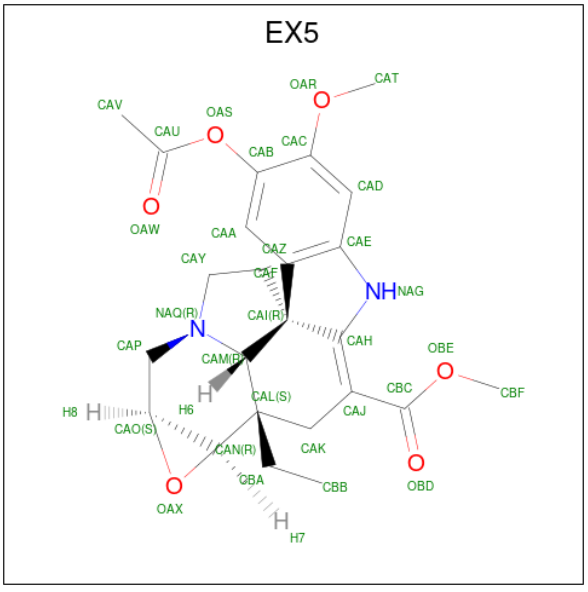
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O P 28 10 5 11 2	0	0
9	D	1	Total C N O P 28 10 5 11 2	0	0

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



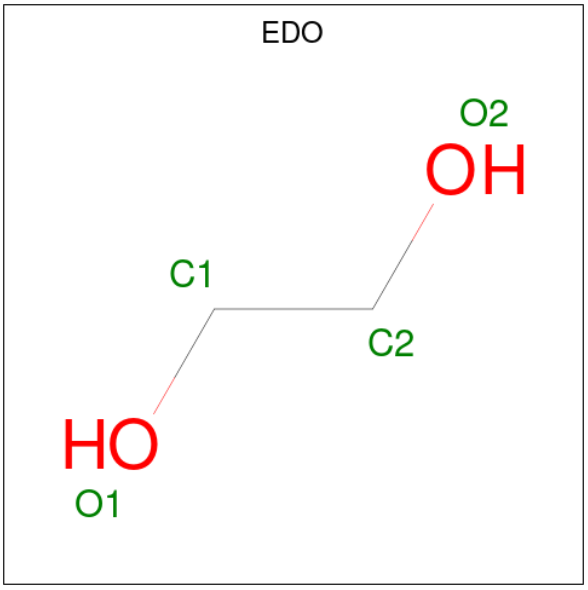
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is Jerantinine B (three-letter code: EX5) (formula: $C_{24}H_{28}N_2O_6$).



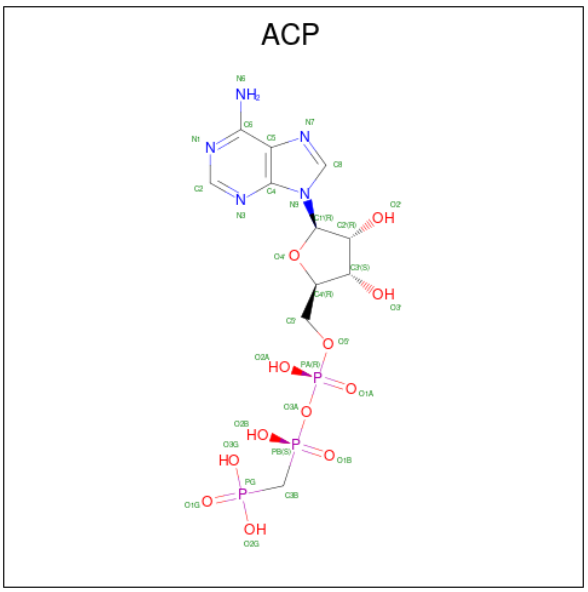
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			32	24	2	6		

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 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
13	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 14 is water.

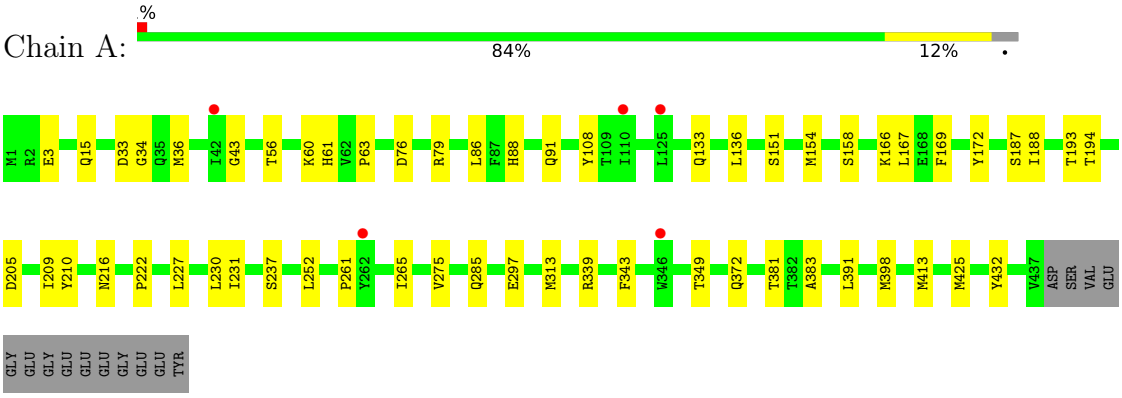
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	30	Total	O	0	0
			30	30		
14	B	30	Total	O	0	0
			30	30		
14	C	63	Total	O	0	0
			63	63		
14	D	9	Total	O	0	0
			9	9		
14	E	8	Total	O	0	0
			8	8		
14	F	13	Total	O	0	0
			13	13		

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.

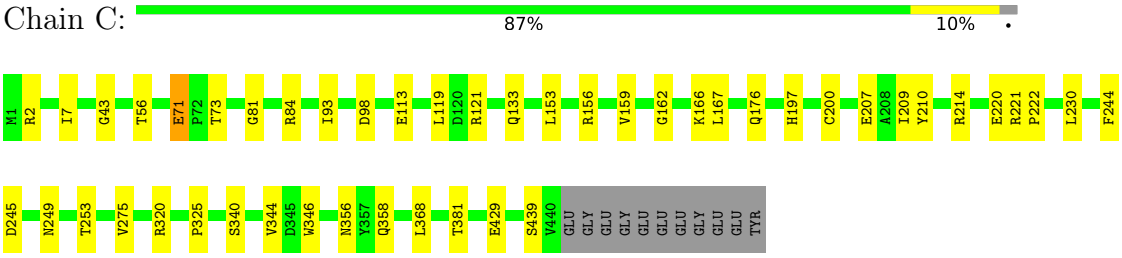
• Molecule 1: Tubulin alpha-1B chain

Chain A:



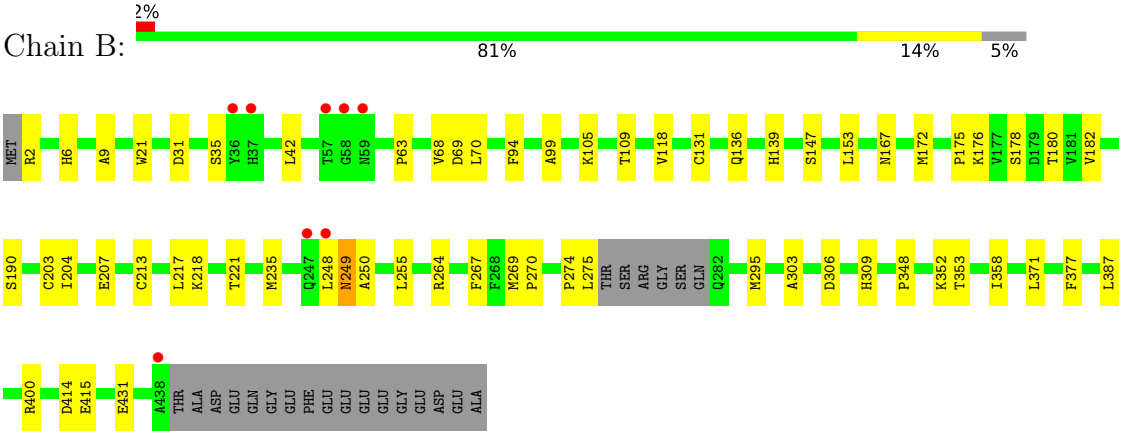
• Molecule 1: Tubulin alpha-1B chain

Chain C:



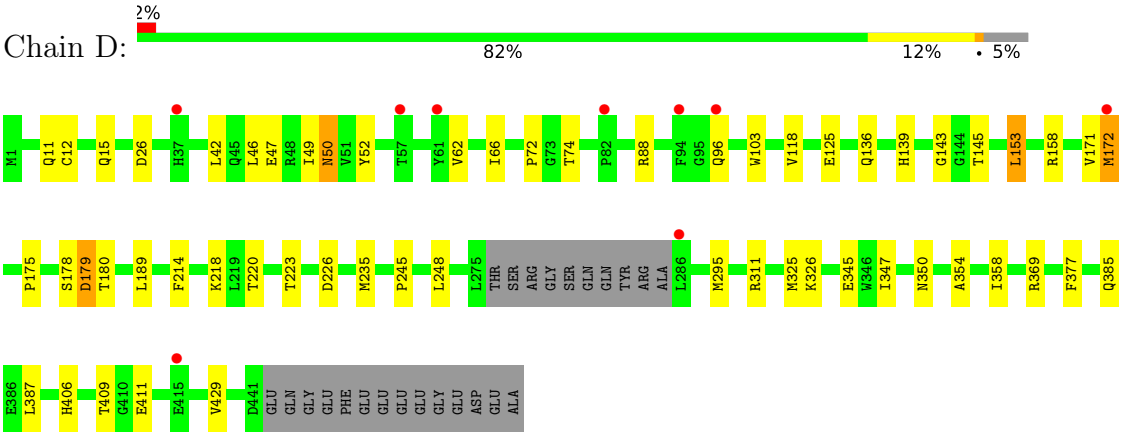
• Molecule 2: Tubulin beta-2B chain

Chain B:



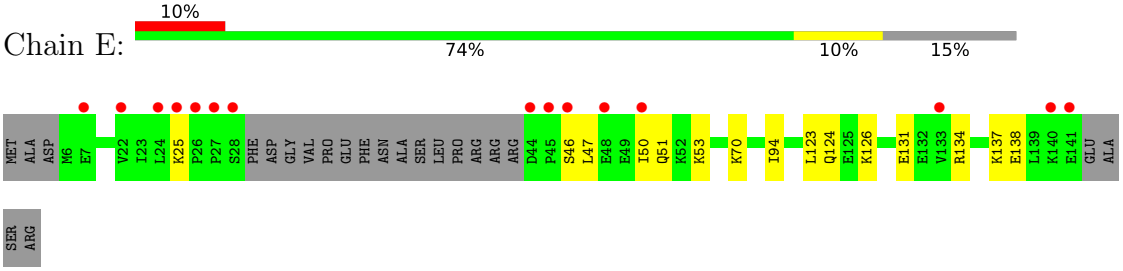
• Molecule 3: Tubulin beta-2B chain

Chain D:



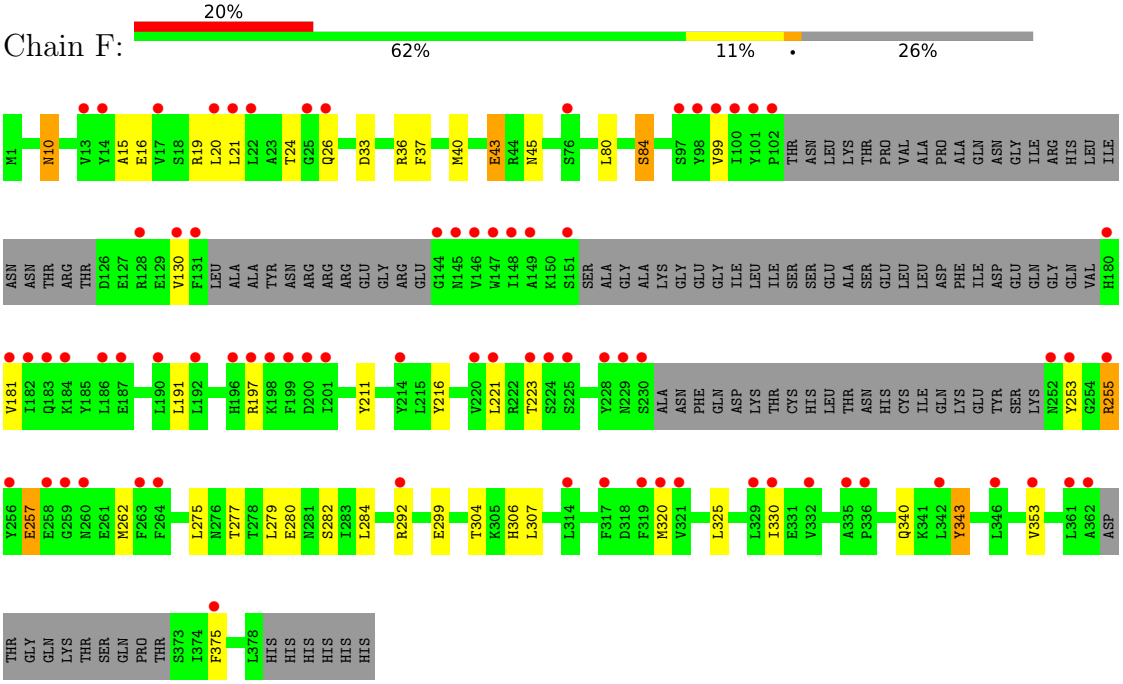
• Molecule 4: Stathmin-4

Chain E:



• Molecule 5: 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	104.72Å 158.15Å 180.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 2.40 52.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.96-2.40) 99.7 (52.27-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.198 , 0.251 0.198 , 0.251	Depositor DCC
R_{free} test set	5877 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	63.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17309	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: CA, MG, GDP, ACP, GTP, MES, EDO, EX5

