Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2022 – 12:46 pm GMT

PDB ID	:	6Y4M
Title	:	Structure of Tubulin Tyrosine Ligase in Complex with Tb111
Authors	:	Gavrilyuk, J.; Nocek, B.; Rigol, S.; Nicolaou, K.C.; Stoll, V.
Deposited on	:	2020-02-21
Resolution	:	3.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

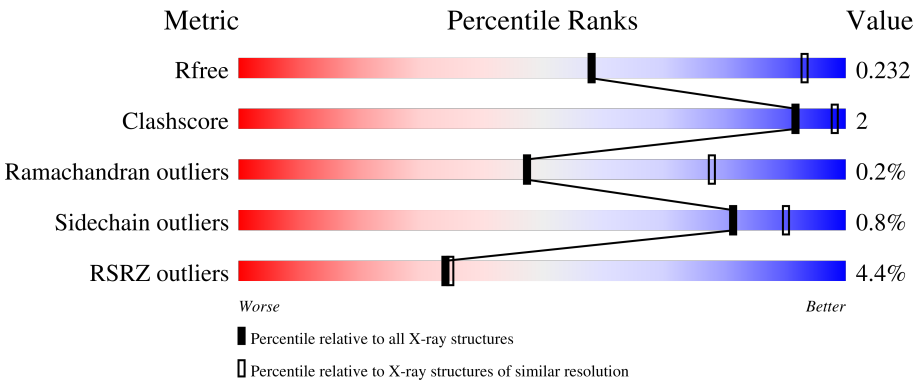
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.34 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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	2% 93%
1	C	451	% 90% 7%
2	B	445	% 94%
2	D	445	6% 92%
3	E	143	8% 83% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	11% 85% 5% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	O9H	B	1005	X	-	-	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 17766 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
			Total	C	N	O	S			
1	A	439	3430	2170	583	655	22	0	0	0
1	C	440	3467	2192	592	661	22	0	3	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	3384	2124	580	654	26	0	0	0
2	D	427	3347	2101	572	648	26	0	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1014	625	183	201	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	47	MET	-	expression tag	UNP P63043
E	48	ALA	-	expression tag	UNP P63043

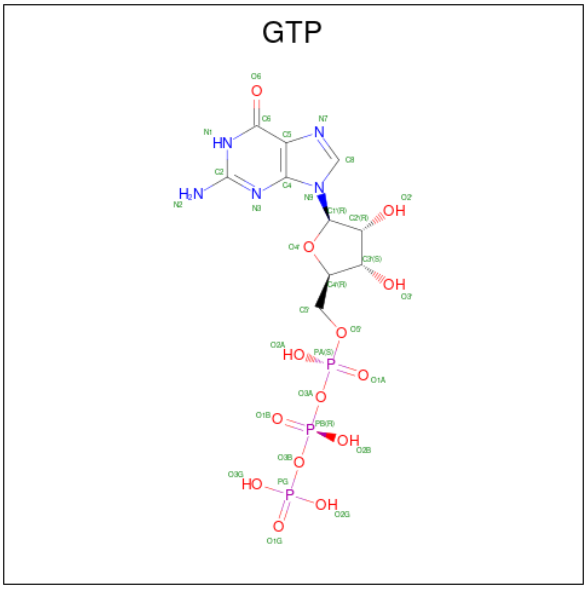
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	346	2848	1824	487	522	15	0	1	0

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

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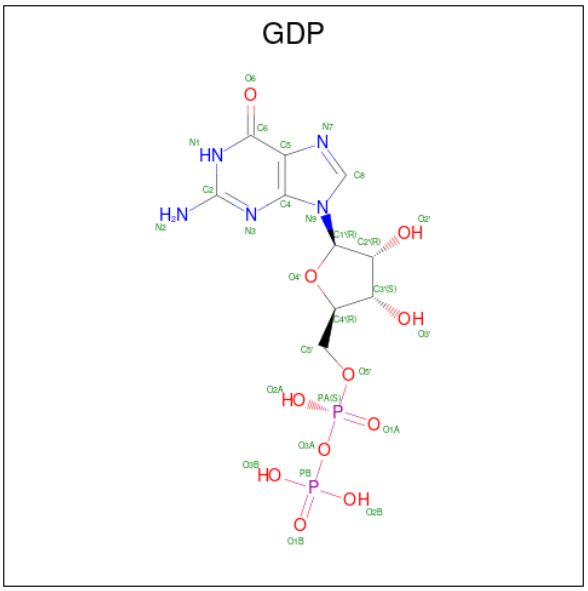
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	D	1	1	1	0	0

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

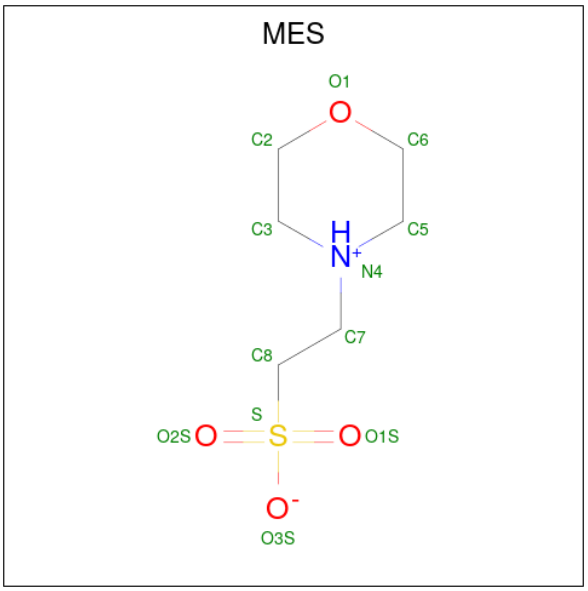
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0

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



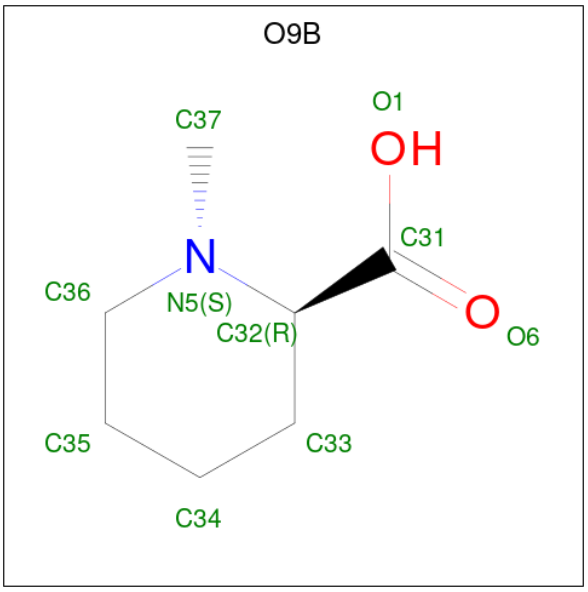
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0

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



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

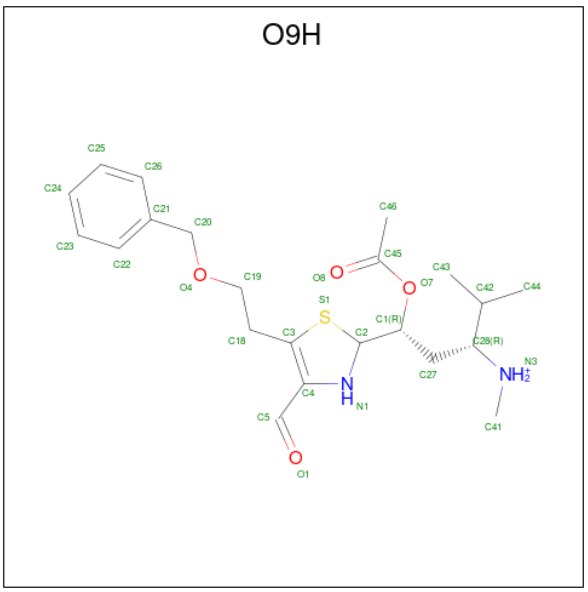
- Molecule 10 is (2 {R})-1-methylpiperidine-2-carboxylic acid (three-letter code: O9B) (formula: $C_7H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	9	7	1	1	0	0

