Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 08:40 PM JST

PDB ID	:	4ZHQ
Title	:	Crystal structure of Tubulin-Stathmin-TTL-MMAE Complex
Authors	:	Wang, Y.; Zhang, R.
Deposited on	:	2015-04-26
Resolution	:	2.55 Å(reported)

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

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

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

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

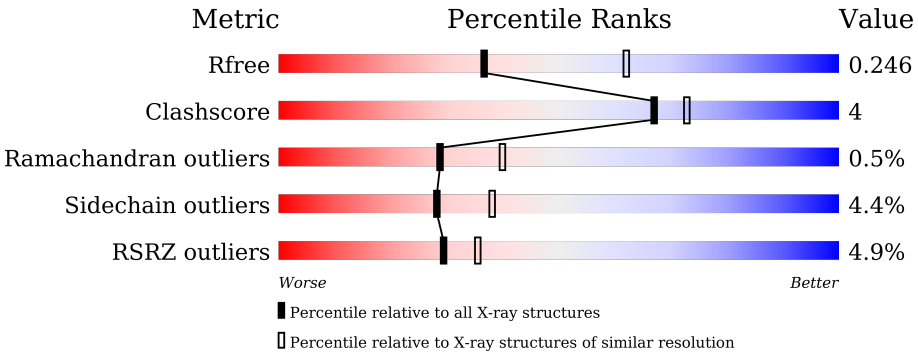
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	89% 8%
1	C	451	89% 8%
2	B	445	83% 12%
2	D	445	6% 79% 15% 5%
3	E	143	7% 77% 8% 14%
4	F	384	15% 74% 14% 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
8	GOL	C	506	-	-	X	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 17988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3360	2111	576	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

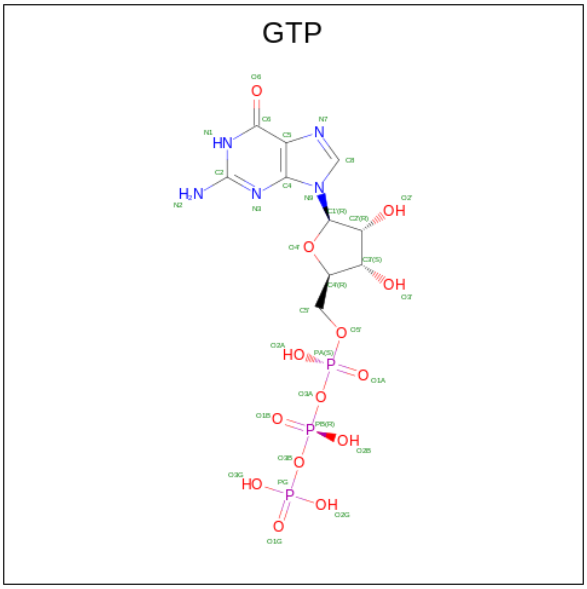
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

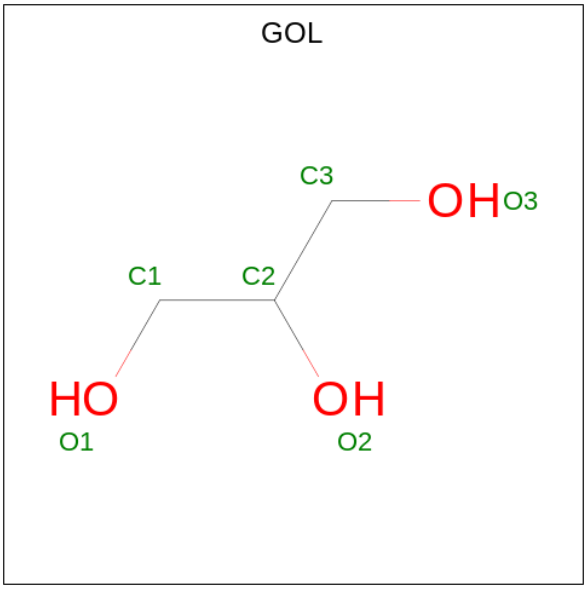
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

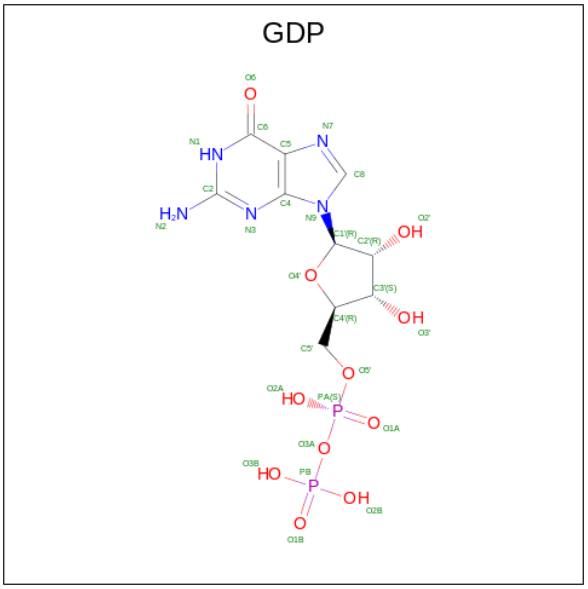
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



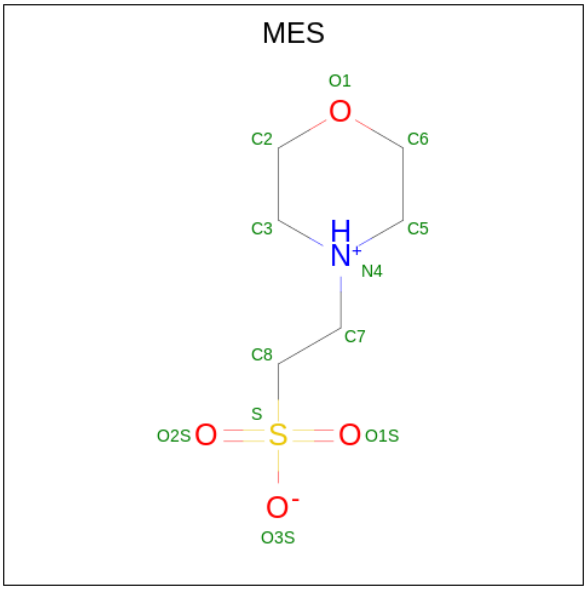
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

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



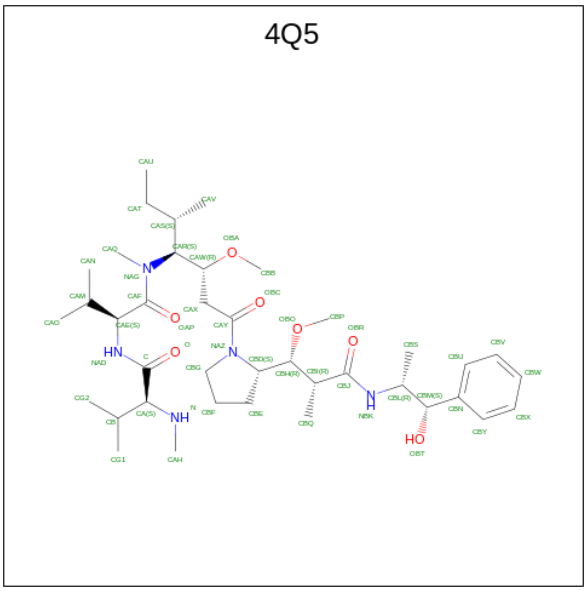
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



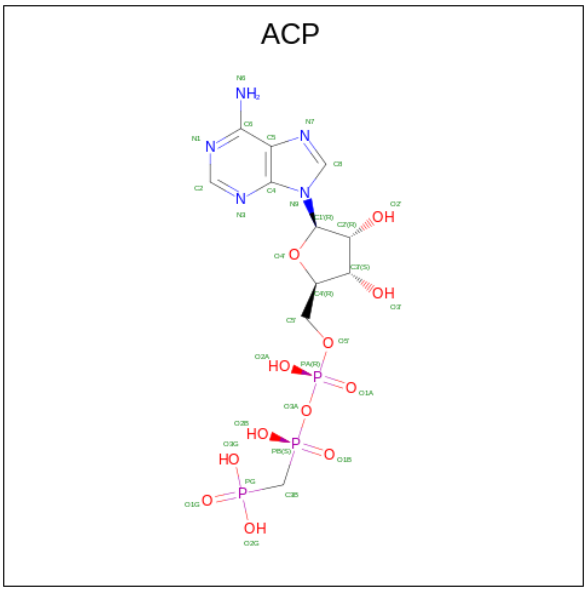
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is N-methyl-L-valyl-N-[(3R,4S,5S)-1-{(2S)-2-[(1R,2R)-3-{[(1S,2R)-1-hydroxy-1-phenylpropan-2-yl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (three-letter code: 4Q5) (formula: $C_{39}H_{67}N_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			51	39	5	7		

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



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

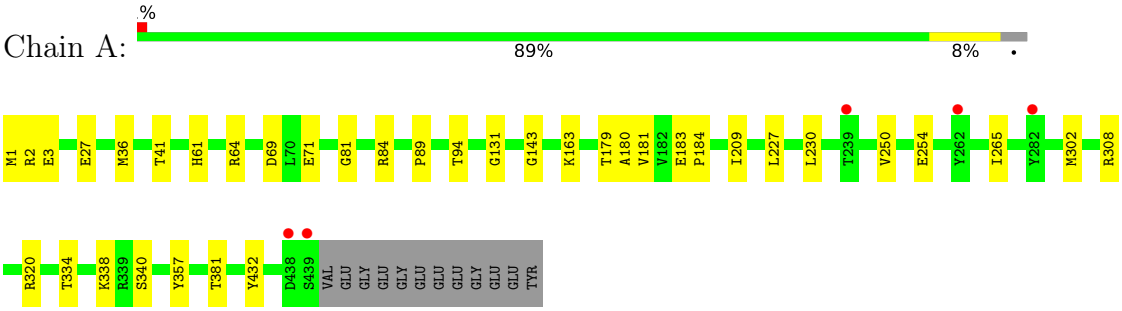
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	63	Total	O	0	0
			63	63		
13	B	66	Total	O	0	0
			66	66		
13	C	110	Total	O	0	0
			110	110		
13	D	19	Total	O	0	0
			19	19		
13	E	2	Total	O	0	0
			2	2		
13	F	37	Total	O	0	0
			37	37		

