



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:37 AM UTC

PDB ID : 9IM5 / pdb_00009im5
Title : Tubulin-RB3(MUT)-TTL-Y12
Authors : Yan, W.; Yang, J.H.
Deposited on : 2024-07-02
Resolution : 2.86 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

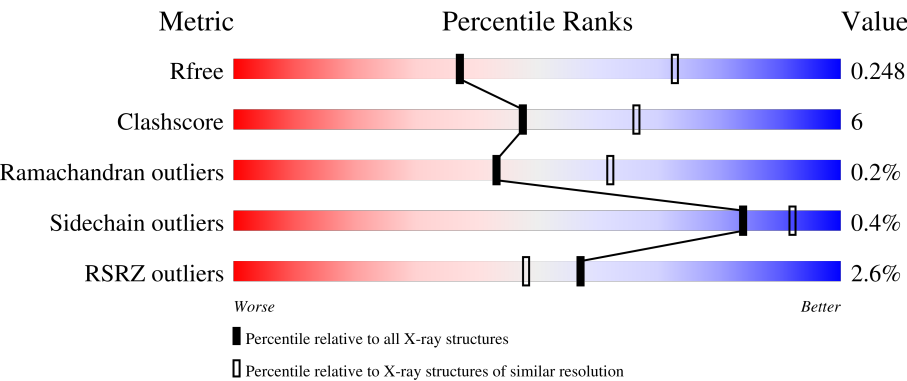
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	% 86%11%.
1	C	451	% 89%8%.
2	B	445	% 83%12%5%.
2	D	445	3% 82%12%6%.
3	E	143	% 73%10%16%.

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Mol	Chain	Length	Quality of chain
4	F	384	6% 70% 10% 20%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17251 atoms, of which 34 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	2	0
			3422	2167	581	650	24			
1	C	440	Total	C	N	O	S	0	1	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3322	2089	567	641	25			
2	D	420	Total	C	N	O	S	0	1	0
			3262	2052	556	630	24			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	1	0
			997	617	179	196	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	71	GLN	HIS	engineered mutation	UNP P63043

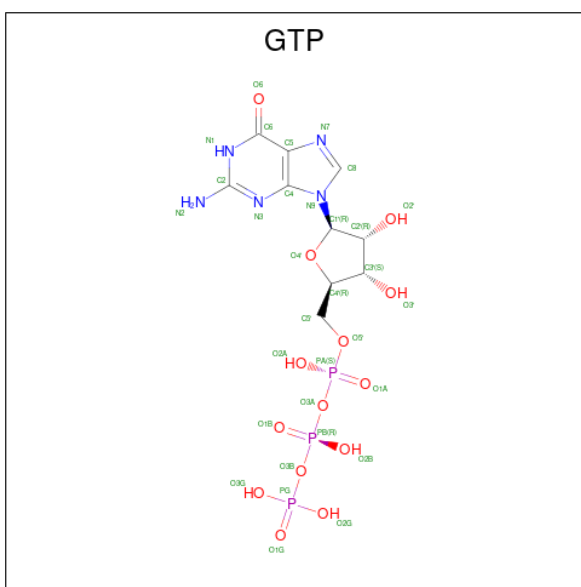
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	0	0
			2530	1631	435	450	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

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



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: 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

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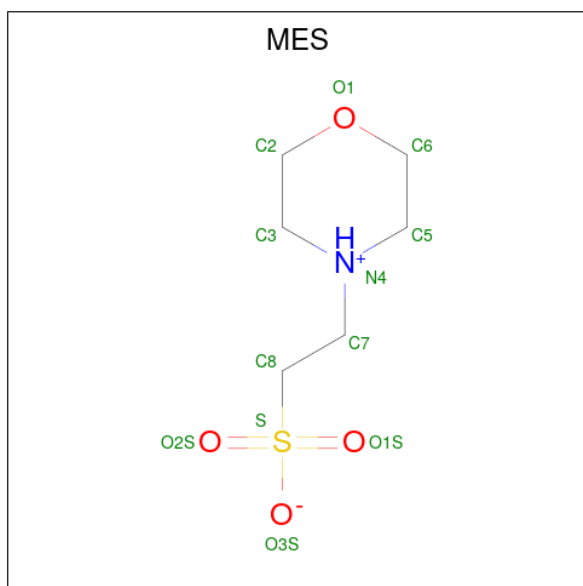
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

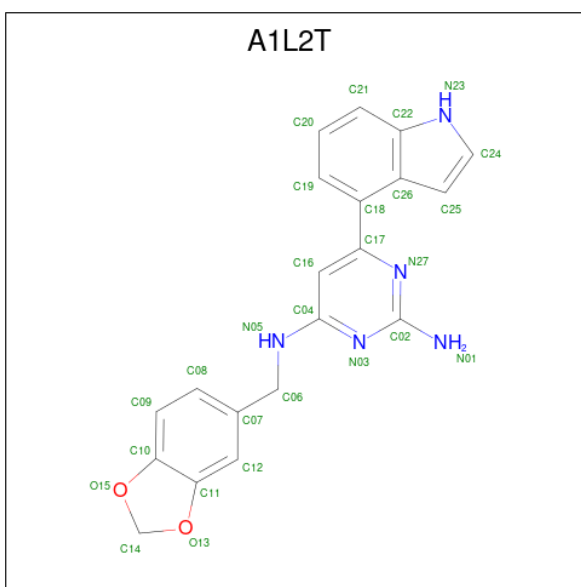
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



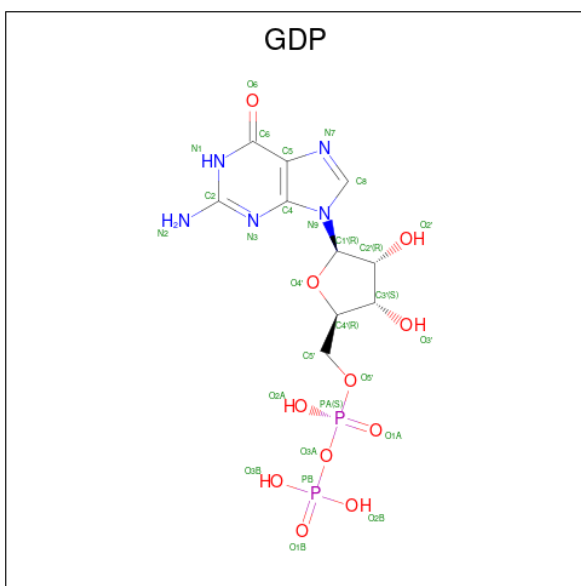
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is {N}4-(1,3-benzodioxol-5-ylmethyl)-6-(1 {H}-indol-4-yl)pyrimidine-2,4-diamine (CCD ID: A1L2T) (formula: C₂₀H₁₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			44	20	17	5	2		
10	D	1	Total	C	H	N	O	0	0
			44	20	17	5	2		

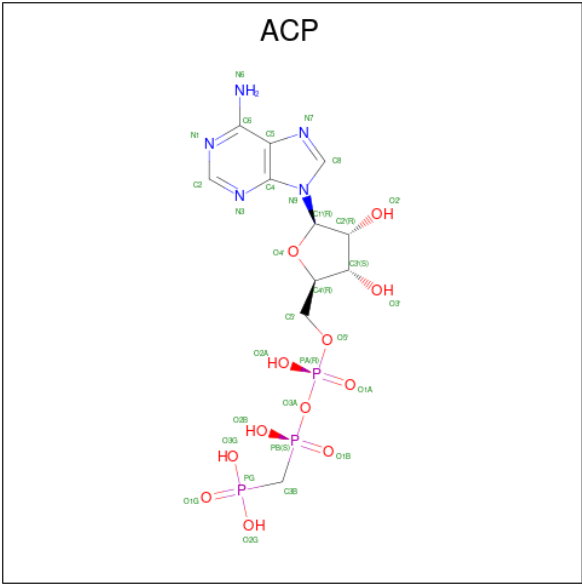
- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD

ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

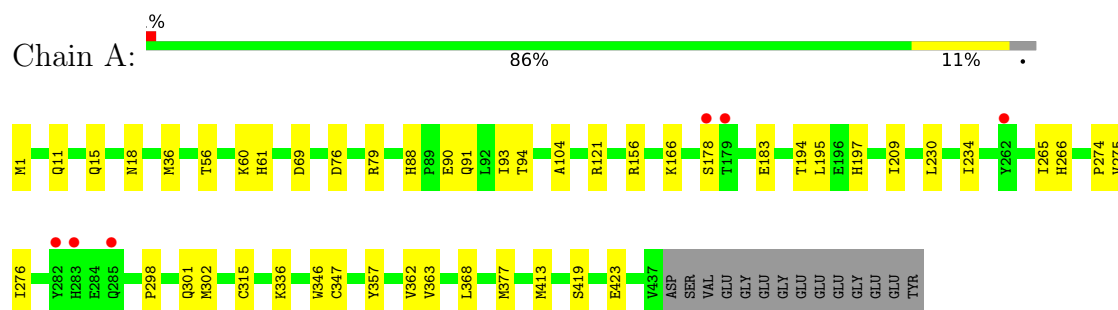
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	O	0	0
			1	1		
13	B	5	Total	O	0	0
			5	5		

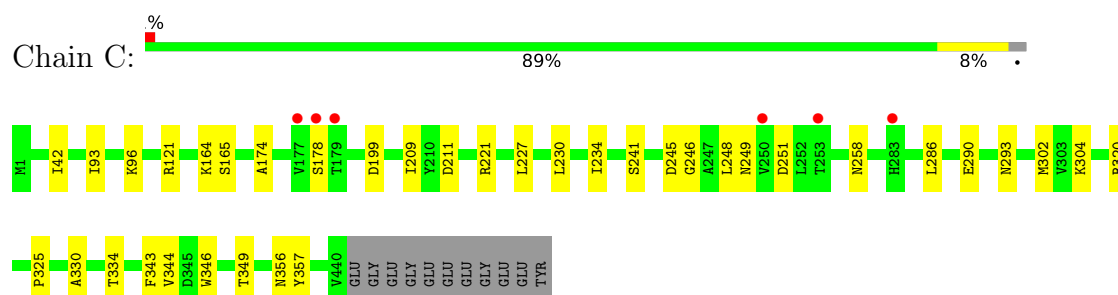
3 Residue-property plots [i](#)

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.