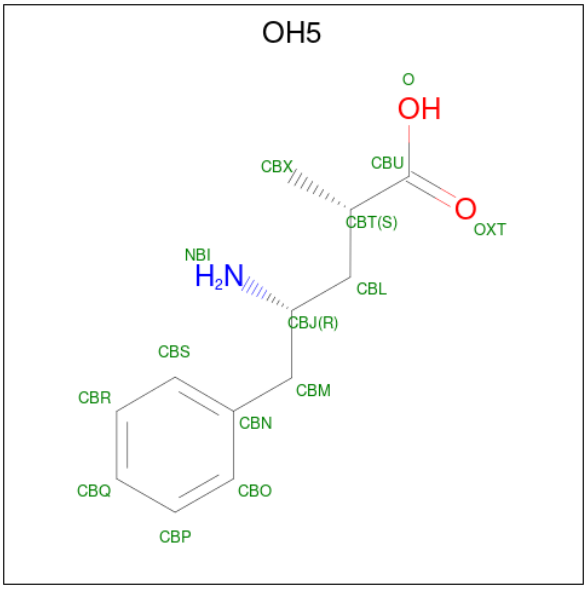
- Molecule 11 is [(1 {R},3 {R})-1-acetyloxy-1-[4-methanoyl-5-(2-phenylmethoxyethyl)-2,3-dihydro-1,3-thiazol-2-yl]-4-methyl-pentan-3-yl]-methyl-azanium (three-letter code: O9H)

(formula: $C_{22}H_{33}N_2O_4S$).



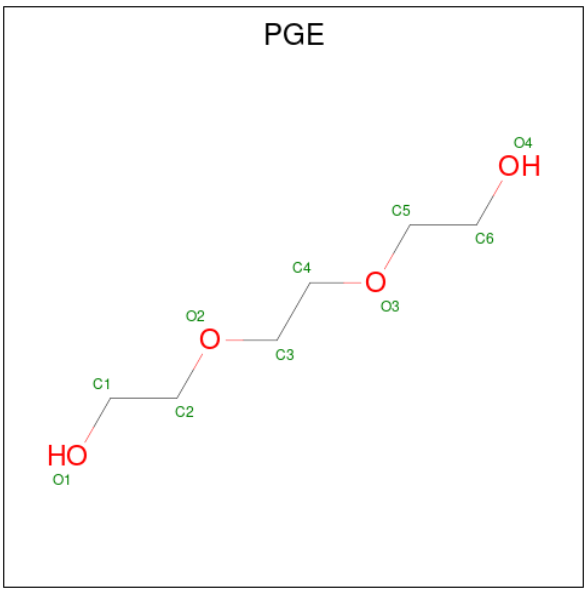
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
11	B	1	29	22	2	4	1	0	0

- Molecule 12 is (2 {S},4 {R})-4-azanyl-2-methyl-5-phenyl-pentanoic acid (three-letter code: OH5) (formula: $C_{12}H_{17}NO_2$).



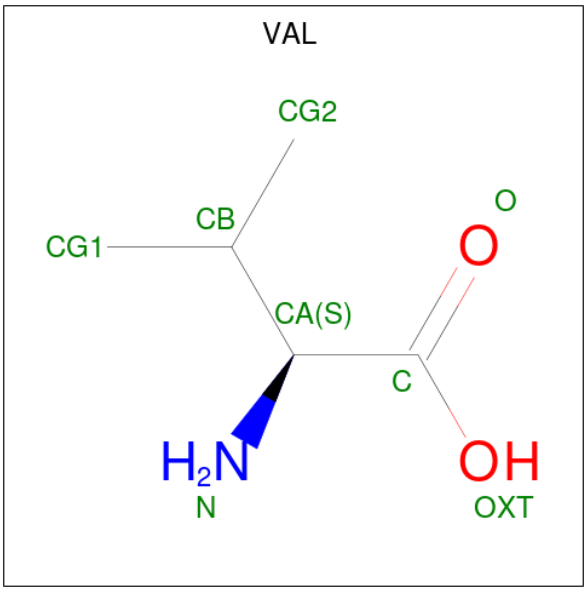
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	B	1	15	12	1	2	0	0

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	C	1	10	6	4	0	0

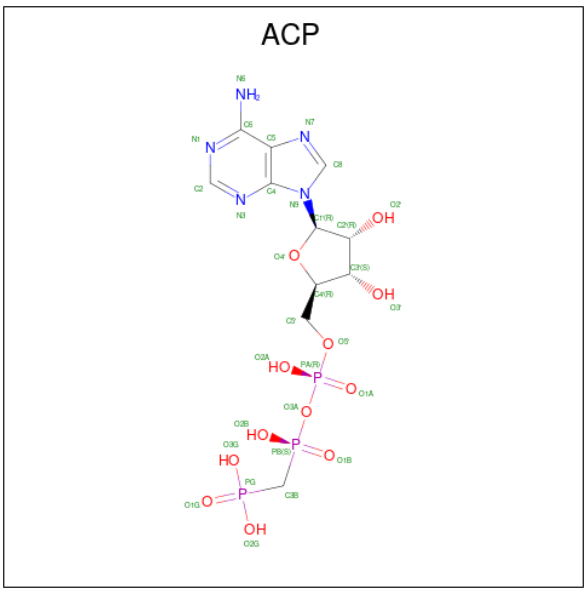
- Molecule 14 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	C	1	7	5	1	1	0	0

- Molecule 15 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
			Total	C	N	O	P		
15	F	1	31	11	5	12	3	0	0

- Molecule 16 is water.

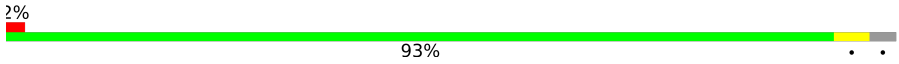
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	A	9	9	9	0	0
			Total	O		
16	B	11	11	11	0	0
			Total	O		
16	C	7	7	7	0	0
			Total	O		
16	D	5	5	5	0	0
			Total	O		
16	E	1	1	1	0	0

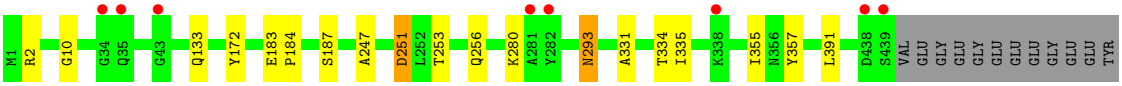
3 Residue-property plots (i)

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

• Molecule 1: Tubulin alpha-1B chain

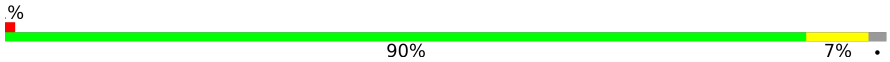
Chain A:

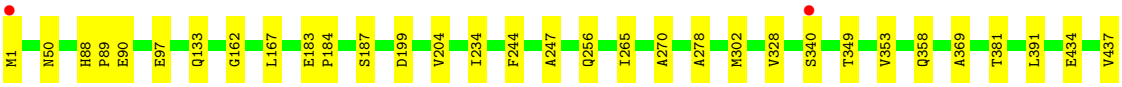


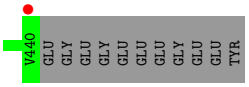


• Molecule 1: Tubulin alpha-1B chain

Chain C:

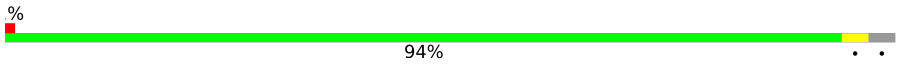






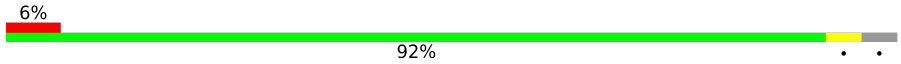
• Molecule 2: Tubulin beta chain

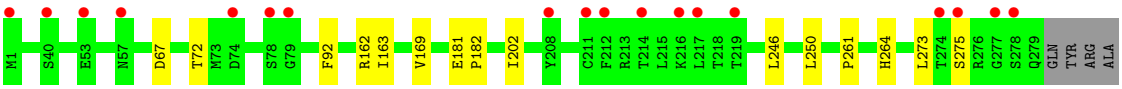
Chain B:

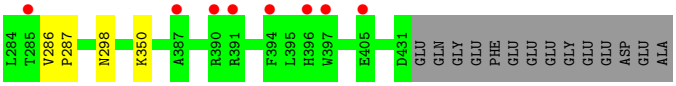


• Molecule 2: Tubulin beta chain

Chain D:





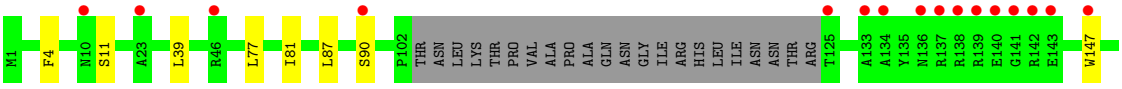


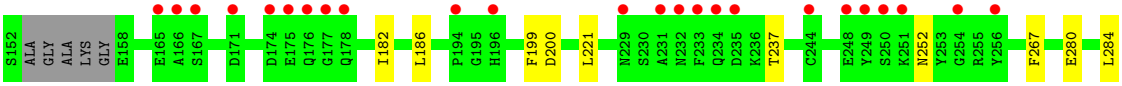
• Molecule 3: Stathmin-4

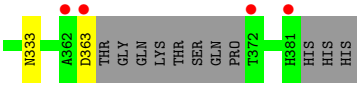
Chain E:

- 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	103.96Å 152.59Å 185.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.34 29.88 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.90-3.34) 99.5 (29.88-3.34)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.207 , 0.234 0.208 , 0.232	Depositor DCC
R_{free} test set	2168 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17766	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: O9H, ACP, PGE, MES, GTP, O9B, CA, OH5, GDP, MG

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	0.65	0/3508	0.73	0/4762
1	C	0.65	0/3546	0.72	0/4814
2	B	0.65	0/3459	0.70	0/4687
2	D	0.65	0/3420	0.70	0/4633
3	E	0.64	0/1022	0.69	0/1356
4	F	0.66	0/2913	0.70	0/3934
All	All	0.65	0/17868	0.71	0/24186

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3339	13	0
1	C	3467	0	3372	19	0
2	B	3384	0	3262	9	0
2	D	3347	0	3226	9	0
3	E	1014	0	1029	3	0
4	F	2848	0	2805	7	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	12	0	13	3	0
10	B	9	0	0	0	0
11	B	29	0	0	1	0
12	B	15	0	0	0	0
13	C	10	0	14	0	0
14	C	7	0	8	0	0
15	F	31	0	14	0	0
16	A	9	0	0	0	0
16	B	11	0	0	0	0
16	C	7	0	0	0	0
16	D	5	0	0	0	0
16	E	1	0	0	0	0
All	All	17766	0	17130	56	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 2.

All (56) 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:88[A]:HIS:NE2	1:C:90[A]:GLU:OE2	1.91	0.89
1:C:234:ILE:HG21	1:C:302:MET:SD	2.38	0.64
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.64	0.63
1:C:434:GLU:O	1:C:437:VAL:HG22	2.02	0.60
1:A:247:ALA:HB3	3:E:63:SER:OG	2.02	0.60
1:A:331:ALA:O	1:A:334:THR:HG22	2.05	0.57
2:B:156:ARG:CZ	9:B:1003:MES:H21	2.36	0.56
2:B:197:ASP:OD2	9:B:1003:MES:H52	2.06	0.54
2:B:197:ASP:OD1	9:B:1003:MES:H32	2.10	0.51
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.91	0.51
1:C:88[A]:HIS:CD2	1:C:89:PRO:HD2	2.46	0.50
1:C:265:ILE:HD12	1:C:265:ILE:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.93	0.49
1:C:204:VAL:HG22	1:C:302:MET:CE	2.43	0.48
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.94	0.48
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.48	0.48
2:D:169:VAL:HA	2:D:202:ILE:O	2.14	0.47
1:A:357:TYR:CE2	3:E:61:GLY:HA2	2.50	0.47
1:A:2:ARG:CB	1:A:133:GLN:HE21	2.27	0.47
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.97	0.46
1:C:167:LEU:HD11	1:C:256:GLN:NE2	2.30	0.46
2:D:181:GLU:N	2:D:182:PRO:CD	2.78	0.46
2:B:169:VAL:HA	2:B:202:ILE:O	2.14	0.46
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.97	0.46
2:B:181:GLU:N	2:B:182:PRO:CD	2.78	0.46
1:C:183:GLU:N	1:C:184:PRO:CD	2.79	0.46
1:A:133:GLN:OE1	1:A:251:ASP:HA	2.16	0.45
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.97	0.45
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.98	0.45
2:B:261:PRO:O	2:B:264:HIS:HD2	2.00	0.45
1:A:253:THR:O	1:A:256:GLN:HG2	2.17	0.45
1:A:183:GLU:N	1:A:184:PRO:CD	2.79	0.45
1:C:97:GLU:OE1	2:D:162:ARG:NH2	2.50	0.44
2:D:261:PRO:O	2:D:264:HIS:HD2	2.00	0.44
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.99	0.44
1:A:355:ILE:O	3:E:61:GLY:HA3	2.18	0.44
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.52	0.44
1:C:265:ILE:N	1:C:265:ILE:CD1	2.81	0.44
11:B:1005:O9H:C19	1:C:247:ALA:HB1	2.47	0.43
1:A:10:GLY:HA3	5:A:1001:GTP:O2B	2.18	0.43
1:C:1:MET:HE1	1:C:50:ASN:HB3	1.99	0.43
2:B:67:ASP:O	2:B:92:PHE:HA	2.19	0.43
2:D:67:ASP:O	2:D:92:PHE:HA	2.18	0.43
4:F:199:PHE:CD1	4:F:221:LEU:CD2	3.02	0.43
4:F:81:ILE:HD13	4:F:87:LEU:HD13	2.01	0.43
2:B:1:MET:HE2	2:B:48:ASN:HB2	2.01	0.42
1:A:293:ASN:ND2	1:A:335:ILE:HG12	2.35	0.42
2:D:163:ILE:HG21	2:D:250:LEU:HB3	2.01	0.41
1:C:265:ILE:O	1:C:265:ILE:HG22	2.20	0.41
2:D:246:LEU:HD21	2:D:350:LYS:HB3	2.02	0.41
4:F:77:LEU:O	4:F:81:ILE:HG12	2.21	0.41
4:F:147:TRP:CE3	4:F:182:ILE:HG22	2.55	0.41
2:D:273:LEU:HD11	2:D:298:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.56	0.40
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.03	0.40
4:F:4:PHE:HA	4:F:39:LEU:O	2.21	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	437/451 (97%)	420 (96%)	16 (4%)	1 (0%)	47	78
1	C	441/451 (98%)	420 (95%)	19 (4%)	2 (0%)	29	63
2	B	429/445 (96%)	418 (97%)	11 (3%)	0	100	100
2	D	423/445 (95%)	414 (98%)	9 (2%)	0	100	100
3	E	119/143 (83%)	116 (98%)	3 (2%)	0	100	100
4	F	339/384 (88%)	322 (95%)	15 (4%)	2 (1%)	25	60
All	All	2188/2319 (94%)	2110 (96%)	73 (3%)	5 (0%)	47	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	LYS
1	C	162	GLY
4	F	11	SER
4	F	186	LEU
1	C	349	THR

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	370/379 (98%)	368 (100%)	2 (0%)	88	93
1	C	374/379 (99%)	370 (99%)	4 (1%)	73	86
2	B	370/381 (97%)	370 (100%)	0	100	100
2	D	367/381 (96%)	365 (100%)	2 (0%)	88	93
3	E	110/127 (87%)	108 (98%)	2 (2%)	59	79
4	F	313/342 (92%)	307 (98%)	6 (2%)	57	79
All	All	1904/1989 (96%)	1888 (99%)	16 (1%)	81	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ASP
1	A	293	ASN
1	C	133	GLN
1	C	199	ASP
1	C	340	SER
1	C	381	THR
2	D	72	THR
2	D	275	SER
3	E	136	ASN
3	E	170	LYS
4	F	90	SER
4	F	200	ASP
4	F	237	THR
4	F	252	ASN
4	F	333	ASN
4	F	363	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	ASN