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/3541	0.42	0/4808
1	C	0.27	0/3573	0.44	0/4852
2	B	0.26	0/3430	0.43	0/4646
3	D	0.25	0/3395	0.42	0/4599
4	E	0.24	0/1017	0.36	0/1349
5	F	0.25	0/2419	0.42	0/3266
All	All	0.26	0/17375	0.42	0/23520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3445	0	3384	33	0
1	C	3474	0	3393	29	0
2	B	3344	0	3224	36	0
3	D	3316	0	3201	36	0
4	E	1006	0	1026	11	0
5	F	2354	0	2361	26	0
6	A	32	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	32	0	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	5	0
10	B	12	0	12	1	0
10	D	12	0	12	1	0
11	B	32	0	0	0	0
12	C	4	0	6	1	0
13	F	31	0	14	2	0
14	A	30	0	0	1	0
14	B	30	0	0	0	0
14	C	63	0	0	0	0
14	D	9	0	0	1	0
14	E	8	0	0	0	0
14	F	13	0	0	1	0
All	All	17309	0	16681	163	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 (163) 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)
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.24	0.71
13:F:401:ACP:H8	13:F:401:ACP:H5'1	1.75	0.69
3:D:11:GLN:HA	3:D:74:THR:HG21	1.75	0.67
3:D:66:ILE:HD11	3:D:125:GLU:HG3	1.77	0.67
1:A:381:THR:HG22	1:A:383:ALA:H	1.61	0.66
4:E:131:GLU:OE1	4:E:134:ARG:NH1	2.28	0.66
3:D:62:VAL:HG11	3:D:88:ARG:HG3	1.79	0.64
5:F:292:ARG:NH2	14:F:502:HOH:O	2.30	0.64
5:F:280:GLU:HA	5:F:284[B]:LEU:HB2	1.80	0.64
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.79	0.63
2:B:118:VAL:HG11	2:B:153:LEU:HD21	1.80	0.62
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.80	0.62
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:24:THR:HG23	5:F:26:GLN:H	1.65	0.61
3:D:11:GLN:NE2	14:D:602:HOH:O	2.34	0.60
3:D:385:GLN:HB2	3:D:429:VAL:HG13	1.82	0.59
5:F:275:LEU:HD23	5:F:325:LEU:HD12	1.84	0.59
5:F:197:ARG:NH1	5:F:257:GLU:OE2	2.31	0.58
3:D:179:ASP:HB2	9:D:501:GDP:H3'	1.85	0.58
2:B:180:THR:HG22	2:B:182:VAL:H	1.69	0.57
3:D:118:VAL:HG11	3:D:153:LEU:HD11	1.86	0.57
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.23	0.57
1:C:162:GLY:HA2	4:E:94:ILE:HD11	1.88	0.56
3:D:47:GLU:HG2	3:D:245:PRO:HG3	1.87	0.55
5:F:279:LEU:HG	5:F:284[B]:LEU:HG	1.88	0.55
3:D:411:GLU:HA	4:E:137:LYS:HD2	1.89	0.55
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.89	0.55
3:D:46:LEU:HA	3:D:49:ILE:HB	1.91	0.53
5:F:255:ARG:CZ	5:F:255:ARG:HA	2.39	0.53
2:B:175:PRO:HA	2:B:178:SER:HB2	1.89	0.53
3:D:145:THR:N	9:D:501:GDP:O2B	2.39	0.53
3:D:158:ARG:HH21	10:D:503:MES:H52	1.73	0.52
3:D:406:HIS:HA	3:D:409:THR:HG22	1.90	0.52
3:D:347:ILE:HG22	3:D:350:ASN:HB3	1.92	0.52
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.92	0.51
3:D:175:PRO:HA	3:D:178:SER:HB3	1.92	0.51
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.43	0.50
5:F:223:THR:OG1	5:F:257:GLU:OE2	2.24	0.50
2:B:249:ASN:H	2:B:249:ASN:HD22	1.58	0.50
1:C:71:GLU:HG2	1:C:73:THR:H	1.76	0.50
1:A:3:GLU:O	1:A:133:GLN:HG2	2.12	0.50
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.94	0.50
5:F:216:TYR:HA	5:F:375:PHE:HD1	1.76	0.50
1:A:154:MET:HG3	1:A:194:THR:HG23	1.93	0.50
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.94	0.50
5:F:99:VAL:HG12	5:F:181:VAL:HG12	1.93	0.49
5:F:340:GLN:HA	5:F:343:TYR:HD2	1.77	0.49
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.93	0.49
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.95	0.49
3:D:172:MET:HG2	3:D:387:LEU:HD11	1.95	0.48
5:F:282:SER:HB2	5:F:325:LEU:HD13	1.95	0.48
5:F:80:LEU:O	5:F:84:SER:HB2	2.13	0.48
1:A:158:SER:OG	1:A:166:LYS:NZ	2.46	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:HA3	1:A:60:LYS:HD3	1.95	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.48
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.49	0.48
3:D:248:LEU:HD23	3:D:354:ALA:HB2	1.95	0.48
1:A:151:SER:HB2	1:A:193:THR:HB	1.95	0.48
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.23	0.48
5:F:320:MET:HB2	5:F:330:ILE:HD11	1.95	0.48
5:F:21:LEU:O	5:F:24:THR:HG22	2.13	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.96	0.47
3:D:72:PRO:HG3	3:D:96:GLN:HE22	1.79	0.47
3:D:158:ARG:HD3	4:E:123:LEU:HD11	1.95	0.47
3:D:26:ASP:CG	3:D:369:ARG:HE	2.18	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.47
5:F:43:GLU:HG3	5:F:45:ASN:O	2.15	0.47
1:C:159:VAL:HA	4:E:94:ILE:HG23	1.97	0.47
4:E:126:LYS:HE3	4:E:126:LYS:HB3	1.73	0.47
1:C:221:ARG:NH1	3:D:325:MET:HB3	2.30	0.47
1:A:136[B]:LEU:HD23	1:A:169:PHE:HE2	1.80	0.47
2:B:69:ASP:O	2:B:94:PHE:HA	2.15	0.46
1:C:245:ASP:N	1:C:245:ASP:OD1	2.48	0.46
2:B:136:GLN:HA	2:B:167:ASN:O	2.15	0.46
1:C:244:PHE:CD1	1:C:358[B]:GLN:HG2	2.51	0.46
1:A:349:THR:HB	4:E:25:LYS:HB3	1.97	0.46
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.97	0.46
1:C:166:LYS:HE2	1:C:197:HIS:O	2.16	0.46
2:B:274:PRO:HD2	2:B:371:LEU:HD13	1.97	0.46
1:C:244:PHE:HB2	1:C:356[B]:ASN:HD21	1.80	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.45
3:D:214:PHE:CE2	3:D:220:THR:HA	2.51	0.45
1:C:98:ASP:HB2	6:C:501:GTP:O3G	2.17	0.45
1:C:220:GLU:HB3	3:D:326:LYS:HD2	1.99	0.45
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.82	0.44
3:D:11:GLN:N	9:D:501:GDP:O3B	2.46	0.44
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.83	0.44
2:B:221:THR:HG21	1:C:325:PRO:HB2	1.98	0.44
2:B:180:THR:CG2	2:B:182:VAL:HG22	2.48	0.44
2:B:250:ALA:HB1	2:B:255:LEU:HD21	2.00	0.44
2:B:269:MET:HG2	2:B:303:ALA:HB3	1.99	0.44
2:B:400:ARG:HE	1:C:439:SER:HB3	1.83	0.44
1:C:81:GLY:O	1:C:84:ARG:NH1	2.47	0.44
5:F:10:ASN:OD1	5:F:10:ASN:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.43
1:A:209[B]:ILE:HG13	1:A:227:LEU:HD22	2.00	0.43
2:B:235:MET:HB3	2:B:235:MET:HE2	1.85	0.43
4:E:46:SER:OG	4:E:47:LEU:N	2.51	0.43
13:F:401:ACP:O2G	13:F:401:ACP:O1A	2.36	0.43
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	2.00	0.43
3:D:235:MET:HB3	3:D:235:MET:HE2	1.89	0.43
2:B:180:THR:HG22	2:B:182:VAL:HG22	1.99	0.43
4:E:50:ILE:HA	4:E:53:LYS:HD3	2.00	0.43
1:A:15:GLN:NE2	6:A:501:GTP:O6	2.51	0.43
1:A:63:PRO:HD3	1:A:86:LEU:HD12	2.01	0.43
3:D:295:MET:HG2	3:D:377:PHE:HB2	2.01	0.43
3:D:143:GLY:HA3	9:D:501:GDP:O3A	2.18	0.43
3:D:52:TYR:OH	3:D:136:GLN:NE2	2.49	0.43
1:A:237:SER:HB2	14:A:614:HOH:O	2.19	0.42
5:F:221:LEU:HD22	5:F:262:MET:HE3	2.00	0.42
2:B:9:ALA:HA	2:B:68:VAL:O	2.20	0.42
3:D:50:ASN:ND2	3:D:50:ASN:H	2.17	0.42
5:F:340:GLN:N	5:F:340:GLN:OE1	2.52	0.42
1:A:285:GLN:HG3	1:A:372[B]:GLN:OE1	2.20	0.42
2:B:264[A]:ARG:NE	2:B:431:GLU:OE1	2.38	0.42
3:D:12:CYS:SG	3:D:171:VAL:HG21	2.59	0.42
5:F:15:ALA:O	5:F:19:ARG:HG3	2.19	0.42
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.01	0.42
2:B:70:LEU:HD12	2:B:99:ALA:HB2	2.01	0.42
3:D:223:THR:HG22	3:D:226:ASP:OD1	2.20	0.42
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.36	0.42
2:B:2:ARG:HA	2:B:131:CYS:O	2.20	0.42
2:B:42:LEU:HB3	2:B:358:ILE:HD11	2.01	0.42
3:D:214:PHE:O	3:D:218:LYS:HD2	2.19	0.42
3:D:218:LYS:HB3	3:D:218:LYS:HE3	1.86	0.42
10:B:502:MES:H81	10:B:502:MES:H51	1.78	0.42
3:D:42:LEU:HB2	3:D:358:ILE:HD11	2.01	0.42
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
4:E:70:LYS:HB2	4:E:70:LYS:HE3	1.72	0.41
5:F:37:PHE:CE1	5:F:40:MET:HB2	2.54	0.41
5:F:216:TYR:HA	5:F:375:PHE:CD1	2.55	0.41
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.01	0.41
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.55	0.41
2:B:414:ASP:OD1	2:B:415:GLU:N	2.52	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:33:ASP:OD1	5:F:33:ASP:N	2.53	0.41
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.56	0.41
2:B:31:ASP:OD2	2:B:35:SER:OG	2.38	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.55	0.41
1:C:244:PHE:CZ	1:C:358[A]:GLN:HG2	2.55	0.41
5:F:16:GLU:OE1	5:F:19:ARG:NH2	2.38	0.41
1:A:43:GLY:HA2	1:A:56:THR:O	2.21	0.41
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.56	0.41
1:A:398:MET:HG3	2:B:348:PRO:HD2	2.03	0.41
2:B:204:ILE:HD13	2:B:270:PRO:HG2	2.02	0.41
1:C:2:ARG:HH21	1:C:133:GLN:NE2	2.19	0.41
1:C:43:GLY:HA2	1:C:56:THR:O	2.21	0.41
2:B:352:LYS:HD3	2:B:353:THR:N	2.35	0.41
1:C:253:THR:HB	12:C:504:EDO:H11	2.03	0.41
3:D:11:GLN:HB2	9:D:501:GDP:O2A	2.21	0.41
2:B:295:MET:CG	2:B:377:PHE:HB2	2.51	0.40
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.86	0.40
1:A:297:GLU:OE1	5:F:306:HIS:ND1	2.43	0.40
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.61	0.40
1:C:210:TYR:HE2	1:C:214:ARG:HH11	1.70	0.40
4:E:47:LEU:O	4:E:51:GLN:HG2	2.22	0.40
5:F:304:THR:HG22	5:F:307:LEU:HD12	2.02	0.40
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.56	0.40
2:B:218:LYS:HD3	2:B:218:LYS:HA	1.94	0.40
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.04	0.40
3:D:103:TRP:CE3	3:D:189:LEU:HD13	2.56	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	441/451 (98%)	429 (97%)	12 (3%)	0	100	100
1	C	446/451 (99%)	438 (98%)	8 (2%)	0	100	100
2	B	423/445 (95%)	410 (97%)	12 (3%)	1 (0%)	47	62
3	D	419/445 (94%)	404 (96%)	15 (4%)	0	100	100
4	E	118/143 (82%)	115 (98%)	3 (2%)	0	100	100
5	F	275/384 (72%)	257 (94%)	17 (6%)	1 (0%)	34	48
All	All	2122/2319 (92%)	2053 (97%)	67 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	253	TYR
2	B	248	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	374/379 (99%)	373 (100%)	1 (0%)	92	97
1	C	379/379 (100%)	374 (99%)	5 (1%)	69	84
2	B	369/383 (96%)	366 (99%)	3 (1%)	81	91
3	D	366/383 (96%)	357 (98%)	9 (2%)	47	67
4	E	110/127 (87%)	108 (98%)	2 (2%)	59	76
5	F	261/342 (76%)	246 (94%)	15 (6%)	20	33
All	All	1859/1993 (93%)	1824 (98%)	35 (2%)	57	75