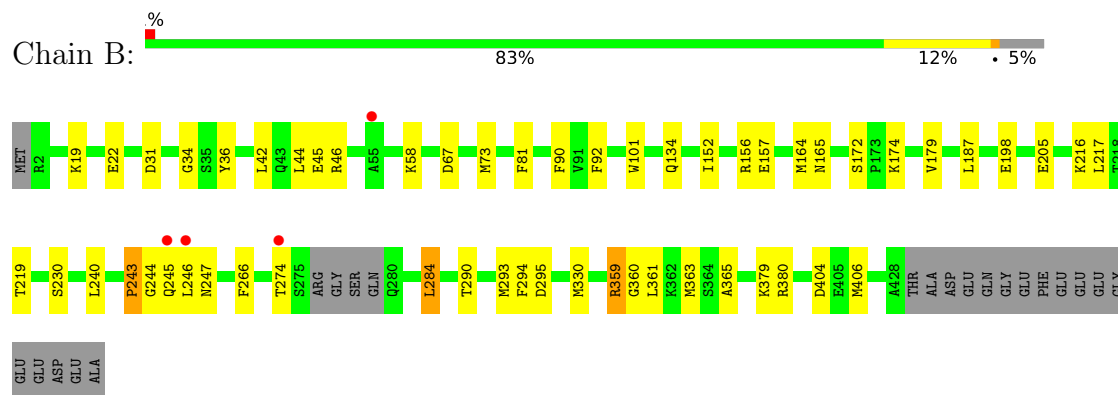
- Molecule 1: Tubulin alpha-1B chain



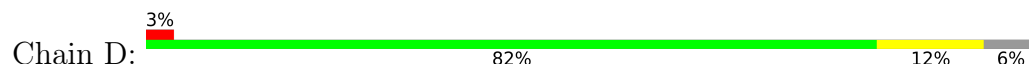
- Molecule 1: Tubulin alpha-1B chain

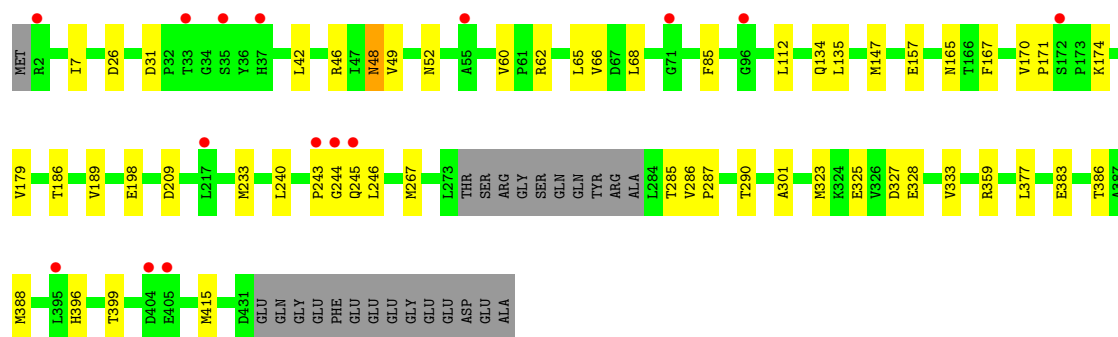


- Molecule 2: Tubulin beta chain

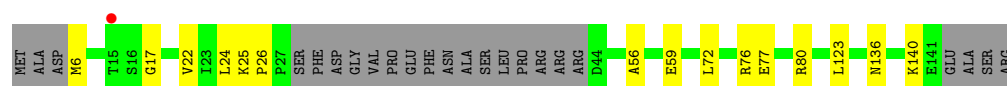
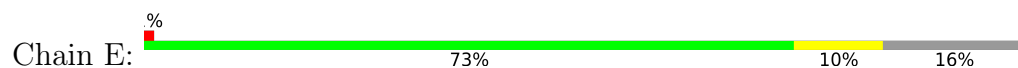


- Molecule 2: Tubulin beta chain

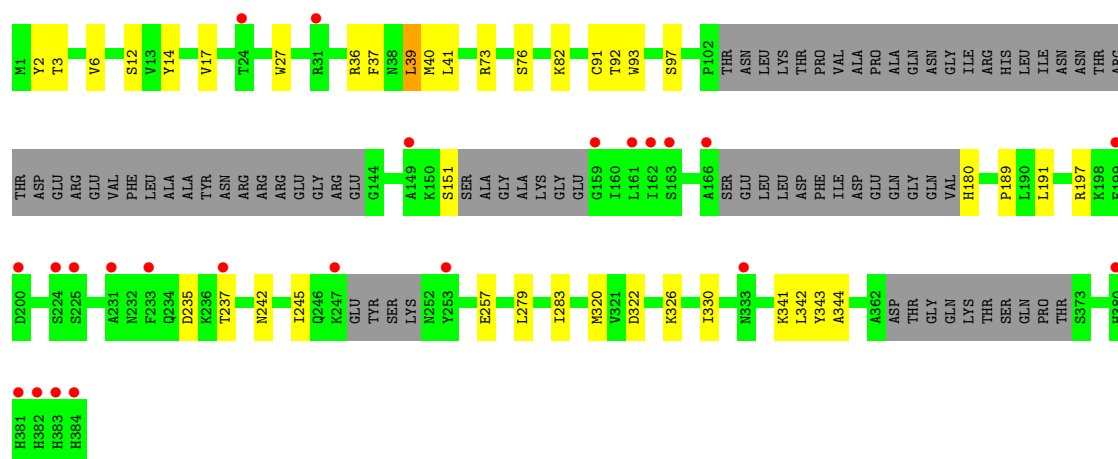




- Molecule 3: Stathmin-4



- Molecule 4: Tubulin-tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.35Å 160.78Å 184.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.15 – 2.86 37.15 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.15-2.86) 99.9 (37.15-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.209 , 0.246 0.212 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17251	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: A1L2T, GTP, MES, CA, ACP, CL, 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	0.31	0/3506	0.66	0/4759
1	C	0.33	0/3515	0.67	0/4772
2	B	0.34	0/3396	0.69	0/4603
2	D	0.31	0/3334	0.68	0/4524
3	E	0.36	0/1004	0.67	0/1332
4	F	0.28	0/2592	0.65	0/3503
All	All	0.32	0/17347	0.67	0/23493

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3422	0	3340	39	0
1	C	3437	0	3347	25	0
2	B	3322	0	3192	49	0
2	D	3262	0	3121	42	0
3	E	997	0	1018	13	0
4	F	2530	0	2498	28	0
5	A	32	0	12	0	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	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	24	0	24	3	0
10	B	27	17	0	1	0
10	D	27	17	0	1	0
11	B	28	0	12	0	0
12	F	31	0	14	0	0
13	A	1	0	0	0	0
13	B	5	0	0	2	0
All	All	17217	34	16602	190	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 6.