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	358	GLN
2	B	99	ASN
2	B	137	HIS
2	B	191	GLN
2	B	264	HIS
1	C	256	GLN
1	C	358	GLN
2	D	15	GLN
2	D	83	GLN
2	D	99	ASN
2	D	137	HIS
2	D	191	GLN
2	D	264	HIS
2	D	291	GLN
3	E	152	ASN
4	F	269	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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
11	O9H	B	1005	12,14	25,30,30	1.15	2 (8%)	27,39,39	1.03	2 (7%)
13	PGE	C	1004	-	9,9,9	0.17	0	8,8,8	0.13	0
10	O9B	B	1004	14	7,9,10	0.42	0	7,11,13	0.68	0
8	GDP	B	1001	-	24,30,30	0.92	0	30,47,47	1.13	4 (13%)
14	VAL	C	1005	10,11	4,6,7	0.58	0	6,7,9	0.98	1 (16%)
15	ACP	F	401	-	27,33,33	1.44	5 (18%)	32,52,52	1.36	5 (15%)
9	MES	B	1003	-	12,12,12	0.75	0	14,16,16	0.70	0
5	GTP	C	1001	6	26,34,34	0.95	2 (7%)	32,54,54	0.69	1 (3%)
5	GTP	A	1001	6	26,34,34	0.96	2 (7%)	32,54,54	0.66	0
5	GTP	D	1001	6	26,34,34	0.95	2 (7%)	32,54,54	0.69	0
12	OH5	B	1006	11	15,15,15	0.55	0	15,19,19	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	O9H	B	1005	12,14	1/1/7/9	4/23/39/39	0/2/2/2
13	PGE	C	1004	-	-	3/7/7/7	-
10	O9B	B	1004	14	-	0/1/13/15	0/1/1/1
8	GDP	B	1001	-	-	4/12/32/32	0/3/3/3
14	VAL	C	1005	10,11	-	0/5/6/8	-
15	ACP	F	401	-	-	6/15/38/38	0/3/3/3
9	MES	B	1003	-	-	0/6/14/14	0/1/1/1
5	GTP	C	1001	6	-	7/18/38/38	0/3/3/3
5	GTP	A	1001	6	-	6/18/38/38	0/3/3/3
5	GTP	D	1001	6	-	5/18/38/38	0/3/3/3
12	OH5	B	1006	11	-	7/12/12/12	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1005	O9H	C2-S1	-4.77	1.73	1.83
15	F	401	ACP	PB-O3A	3.49	1.62	1.58
15	F	401	ACP	PG-O2G	2.85	1.61	1.54
11	B	1005	O9H	C5-C4	2.77	1.48	1.42
15	F	401	ACP	PG-O3G	2.76	1.61	1.54
5	A	1001	GTP	C5-C6	-2.64	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1001	GTP	C5-C6	-2.57	1.42	1.47
5	C	1001	GTP	C5-C6	-2.55	1.42	1.47
15	F	401	ACP	C5-C4	2.49	1.47	1.40
15	F	401	ACP	PB-O2B	2.22	1.61	1.56
5	A	1001	GTP	C8-N7	-2.09	1.31	1.35
5	D	1001	GTP	C8-N7	-2.07	1.31	1.35
5	C	1001	GTP	C8-N7	-2.00	1.31	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	1005	O9H	O1-C5-C4	-4.37	119.61	125.22
15	F	401	ACP	N3-C2-N1	-3.66	122.96	128.68
15	F	401	ACP	C3'-C2'-C1'	3.01	105.52	100.98
8	B	1001	GDP	PA-O3A-PB	-2.78	123.30	132.83
15	F	401	ACP	PB-O3A-PA	-2.42	124.88	132.56
11	B	1005	O9H	C5-C4-N1	-2.39	118.25	122.33
15	F	401	ACP	C4-C5-N7	-2.38	106.92	109.40
15	F	401	ACP	C2-N1-C6	2.19	122.49	118.75
8	B	1001	GDP	C8-N7-C5	2.18	107.15	102.99
8	B	1001	GDP	C5-C6-N1	2.16	117.77	113.95
8	B	1001	GDP	O6-C6-C5	-2.14	120.20	124.37
14	C	1005	VAL	O-C-CA	-2.13	119.19	124.78
5	C	1001	GTP	O6-C6-C5	2.02	128.31	124.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	B	1005	O9H	C2

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	GTP	C5'-O5'-PA-O1A
5	A	1001	GTP	C5'-O5'-PA-O2A
5	C	1001	GTP	C5'-O5'-PA-O1A
5	C	1001	GTP	C5'-O5'-PA-O2A
5	D	1001	GTP	C5'-O5'-PA-O1A
8	B	1001	GDP	C5'-O5'-PA-O1A
11	B	1005	O9H	N1-C4-C5-O1
11	B	1005	O9H	C3-C4-C5-O1
12	B	1006	OH5	NBI-CBJ-CBL-CBT

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Mol	Chain	Res	Type	Atoms
15	F	401	ACP	PG-C3B-PB-O1B
15	F	401	ACP	PG-C3B-PB-O2B
15	F	401	ACP	PG-C3B-PB-O3A
13	C	1004	PGE	O2-C3-C4-O3
12	B	1006	OH5	CBM-CBJ-CBL-CBT
11	B	1005	O9H	C27-C28-C42-C44
12	B	1006	OH5	CBL-CBT-CBU-O
5	A	1001	GTP	PB-O3B-PG-O1G
5	C	1001	GTP	PB-O3B-PG-O1G
13	C	1004	PGE	O1-C1-C2-O2
8	B	1001	GDP	C5'-O5'-PA-O3A
13	C	1004	PGE	C1-C2-O2-C3
5	D	1001	GTP	C5'-O5'-PA-O2A
8	B	1001	GDP	C5'-O5'-PA-O2A
12	B	1006	OH5	CBJ-CBL-CBT-CBX
15	F	401	ACP	O4'-C4'-C5'-O5'
5	D	1001	GTP	PB-O3A-PA-O2A
12	B	1006	OH5	CBX-CBT-CBU-O
12	B	1006	OH5	CBX-CBT-CBU-OXT
12	B	1006	OH5	CBL-CBT-CBU-OXT
11	B	1005	O9H	C27-C28-C42-C43
15	F	401	ACP	C3'-C4'-C5'-O5'
8	B	1001	GDP	C3'-C4'-C5'-O5'
5	A	1001	GTP	PB-O3B-PG-O2G
5	A	1001	GTP	PB-O3B-PG-O3G
5	C	1001	GTP	PB-O3B-PG-O2G
5	C	1001	GTP	PB-O3B-PG-O3G
5	D	1001	GTP	PB-O3B-PG-O3G
5	A	1001	GTP	C5'-O5'-PA-O3A
5	C	1001	GTP	C5'-O5'-PA-O3A
5	D	1001	GTP	C5'-O5'-PA-O3A
5	C	1001	GTP	PB-O3A-PA-O2A
15	F	401	ACP	C5'-O5'-PA-O1A