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
2	B	139	HIS
2	B	249	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	275	LEU
1	C	71	GLU
1	C	113	GLU
1	C	340	SER
1	C	381	THR
1	C	429	GLU
3	D	15	GLN
3	D	50	ASN
3	D	139	HIS
3	D	153	LEU
3	D	172	MET
3	D	179	ASP
3	D	180	THR
3	D	311	ARG
3	D	345	GLU
4	E	124	GLN
4	E	138	GLU
5	F	10	ASN
5	F	20	LEU
5	F	36	ARG
5	F	43	GLU
5	F	84	SER
5	F	130	VAL
5	F	191	LEU
5	F	211	TYR
5	F	255	ARG
5	F	257	GLU
5	F	277	THR
5	F	299	GLU
5	F	343	TYR
5	F	353[A]	VAL
5	F	353[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	HIS
2	B	11	GLN
2	B	247	GLN
2	B	249	ASN
1	C	133	GLN
1	C	285	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	372	GLN
3	D	96	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	GDP	B	501	7	24,30,30	0.96	1 (4%)	30,47,47	1.11	3 (10%)
10	MES	D	503	-	12,12,12	2.27	1 (8%)	14,16,16	1.91	4 (28%)
9	GDP	D	501	7	24,30,30	0.95	1 (4%)	30,47,47	1.22	4 (13%)
12	EDO	C	504	-	3,3,3	0.47	0	2,2,2	0.33	0
10	MES	B	502	-	12,12,12	2.21	1 (8%)	14,16,16	1.82	2 (14%)
6	GTP	A	501	7	26,34,34	1.15	2 (7%)	32,54,54	1.43	6 (18%)
13	ACP	F	401	-	27,33,33	1.82	6 (22%)	32,52,52	1.28	4 (12%)
11	EX5	B	503	-	36,37,37	3.01	12 (33%)	49,60,60	2.27	18 (36%)
6	GTP	C	501	7	26,34,34	1.17	2 (7%)	32,54,54	1.38	6 (18%)

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	GDP	B	501	7	-	3/12/32/32	0/3/3/3
10	MES	D	503	-	-	1/6/14/14	0/1/1/1
9	GDP	D	501	7	-	2/12/32/32	0/3/3/3
12	EDO	C	504	-	-	0/1/1/1	-
10	MES	B	502	-	-	0/6/14/14	0/1/1/1
6	GTP	A	501	7	-	7/18/38/38	0/3/3/3
13	ACP	F	401	-	-	3/15/38/38	0/3/3/3
11	EX5	B	503	-	-	6/15/77/77	0/6/6/6
6	GTP	C	501	7	-	6/18/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	503	EX5	CAI-CAF	-8.92	1.38	1.51
11	B	503	EX5	CAK-CAL	8.44	1.67	1.54
10	D	503	MES	C8-S	-7.59	1.66	1.77
10	B	502	MES	C8-S	-7.39	1.67	1.77
11	B	503	EX5	CAI-CAH	-6.50	1.40	1.52
13	F	401	ACP	PG-O1G	5.39	1.61	1.50
11	B	503	EX5	CAE-NAG	-4.67	1.30	1.38
11	B	503	EX5	CAZ-CAY	4.47	1.61	1.52
6	C	501	GTP	C5-C6	-4.23	1.38	1.47
13	F	401	ACP	PB-O3A	4.13	1.63	1.58
11	B	503	EX5	CAH-NAG	-4.02	1.31	1.38
6	A	501	GTP	C5-C6	-4.01	1.39	1.47
11	B	503	EX5	CAK-CAJ	-3.69	1.44	1.50
11	B	503	EX5	CBC-CAJ	-3.49	1.39	1.47
11	B	503	EX5	CAD-CAC	3.40	1.45	1.38
11	B	503	EX5	CAA-CAB	3.03	1.44	1.38
13	F	401	ACP	PG-O3G	-2.64	1.48	1.54
13	F	401	ACP	C2'-C1'	-2.59	1.49	1.53
13	F	401	ACP	PG-O2G	2.54	1.60	1.54
11	B	503	EX5	CAI-CAM	2.48	1.61	1.56
9	D	501	GDP	C6-N1	-2.31	1.34	1.37
9	B	501	GDP	C6-N1	-2.28	1.34	1.37
6	C	501	GTP	C2-N3	2.17	1.38	1.33
6	A	501	GTP	C2-N3	2.14	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	503	EX5	CAZ-CAI	2.10	1.59	1.55
13	F	401	ACP	C5-C4	2.10	1.46	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	503	EX5	CAF-CAI-CAH	6.50	106.91	101.25
11	B	503	EX5	CAI-CAM-NAQ	5.64	111.18	104.39
11	B	503	EX5	CAZ-CAI-CAM	-4.74	97.76	102.87
10	D	503	MES	C5-N4-C3	4.51	118.98	108.83
10	B	502	MES	C5-N4-C3	4.51	118.97	108.83
11	B	503	EX5	CAB-OAS-CAU	4.21	126.63	117.65
11	B	503	EX5	CBF-OBE-CBC	-3.68	108.90	115.86
11	B	503	EX5	CAK-CAL-CAM	-3.54	101.05	109.53
11	B	503	EX5	CAZ-CAI-CAF	-3.41	98.65	110.41
6	C	501	GTP	C5-C6-N1	3.32	119.82	113.95
9	D	501	GDP	PA-O3A-PB	-3.30	121.49	132.83
11	B	503	EX5	CAF-CAI-CAM	3.13	124.09	118.55
10	B	502	MES	O1S-S-C8	3.07	110.62	106.92
6	A	501	GTP	C5-C6-N1	3.05	119.34	113.95
6	A	501	GTP	C8-N7-C5	3.04	108.79	102.99
13	F	401	ACP	N3-C2-N1	-3.04	123.93	128.68
11	B	503	EX5	CBB-CBA-CAL	-2.96	110.81	116.59
6	C	501	GTP	C8-N7-C5	2.95	108.61	102.99
11	B	503	EX5	CAY-NAQ-CAM	-2.93	98.99	105.89
6	C	501	GTP	C2-N1-C6	-2.87	119.81	125.10
6	A	501	GTP	PA-O3A-PB	-2.86	123.00	132.83
6	A	501	GTP	C2-N1-C6	-2.86	119.83	125.10
6	A	501	GTP	PB-O3B-PG	-2.79	123.24	132.83
11	B	503	EX5	CBA-CAL-CAM	2.79	114.02	109.63
11	B	503	EX5	OBE-CBC-CAJ	2.69	116.83	112.29
10	D	503	MES	O3S-S-C8	2.68	110.11	105.77
11	B	503	EX5	CAI-CAF-CAE	-2.66	105.66	108.35
9	B	501	GDP	PA-O3A-PB	-2.60	123.89	132.83
6	C	501	GTP	PB-O3B-PG	-2.60	123.89	132.83
13	F	401	ACP	C4-C5-N7	-2.54	106.75	109.40
9	D	501	GDP	C3'-C2'-C1'	2.41	104.61	100.98
9	B	501	GDP	C8-N7-C5	2.39	107.54	102.99
9	B	501	GDP	C5-C6-N1	2.38	118.15	113.95
9	D	501	GDP	C8-N7-C5	2.35	107.47	102.99
11	B	503	EX5	CAK-CAJ-CAH	2.29	121.50	117.34
6	C	501	GTP	O6-C6-C5	-2.25	119.97	124.37

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	2.22	117.87	113.95
6	A	501	GTP	O6-C6-C5	-2.17	120.13	124.37
11	B	503	EX5	CAZ-CAY-NAQ	-2.16	99.73	104.48
13	F	401	ACP	C3'-C2'-C1'	2.16	104.22	100.98
11	B	503	EX5	CAO-OAX-CAN	2.12	64.10	60.99
10	D	503	MES	O2S-S-C8	2.09	109.43	106.92
13	F	401	ACP	O2G-PG-C3B	2.09	111.46	106.40
6	C	501	GTP	PA-O3A-PB	-2.08	125.68	132.83
10	D	503	MES	C7-N4-C5	2.05	116.47	111.23
11	B	503	EX5	OBD-CBC-CAJ	-2.04	120.94	125.14
11	B	503	EX5	CAL-CAM-NAQ	2.02	115.92	111.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	GTP	PB-O3B-PG-O3G
6	A	501	GTP	C5'-O5'-PA-O1A
6	C	501	GTP	PB-O3B-PG-O2G
6	C	501	GTP	C5'-O5'-PA-O1A
6	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O2A
13	F	401	ACP	PG-C3B-PB-O1B
13	F	401	ACP	PG-C3B-PB-O2B
11	B	503	EX5	CAJ-CBC-OBE-CBF
11	B	503	EX5	OBD-CBC-OBE-CBF
11	B	503	EX5	CAV-CAU-OAS-CAB
11	B	503	EX5	OAW-CAU-OAS-CAB
13	F	401	ACP	O4'-C4'-C5'-O5'
10	D	503	MES	C8-C7-N4-C3
11	B	503	EX5	CAM-CAL-CBA-CBB
6	A	501	GTP	C5'-O5'-PA-O3A
11	B	503	EX5	CAN-CAL-CBA-CBB
6	A	501	GTP	PB-O3A-PA-O2A
6	C	501	GTP	PB-O3A-PA-O2A
6	A	501	GTP	C5'-O5'-PA-O2A
6	C	501	GTP	C4'-C5'-O5'-PA
6	A	501	GTP	PB-O3B-PG-O1G
6	A	501	GTP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A

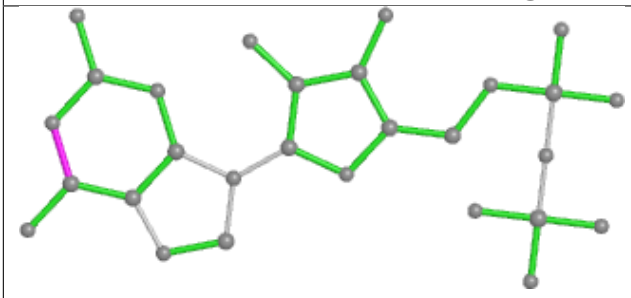
There are no ring outliers.