All (190) 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)
2:D:244:GLY:O	2:D:246:LEU:N	1.99	0.96
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.47	0.95
2:B:157:GLU:HB2	3:E:72:LEU:HD13	1.50	0.94
3:E:25:LYS:HD2	3:E:26:PRO:O	1.72	0.90
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.55	0.89
2:B:244:GLY:O	2:B:246:LEU:N	2.06	0.86
1:A:274:PRO:HB2	1:A:276:ILE:HD11	1.58	0.86
2:D:165:ASN:OD1	2:D:198:GLU:HB2	1.76	0.85
2:D:240:LEU:HD12	10:D:503:A1L2T:C24	2.09	0.82
4:F:151:SER:HB3	4:F:180:HIS:ND1	1.96	0.81
4:F:73:ARG:HB2	4:F:76:SER:OG	1.80	0.80
2:B:45:GLU:CD	2:B:243:PRO:HG3	2.04	0.79
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.83	0.79
2:B:198:GLU:HG2	2:B:266:PHE:CE2	2.18	0.78
2:B:290:THR:HG23	2:B:330:MET:CE	2.13	0.78
2:B:240:LEU:HD12	10:B:505:A1L2T:C24	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:MET:HA	2:B:330:MET:HE2	1.65	0.77
2:D:48:ASN:O	2:D:62:ARG:NH2	2.19	0.75
2:D:325:GLU:HA	2:D:328:GLU:HG2	1.68	0.75
4:F:3:THR:HG23	4:F:37:PHE:HA	1.69	0.74
2:D:396:HIS:HA	2:D:399:THR:HG22	1.69	0.74
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.20	0.74
2:B:359:ARG:HA	2:B:359:ARG:HE	1.55	0.71
2:B:290:THR:HG23	2:B:330:MET:HE1	1.73	0.71
4:F:341:LYS:HD2	4:F:341:LYS:O	1.92	0.70
2:D:179:VAL:O	2:D:388:MET:HE1	1.92	0.70
1:A:315[B]:CYS:SG	1:A:377:MET:HE3	2.32	0.70
2:D:66:VAL:CG1	2:D:147:MET:HE1	2.22	0.69
1:A:315[A]:CYS:SG	1:A:377:MET:HE3	2.32	0.68
9:B:503:MES:H52	13:B:601:HOH:O	1.94	0.68
2:D:383:GLU:O	2:D:386:THR:HG22	1.94	0.67
4:F:235:ASP:OD2	4:F:237:THR:HG22	1.95	0.67
2:D:46:ARG:O	2:D:49:VAL:HG12	1.95	0.66
2:B:19:LYS:HG3	2:B:230:SER:CB	2.25	0.65
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.77	0.65
1:C:330:ALA:O	1:C:334:THR:HG23	1.96	0.64
1:A:56:THR:CG2	1:A:60:LYS:HB3	2.28	0.63
1:A:104:ALA:HB2	1:A:413:MET:CE	2.25	0.63
1:A:274:PRO:HB2	1:A:276:ILE:CD1	2.27	0.63
2:B:46:ARG:NH1	2:B:240:LEU:O	2.32	0.62
2:B:294:PHE:O	9:B:504:MES:H81	1.99	0.62
1:C:42:ILE:HD12	1:C:42:ILE:H	1.63	0.62
1:A:419:SER:O	1:A:423:GLU:HG2	1.99	0.62
2:B:172:SER:OG	2:B:205:GLU:OE1	2.16	0.62
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.80	0.62
2:D:48:ASN:OD1	2:D:48:ASN:N	2.25	0.62
3:E:76:ARG:O	3:E:80:ARG:HD3	2.00	0.62
4:F:189:PRO:O	4:F:191:LEU:HD22	1.99	0.62
1:A:166:LYS:HE2	1:A:197:HIS:O	2.00	0.61
2:B:284:LEU:O	2:B:363:MET:HE2	2.00	0.61
2:B:179:VAL:HG13	1:C:258:ASN:OD1	2.00	0.61
1:C:209:ILE:HD11	1:C:302:MET:SD	2.40	0.61
1:A:346:TRP:CD1	1:A:347:CYS:HG	2.19	0.60
1:C:221:ARG:HH21	2:D:323:MET:HE2	1.66	0.60
1:A:234:ILE:HD13	1:A:302:MET:SD	2.42	0.60
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.37	0.60
2:D:66:VAL:HG12	2:D:147:MET:HE1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:CG2	1:C:227:LEU:HD22	2.32	0.58
2:B:34:GLY:C	2:B:58:LYS:HE3	2.29	0.57
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.31	0.57
2:D:323:MET:HE3	2:D:327:ASP:OD2	2.04	0.57
1:A:56:THR:HG22	1:A:60:LYS:HB3	1.87	0.57
1:C:174:ALA:O	1:C:178:SER:HB3	2.04	0.56
2:D:377:LEU:C	2:D:377:LEU:HD23	2.29	0.56
1:A:56:THR:CG2	1:A:60:LYS:H	2.18	0.56
4:F:39:LEU:HD21	4:F:41:LEU:CD2	2.35	0.56
4:F:82:LYS:NZ	4:F:97:SER:O	2.34	0.56
1:A:11:GLN:NE2	2:B:247:ASN:OD1	2.38	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.56
2:D:189:VAL:HG11	2:D:415:MET:HE2	1.88	0.55
2:B:19:LYS:HG3	2:B:230:SER:HB3	1.88	0.55
2:D:26:ASP:OD1	2:D:359:ARG:HD2	2.07	0.55
4:F:242:ASN:O	4:F:245:ILE:HG22	2.07	0.54
1:A:104:ALA:CB	1:A:413:MET:HE3	2.30	0.54
2:B:45:GLU:OE2	2:B:243:PRO:HB3	2.08	0.54
2:D:186:THR:HA	2:D:415:MET:HE1	1.90	0.54
2:D:52:ASN:HB2	2:D:60:VAL:HG13	1.89	0.53
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.20	0.53
2:B:42:LEU:HD23	2:B:243:PRO:HG2	1.90	0.53
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.90	0.53
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.74	0.53
1:C:42:ILE:HD12	1:C:42:ILE:N	2.24	0.53
2:D:325:GLU:HA	2:D:328:GLU:CG	2.38	0.53
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.39	0.52
1:C:245:ASP:OD1	1:C:246:GLY:N	2.42	0.52
2:D:174:LYS:NZ	2:D:209:ASP:OD1	2.40	0.51
2:D:7:ILE:O	2:D:135:LEU:HD12	2.09	0.51
2:B:359:ARG:HE	2:B:360:GLY:H	1.59	0.51
2:D:290:THR:HG22	2:D:333:VAL:HG11	1.92	0.51
2:D:286:VAL:N	2:D:287:PRO:HD2	2.26	0.51
1:C:230:LEU:O	1:C:234:ILE:HD12	2.10	0.50
3:E:136:ASN:OD1	3:E:140:LYS:HE2	2.11	0.50
2:B:42:LEU:CD2	2:B:243:PRO:HG2	2.41	0.50
2:B:404:ASP:OD1	2:B:406:MET:HB3	2.12	0.50
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.75	0.50
1:A:56:THR:HG21	1:A:60:LYS:HB3	1.93	0.50
2:B:198:GLU:HG2	2:B:266:PHE:HE2	1.70	0.49
2:D:396:HIS:HA	2:D:399:THR:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:25:LYS:CD	3:E:26:PRO:O	2.55	0.49
1:A:265:ILE:HG22	1:A:265:ILE:O	2.13	0.49
2:B:274:THR:HG21	2:B:361:LEU:HD21	1.95	0.48
4:F:3:THR:CG2	4:F:37:PHE:HA	2.42	0.48
2:B:295:ASP:HA	9:B:504:MES:S	2.53	0.48
4:F:242:ASN:HB2	4:F:245:ILE:HG22	1.96	0.48
2:D:189:VAL:CG1	2:D:415:MET:HE2	2.43	0.48
4:F:39:LEU:HD23	4:F:39:LEU:C	2.39	0.48
1:A:357:TYR:CE1	3:E:17:GLY:HA2	2.49	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.13	0.48
1:A:178:SER:HB2	1:A:183:GLU:OE2	2.14	0.47
2:D:157:GLU:HG3	3:E:123:LEU:HD13	1.96	0.47
3:E:56:ALA:O	3:E:59:GLU:HG2	2.14	0.47
2:B:156:ARG:NH2	13:B:601:HOH:O	2.13	0.47
2:D:325:GLU:CA	2:D:328:GLU:HG2	2.42	0.47
2:B:58:LYS:HA	2:B:58:LYS:HD2	1.64	0.47
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.49	0.47
2:B:359:ARG:HE	2:B:359:ARG:CA	2.24	0.47
2:D:66:VAL:HG11	2:D:147:MET:HE1	1.97	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
2:B:22:GLU:HG2	2:B:81:PHE:CD2	2.50	0.47
2:B:36:TYR:CE2	2:B:44:LEU:HD11	2.50	0.47
1:A:56:THR:HG22	1:A:60:LYS:H	1.80	0.47
1:C:96:LYS:N	1:C:96:LYS:HD3	2.30	0.47
1:A:362:VAL:HG12	1:A:363:VAL:N	2.30	0.46
2:B:45:GLU:HG3	2:B:46:ARG:HG3	1.97	0.46
2:B:198:GLU:HG2	2:B:266:PHE:CZ	2.50	0.46
2:B:359:ARG:HA	2:B:359:ARG:NE	2.26	0.46
4:F:14:TYR:HA	4:F:17:VAL:HB	1.96	0.46
2:D:66:VAL:HG11	2:D:147:MET:CE	2.46	0.46
1:C:241:SER:HA	1:C:249:ASN:HD21	1.81	0.46
2:D:170:VAL:HG13	2:D:171:PRO:HD2	1.99	0.45
3:E:6:MET:HE3	3:E:6:MET:HB2	1.87	0.45
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.97	0.45
2:B:152:ILE:HD11	2:B:164:MET:HE2	1.98	0.45
1:A:362:VAL:CG1	1:A:363:VAL:N	2.79	0.45
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.98	0.45
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.43	0.45
2:D:65:LEU:HD11	2:D:85:PHE:HD1	1.82	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.45
2:B:31:ASP:OD1	2:B:31:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:22:VAL:O	3:E:22:VAL:HG13	2.16	0.45
4:F:235:ASP:OD2	4:F:235:ASP:C	2.60	0.45
2:B:216:LYS:O	2:B:217:LEU:HD23	2.17	0.44
2:B:219:THR:HG21	1:C:325:PRO:HB2	1.98	0.44
2:B:73:MET:HE3	2:B:90:PHE:CD2	2.53	0.44
1:A:88:HIS:O	1:A:91:GLN:HB2	2.17	0.44
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.82	0.44
2:D:31:ASP:OD1	2:D:31:ASP:C	2.60	0.44
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.53	0.44
2:B:134:GLN:HA	2:B:165:ASN:O	2.17	0.44
2:B:379:LYS:O	2:B:380:ARG:C	2.60	0.44
2:D:285:THR:OG1	2:D:287:PRO:HG2	2.18	0.44
1:A:194:THR:HG22	1:A:194:THR:O	2.17	0.44
2:B:293:MET:CE	2:B:365:ALA:HB1	2.48	0.44
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.11	0.43
2:D:134:GLN:HA	2:D:165:ASN:O	2.18	0.43
4:F:320:MET:HG2	4:F:330:ILE:HG13	1.98	0.43
1:A:298:PRO:HA	1:A:301:GLN:CD	2.44	0.43
2:D:167:PHE:CD2	2:D:233:MET:HE3	2.54	0.43
4:F:92:THR:O	4:F:326:LYS:NZ	2.50	0.43
4:F:322:ASP:OD1	4:F:322:ASP:C	2.62	0.43
4:F:343:TYR:O	4:F:344:ALA:C	2.61	0.43
1:C:286:LEU:HA	1:C:290:GLU:OE2	2.19	0.43
2:D:68:LEU:HD23	2:D:112:LEU:HD22	2.00	0.43
2:D:66:VAL:CG1	2:D:147:MET:CE	2.96	0.42
2:D:42:LEU:HD23	2:D:243:PRO:HG2	2.01	0.42
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.90	0.42
3:E:140:LYS:HD3	3:E:140:LYS:HA	1.65	0.42
4:F:342:LEU:O	4:F:343:TYR:C	2.61	0.42
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.53	0.42
2:B:174:LYS:HD2	2:B:205:GLU:CD	2.44	0.42
2:D:52:ASN:HB2	2:D:60:VAL:CG1	2.50	0.42
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.54	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.19	0.42
1:C:343:PHE:CG	1:C:349:THR:HG22	2.55	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.41
1:A:56:THR:HG22	1:A:60:LYS:N	2.35	0.41
2:D:244:GLY:C	2:D:246:LEU:N	2.76	0.41
2:B:244:GLY:C	2:B:246:LEU:N	2.78	0.41
4:F:6:VAL:HG22	4:F:41:LEU:HD12	2.02	0.41
2:B:240:LEU:HD23	2:B:240:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.41
4:F:3:THR:HG21	4:F:36:ARG:O	2.20	0.41
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.02	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.41
1:A:1:MET:HE3	1:A:1:MET:HB3	1.98	0.41
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.55	0.41
4:F:39:LEU:HD23	4:F:40:MET:N	2.36	0.41
4:F:39:LEU:HD21	4:F:41:LEU:HD23	2.01	0.40
1:A:156:ARG:HA	1:A:156:ARG:HD2	1.93	0.40
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	429 (98%)	8 (2%)	0	100	100
1	C	438/451 (97%)	429 (98%)	8 (2%)	1 (0%)	43	62
2	B	419/445 (94%)	407 (97%)	10 (2%)	2 (0%)	24	42
2	D	416/445 (94%)	409 (98%)	6 (1%)	1 (0%)	43	62
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	297/384 (77%)	287 (97%)	10 (3%)	0	100	100
All	All	2124/2319 (92%)	2076 (98%)	44 (2%)	4 (0%)	43	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	245	GLN
2	D	245	GLN