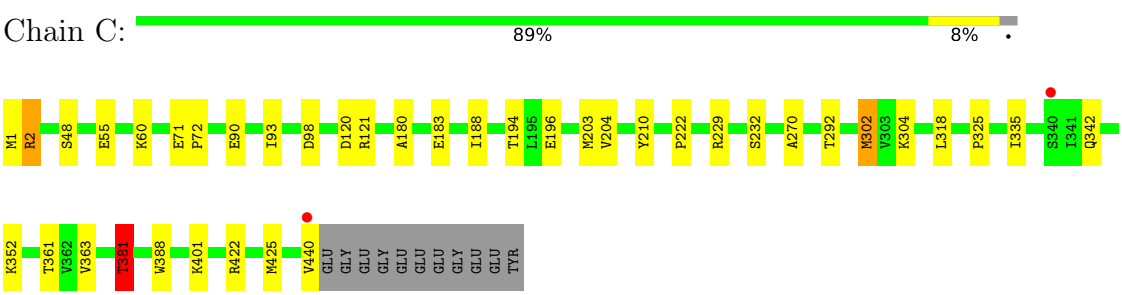
3 Residue-property plots (i)

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

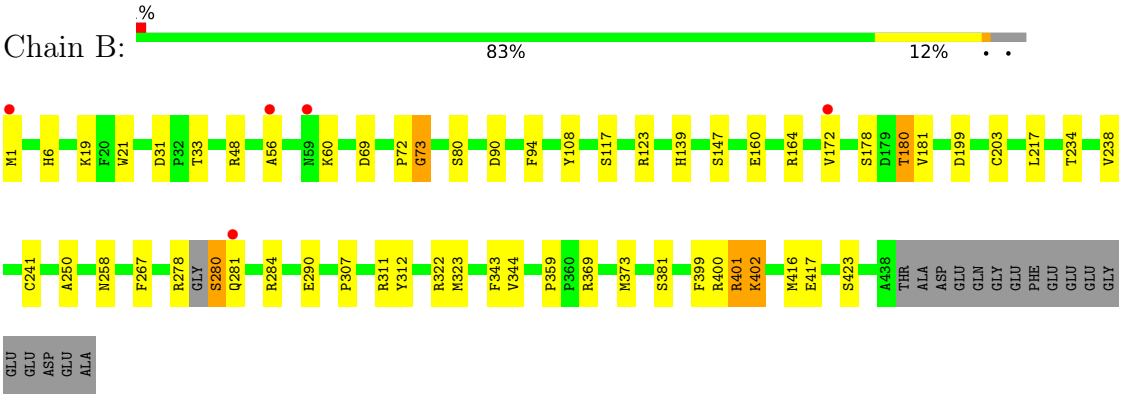
• Molecule 1: Tubulin alpha-1B chain



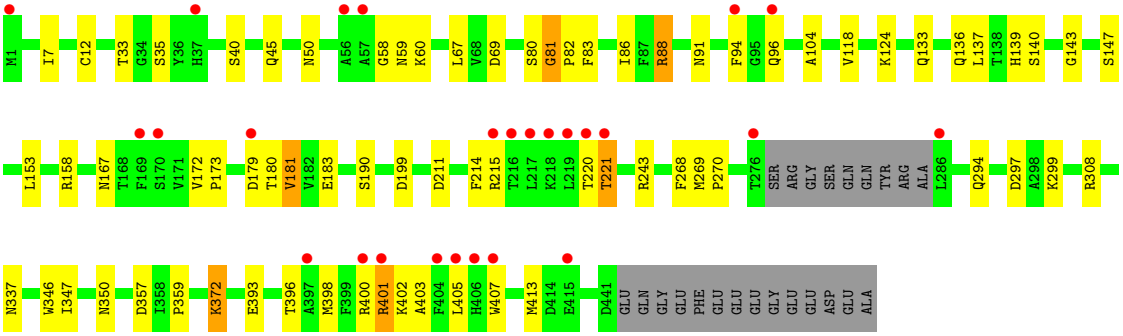
• Molecule 1: Tubulin alpha-1B chain



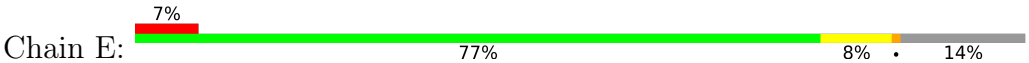
• Molecule 2: Tubulin beta chain

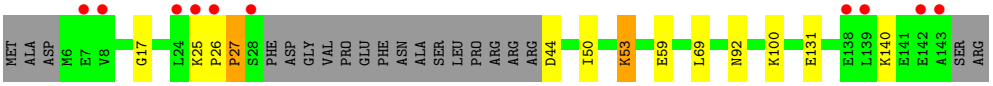


• Molecule 2: Tubulin beta chain

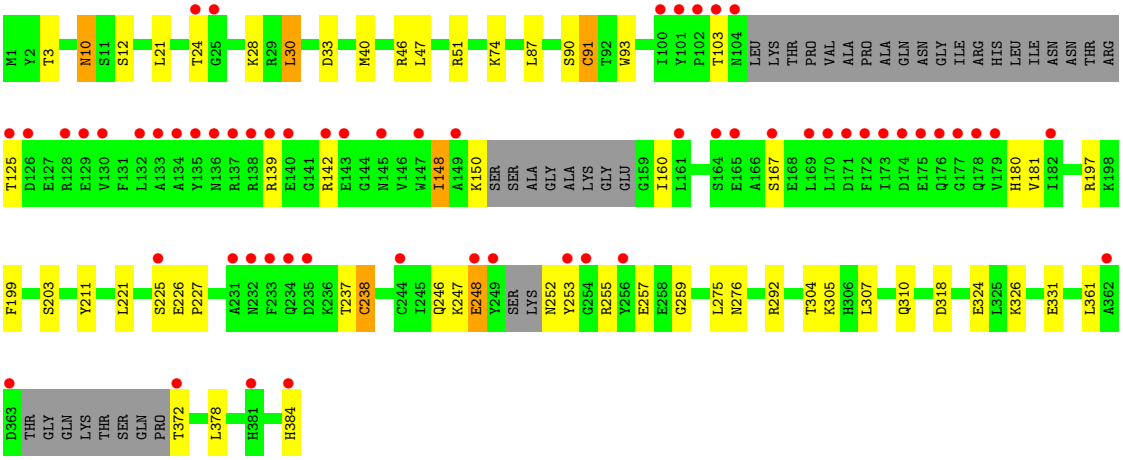


• Molecule 3: Stathmin-4





• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.94Å 156.81Å 182.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.55 39.34 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.34-2.55) 99.7 (39.34-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.190 , 0.245 0.192 , 0.246	Depositor DCC
R_{free} test set	4896 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17988	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GDP, ACP, GTP, 4Q5, CA, MG, GOL