7 monomers are involved in 12 short contacts:

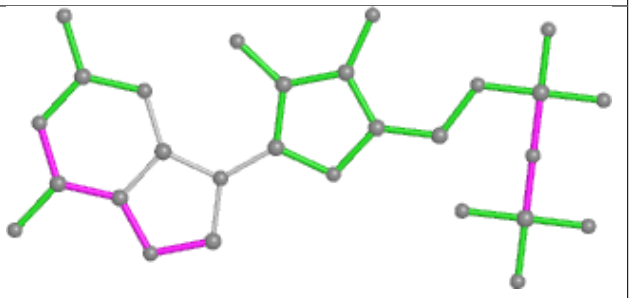
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	MES	1	0
9	D	501	GDP	5	0
12	C	504	EDO	1	0
10	B	502	MES	1	0
6	A	501	GTP	1	0
13	F	401	ACP	2	0
6	C	501	GTP	1	0

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.

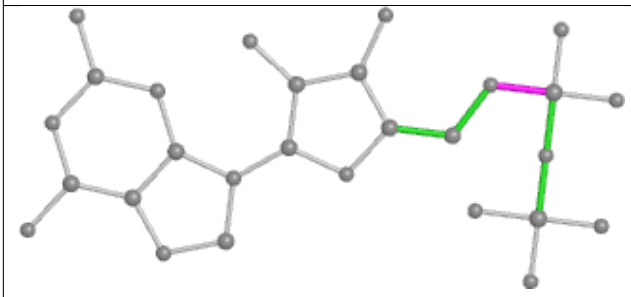
Ligand GDP B 501



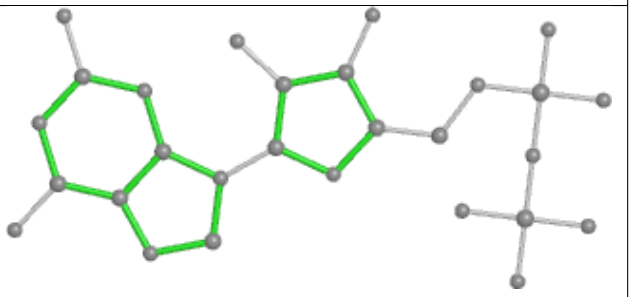
Bond lengths



Bond angles

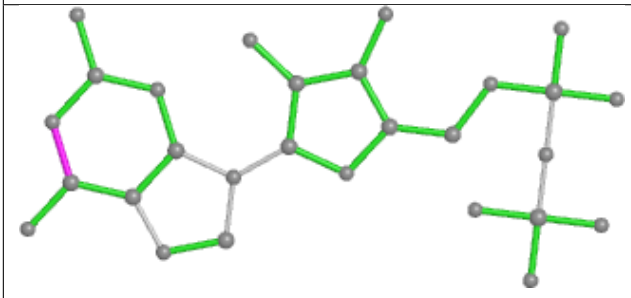


Torsions

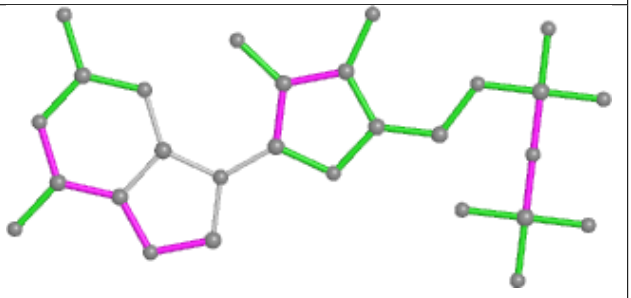


Rings

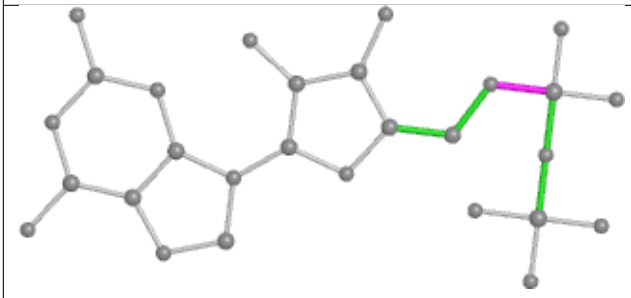
Ligand GDP D 501



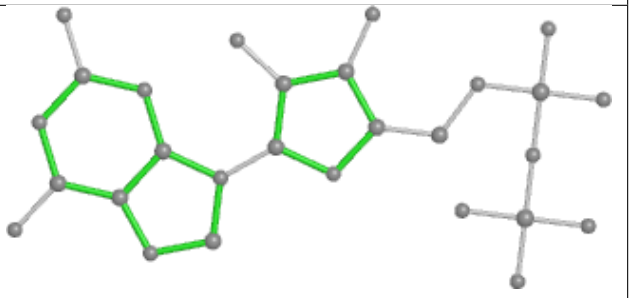
Bond lengths



Bond angles

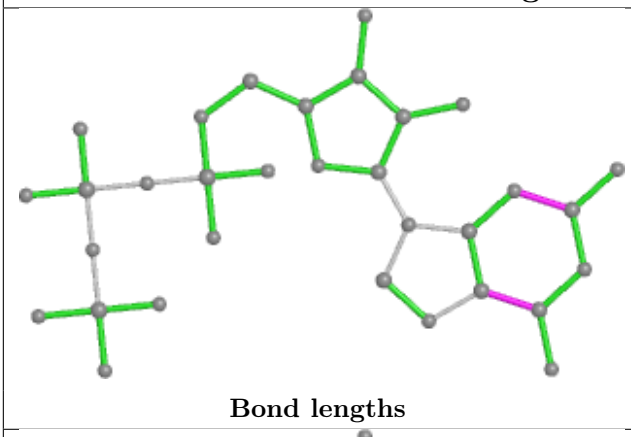


Torsions

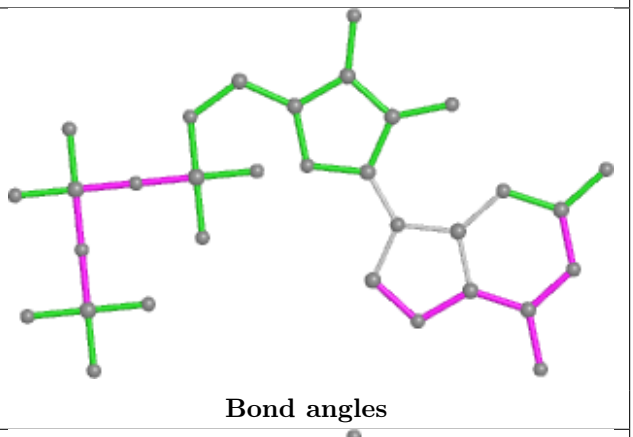


Rings

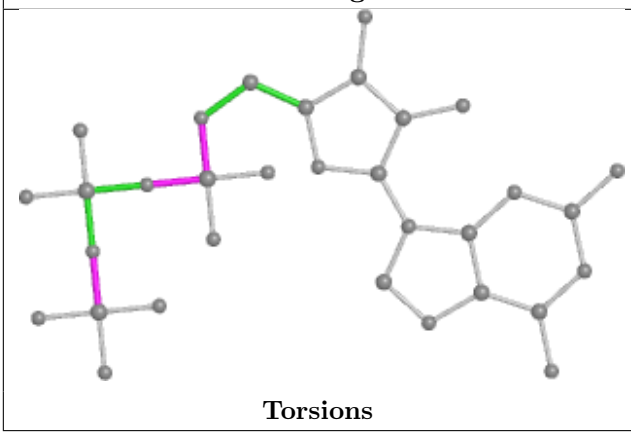
Ligand GTP A 501



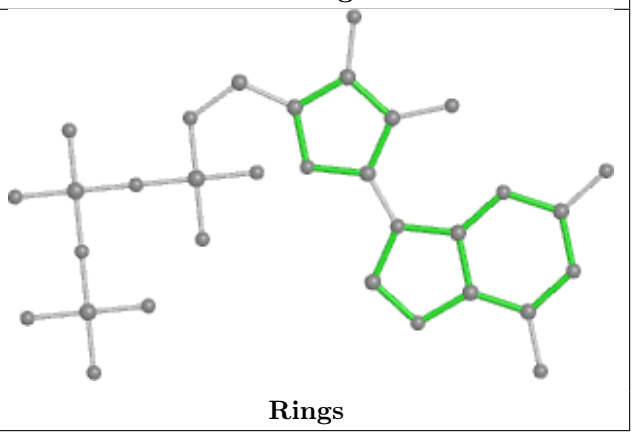
Bond lengths



Bond angles

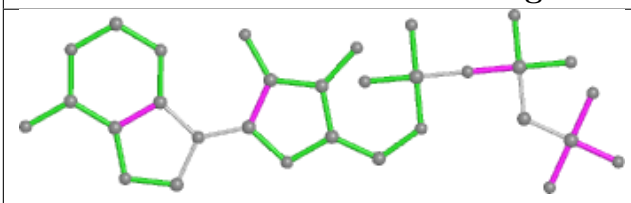


Torsions

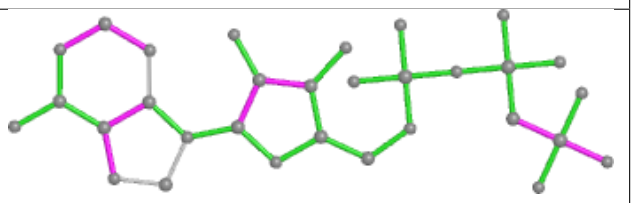


Rings

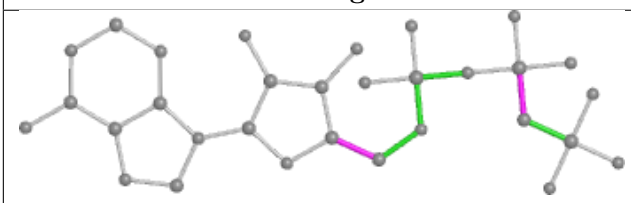
Ligand ACP F 401



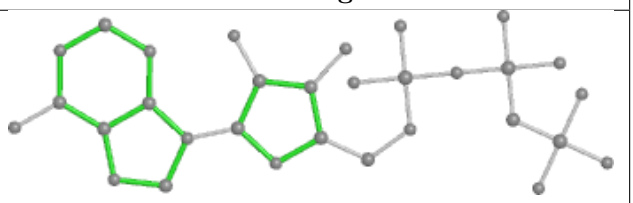
Bond lengths



Bond angles

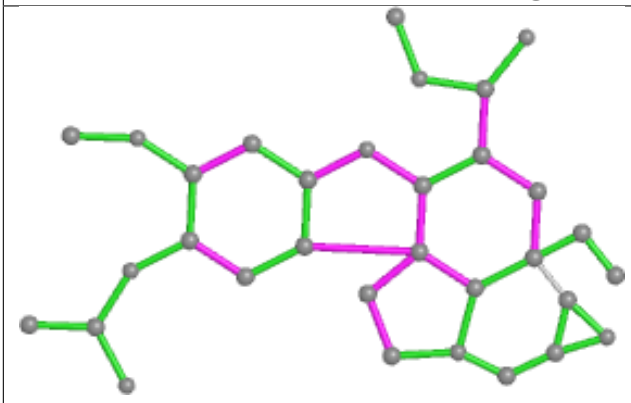


Torsions

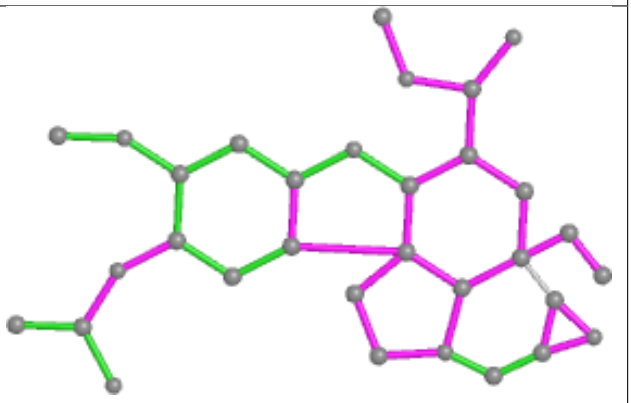


Rings

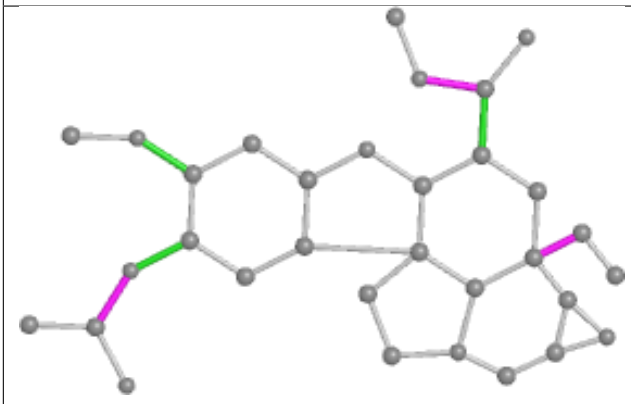
Ligand EX5 B 503



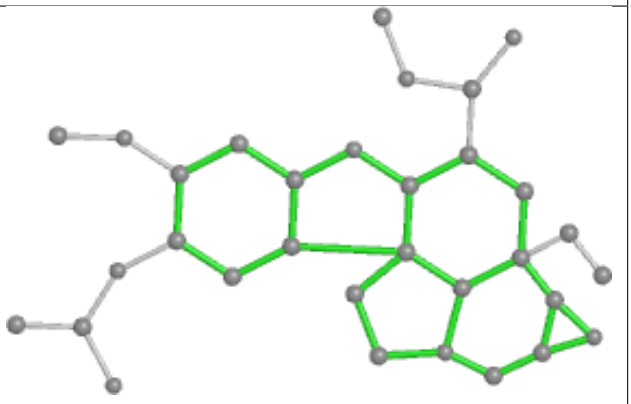
Bond lengths



Bond angles

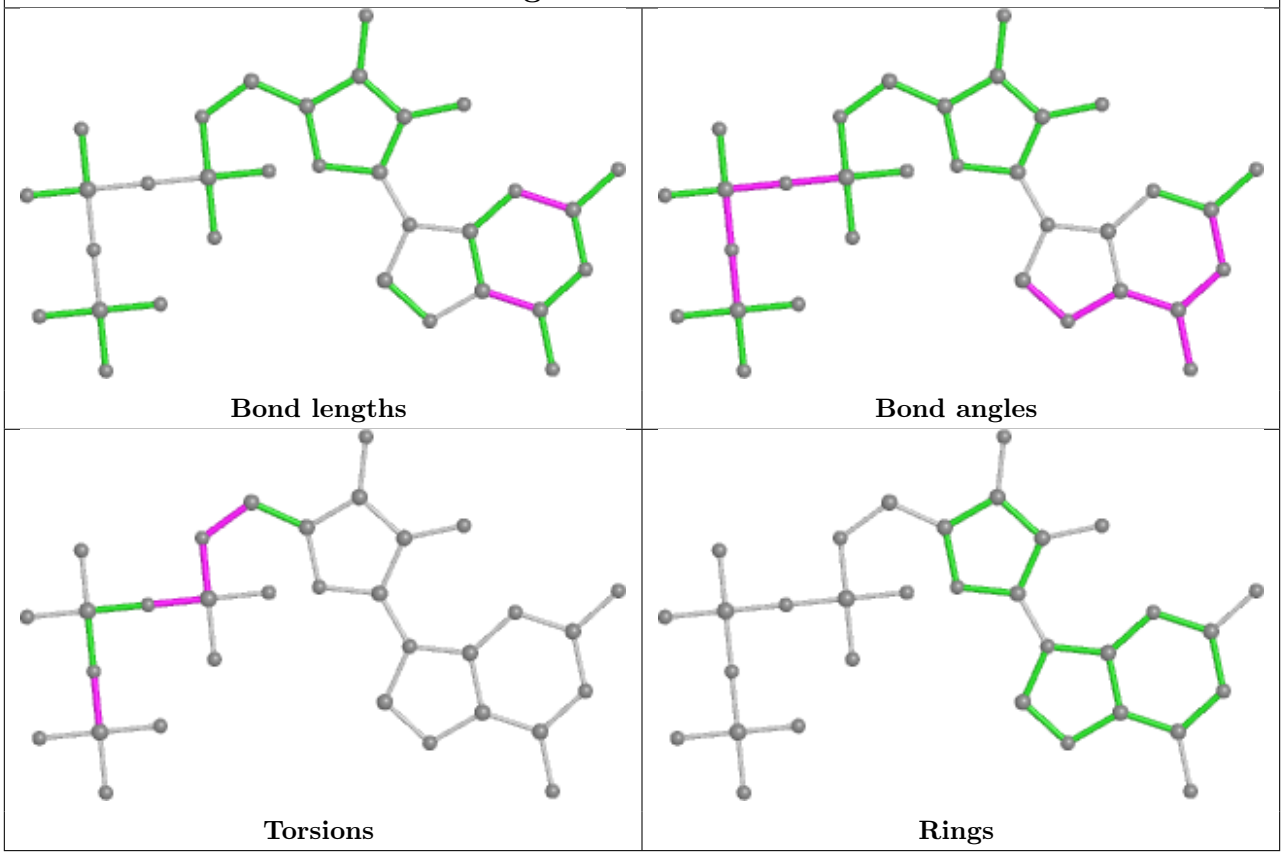


Torsions



Rings

Ligand GTP C 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	437/451 (96%)	-0.00	5 (1%) 80 79	50, 77, 124, 190	0
1	C	440/451 (97%)	-0.28	0 100 100	42, 60, 96, 130	0
2	B	421/445 (94%)	-0.01	8 (1%) 66 64	44, 70, 119, 190	0