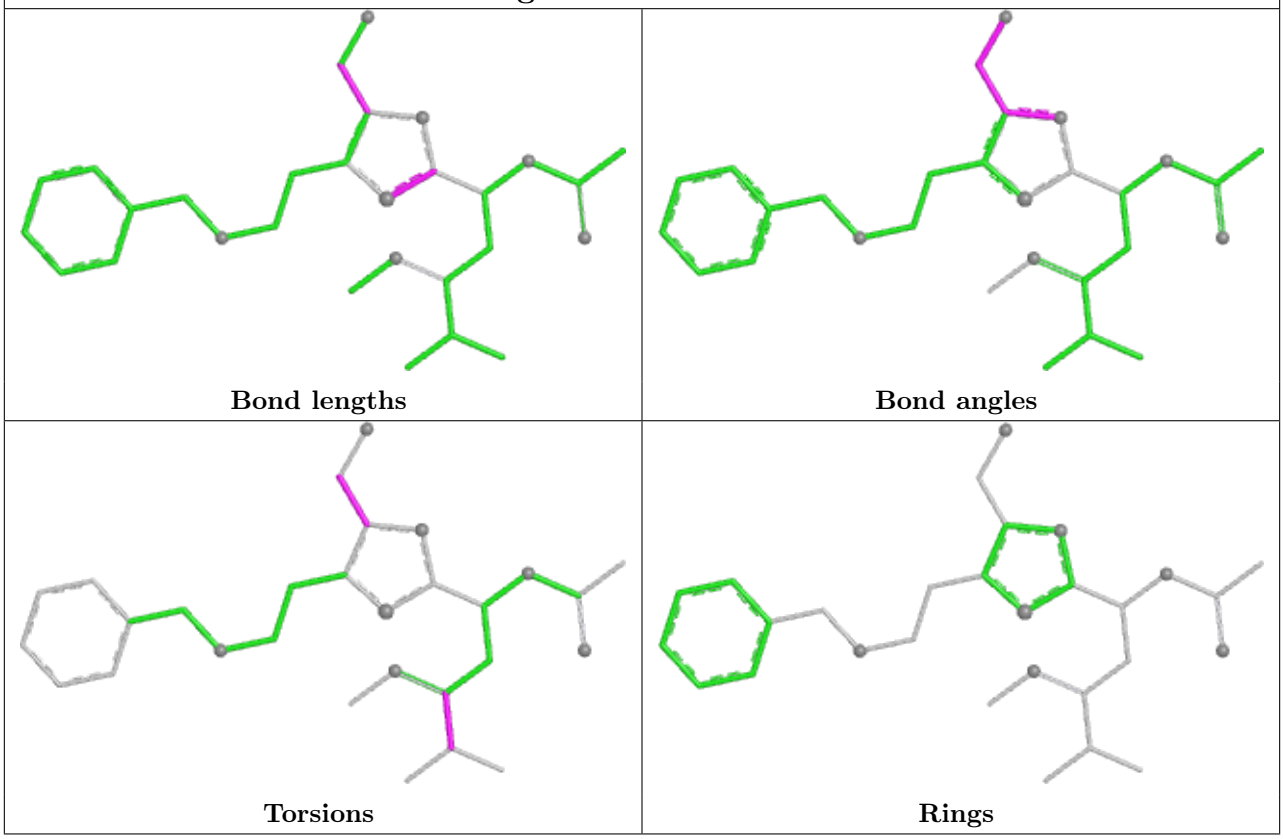
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1005	O9H	1	0
9	B	1003	MES	3	0
5	A	1001	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 O9H B 1005



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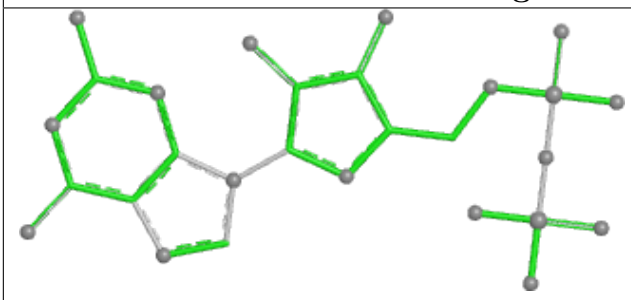
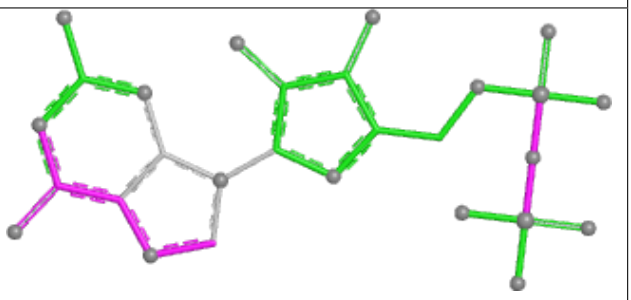
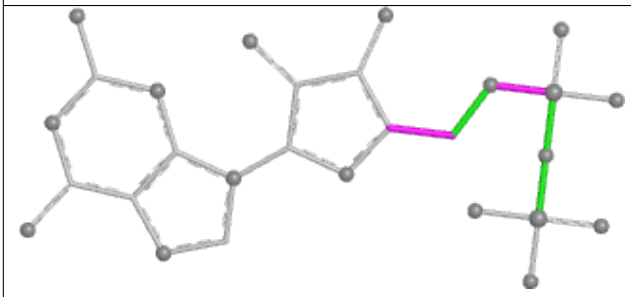
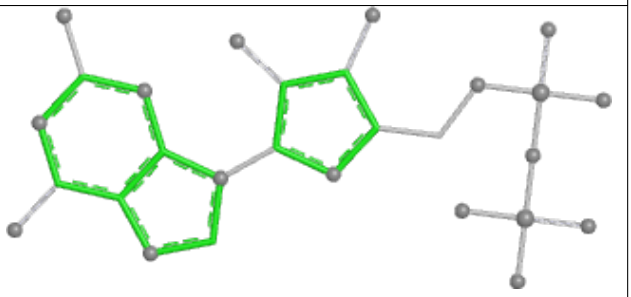
 Bond lengths	 Bond angles
 Torsions	 Rings

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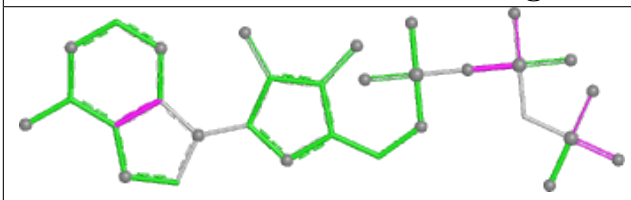
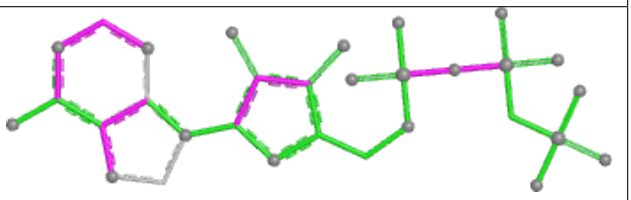
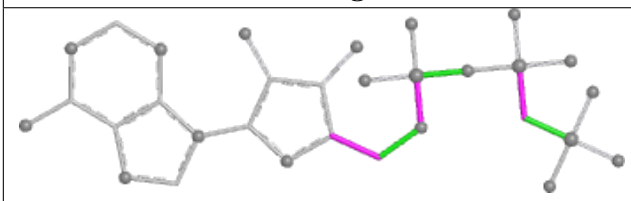
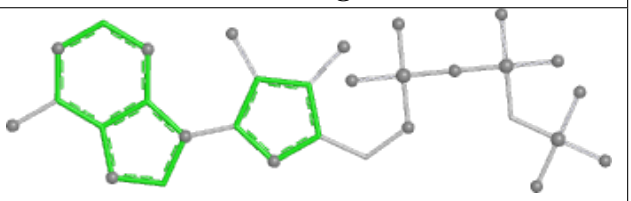
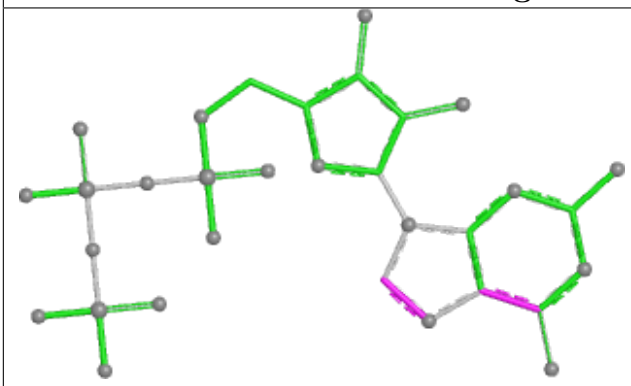
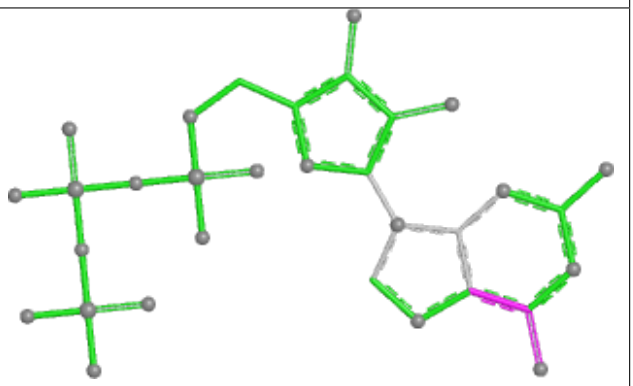
 Bond lengths	 Bond angles
 Torsions	 Rings