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	0.70	0/3508	0.83	1/4762 (0.0%)
1	C	0.79	0/3524	0.88	3/4785 (0.1%)
2	B	0.78	0/3434	0.84	5/4651 (0.1%)
2	D	0.67	1/3384 (0.0%)	0.80	4/4586 (0.1%)
3	E	0.73	0/1022	0.81	0/1356
4	F	0.58	0/2916	0.76	2/3940 (0.1%)
All	All	0.71	1/17788 (0.0%)	0.83	15/24080 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	173	PRO	N-CD	5.17	1.55	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	221	THR	N-CA-C	-8.78	87.29	111.00
1	C	381	THR	CB-CA-C	-6.49	94.09	111.60
1	C	422	ARG	NE-CZ-NH2	-6.28	117.16	120.30
4	F	51	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	D	243	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	D	359	PRO	C-N-CD	6.02	141.04	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	311	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	B	359	PRO	C-N-CD	5.75	140.48	128.40
1	A	308	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	B	48	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	D	172	VAL	C-N-CD	5.29	139.52	128.40
1	C	302	MET	CB-CG-SD	-5.22	96.75	112.40
2	B	172	VAL	C-N-CD	5.16	139.24	128.40
2	B	401	ARG	NE-CZ-NH2	5.04	122.82	120.30
4	F	51	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3340	17	0
1	C	3446	0	3354	35	0
2	B	3360	0	3242	29	0
2	D	3311	0	3192	32	1
3	E	1014	0	1029	5	0
4	F	2849	0	2796	22	1
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	1	0
8	B	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	24	0	32	9	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	24	0	26	2	0
11	B	51	0	0	0	0
12	F	31	0	14	1	0
13	A	63	0	0	1	0
13	B	66	0	0	1	0
13	C	110	0	0	2	0
13	D	19	0	0	0	0
13	E	2	0	0	0	0
13	F	37	0	0	1	0
All	All	17988	0	17105	137	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (137) 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:229:ARG:HG2	8:C:506:GOL:O2	1.50	1.09
1:C:204:VAL:HG22	1:C:302:MET:CE	1.99	0.91
1:C:204:VAL:HG22	1:C:302:MET:HE2	1.51	0.90
1:C:363:VAL:HG21	8:C:506:GOL:H2	1.62	0.80
2:D:33:THR:OG1	2:D:60:LYS:NZ	2.16	0.78
1:C:363:VAL:CG2	8:C:506:GOL:H2	2.18	0.73
2:B:31:ASP:OD1	2:B:33:THR:HB	1.89	0.72
3:E:50:ILE:O	3:E:53:LYS:HB3	1.89	0.72
2:D:33:THR:CB	2:D:60:LYS:NZ	2.55	0.70
1:C:204:VAL:CG2	1:C:302:MET:HE2	2.21	0.69
2:D:136:GLN:HA	2:D:167:ASN:O	1.92	0.68
2:D:33:THR:HB	2:D:60:LYS:NZ	2.10	0.67
2:B:278:ARG:C	2:B:280:SER:N	2.49	0.67
1:C:229:ARG:CG	8:C:506:GOL:O2	2.38	0.64
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.80	0.63
1:C:55:GLU:HA	1:C:60:LYS:O	1.98	0.63
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.79	0.63
1:C:204:VAL:HG13	1:C:302:MET:HE2	1.78	0.63
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.20	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.02	0.59
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:VAL:HG13	2:D:398:MET:HE1	1.85	0.58
4:F:21:LEU:O	4:F:24:THR:OG1	2.15	0.56
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.40	0.56
2:B:180:THR:HG22	1:C:352:LYS:NZ	2.22	0.55
4:F:74:LYS:HB3	4:F:181:VAL:HG21	1.88	0.55
2:B:401:ARG:HE	8:B:506:GOL:C1	2.20	0.55
2:B:323:MET:HB3	2:B:373:MET:HE1	1.89	0.55
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.89	0.55
4:F:237:THR:O	4:F:246:GLN:NE2	2.34	0.54
2:D:104:ALA:HB2	2:D:413:MET:SD	2.48	0.54
1:C:304:LYS:HG3	8:C:505:GOL:H12	1.90	0.54
2:B:399:PHE:O	2:B:402:LYS:HE2	2.09	0.53
2:D:40:SER:O	2:D:45:GLN:HB2	2.07	0.53
4:F:150:LYS:N	4:F:181:VAL:O	2.41	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.44	0.52
1:C:204:VAL:CG1	1:C:302:MET:HE2	2.40	0.52
4:F:10:ASN:N	4:F:10:ASN:OD1	2.43	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.28	0.51
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.46	0.51
4:F:304:THR:O	4:F:310:GLN:NE2	2.42	0.51
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.11	0.50
2:B:72:PRO:O	2:B:73:GLY:C	2.50	0.50
2:B:199:ASP:OD1	10:B:504:MES:H32	2.11	0.50
2:D:393:GLU:O	2:D:396:THR:HG22	2.10	0.50
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.47	0.50
1:C:363:VAL:HG21	8:C:506:GOL:C2	2.36	0.50
2:B:199:ASP:OD2	10:B:504:MES:H52	2.12	0.49
2:B:164:ARG:HD2	13:B:649:HOH:O	2.12	0.49
1:C:1:MET:O	1:C:2:ARG:HB2	2.13	0.49
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.94	0.49
2:B:401:ARG:HH21	8:B:506:GOL:H12	1.77	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.48
2:B:401:ARG:HH21	8:B:506:GOL:C1	2.26	0.48
2:D:33:THR:HB	2:D:60:LYS:HZ2	1.78	0.48
1:C:204:VAL:CB	1:C:302:MET:HE2	2.42	0.48
2:D:82:PRO:O	2:D:83:PHE:HB2	2.13	0.48
2:D:118:VAL:HG11	2:D:153:LEU:HD21	1.94	0.48
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.48	0.48
1:C:204:VAL:HG13	1:C:302:MET:CE	2.41	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.97	0.47
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:CG2	1:C:302:MET:CE	2.82	0.47
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.47	0.47
1:A:183:GLU:N	1:A:184:PRO:CD	2.77	0.47
2:B:278:ARG:O	2:B:280:SER:N	2.48	0.47
2:D:58:GLY:O	2:D:59:ASN:HB2	2.15	0.47
2:D:180:THR:O	2:D:183:GLU:HG3	2.15	0.47
8:C:507:GOL:O1	8:C:507:GOL:O3	2.28	0.46
2:B:180:THR:HG22	1:C:352:LYS:HZ3	1.80	0.46
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.46
4:F:225:SER:OG	4:F:252:ASN:O	2.31	0.46
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.96	0.46
2:D:372:LYS:HE2	2:D:372:LYS:HB2	1.71	0.46
1:A:69:ASP:O	1:A:94:THR:HA	2.16	0.46
2:B:178:SER:HG	2:B:180:THR:HG23	1.80	0.46
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.16	0.45
2:D:35:SER:OG	2:D:60:LYS:HE2	2.16	0.45
1:C:381:THR:CG2	13:C:642:HOH:O	2.64	0.45
4:F:292:ARG:CG	4:F:378:LEU:HB3	2.46	0.45
1:C:90:GLU:HB3	1:C:121:ARG:HD2	1.99	0.45
2:D:211:ASP:O	2:D:215:ARG:HB2	2.16	0.45
4:F:40:MET:HE2	4:F:47:LEU:HG	1.98	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.16	0.45
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.45
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.10	0.45
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.45
1:C:270:ALA:HB3	1:C:302:MET:SD	2.57	0.45
4:F:28:LYS:NZ	13:F:502:HOH:O	2.50	0.44
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.18	0.44
2:B:343:PHE:O	2:B:344:VAL:C	2.54	0.44
2:D:7:ILE:O	2:D:137:LEU:HD12	2.17	0.44
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.51	0.44
2:B:56:ALA:N	2:B:60:LYS:O	2.49	0.44
1:C:381:THR:HG23	13:C:642:HOH:O	2.17	0.44
1:C:71:GLU:HG2	1:C:72:PRO:HD2	2.00	0.43
2:D:80:SER:OG	2:D:81:GLY:N	2.51	0.43
1:A:81:GLY:O	1:A:84:ARG:NH1	2.49	0.43
1:C:194:THR:O	1:C:194:THR:HG22	2.18	0.43
4:F:247:LYS:HE3	4:F:253:TYR:CZ	2.54	0.43
4:F:275:LEU:O	4:F:276:ASN:HB3	2.18	0.43
1:A:209:ILE:HD11	1:A:302:MET:SD	2.58	0.43
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:NH2	2:B:290:GLU:OE1	2.51	0.43
1:A:2:ARG:HB3	1:A:131:GLY:O	2.18	0.43
1:C:232:SER:OG	8:C:506:GOL:C3	2.67	0.43
2:D:268:PHE:O	2:D:270:PRO:HD3	2.19	0.43
2:B:123:ARG:NH2	2:B:160:GLU:OE1	2.50	0.42
2:B:241:CYS:O	2:B:250:ALA:HA	2.19	0.42
8:A:504:GOL:H12	13:A:639:HOH:O	2.18	0.42
2:D:214:PHE:HD1	2:D:220:THR:HA	1.83	0.42
2:B:178:SER:OG	2:B:180:THR:HG23	2.19	0.42
2:D:401:ARG:O	2:D:403:ALA:N	2.52	0.42
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.02	0.42
4:F:226:GLU:O	4:F:238:CYS:HB2	2.19	0.42
1:C:232:SER:OG	8:C:506:GOL:H31	2.20	0.41
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.60	0.41
2:B:234:THR:O	2:B:238:VAL:HG13	2.20	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.20	0.41
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.56	0.41
2:D:158:ARG:NH1	2:D:199:ASP:OD2	2.53	0.41
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.41
3:E:26:PRO:O	3:E:27:PRO:O	2.38	0.41
3:E:69:LEU:HD23	3:E:69:LEU:HA	1.95	0.41
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.24	0.41
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.02	0.41
2:D:12:CYS:CB	2:D:140:SER:HB3	2.50	0.41
4:F:90:SER:OG	4:F:91:CYS:N	2.53	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.41
1:C:203:MET:SD	1:C:388:TRP:CH2	3.14	0.41
2:D:294:GLN:O	2:D:297:ASP:HB2	2.21	0.41
3:E:131:GLU:OE2	3:E:131:GLU:HA	2.21	0.41
1:A:1:MET:C	1:A:1:MET:SD	2.99	0.40
2:D:405:LEU:HD12	2:D:405:LEU:HA	1.92	0.40
4:F:3:THR:HB	4:F:30:LEU:HD21	2.03	0.40
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.23	0.40
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:ASN:OD1	4:F:384:HIS:NE2[3_555]	2.17	0.03

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%)	419 (96%)	17 (4%)	1 (0%)	47	60
1	C	439/451 (97%)	424 (97%)	14 (3%)	1 (0%)	47	60
2	B	423/445 (95%)	409 (97%)	13 (3%)	1 (0%)	47	60
2	D	418/445 (94%)	401 (96%)	14 (3%)	3 (1%)	22	30
3	E	119/143 (83%)	112 (94%)	6 (5%)	1 (1%)	19	27
4	F	336/384 (88%)	308 (92%)	24 (7%)	4 (1%)	13	17
All	All	2172/2319 (94%)	2073 (95%)	88 (4%)	11 (0%)	29	40

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	402	LYS
3	E	27	PRO
4	F	91	CYS
4	F	142	ARG
2	B	73	GLY
2	D	81	GLY
1	C	2	ARG
4	F	248	GLU
1	A	89	PRO
4	F	227	PRO
2	D	143	GLY

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%)	361 (98%)	9 (2%)	49	64
1	C	372/379 (98%)	363 (98%)	9 (2%)	49	64
2	B	368/381 (97%)	350 (95%)	18 (5%)	25	34
2	D	363/381 (95%)	346 (95%)	17 (5%)	26	35
3	E	110/127 (87%)	103 (94%)	7 (6%)	17	23
4	F	312/342 (91%)	289 (93%)	23 (7%)	13	18
All	All	1895/1989 (95%)	1812 (96%)	83 (4%)	28	38

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	71	GLU
1	A	163	LYS
1	A	179	THR
1	A	181	VAL
1	A	334	THR
1	A	338	LYS
1	A	340	SER
1	A	381	THR
2	B	19	LYS
2	B	80	SER
2	B	90	ASP
2	B	117	SER
2	B	139	HIS
2	B	147	SER
2	B	180	THR
2	B	181	VAL
2	B	217	LEU
2	B	280	SER
2	B	281	GLN
2	B	307	PRO
2	B	322	ARG
2	B	369	ARG
2	B	400	ARG
2	B	402	LYS
2	B	416	MET
2	B	423	SER
1	C	48	SER
1	C	120	ASP
1	C	196	GLU