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Mol	Chain	Res	Type
1	C	164	LYS
2	B	243	PRO

5.3.2 Protein sidechains ⓘ

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%)	370 (100%)	0	100	100
1	C	371/379 (98%)	369 (100%)	2 (0%)	81	90
2	B	363/381 (95%)	361 (99%)	2 (1%)	78	89
2	D	353/381 (93%)	352 (100%)	1 (0%)	86	93
3	E	108/127 (85%)	107 (99%)	1 (1%)	70	84
4	F	278/342 (81%)	276 (99%)	2 (1%)	76	87
All	All	1843/1989 (93%)	1835 (100%)	8 (0%)	84	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	284	LEU
2	B	359	ARG
1	C	251	ASP
1	C	293	ASN
2	D	48	ASN
3	E	77	GLU
4	F	12	SER
4	F	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	393	HIS
2	B	48	ASN

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	99	ASN
2	B	191	GLN
2	B	329	GLN
2	B	426	GLN
1	C	107	HIS
1	C	358	GLN
2	D	15	GLN
2	D	195	ASN
2	D	256	ASN
3	E	115	HIS
4	F	379	HIS
4	F	382	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	MES	B	503	-	12,12,12	2.22	1 (8%)	15,16,16	1.94	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ACP	F	401	-	31,33,33	1.83	9 (29%)	47,52,52	1.77	10 (21%)
10	A1L2T	B	505	-	31,31,31	1.67	7 (22%)	42,44,44	1.80	9 (21%)
5	GTP	D	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.63	9 (18%)
10	A1L2T	D	503	-	31,31,31	1.03	2 (6%)	42,44,44	1.11	2 (4%)
5	GTP	C	501	6	33,34,34	1.14	3 (9%)	50,54,54	1.49	9 (18%)
11	GDP	B	506	6	29,30,30	1.20	3 (10%)	45,47,47	1.78	6 (13%)
9	MES	B	504	-	12,12,12	2.17	2 (16%)	15,16,16	1.81	2 (13%)
5	GTP	A	501	6	33,34,34	1.20	4 (12%)	50,54,54	1.51	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
12	ACP	F	401	-	-	6/19/38/38	0/3/3/3
10	A1L2T	B	505	-	-	2/9/15/15	0/5/5/5
5	GTP	D	501	-	-	5/22/38/38	0/3/3/3
10	A1L2T	D	503	-	-	0/9/15/15	0/5/5/5
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
11	GDP	B	506	6	-	3/16/32/32	0/3/3/3
9	MES	B	504	-	-	5/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.36	1.67	1.77
9	B	504	MES	C8-S	-6.98	1.67	1.77
10	B	505	A1L2T	C04-N05	5.31	1.44	1.36
12	F	401	ACP	C5-C4	4.77	1.47	1.39
12	F	401	ACP	PB-O3A	4.06	1.62	1.58
5	A	501	GTP	PB-O3B	3.27	1.63	1.59
5	C	501	GTP	PB-O3B	3.21	1.63	1.59
11	B	506	GDP	C5-C4	3.16	1.47	1.38
12	F	401	ACP	PA-O3A	3.14	1.62	1.59
12	F	401	ACP	PG-O2G	3.00	1.61	1.55
10	B	505	A1L2T	C02-N03	2.98	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PG-O3G	2.95	1.61	1.55
5	A	501	GTP	PA-O3A	2.91	1.62	1.59
5	A	501	GTP	PB-O3A	2.83	1.62	1.59
12	F	401	ACP	C5-C6	2.77	1.48	1.41
10	B	505	A1L2T	C04-N03	2.65	1.39	1.34
10	B	505	A1L2T	C26-C22	2.60	1.44	1.41
5	C	501	GTP	PA-O3A	2.49	1.62	1.59
10	D	503	A1L2T	C02-N01	2.47	1.38	1.33
5	D	501	GTP	PA-O3A	2.46	1.62	1.59
12	F	401	ACP	C8-N7	2.46	1.36	1.31
11	B	506	GDP	C6-N1	-2.37	1.34	1.38
12	F	401	ACP	C5-N7	-2.23	1.35	1.39
5	D	501	GTP	C2-N3	2.23	1.38	1.33
11	B	506	GDP	PA-O3A	2.21	1.61	1.59
10	B	505	A1L2T	C16-C04	2.19	1.45	1.39
10	D	503	A1L2T	C02-N27	2.17	1.39	1.35
5	C	501	GTP	PB-O3A	2.16	1.61	1.59
10	B	505	A1L2T	C16-C17	2.15	1.43	1.39
10	B	505	A1L2T	C02-N01	2.08	1.38	1.33
9	B	504	MES	O1S-S	2.06	1.50	1.45
12	F	401	ACP	PB-O2B	2.05	1.61	1.56
5	A	501	GTP	C2-N3	2.02	1.38	1.33