3	D	421/445 (94%)	0.02	9 (2%) 63 61	55, 94, 133, 170	0
4	E	121/143 (84%)	0.44	15 (12%) 4 3	59, 90, 143, 207	0
5	F	284/384 (73%)	1.09	75 (26%) 0 0	71, 113, 172, 212	0
All	All	2124/2319 (91%)	0.11	112 (5%) 26 25	42, 80, 138, 212	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	26	PRO	11.4
5	F	102	PRO	8.6
5	F	182	ILE	7.4
3	D	286	LEU	7.0
5	F	101	TYR	6.7
5	F	199	PHE	6.6
4	E	27	PRO	6.2
5	F	100	ILE	5.8
2	B	438	ALA	5.7
2	B	59	ASN	5.4
5	F	186	LEU	5.3
5	F	253	TYR	5.2
3	D	57	THR	5.0
4	E	25	LYS	4.9
5	F	225	SER	4.8
5	F	181	VAL	4.7
5	F	256	TYR	4.7
5	F	99	VAL	4.5
3	D	94	PHE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	255	ARG	4.3
5	F	22	LEU	4.3
5	F	353[A]	VAL	4.3
5	F	147	TRP	4.2
4	E	45	PRO	4.2
5	F	228	TYR	4.2
5	F	148	ILE	4.2
5	F	346	LEU	4.1
5	F	128	ARG	4.1
5	F	183	GLN	4.1
5	F	361	LEU	4.1
5	F	149	ALA	4.0
5	F	342	LEU	3.9
4	E	46	SER	3.9
5	F	21	LEU	3.9
5	F	131	PHE	3.9
5	F	130	VAL	3.8
5	F	259	GLY	3.7
5	F	223	THR	3.7
1	A	262	TYR	3.7
4	E	28	SER	3.6
5	F	224	SER	3.6
5	F	98	TYR	3.4
5	F	198	LYS	3.4
5	F	197	ARG	3.3
5	F	314	LEU	3.3
5	F	201	ILE	3.3
2	B	58	GLY	3.3
5	F	362	ALA	3.2
5	F	330	ILE	3.2
3	D	96	GLN	3.1
2	B	57	THR	3.1
5	F	190	LEU	3.1
4	E	7	GLU	3.1
4	E	50	ILE	3.1
5	F	180	HIS	3.1
5	F	146	VAL	3.0
4	E	44	ASP	2.9
5	F	151	SER	2.9
5	F	263	PHE	2.9
5	F	252	ASN	2.9
5	F	329	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	320	MET	2.9
5	F	292	ARG	2.8
5	F	317	PHE	2.8
5	F	230	SER	2.8
5	F	264	PHE	2.7
4	E	24	LEU	2.7
5	F	196	HIS	2.7
5	F	14	TYR	2.6
5	F	20	LEU	2.6
2	B	247	GLN	2.6
3	D	415	GLU	2.5
5	F	76[A]	SER	2.5
5	F	335	ALA	2.4
5	F	332	VAL	2.4
5	F	214	TYR	2.4
5	F	375	PHE	2.4
5	F	13	VAL	2.4
5	F	220	VAL	2.3
5	F	319	PHE	2.3