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Mol	Chain	Res	Type
1	C	318	LEU
1	C	325	PRO
1	C	342	GLN
1	C	361	THR
1	C	381	THR
1	C	440	VAL
2	D	50	ASN
2	D	88	ARG
2	D	96	GLN
2	D	124	LYS
2	D	133	GLN
2	D	139	HIS
2	D	179	ASP
2	D	181	VAL
2	D	221	THR
2	D	269	MET
2	D	299	LYS
2	D	308	ARG
2	D	357	ASP
2	D	372	LYS
2	D	400	ARG
2	D	401	ARG
2	D	407	TRP
3	E	25	LYS
3	E	44	ASP
3	E	53	LYS
3	E	59	GLU
3	E	92	ASN
3	E	100	LYS
3	E	140	LYS
4	F	10	ASN
4	F	12	SER
4	F	30	LEU
4	F	33	ASP
4	F	46	ARG
4	F	87	LEU
4	F	103	THR
4	F	125	THR
4	F	139	ARG
4	F	148	ILE
4	F	167	SER
4	F	180	HIS

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Mol	Chain	Res	Type
4	F	203	SER
4	F	211	TYR
4	F	238	CYS
4	F	248	GLU
4	F	255	ARG
4	F	305	LYS
4	F	324	GLU
4	F	326	LYS
4	F	331	GLU
4	F	361	LEU
4	F	372	THR

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

Mol	Chain	Res	Type
4	F	383	HIS

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 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 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	4Q5	B	507	-	52,52,52	1.33	4 (7%)	55,72,72	1.74	13 (23%)
8	GOL	A	506	-	5,5,5	0.55	0	5,5,5	0.30	0
9	GDP	D	501	6	24,30,30	1.01	2 (8%)	30,47,47	1.22	3 (10%)
10	MES	B	504	-	12,12,12	2.04	3 (25%)	14,16,16	6.37	8 (57%)
10	MES	B	505	-	12,12,12	2.29	2 (16%)	14,16,16	2.08	4 (28%)
8	GOL	A	504	-	5,5,5	0.48	0	5,5,5	0.53	0
8	GOL	C	506	-	5,5,5	0.65	0	5,5,5	0.95	0
8	GOL	C	505	-	5,5,5	0.66	0	5,5,5	0.88	0
8	GOL	A	505	-	5,5,5	0.45	0	5,5,5	1.08	0
8	GOL	B	506	-	5,5,5	0.86	0	5,5,5	0.85	0
5	GTP	C	501	6	26,34,34	0.92	0	32,54,54	1.52	6 (18%)
8	GOL	C	507	-	5,5,5	0.36	0	5,5,5	0.71	0
9	GDP	B	501	6	24,30,30	1.25	2 (8%)	30,47,47	1.44	6 (20%)
8	GOL	C	503	-	5,5,5	0.57	0	5,5,5	0.87	0
12	ACP	F	401	-	27,33,33	2.17	8 (29%)	32,52,52	1.21	3 (9%)
5	GTP	A	501	6	26,34,34	1.09	2 (7%)	32,54,54	1.48	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
11	4Q5	B	507	-	-	11/76/86/86	0/2/2/2
8	GOL	A	506	-	-	1/4/4/4	-
9	GDP	D	501	6	-	5/12/32/32	0/3/3/3
10	MES	B	504	-	-	5/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
8	GOL	A	504	-	-	3/4/4/4	-
8	GOL	C	506	-	-	2/4/4/4	-
8	GOL	C	505	-	-	2/4/4/4	-
8	GOL	A	505	-	-	3/4/4/4	-
8	GOL	B	506	-	-	2/4/4/4	-
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
8	GOL	C	507	-	-	2/4/4/4	-
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
8	GOL	C	503	-	-	2/4/4/4	-
12	ACP	F	401	-	-	5/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-7.36	1.67	1.77
12	F	401	ACP	PB-O3A	6.16	1.65	1.58
12	F	401	ACP	PG-O1G	6.07	1.62	1.50
10	B	504	MES	C8-S	-5.84	1.69	1.77
11	B	507	4Q5	CBN-CBM	-5.14	1.44	1.51
9	B	501	GDP	C2'-C1'	-3.82	1.48	1.53
12	F	401	ACP	PG-O3G	3.27	1.62	1.54
11	B	507	4Q5	CBY-CBN	3.13	1.44	1.39
12	F	401	ACP	C5-C4	2.82	1.48	1.40
5	A	501	GTP	C6-N1	-2.82	1.33	1.37
5	A	501	GTP	C2'-C1'	-2.72	1.49	1.53
9	B	501	GDP	C6-N1	-2.64	1.33	1.37
10	B	504	MES	O2S-S	2.54	1.52	1.45
12	F	401	ACP	PB-O2B	2.49	1.62	1.56
12	F	401	ACP	PG-O2G	-2.45	1.49	1.54
10	B	505	MES	O1S-S	2.22	1.51	1.45
12	F	401	ACP	O4'-C1'	2.22	1.44	1.41
12	F	401	ACP	C2-N3	2.16	1.35	1.32
11	B	507	4Q5	OBO-CBH	2.13	1.48	1.42
9	D	501	GDP	C6-N1	-2.12	1.34	1.37
10	B	504	MES	O1S-S	2.09	1.51	1.45
11	B	507	4Q5	CBM-CBL	2.07	1.55	1.54
9	D	501	GDP	C2-N3	2.04	1.38	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	MES	O3S-S-O2S	-11.68	82.73	111.27
10	B	504	MES	O1S-S-C8	11.34	120.57	106.92
10	B	504	MES	O3S-S-O1S	-10.95	84.53	111.27
10	B	504	MES	O3S-S-C8	-9.76	89.98	105.77
10	B	504	MES	O2S-S-C8	7.64	116.11	106.92
10	B	505	MES	O1S-S-C8	5.81	113.91	106.92
11	B	507	4Q5	CB-CA-C	-5.49	97.65	111.38
11	B	507	4Q5	CAW-CAX-CAY	-4.03	106.19	112.42
11	B	507	4Q5	CBI-CBJ-NBK	-3.84	110.62	116.44
10	B	504	MES	C6-C5-N4	3.39	115.25	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	501	GDP	O6-C6-C5	-3.29	117.95	124.37
11	B	507	4Q5	CBS-CBL-CBM	-3.28	109.57	112.67
9	D	501	GDP	C8-N7-C5	3.21	109.10	102.99
10	B	505	MES	O3S-S-O1S	-3.17	103.53	111.27
5	C	501	GTP	PA-O3A-PB	-3.17	121.96	132.83
5	A	501	GTP	C8-N7-C5	3.02	108.74	102.99
11	B	507	4Q5	OAP-CAF-CAE	2.99	125.83	119.99
12	F	401	ACP	N3-C2-N1	-2.99	124.01	128.68
5	C	501	GTP	C8-N7-C5	2.91	108.54	102.99
5	C	501	GTP	O6-C6-C5	-2.89	118.72	124.37
11	B	507	4Q5	CAM-CAE-CAF	2.82	116.44	110.73
12	F	401	ACP	C3'-C2'-C1'	2.79	105.19	100.98
9	D	501	GDP	O3B-PB-O1B	2.75	121.45	110.68
5	C	501	GTP	C5-C6-N1	2.71	118.74	113.95
11	B	507	4Q5	CBW-CBV-CBU	2.65	124.22	120.19
11	B	507	4Q5	CAM-CAE-NAD	2.64	117.97	111.43
9	B	501	GDP	C5-C6-N1	2.62	118.58	113.95
5	A	501	GTP	O6-C6-C5	-2.60	119.30	124.37
10	B	505	MES	O3S-S-C8	2.58	109.94	105.77
9	B	501	GDP	C8-N7-C5	2.56	107.87	102.99
5	A	501	GTP	C3'-C2'-C1'	-2.54	97.15	100.98
5	A	501	GTP	O4'-C1'-C2'	2.46	110.53	106.93
11	B	507	4Q5	CBP-OBO-CBH	-2.46	108.07	114.52
5	A	501	GTP	O3G-PG-O1G	2.43	120.18	110.68
9	B	501	GDP	PA-O3A-PB	-2.41	124.54	132.83
10	B	505	MES	O2S-S-C8	-2.40	104.02	106.92
9	B	501	GDP	O6-C6-N1	2.39	123.47	120.65
9	D	501	GDP	C5-C6-N1	2.38	118.16	113.95
11	B	507	4Q5	OBR-CBJ-NBK	2.27	127.13	122.93
10	B	504	MES	C2-C3-N4	2.26	113.53	110.10
5	A	501	GTP	O6-C6-N1	2.24	123.30	120.65
10	B	504	MES	O2S-S-O1S	2.22	121.64	113.95
11	B	507	4Q5	CAQ-NAG-CAR	2.16	123.70	119.46
11	B	507	4Q5	O-C-CA	-2.13	116.34	120.74
12	F	401	ACP	C4-C5-N7	-2.11	107.20	109.40
5	C	501	GTP	PB-O3B-PG	-2.11	125.58	132.83
9	B	501	GDP	C2-N1-C6	-2.10	121.23	125.10
11	B	507	4Q5	OAP-CAF-NAG	-2.10	118.19	121.71
5	C	501	GTP	O3'-C3'-C4'	-2.07	105.06	111.05