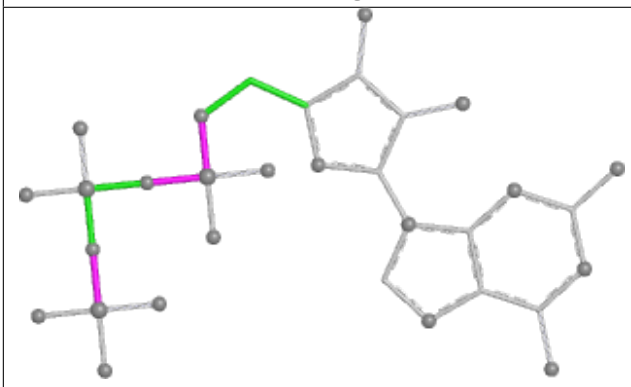
Ligand GTP C 1001



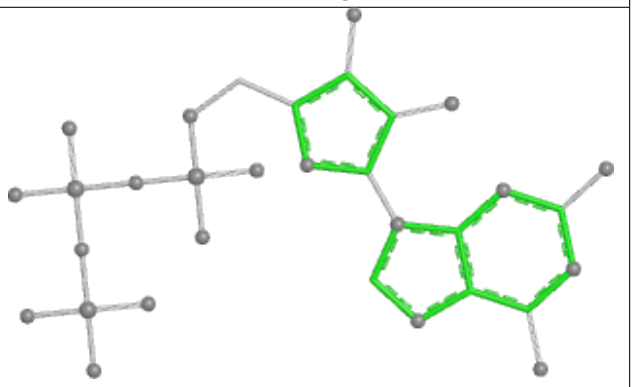
Bond lengths



Bond angles

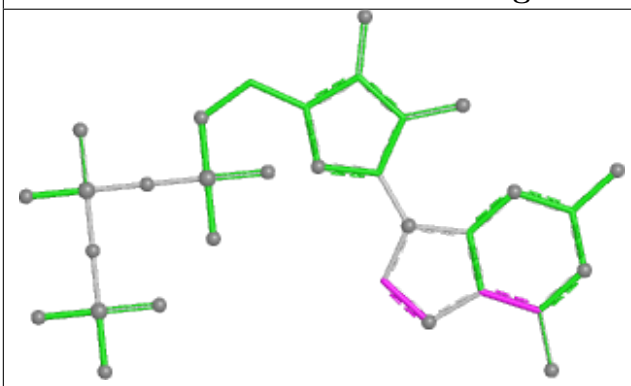


Torsions

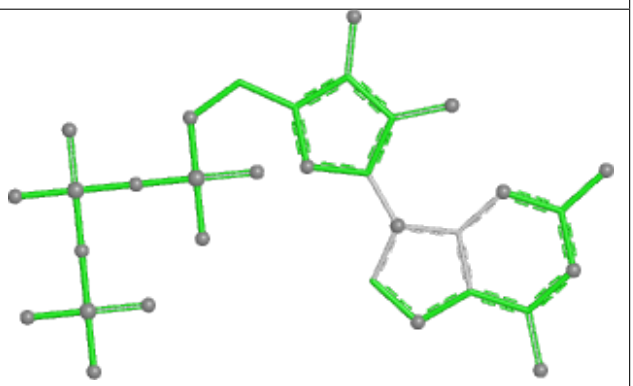


Rings

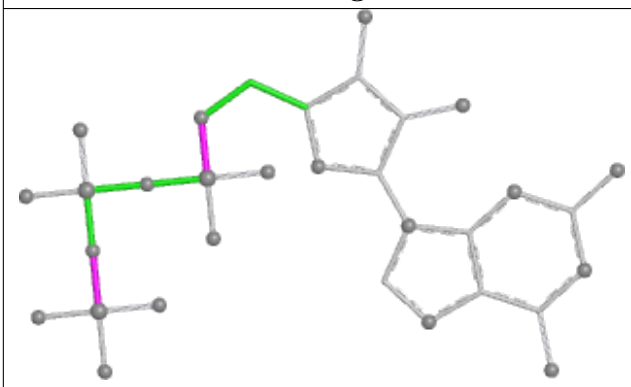
Ligand GTP A 1001



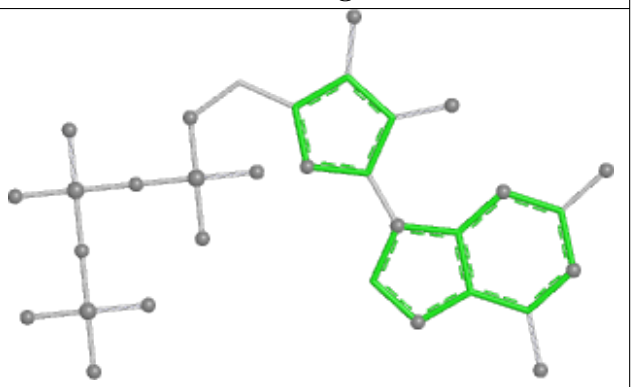
Bond lengths



Bond angles

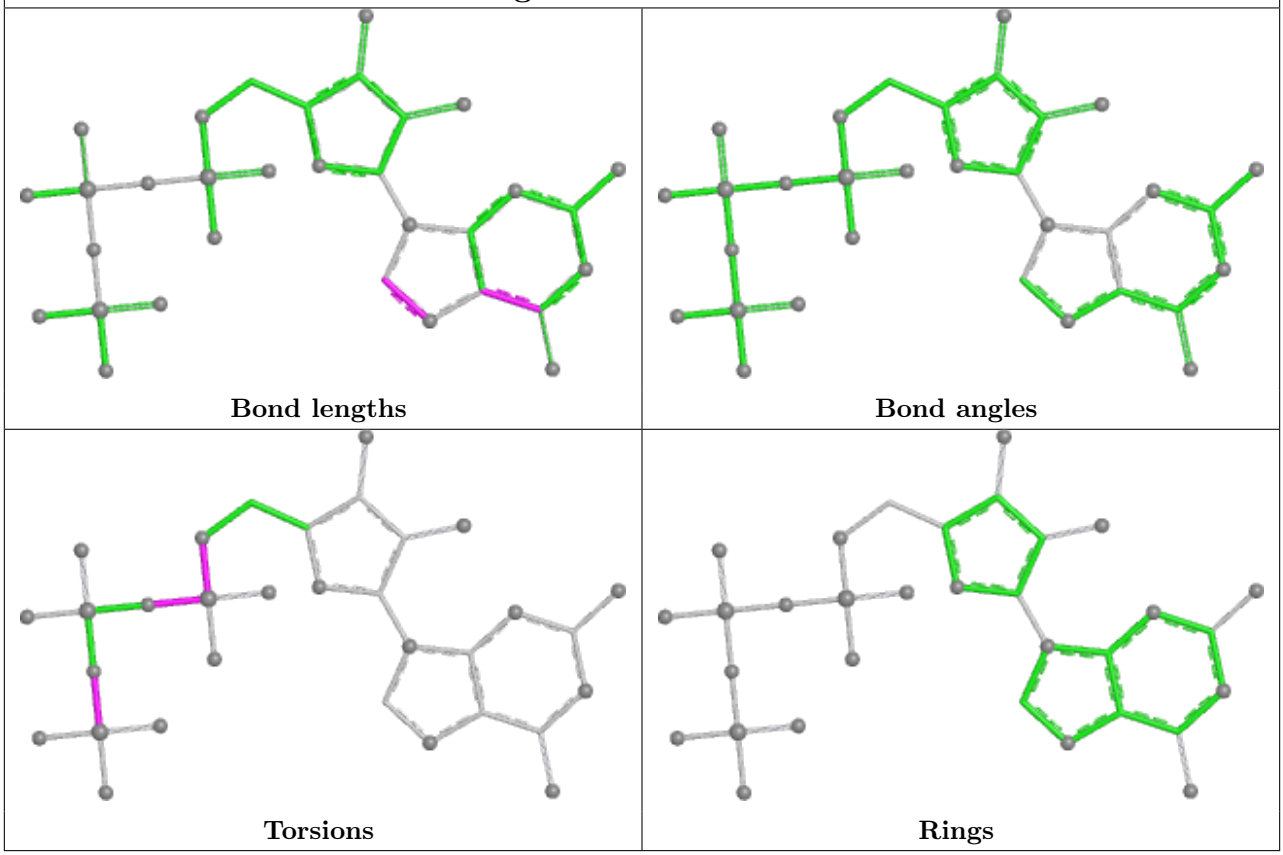


Torsions



Rings

Ligand GTP D 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	439/451 (97%)	0.03	8 (1%)	68	67	53, 75, 105, 145	0
1	C	440/451 (97%)	-0.17	3 (0%)	87	90	46, 63, 86, 106	0
2	B	431/445 (96%)	-0.09	5 (1%)	79	79	40, 63, 100, 133	0
2	D	427/445 (95%)	0.29	26 (6%)	21	22	62, 92, 127, 166	0
3	E	123/143 (86%)	0.64	11 (8%)	9	10	63, 88, 124, 143	0
4	F	346/384 (90%)	0.53	44 (12%)	3	3	66, 103, 155, 172	0
All	All	2206/2319 (95%)	0.13	97 (4%)	34	35	40, 78, 129, 172	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	277	GLY	6.0
2	D	278	SER	5.7
1	A	439	SER	5.7
4	F	249	TYR	5.1
2	B	1	MET	5.1
4	F	232	ASN	4.8
1	A	438	ASP	4.6
3	E	88	ASP	4.3
3	E	184	LYS	4.2
4	F	178	GLN	4.0
4	F	244	CYS	4.0
4	F	250	SER	4.0
3	E	187	ALA	3.9
4	F	362	ALA	3.9
2	D	40	SER	3.7
4	F	175	GLU	3.6
4	F	234	GLN	3.6
4	F	140	GLU	3.5
2	B	57	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	372	THR	3.4
3	E	183	LEU	3.4
1	A	281	ALA	3.3
2	D	387	ALA	3.2
2	D	274	THR	3.2
2	D	78	SER	3.2
4	F	167	SER	3.2
2	D	397	TRP	3.2
4	F	142	ARG	3.1
2	D	396	HIS	3.1
4	F	143	GLU	3.1
1	A	282	TYR	3.0
2	B	281	TYR	3.0
4	F	139	ARG	3.0
4	F	166	ALA	2.9
2	D	275	SER	2.9
2	D	74	ASP	2.8
4	F	171	ASP	2.8
4	F	10	ASN	2.7
4	F	251	LYS	2.7
2	D	394	PHE	2.7
2	D	1	MET	2.7
4	F	235	ASP	2.6
2	D	208	TYR	2.6
1	C	440	VAL	2.6
3	E	186	GLU	2.6
1	C	1	MET	2.6
4	F	248	GLU	2.6
3	E	92	GLU	2.5
4	F	90	SER	2.5
4	F	381	HIS	2.5
2	D	212	PHE	2.5
2	D	390	ARG	2.5