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	506	GDP	C5-C4-N3	-6.09	118.70	128.39
12	F	401	ACP	C5-C4-N3	-5.91	118.58	126.72
10	B	505	A1L2T	C26-C18-C17	5.77	127.87	123.02
5	D	501	GTP	C5-C4-N3	-5.36	119.86	128.39
9	B	503	MES	C5-N4-C3	5.18	120.00	108.84
11	B	506	GDP	C2-N3-C4	5.14	121.15	112.30
9	B	504	MES	C5-N4-C3	5.13	119.89	108.84
5	D	501	GTP	C2-N3-C4	4.76	120.51	112.30
5	A	501	GTP	C5-C4-N3	-4.76	120.81	128.39
12	F	401	ACP	N3-C4-N9	4.64	135.06	127.17
5	A	501	GTP	C2-N3-C4	4.48	120.02	112.30
5	C	501	GTP	C5-C4-N3	-4.36	121.45	128.39
11	B	506	GDP	N9-C4-N3	4.34	134.63	125.95
10	B	505	A1L2T	C06-N05-C04	4.22	131.45	123.04
5	C	501	GTP	C2-N3-C4	4.22	119.57	112.30
12	F	401	ACP	C2-N3-C4	3.71	120.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	506	GDP	C6-C5-N7	3.65	136.93	130.29
12	F	401	ACP	C4-C5-N7	-3.60	106.47	110.58
5	D	501	GTP	N9-C4-N3	3.32	132.60	125.95
10	B	505	A1L2T	C26-C22-N23	3.21	108.92	107.09
12	F	401	ACP	N3-C2-N1	-3.18	123.77	128.58
10	D	503	A1L2T	C17-N27-C02	-3.15	114.49	116.35
5	D	501	GTP	C2-N1-C6	-3.01	119.66	125.11
10	B	505	A1L2T	C17-N27-C02	-3.01	114.57	116.35
5	A	501	GTP	N9-C4-N3	2.94	131.84	125.95
5	C	501	GTP	N9-C8-N7	-2.92	107.98	113.40
5	D	501	GTP	C8-N7-C5	2.84	109.32	104.26
5	C	501	GTP	O2B-PB-O3A	2.81	114.86	107.27
5	C	501	GTP	C8-N7-C5	2.80	109.25	104.26
5	A	501	GTP	N9-C8-N7	-2.76	108.28	113.40
5	A	501	GTP	C2-N1-C6	-2.74	120.14	125.11
5	D	501	GTP	N9-C8-N7	-2.71	108.38	113.40
12	F	401	ACP	C4-N9-C8	2.69	108.57	105.74
12	F	401	ACP	C5-N7-C8	2.66	107.64	103.45
5	C	501	GTP	N9-C4-N3	2.65	131.25	125.95
5	A	501	GTP	C8-N7-C5	2.64	108.96	104.26
11	B	506	GDP	C4-C5-N7	-2.62	106.51	110.67
10	B	505	A1L2T	C22-C26-C25	-2.60	105.13	107.02
9	B	503	MES	O1S-S-C8	2.59	110.64	106.73
9	B	504	MES	O1S-S-C8	2.57	110.62	106.73
10	D	503	A1L2T	C26-C22-N23	2.54	108.54	107.09
5	D	501	GTP	C5-C6-N1	2.49	119.60	113.25
5	A	501	GTP	C5-C6-N1	2.41	119.39	113.25
10	B	505	A1L2T	C18-C17-N27	-2.28	111.30	116.69
5	C	501	GTP	C2-N1-C6	-2.26	121.01	125.11
10	B	505	A1L2T	C09-C08-C07	2.23	123.93	121.00
11	B	506	GDP	C5-C6-N1	2.18	118.80	113.25
9	B	503	MES	O2S-S-C8	2.14	109.96	106.73
5	A	501	GTP	O6-C6-C5	-2.13	120.90	126.53
5	D	501	GTP	C4-C5-N7	-2.13	107.30	110.67
10	B	505	A1L2T	C16-C17-C18	2.12	126.00	121.98
10	B	505	A1L2T	N27-C02-N03	2.10	128.70	125.48
12	F	401	ACP	N9-C8-N7	-2.09	110.97	113.94
5	C	501	GTP	C4-C5-N7	-2.08	107.37	110.67
12	F	401	ACP	C6-C5-N7	2.07	136.09	132.09
5	D	501	GTP	O2B-PB-O3A	2.04	112.78	107.27
12	F	401	ACP	PB-O3A-PA	-2.03	125.76	132.37
5	C	501	GTP	C5-C6-N1	2.02	118.39	113.25

There are no chirality outliers.

All (38) torsion outliers are listed below:

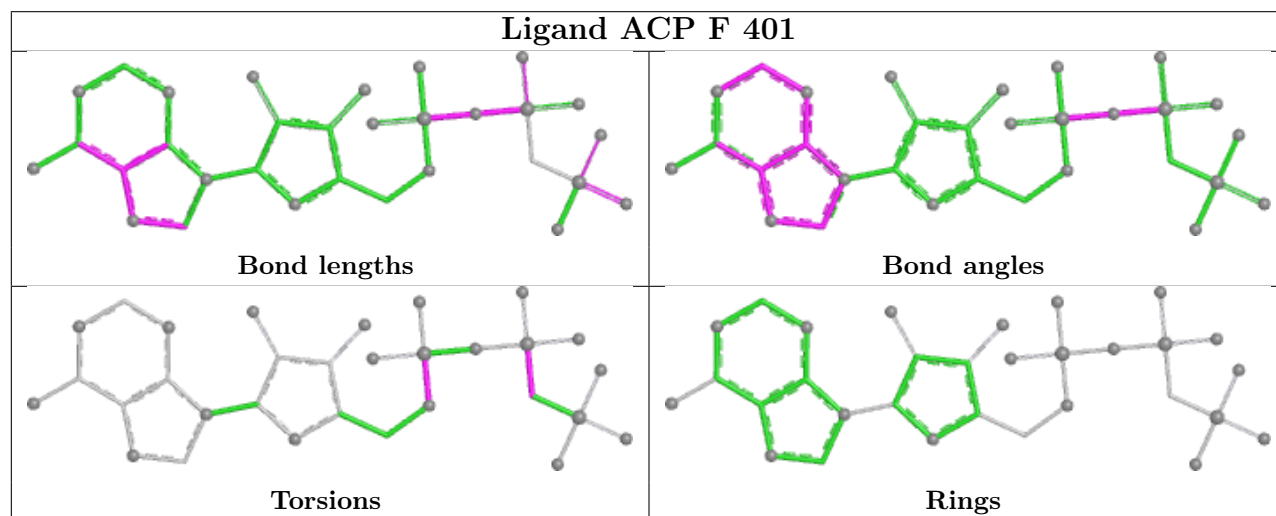
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
10	B	505	A1L2T	C16-C04-N05-C06
10	B	505	A1L2T	N03-C04-N05-C06
11	B	506	GDP	C5'-O5'-PA-O3A
11	B	506	GDP	C5'-O5'-PA-O1A
11	B	506	GDP	C5'-O5'-PA-O2A
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O3A
9	B	503	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O3S
9	B	503	MES	C8-C7-N4-C3
9	B	504	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C3
5	D	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

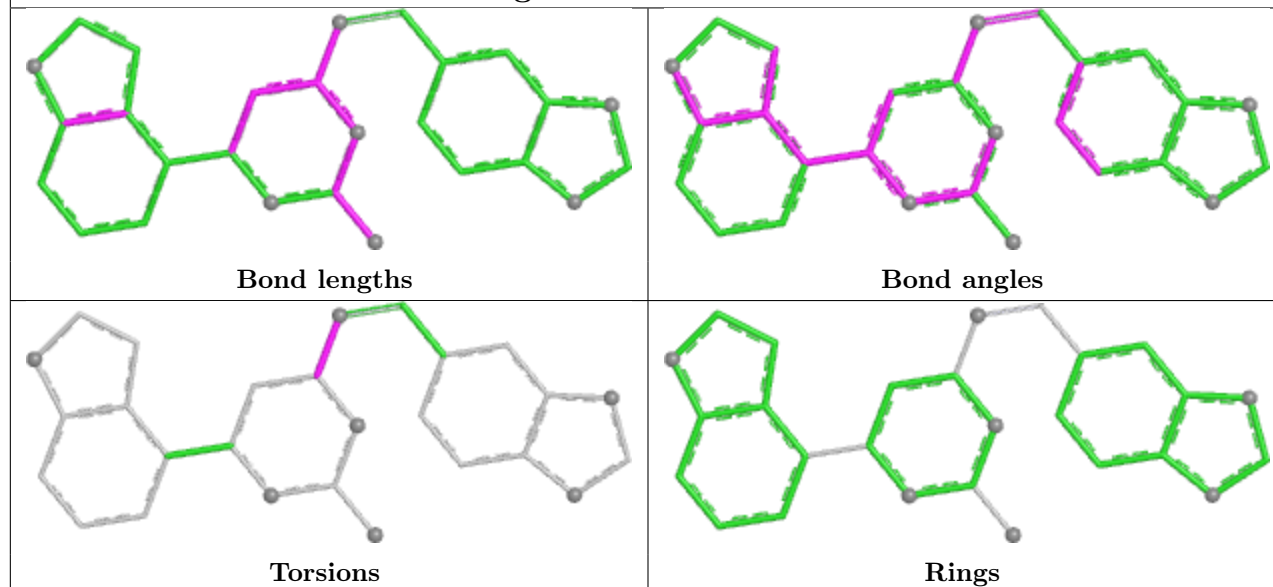
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	1	0
10	B	505	A1L2T	1	0
10	D	503	A1L2T	1	0
9	B	504	MES	2	0