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
8	B	506	GOL	O1-C1-C2-C3
8	C	507	GOL	C1-C2-C3-O3
8	C	507	GOL	O2-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	N4-C7-C8-S
10	B	504	MES	C7-C8-S-O2S
11	B	507	4Q5	C-CA-CB-CG1
11	B	507	4Q5	C-CA-CB-CG2
11	B	507	4Q5	CAF-CAE-CAM-CAN
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
11	B	507	4Q5	N-CA-CB-CG1
11	B	507	4Q5	N-CA-CB-CG2
11	B	507	4Q5	NAD-CAE-CAM-CAN
11	B	507	4Q5	NAD-CAE-CAM-CAO
11	B	507	4Q5	CAF-CAE-CAM-CAO
8	A	505	GOL	O1-C1-C2-C3
8	C	503	GOL	C1-C2-C3-O3
8	C	505	GOL	O1-C1-C2-C3
8	B	506	GOL	O1-C1-C2-O2
8	C	505	GOL	O1-C1-C2-O2
11	B	507	4Q5	CAR-CAS-CAT-CAU
11	B	507	4Q5	CAV-CAS-CAT-CAU
8	A	504	GOL	O1-C1-C2-O2
8	A	506	GOL	O1-C1-C2-C3
8	A	505	GOL	O1-C1-C2-O2
8	A	505	GOL	O2-C2-C3-O3
8	C	506	GOL	O1-C1-C2-O2
11	B	507	4Q5	CBS-CBL-CBM-CBN
8	C	503	GOL	O2-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
10	B	504	MES	C7-C8-S-O1S
9	D	501	GDP	C4'-C5'-O5'-PA
10	B	504	MES	C8-C7-N4-C3
8	A	504	GOL	C1-C2-C3-O3
8	C	506	GOL	O1-C1-C2-C3
12	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
12	F	401	ACP	C3'-C4'-C5'-O5'
9	B	501	GDP	PB-O3A-PA-O1A
9	D	501	GDP	PB-O3A-PA-O1A

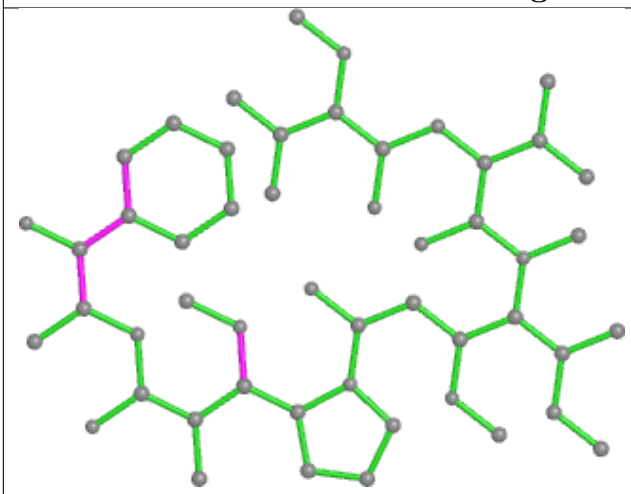
There are no ring outliers.

8 monomers are involved in 17 short contacts:

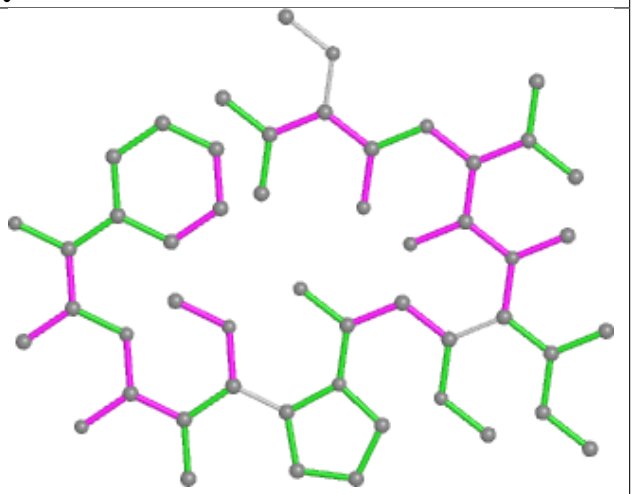
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	2	0
8	A	504	GOL	1	0
8	C	506	GOL	7	0
8	C	505	GOL	1	0
8	B	506	GOL	3	0
8	C	507	GOL	1	0
12	F	401	ACP	1	0
5	A	501	GTP	1	0

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.

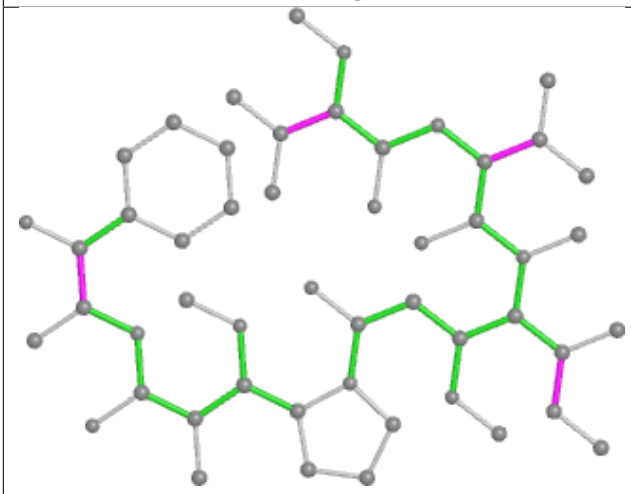
Ligand 4Q5 B 507



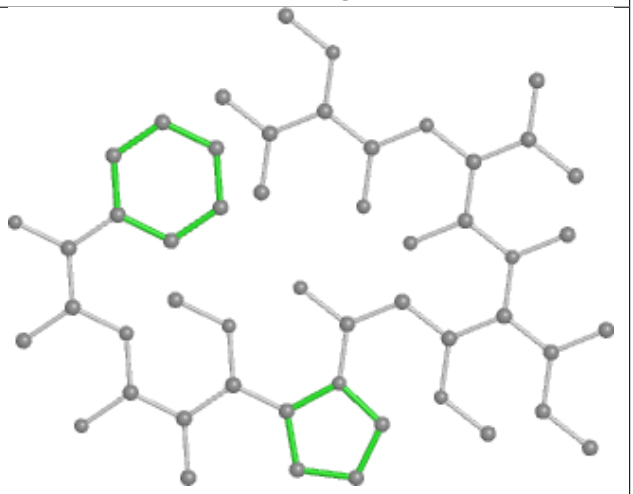
Bond lengths



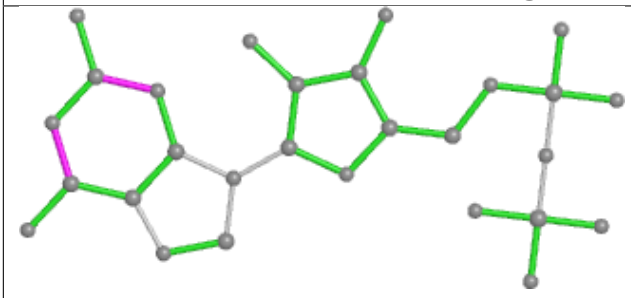
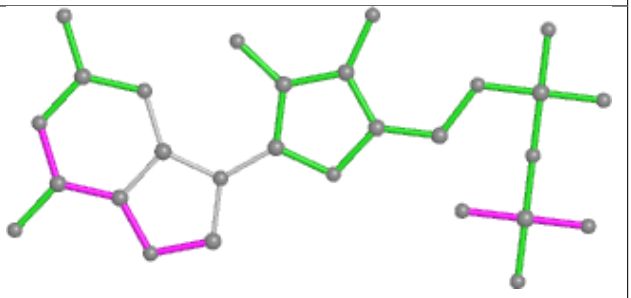
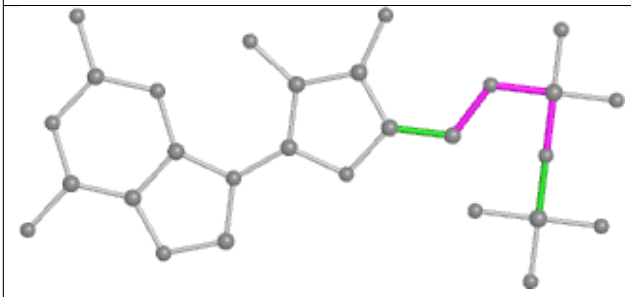
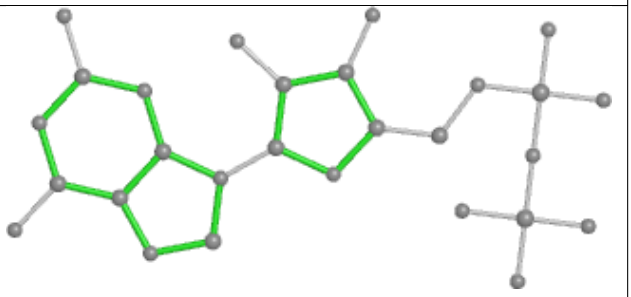
Bond angles