3	E	50	MET	2.5
4	F	46	ARG	2.5
4	F	141	GLY	2.5
4	F	176	GLN	2.4
4	F	177	GLY	2.4
2	B	78	SER	2.4
1	A	34	GLY	2.4
4	F	136	ASN	2.4
1	A	35	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	254	GLY	2.4
4	F	137	ARG	2.4
4	F	229	ASN	2.4
4	F	363	ASP	2.3
1	A	338	LYS	2.3
4	F	23	ALA	2.3
4	F	138	ARG	2.3
4	F	194	PRO	2.3
2	D	391	ARG	2.3
3	E	172	LYS	2.3
2	D	405	GLU	2.2
4	F	147	TRP	2.2
2	D	211	CYS	2.2
4	F	233	PHE	2.2
4	F	125	THR	2.2
1	C	340	SER	2.2
2	B	279	GLN	2.2
4	F	231	ALA	2.2
1	A	43	GLY	2.2
2	D	217	LEU	2.2
2	D	57	ASN	2.2
2	D	214	THR	2.2
2	D	53	GLU	2.2
2	D	219	THR	2.2
2	D	216	LYS	2.1
4	F	133	ALA	2.1
4	F	134	ALA	2.1
4	F	256	TYR	2.1
2	D	285	THR	2.1
2	D	79	GLY	2.1
4	F	165	GLU	2.1
3	E	179	LYS	2.1
3	E	72	SER	2.1
4	F	196	HIS	2.1
4	F	174	ASP	2.0
3	E	51	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

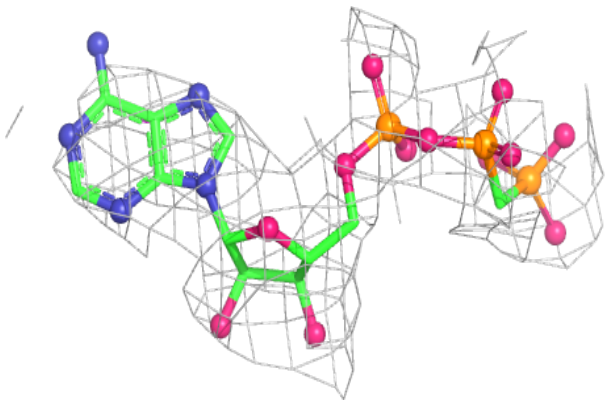
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

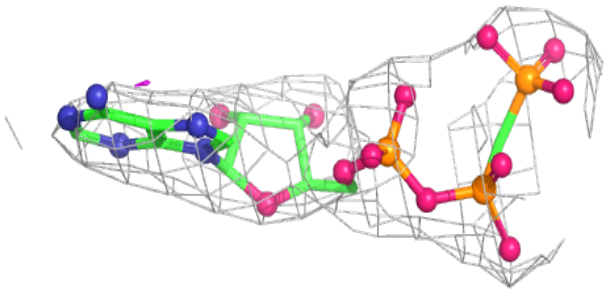
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	PGE	C	1004	10/10	0.82	0.26	68,71,76,77	0
7	CA	A	1003	1/1	0.90	0.13	132,132,132,132	0
6	MG	B	1002	1/1	0.90	0.18	34,34,34,34	0
15	ACP	F	401	31/31	0.90	0.27	116,120,129,131	0
12	OH5	B	1006	15/15	0.93	0.37	65,69,74,80	0
11	O9H	B	1005	29/29	0.94	0.33	53,62,72,73	0
5	GTP	D	1001	32/32	0.94	0.17	91,99,104,105	0
5	GTP	C	1001	32/32	0.95	0.19	54,56,57,58	0
6	MG	D	1002	1/1	0.96	0.08	96,96,96,96	0
9	MES	B	1003	12/12	0.96	0.20	67,68,69,70	0
6	MG	C	1002	1/1	0.97	0.06	51,51,51,51	0
8	GDP	B	1001	28/28	0.97	0.15	49,51,54,55	0
5	GTP	A	1001	32/32	0.97	0.15	51,53,56,57	0
14	VAL	C	1005	7/8	0.97	0.18	46,48,49,50	0
10	O9B	B	1004	9/10	0.97	0.22	43,44,45,45	0
6	MG	A	1002	1/1	0.98	0.06	47,47,47,47	0
7	CA	C	1003	1/1	0.98	0.15	86,86,86,86	0

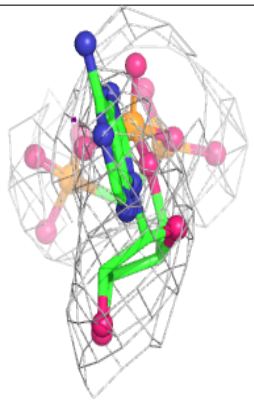
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