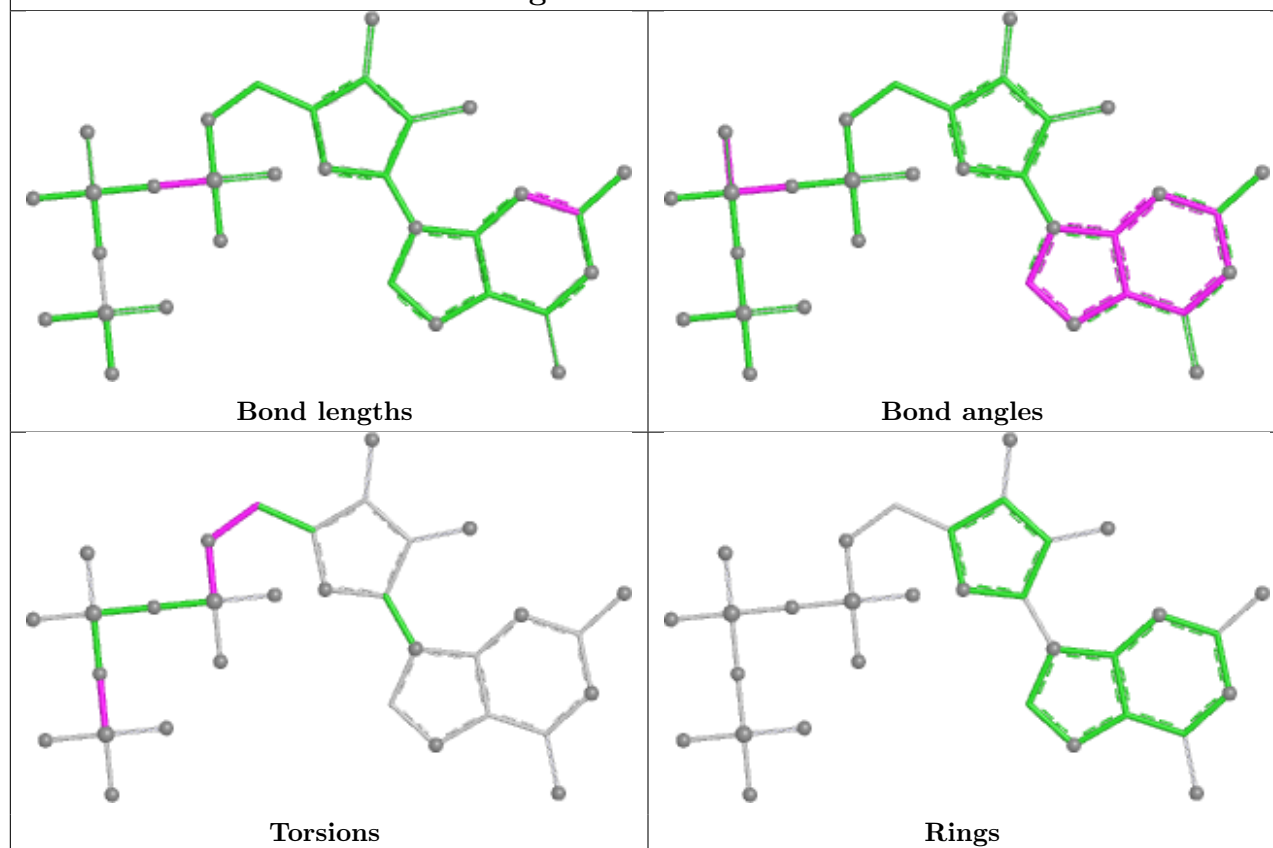
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