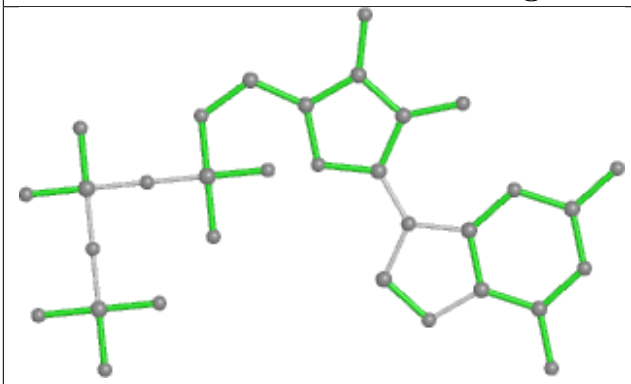
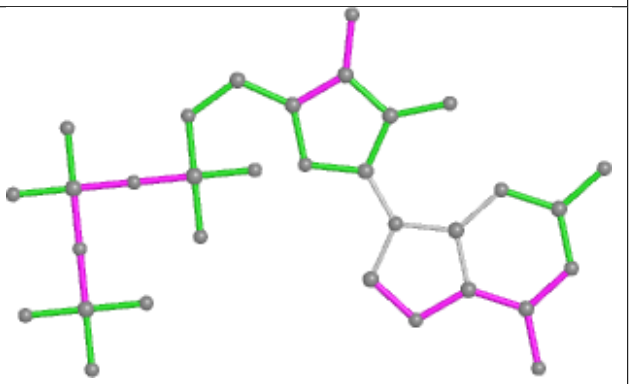
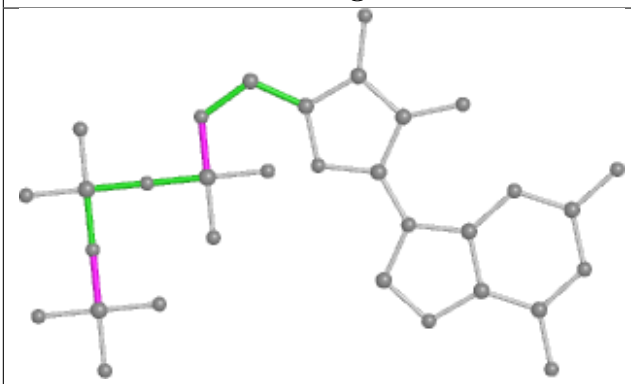
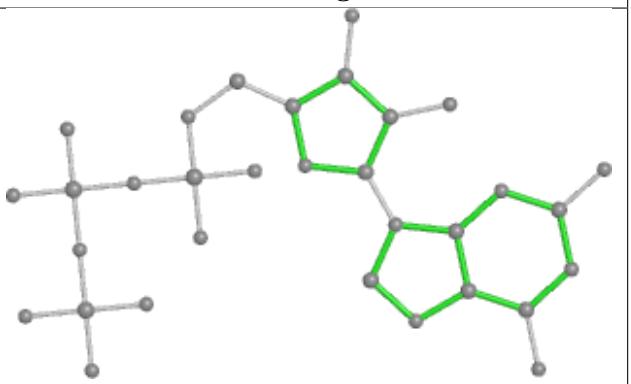


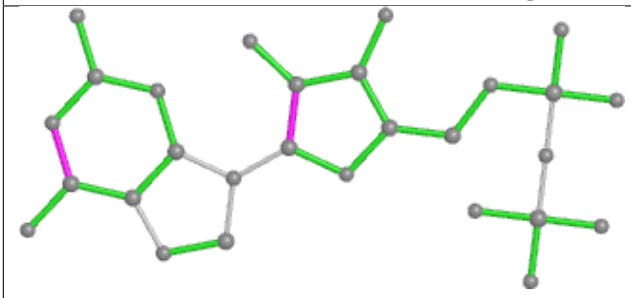
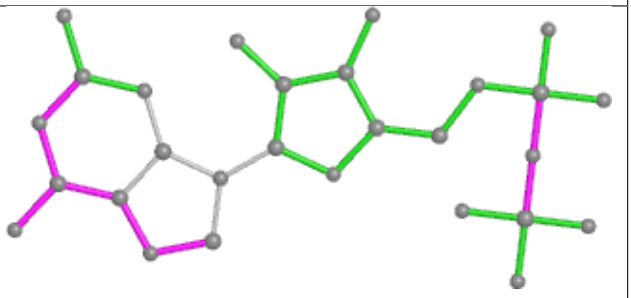
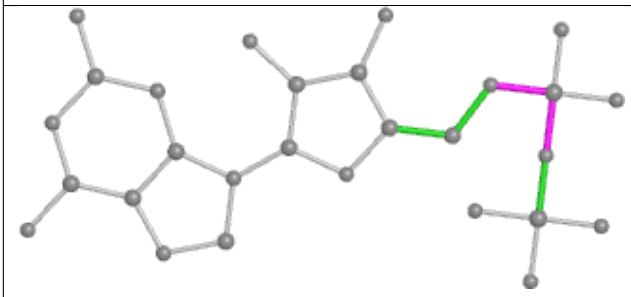
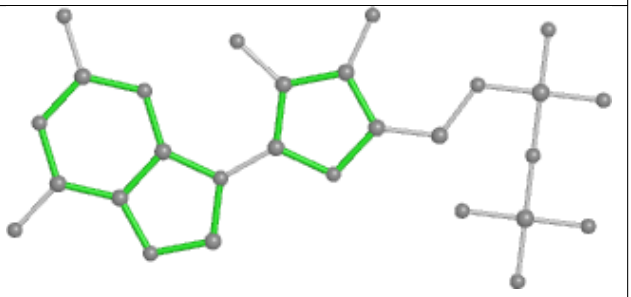
Torsions

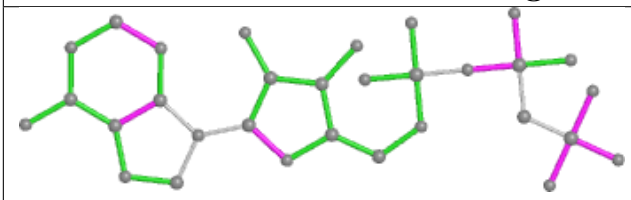
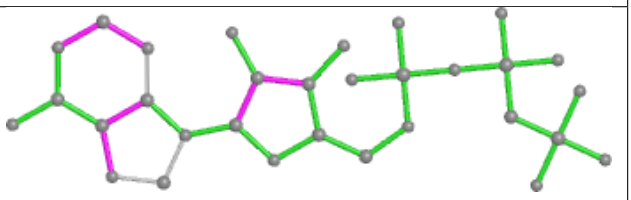
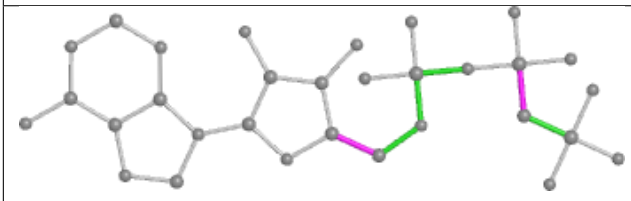
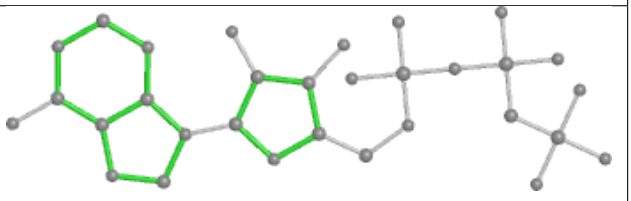