5	F	321	VAL	2.3
2	B	248	LEU	2.3
5	F	336	PRO	2.3
5	F	260	ASN	2.3
1	A	42	ILE	2.3
5	F	26	GLN	2.3
3	D	37	HIS	2.3
5	F	97	SER	2.2
5	F	145	ASN	2.2
5	F	25	GLY	2.2
4	E	48	GLU	2.2
5	F	200	ASP	2.2
5	F	17	VAL	2.2
4	E	140	LYS	2.2
1	A	346	TRP	2.2
5	F	187	GLU	2.2
1	A	125	LEU	2.1
4	E	133	VAL	2.1
2	B	37	HIS	2.1
5	F	258	GLU	2.1
2	B	36	TYR	2.1
3	D	61	TYR	2.1
4	E	22	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	192	LEU	2.1
5	F	229	ASN	2.1
5	F	221	LEU	2.1
5	F	144	GLY	2.1
4	E	141	GLU	2.1
5	F	184	LYS	2.1
3	D	172	MET	2.0
1	A	110	ILE	2.0
3	D	82	PRO	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
13	ACP	F	401	31/31	0.85	0.20	120,132,190,191	0
10	MES	D	503	12/12	0.86	0.24	115,129,133,135	0
7	MG	D	502	1/1	0.86	0.19	126,126,126,126	0
12	EDO	C	504	4/4	0.94	0.22	78,79,81,83	0
9	GDP	D	501	28/28	0.94	0.13	69,87,102,118	0
8	CA	C	503	1/1	0.95	0.12	81,81,81,81	0
11	EX5	B	503	32/32	0.95	0.19	58,72,83,86	0
7	MG	B	504	1/1	0.95	0.17	52,52,52,52	0
10	MES	B	502	12/12	0.95	0.19	51,66,85,87	0
8	CA	A	503	1/1	0.97	0.05	113,113,113,113	0
6	GTP	C	501	32/32	0.97	0.17	45,52,62,72	0
7	MG	C	502	1/1	0.98	0.13	52,52,52,52	0
7	MG	A	502	1/1	0.98	0.17	57,57,57,57	0
6	GTP	A	501	32/32	0.99	0.21	50,59,67,71	0

Continued on next page...

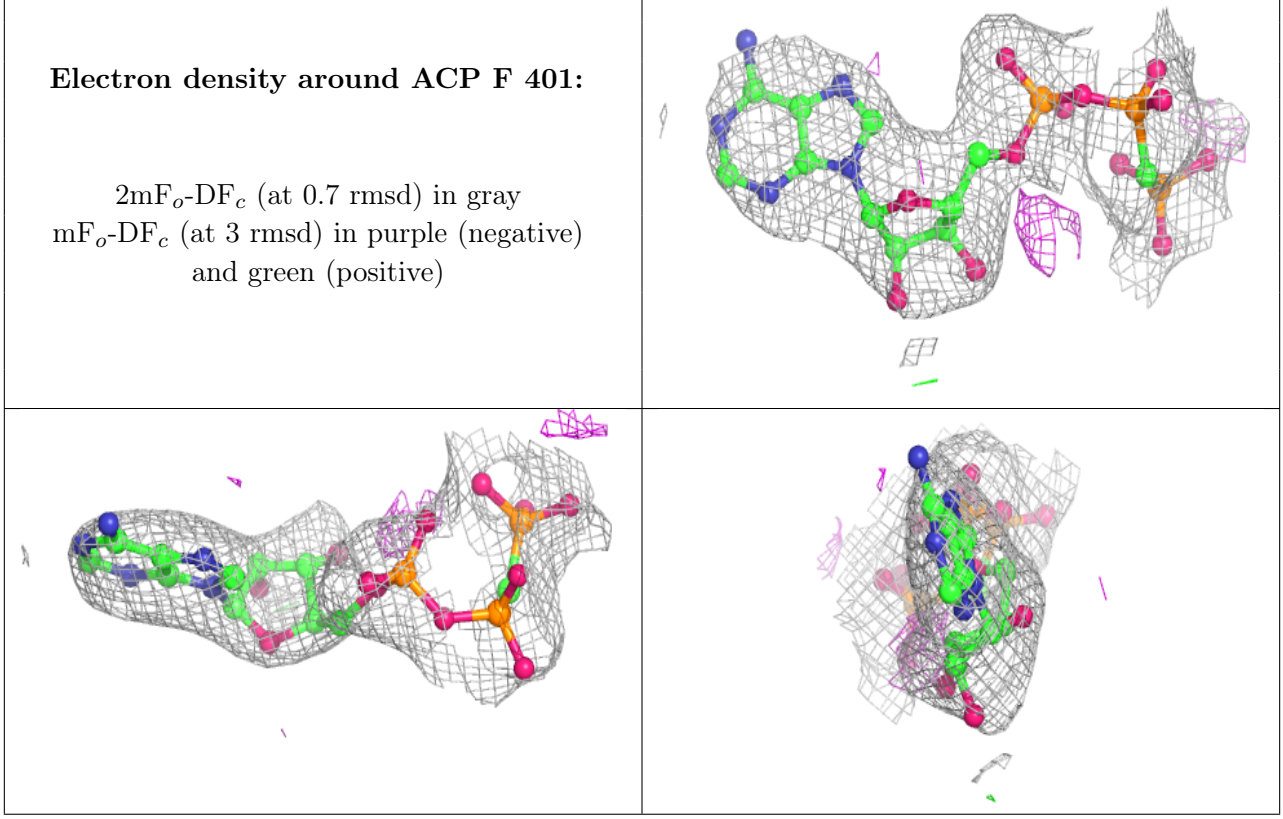
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GDP	B	501	28/28	0.99	0.16	44,54,63,67	0

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

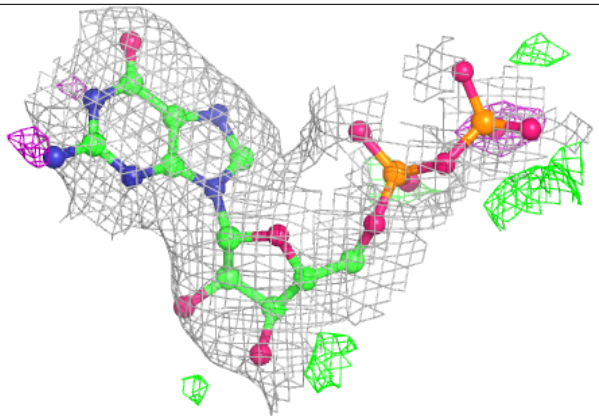
Electron density around ACP F 401:

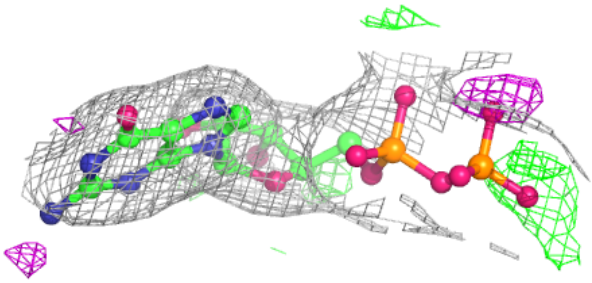
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

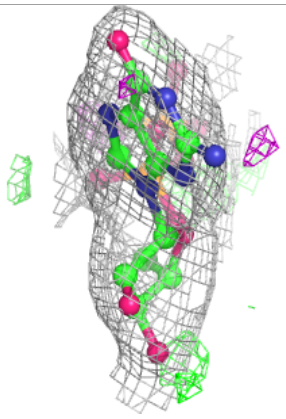


Electron density around GDP D 501:

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

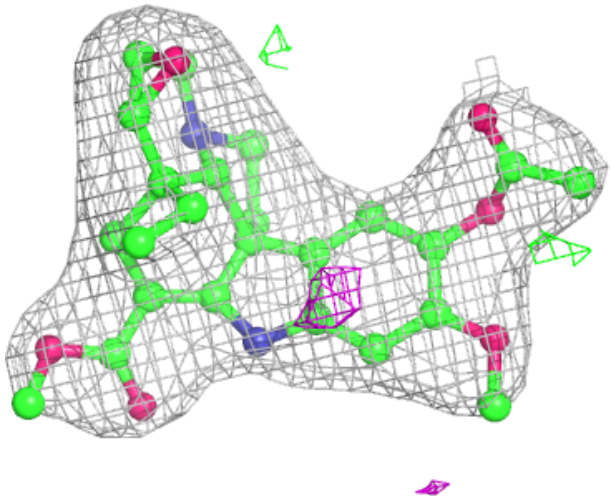


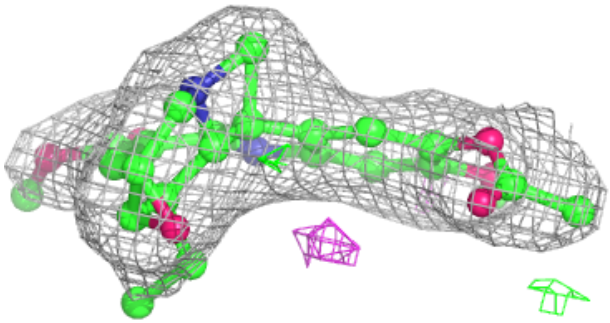


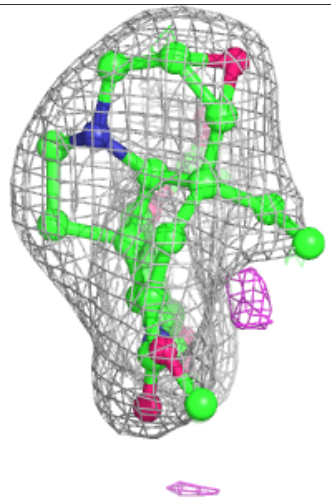


Electron density around EX5 B 503:

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

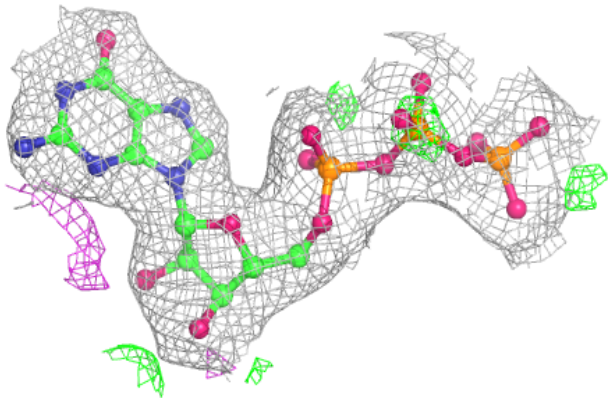


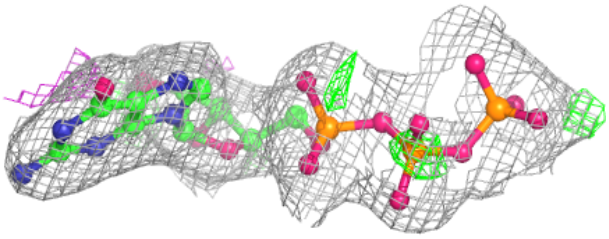


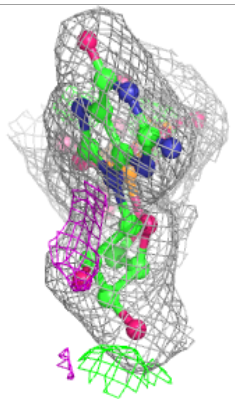


Electron density around GTP C 501:

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

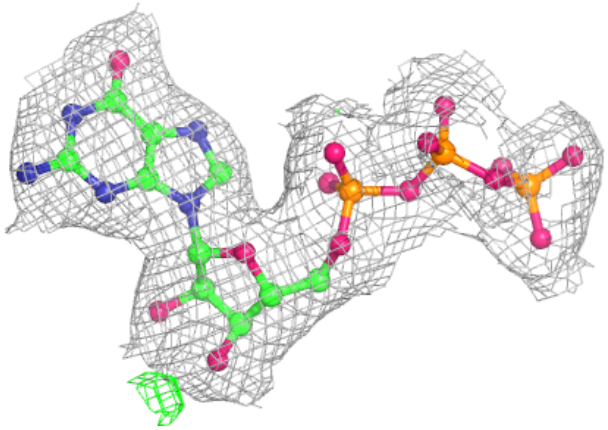


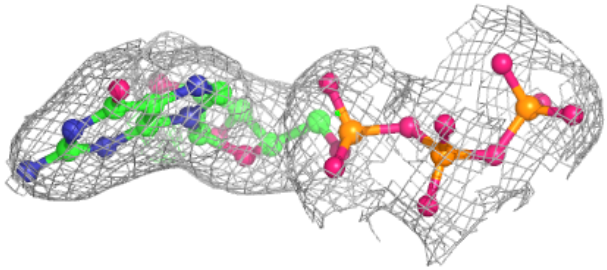


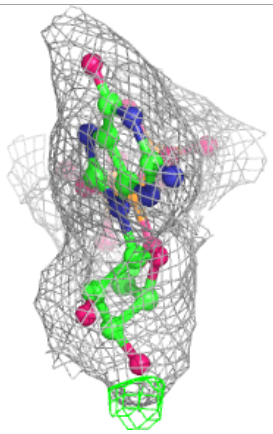


Electron density around GTP A 501:

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

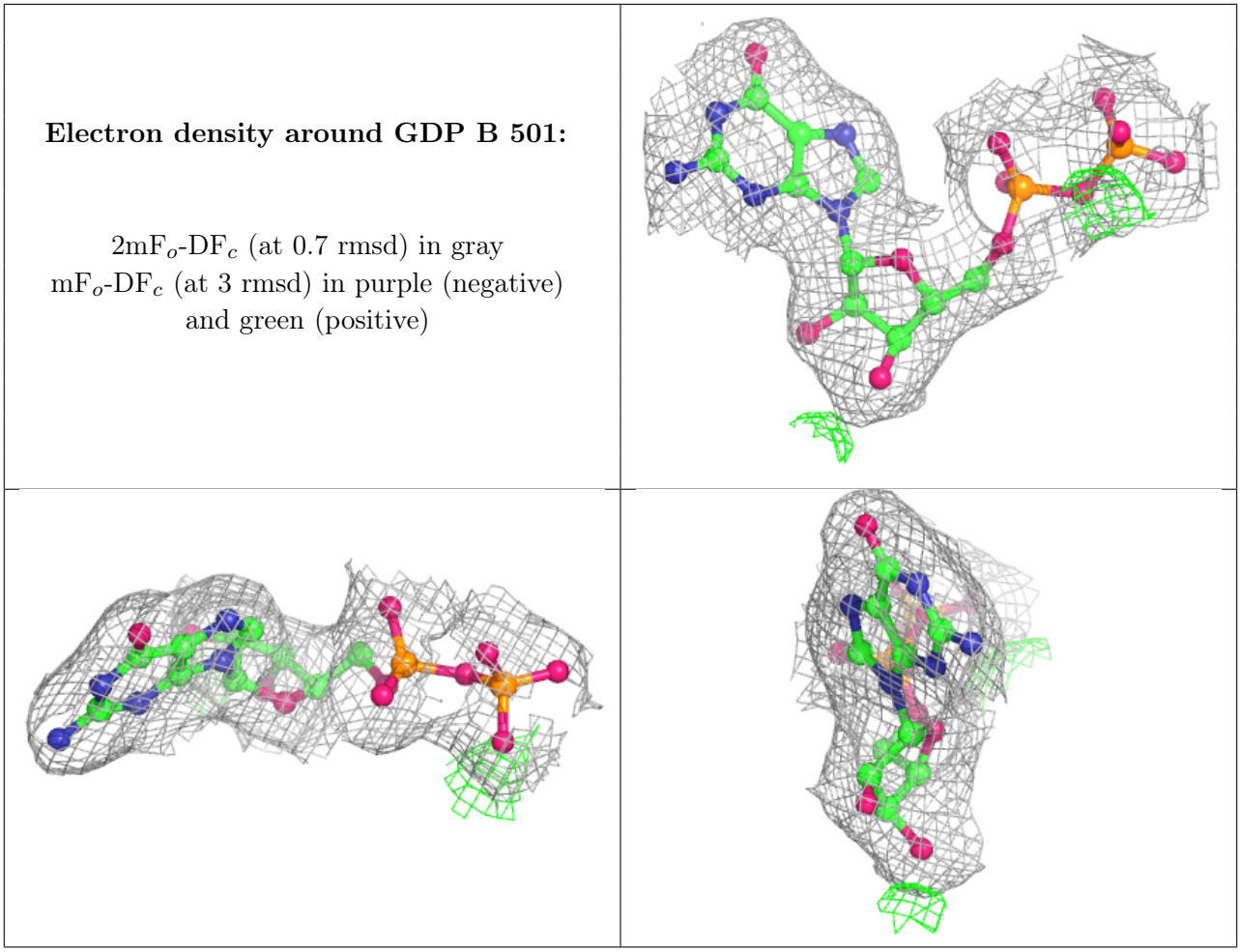






Electron density around GDP B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.