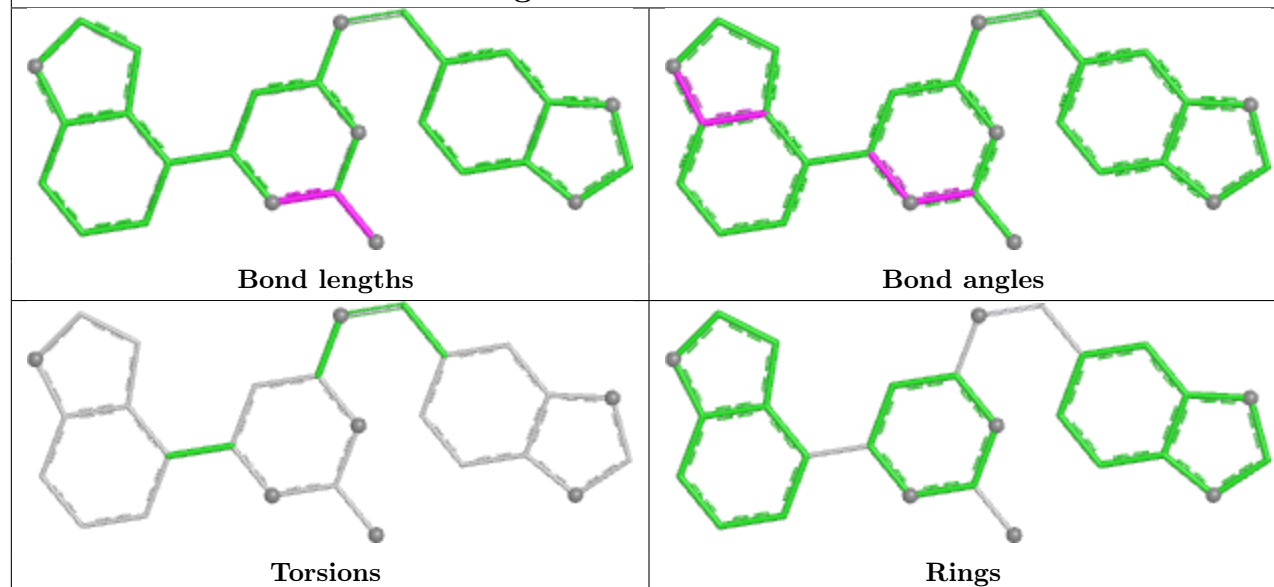
Ligand A1L2T B 505



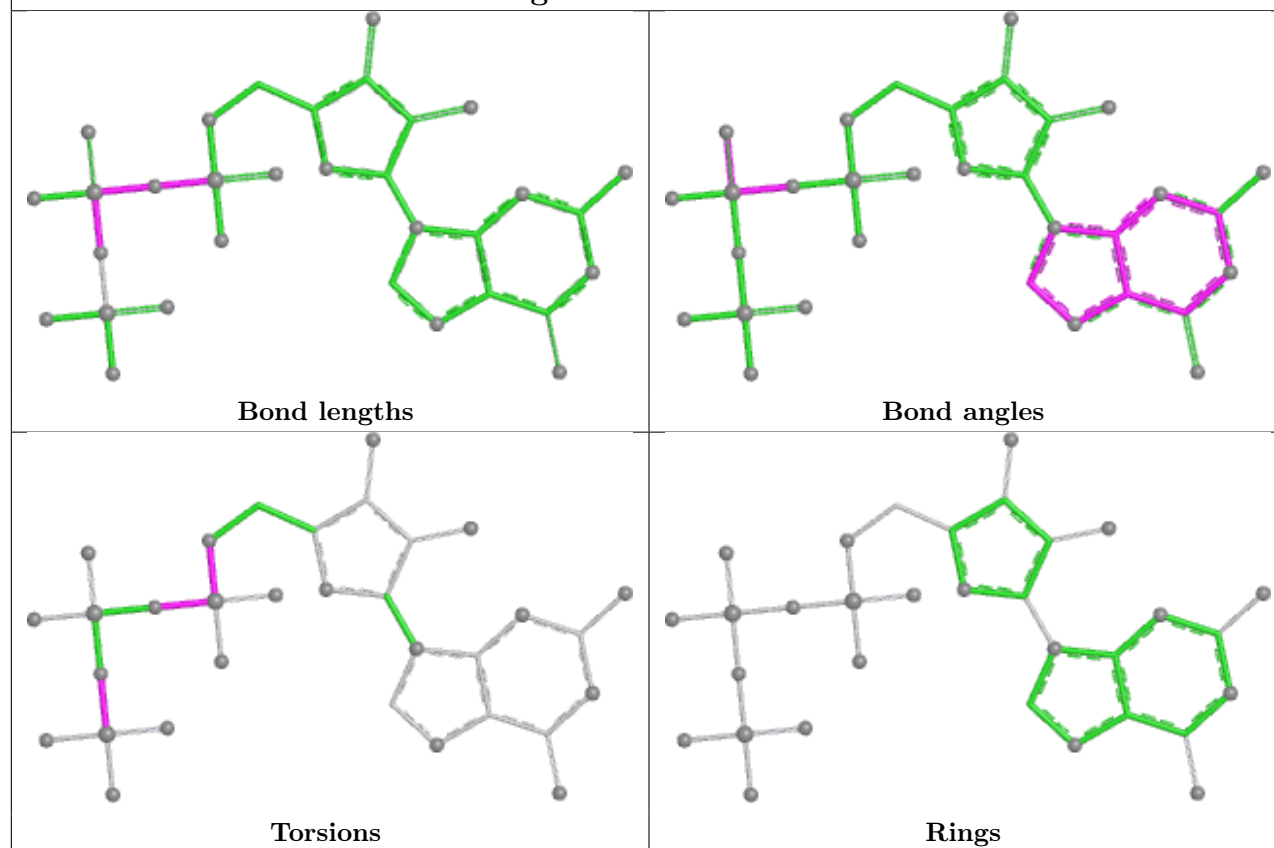
Ligand GTP D 501

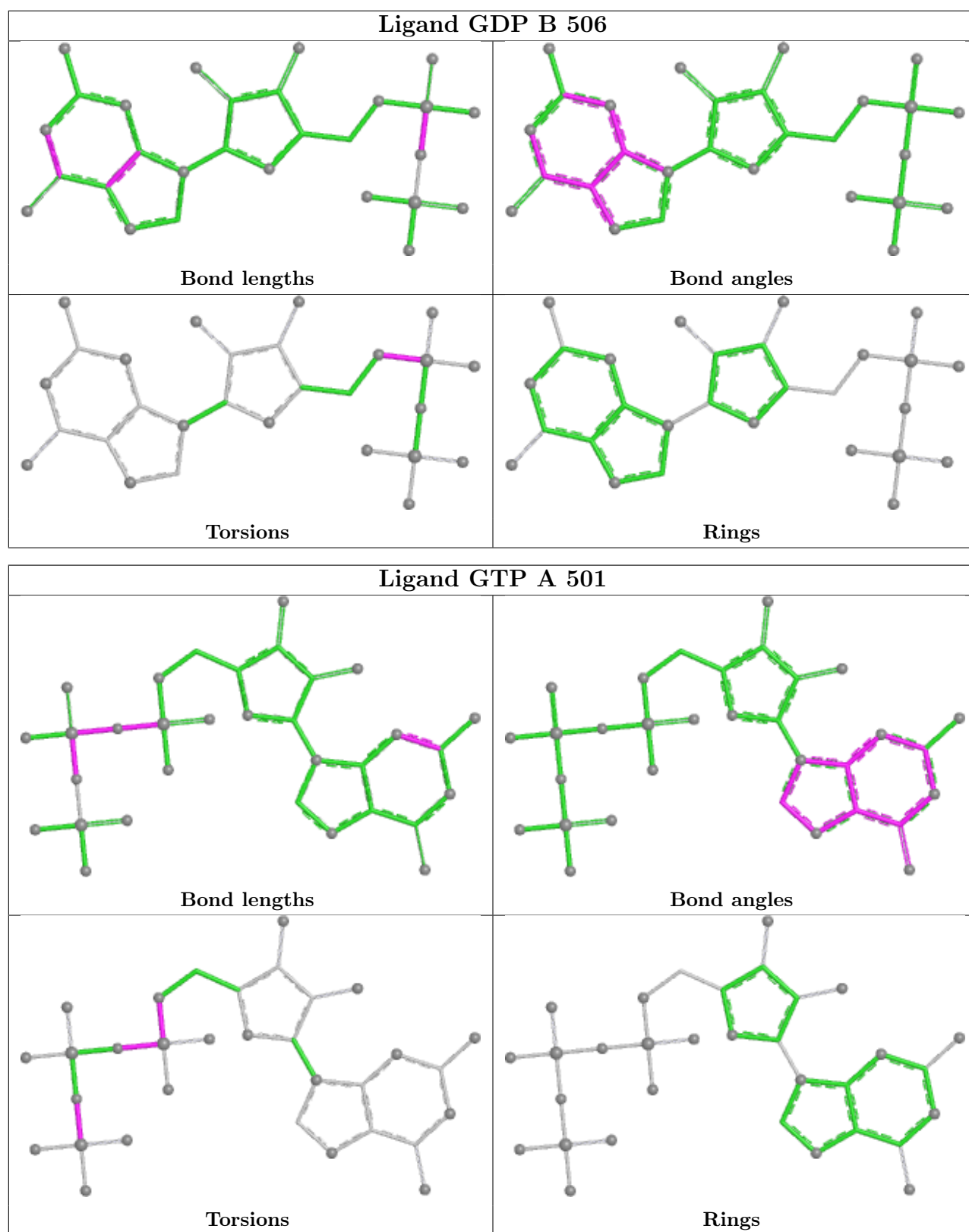


Ligand A1L2T D 503



Ligand GTP C 501





5.7 Other polymers [i](#)

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, 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(Å²)	Q<0.9
1	A	437/451 (96%)	-0.08	6 (1%)	73	67	28, 47, 76, 104	2 (0%)
1	C	440/451 (97%)	-0.27	6 (1%)	73	67	23, 38, 67, 95	0
2	B	423/445 (95%)	-0.08	4 (0%)	81	76	22, 46, 81, 106	0
2	D	420/445 (94%)	0.35	15 (3%)	46	36	31, 61, 91, 108	2 (0%)
3	E	120/143 (83%)	0.43	1 (0%)	82	78	35, 63, 97, 110	1 (0%)
4	F	309/384 (80%)	0.58	23 (7%)	20	14	40, 71, 110, 132	0
All	All	2149/2319 (92%)	0.09	55 (2%)	57	48	22, 52, 92, 132	5 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	THR	8.4
1	A	179	THR	5.8
4	F	382	HIS	4.7
4	F	166	ALA	4.2
4	F	159	GLY	4.2
1	C	178	SER	3.9
1	A	178	SER	3.9
4	F	161	LEU	3.7
2	B	274	THR	3.3
4	F	383	HIS	3.3
1	C	177	VAL	3.2
4	F	384	HIS	3.1
2	D	245	GLN	3.0
4	F	247	LYS	3.0
4	F	24	THR	3.0
4	F	163	SER	2.9
2	D	243	PRO	2.7
2	D	33	THR	2.6
2	D	244	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	2.5
2	D	217	LEU	2.4
1	A	262	TYR	2.4
1	C	253	THR	2.4
4	F	380	HIS	2.4
2	D	96	GLY	2.4
4	F	199	PHE	2.4
2	B	245	GLN	2.4
2	B	55	ALA	2.3
2	D	395	LEU	2.3
4	F	162	ILE	2.3
4	F	231	ALA	2.3
1	A	283	HIS	2.3
4	F	31	ARG	2.3
2	D	37	HIS	2.2
2	D	404	ASP	2.2
4	F	200	ASP	2.2
2	D	71	GLY	2.2
2	D	35	SER	2.2
4	F	225	SER	2.2
4	F	233	PHE	2.2
1	A	285	GLN	2.1
2	D	172	SER	2.1
4	F	381	HIS	2.1
2	D	55	ALA	2.1
4	F	237	THR	2.1
4	F	149	ALA	2.1
4	F	333	ASN	2.1
2	B	246	LEU	2.1
2	D	2	ARG	2.1
4	F	224	SER	2.0
1	C	250	VAL	2.0
3	E	15	THR	2.0
2	D	405	GLU	2.0
1	C	283	HIS	2.0
4	F	253	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

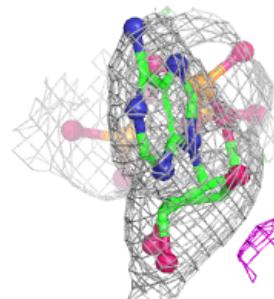
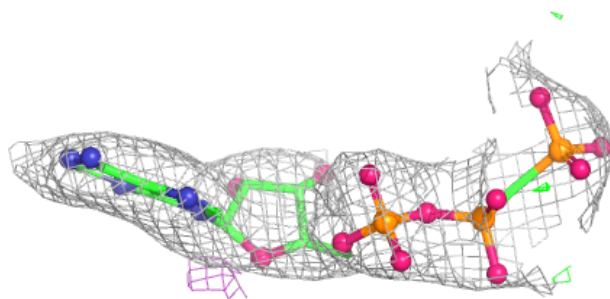
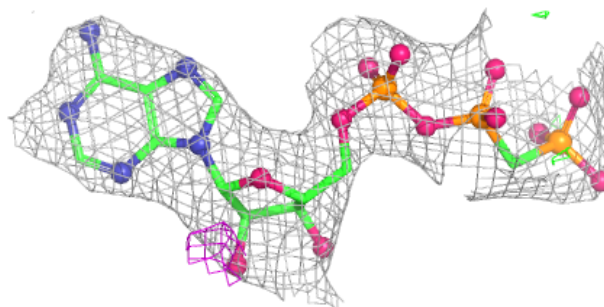
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MES	B	503	12/12	0.70	0.19	47,64,84,90	0
6	MG	D	502	1/1	0.76	0.19	70,70,70,70	0
12	ACP	F	401	31/31	0.82	0.13	85,94,119,120	0
8	CL	A	504	1/1	0.83	0.12	84,84,84,84	0
9	MES	B	504	12/12	0.85	0.15	69,78,84,92	0
5	GTP	D	501	32/32	0.91	0.10	43,55,75,91	0
7	CA	B	502	1/1	0.91	0.08	77,77,77,77	0
10	A1L2T	B	505	27/27	0.92	0.09	34,45,69,82	0
6	MG	C	502	1/1	0.94	0.29	36,36,36,36	0
6	MG	B	501	1/1	0.94	0.13	46,46,46,46	0
7	CA	C	503	1/1	0.95	0.07	53,53,53,53	0
7	CA	A	503	1/1	0.96	0.05	75,75,75,75	0
10	A1L2T	D	503	27/27	0.96	0.07	33,46,60,69	0
6	MG	A	502	1/1	0.96	0.27	35,35,35,35	0
5	GTP	A	501	32/32	0.97	0.06	25,33,40,49	0
5	GTP	C	501	32/32	0.97	0.07	23,30,33,36	0
11	GDP	B	506	28/28	0.98	0.06	26,33,38,45	0

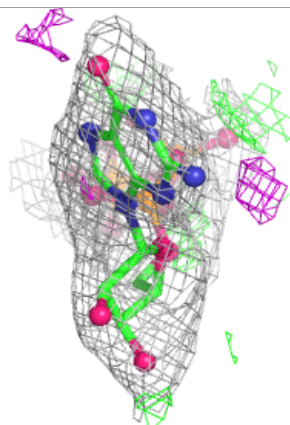
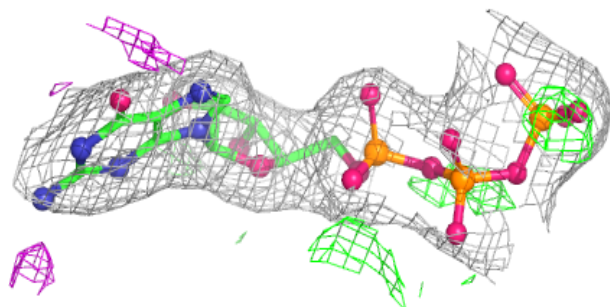
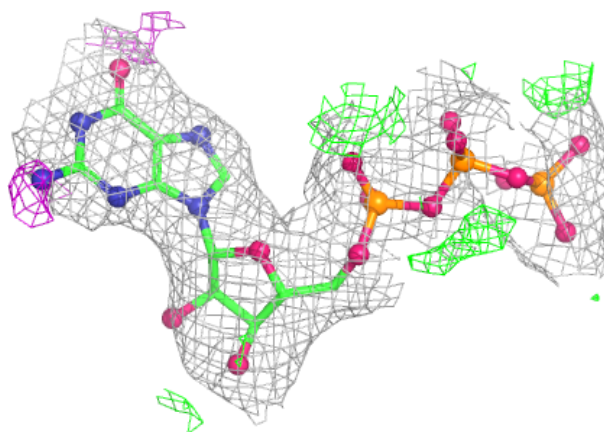
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