Rings

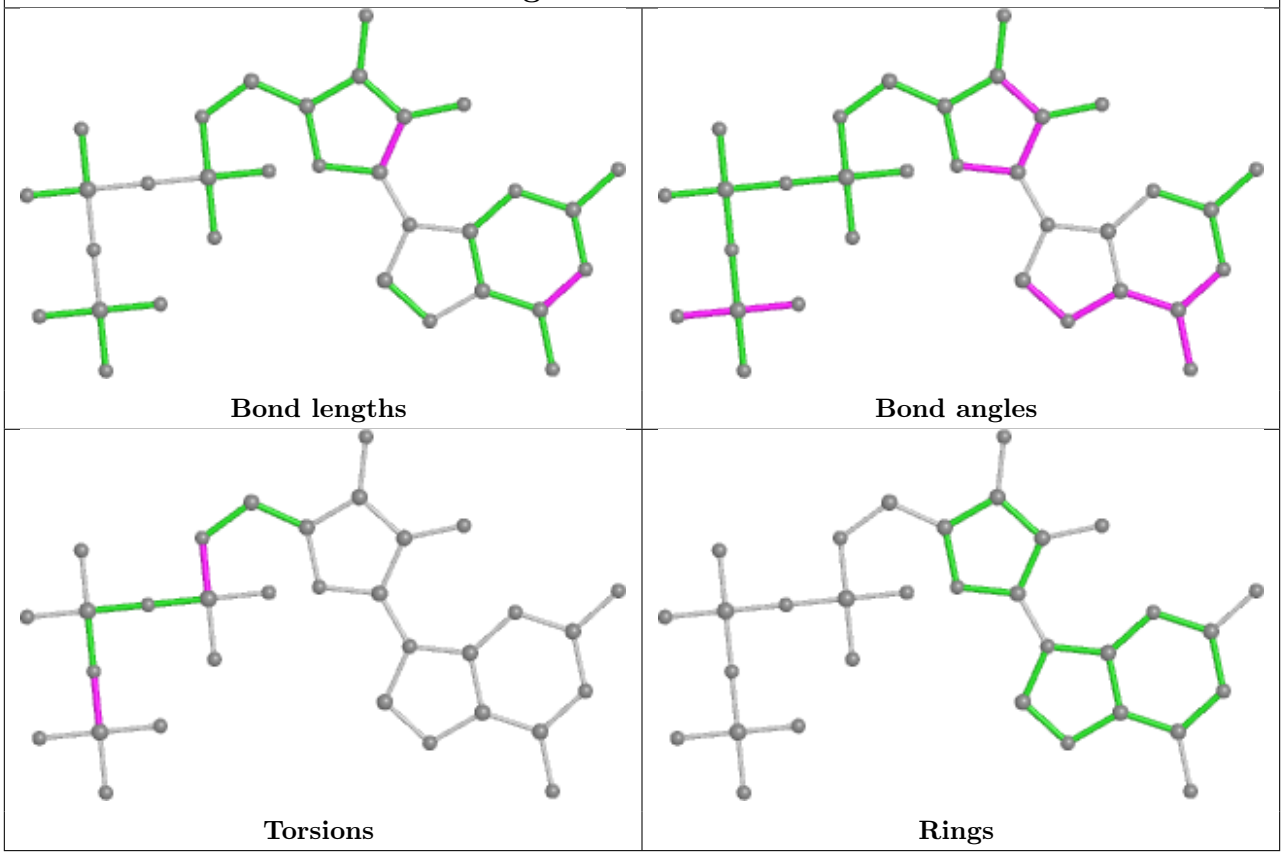
Ligand GDP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACP F 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP A 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	439/451 (97%)	-0.17	5 (1%) 80 85	18, 35, 61, 98	0
1	C	440/451 (97%)	-0.49	2 (0%) 91 94	16, 28, 51, 79	0
2	B	427/445 (95%)	-0.26	5 (1%) 79 84	16, 30, 61, 101	0
2	D	422/445 (94%)	0.17	26 (6%) 20 24	25, 47, 80, 93	0
3	E	123/143 (86%)	0.32	10 (8%) 12 15	29, 51, 85, 109	0
4	F	346/384 (90%)	0.53	59 (17%) 1 1	27, 59, 116, 135	0
All	All	2197/2319 (94%)	-0.05	107 (4%) 29 35	16, 39, 85, 135	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	372	THR	6.8
4	F	133	ALA	6.2
4	F	101	TYR	5.2
4	F	235	ASP	4.7
1	A	439	SER	4.5
4	F	104	ASN	4.5
4	F	135	TYR	4.5
4	F	132	LEU	4.3
4	F	103	THR	4.2
4	F	170	LEU	4.1
4	F	139	ARG	4.1
4	F	182	ILE	4.0
4	F	100	ILE	4.0
4	F	136	ASN	4.0
4	F	233	PHE	3.9
4	F	176	GLN	3.8
2	D	221	THR	3.8
4	F	232	ASN	3.7
4	F	140	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	167	SER	3.6
2	D	218	LYS	3.6
2	D	407	TRP	3.6
4	F	137	ARG	3.5
2	D	57	ALA	3.5
4	F	169	LEU	3.5
4	F	225	SER	3.5
2	D	286	LEU	3.5
4	F	234	GLN	3.5
2	D	400	ARG	3.4
4	F	363	ASP	3.4
4	F	178	GLN	3.3
2	D	276	THR	3.3
4	F	125	THR	3.3
2	D	1	MET	3.3
2	D	220	THR	3.3
4	F	142	ARG	3.3
4	F	175	GLU	3.3
3	E	143	ALA	3.2
4	F	171	ASP	3.1
4	F	102	PRO	3.1
4	F	362	ALA	3.1
4	F	161	LEU	3.1
4	F	177	GLY	3.1
4	F	244	CYS	3.1
4	F	179	VAL	3.0
1	A	262	TYR	3.0
4	F	249	TYR	3.0
4	F	173	ILE	3.0
2	B	59	ASN	3.0
4	F	174	ASP	2.9
4	F	248	GLU	2.9
2	D	405	LEU	2.8
2	B	1	MET	2.8
4	F	147	TRP	2.8
2	D	216	THR	2.8
3	E	139	LEU	2.7
4	F	256	TYR	2.7
2	D	96	GLN	2.7
4	F	231	ALA	2.7
4	F	130	VAL	2.7
4	F	165	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	172	PHE	2.6
3	E	26	PRO	2.6
3	E	25	LYS	2.6
2	B	281	GLN	2.6
4	F	149	ALA	2.5
3	E	8	VAL	2.5
2	D	217	LEU	2.5
2	D	94	PHE	2.5
4	F	254	GLY	2.5
4	F	253	TYR	2.5
2	D	179	ASP	2.4
2	D	406	HIS	2.4
2	D	37	HIS	2.3
1	A	438	ASP	2.3
2	B	56	ALA	2.3
3	E	142	GLU	2.3
4	F	143	GLU	2.3
3	E	138	GLU	2.3
4	F	134	ALA	2.3
4	F	24	THR	2.3
2	D	56	ALA	2.3
2	D	169	PHE	2.2
2	D	397	ALA	2.2
3	E	24	LEU	2.2
2	D	415	GLU	2.2
2	D	170	SER	2.2
2	D	401	ARG	2.2
4	F	384	HIS	2.2
3	E	28	SER	2.2
4	F	25	GLY	2.2
4	F	126	ASP	2.1
4	F	381	HIS	2.1
1	A	239	THR	2.1
2	B	172	VAL	2.1
4	F	138	ARG	2.1
4	F	164	SER	2.1
4	F	145	ASN	2.1
4	F	129	GLU	2.1
3	E	7	GLU	2.1
2	D	215	ARG	2.1
1	C	440	VAL	2.0
1	A	282	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	404	PHE	2.0
1	C	340	SER	2.0
2	D	219	LEU	2.0
4	F	128	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
8	GOL	C	506	6/6	0.73	0.53	50,68,69,82	0
8	GOL	A	506	6/6	0.82	0.22	54,61,65,67	0
8	GOL	B	506	6/6	0.84	0.26	49,51,54,55	0
7	CA	B	503	1/1	0.84	0.15	82,82,82,82	0
8	GOL	A	504	6/6	0.85	0.19	63,69,72,81	0
8	GOL	C	503	6/6	0.87	0.27	54,69,72,77	0
8	GOL	C	505	6/6	0.90	0.34	44,53,55,63	0
7	CA	A	503	1/1	0.90	0.04	57,57,57,57	0
12	ACP	F	401	31/31	0.90	0.17	66,83,96,109	0
8	GOL	A	505	6/6	0.91	0.20	46,59,60,67	0
6	MG	D	502	1/1	0.92	0.08	46,46,46,46	0
10	MES	B	504	12/12	0.95	0.13	45,49,56,60	0
10	MES	B	505	12/12	0.96	0.17	49,52,53,55	0
6	MG	B	502	1/1	0.96	0.08	63,63,63,63	0
6	MG	A	502	1/1	0.97	0.05	25,25,25,25	0
8	GOL	C	507	6/6	0.97	0.15	45,51,53,55	0
11	4Q5	B	507	51/51	0.97	0.11	18,22,25,25	0
9	GDP	D	501	28/28	0.97	0.12	34,38,48,60	0
7	CA	C	504	1/1	0.98	0.03	35,35,35,35	0

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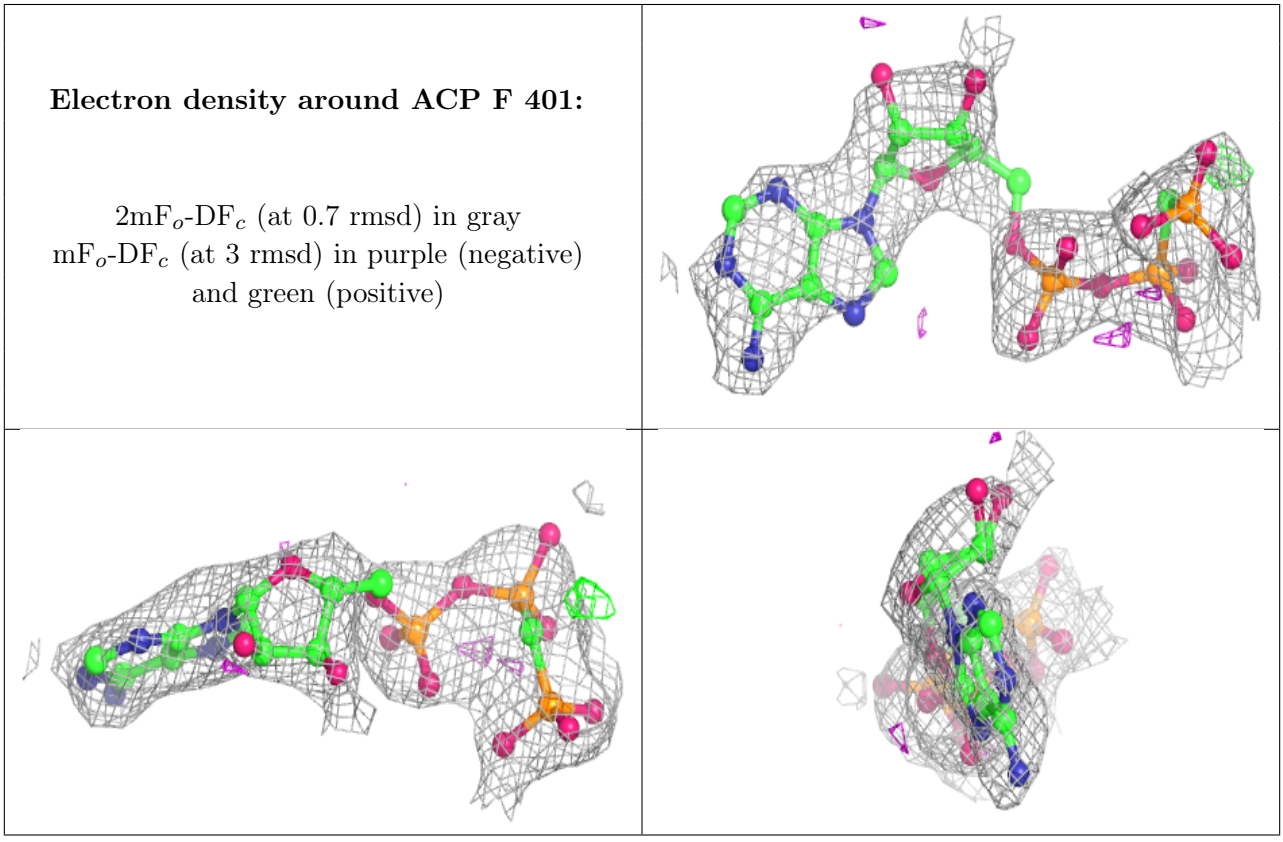
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	C	502	1/1	0.98	0.07	23,23,23,23	0
9	GDP	B	501	28/28	0.99	0.13	15,18,19,20	0
5	GTP	C	501	32/32	0.99	0.12	17,20,23,23	0
5	GTP	A	501	32/32	0.99	0.14	18,22,25,26	0

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

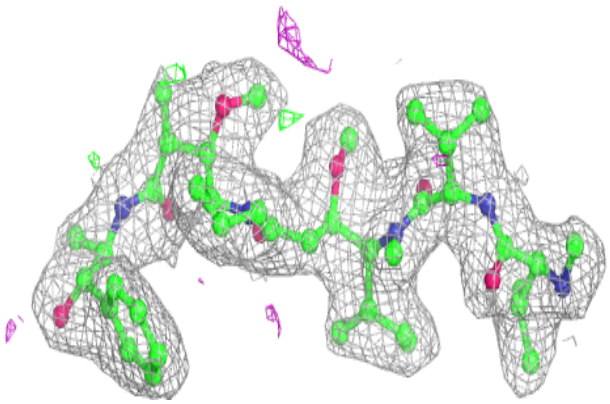
Electron density around ACP F 401:

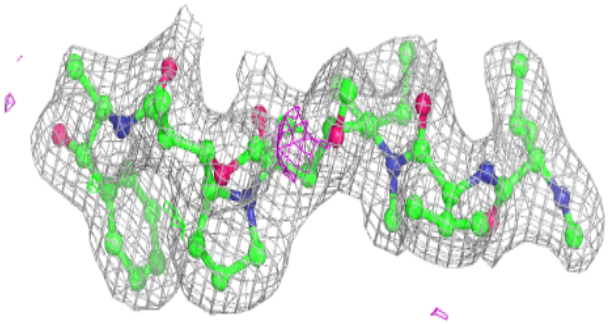
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

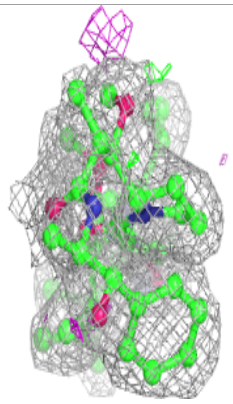


Electron density around 4Q5 B 507:

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

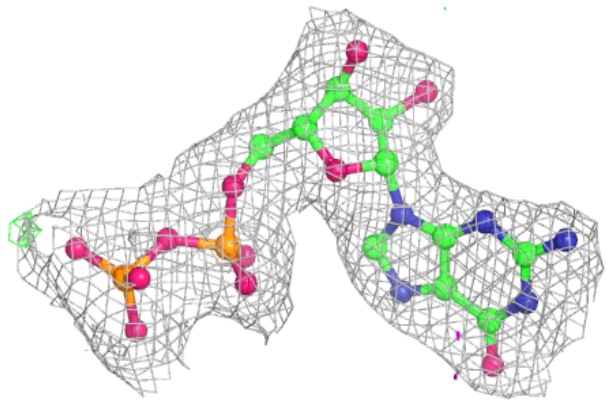


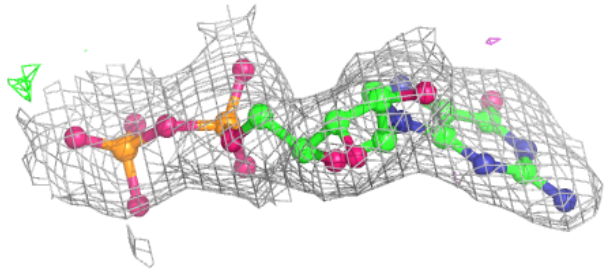


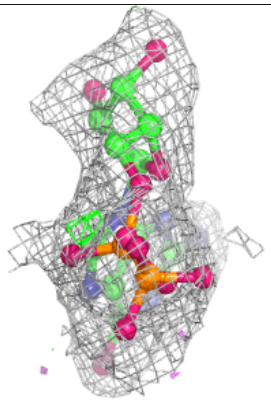


Electron density around GDP D 501:

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

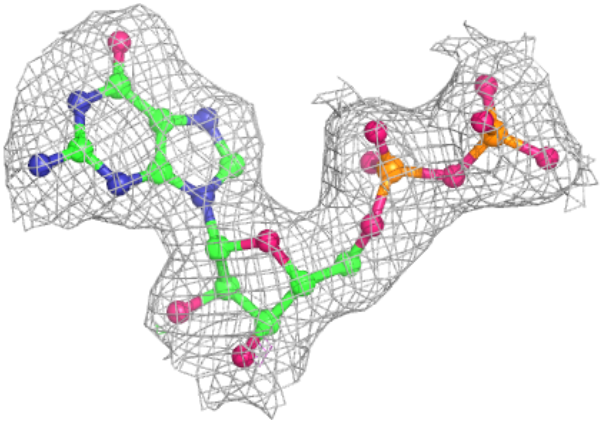


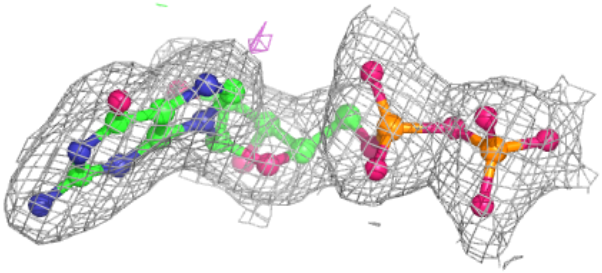


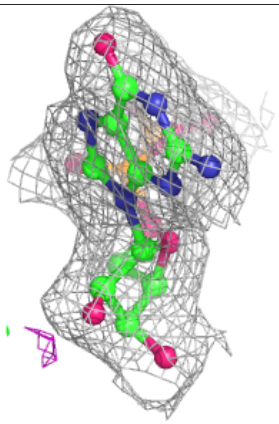


Electron density around GDP B 501:

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

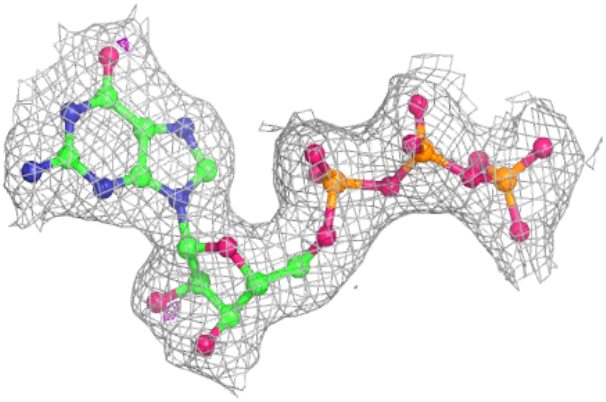


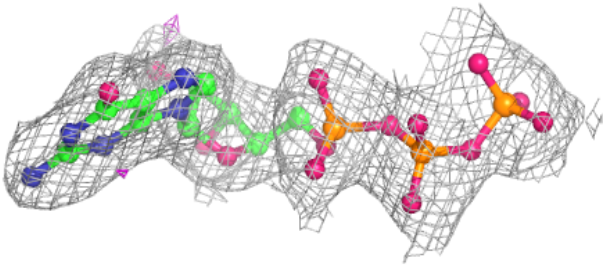


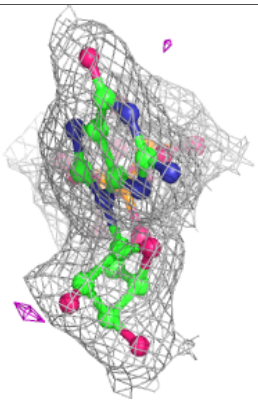


Electron density around GTP C 501:

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

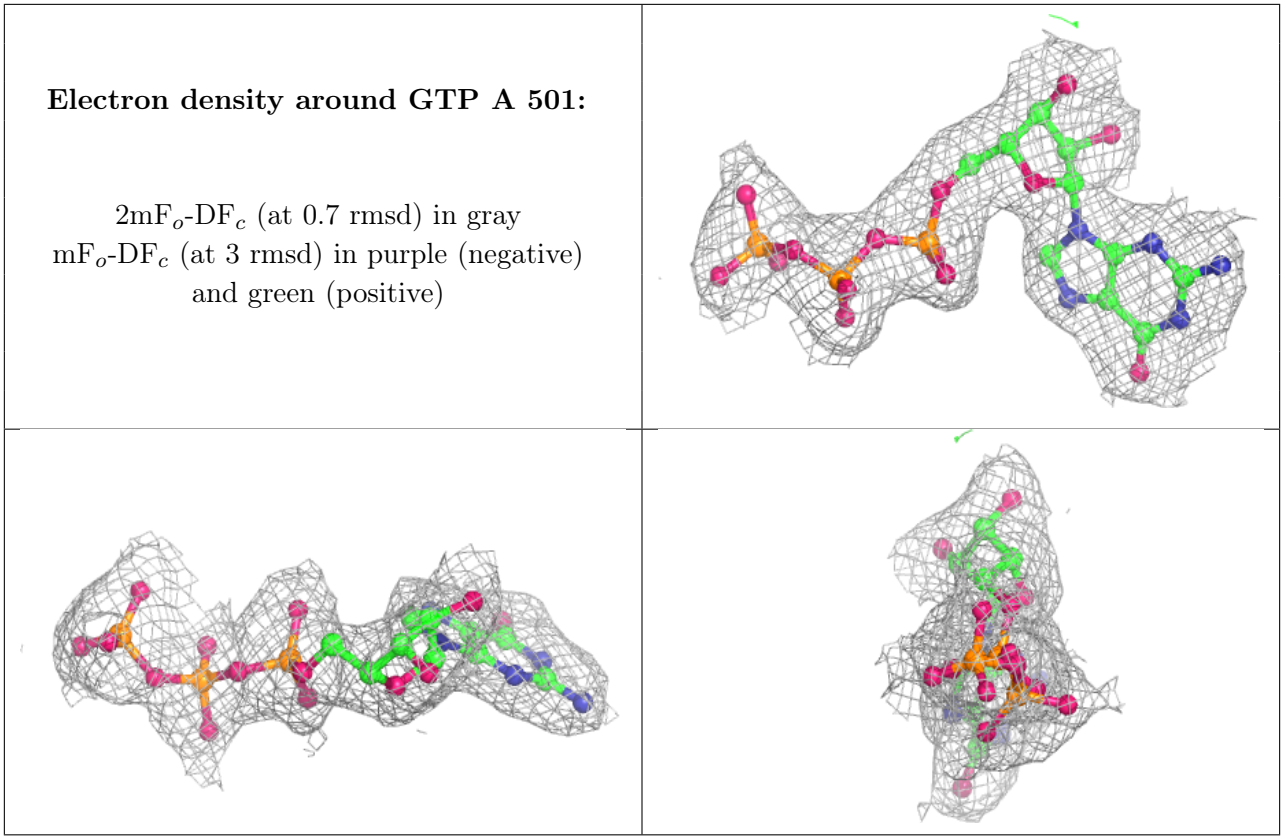






Electron density around GTP A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.