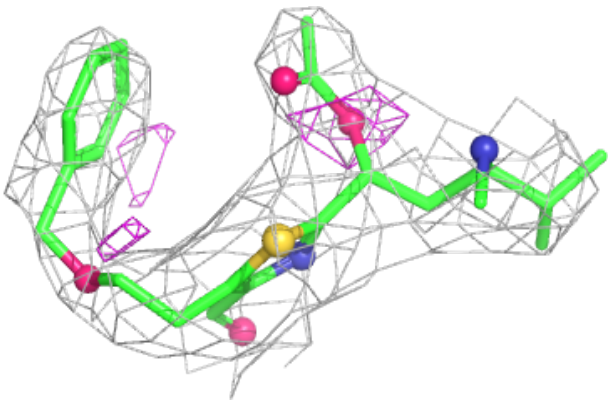


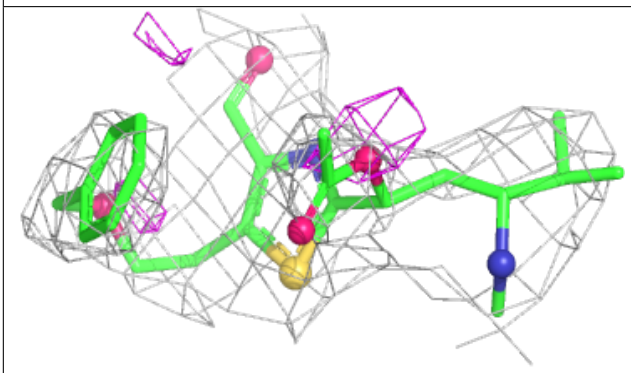


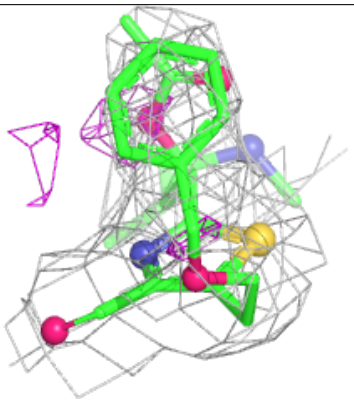


Electron density around O9H B 1005:

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

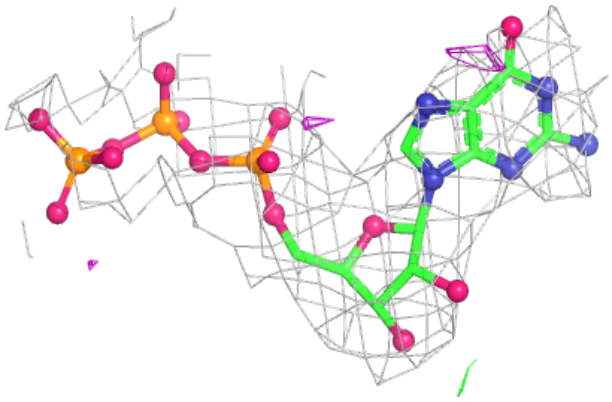


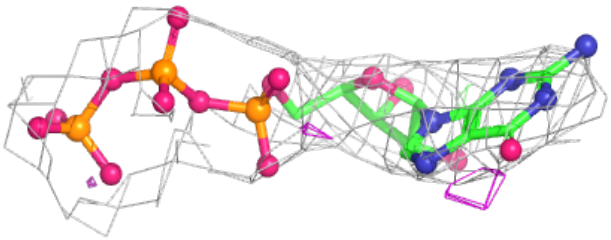


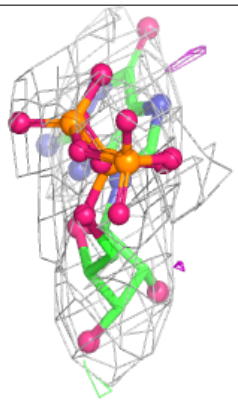


Electron density around GTP D 1001:

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

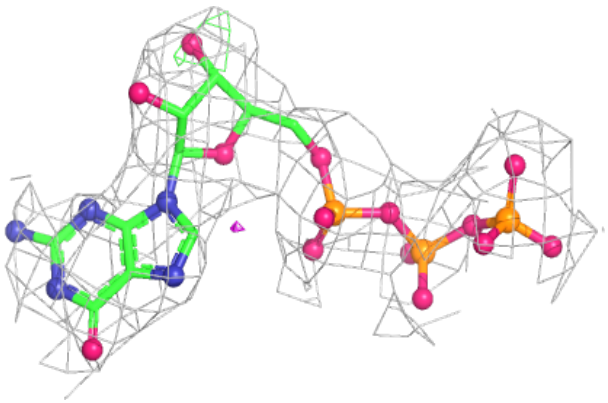


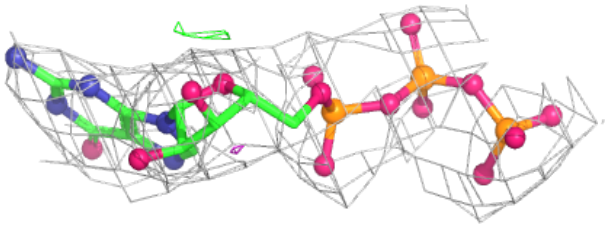


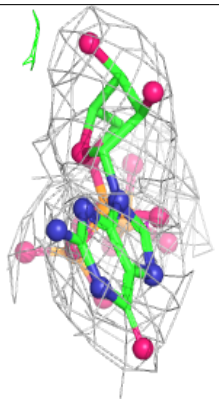


Electron density around GTP C 1001:

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

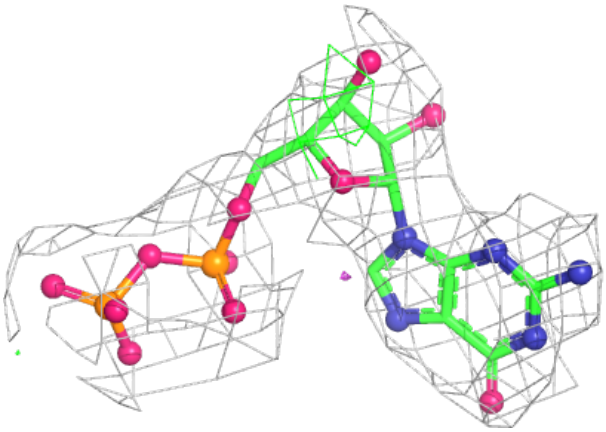


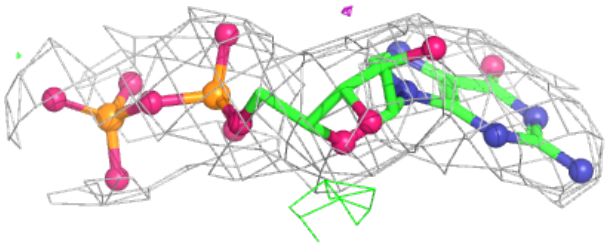


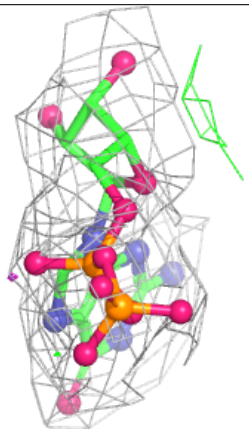


Electron density around GDP B 1001:

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

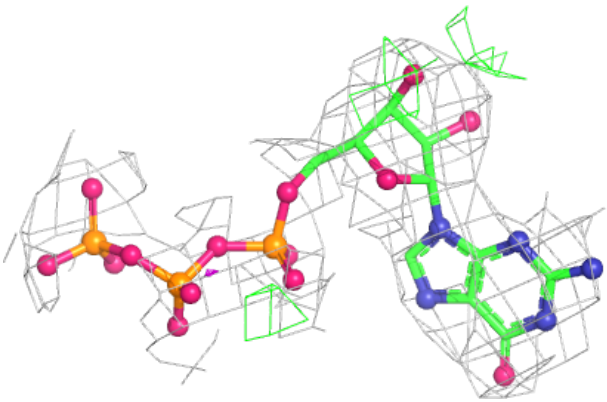


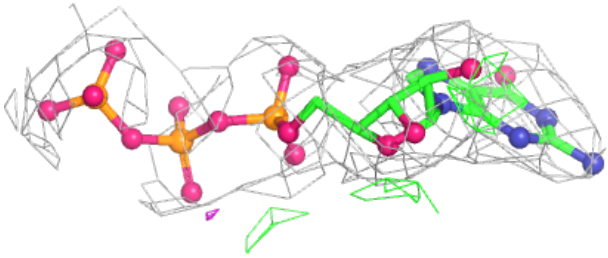


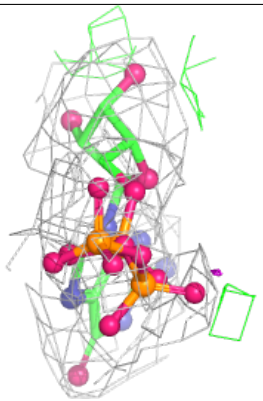


Electron density around GTP A 1001:

$2mF_o$-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.