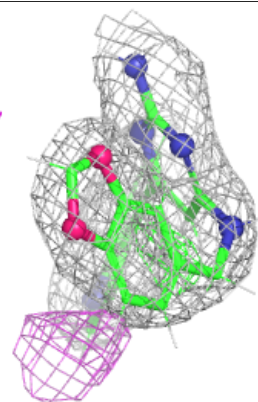
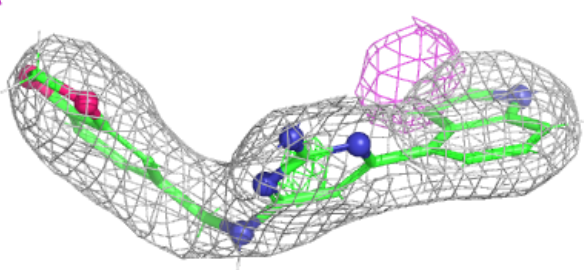
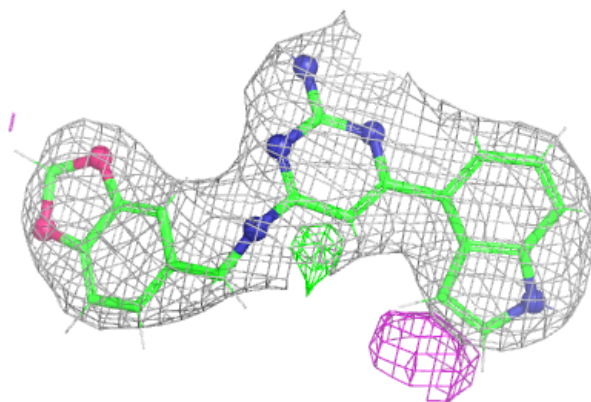
**Electron density around GTP D 501:**

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

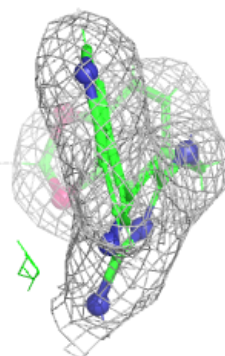
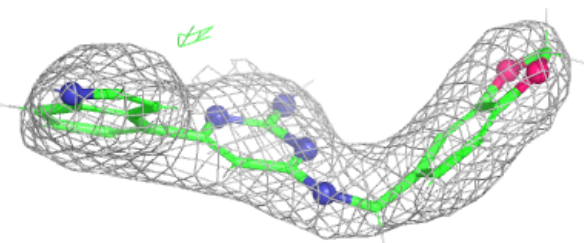
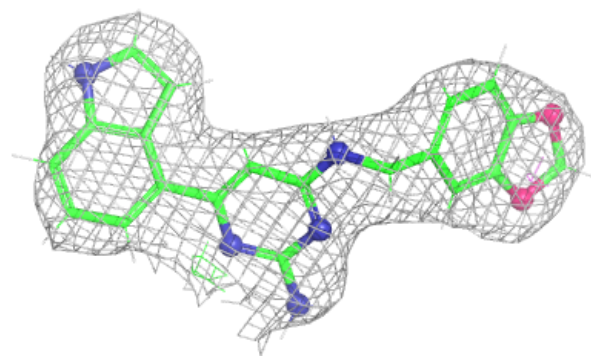


Electron density around A1L2T B 505:

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

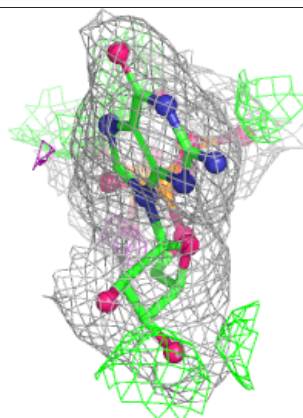
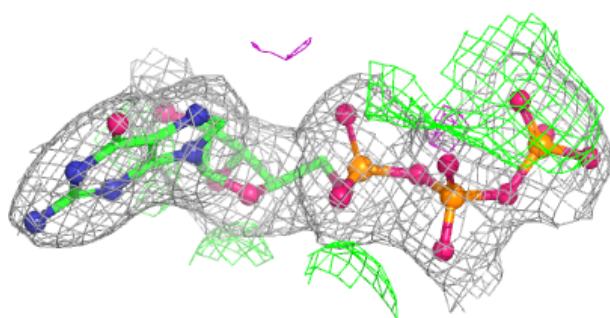
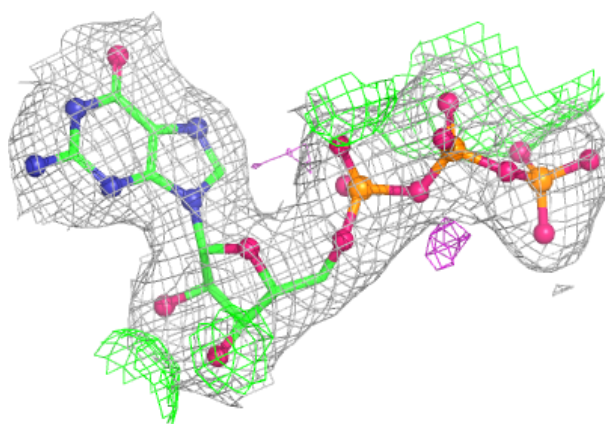
**Electron density around A1L2T D 503:**

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

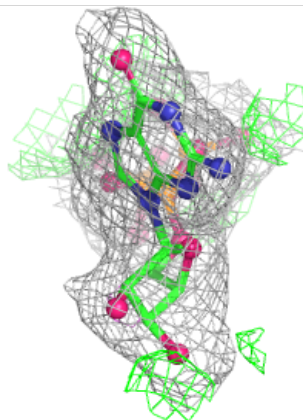
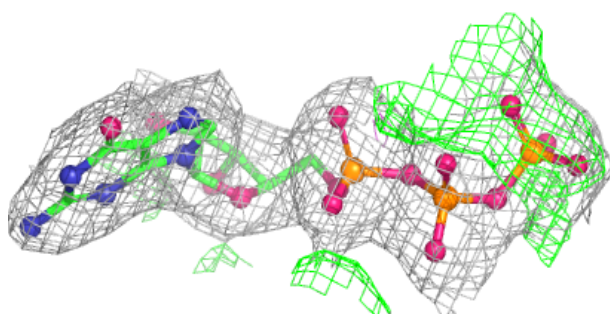
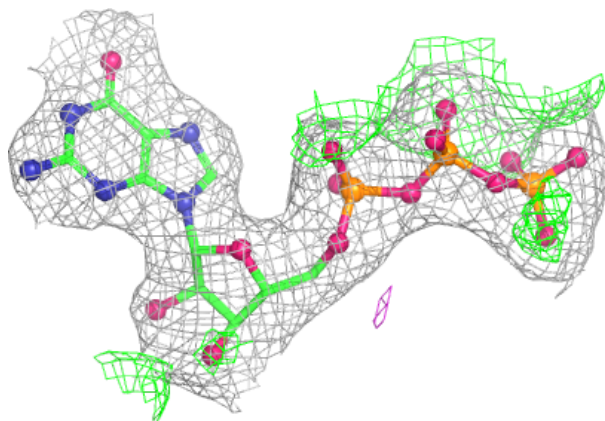


Electron density around GTP A 501:

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

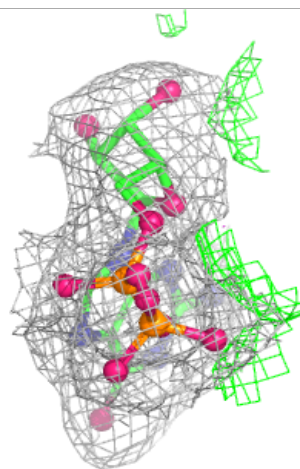
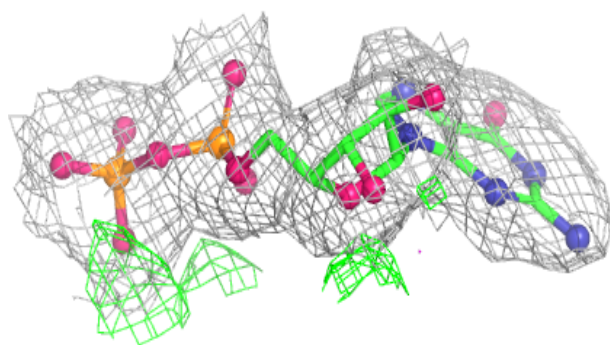
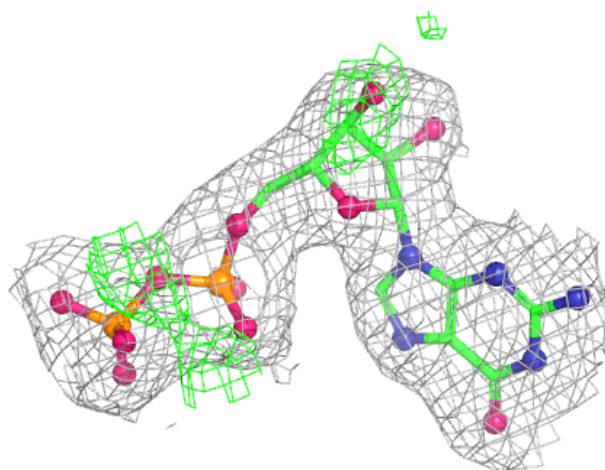
**Electron density around GTP C 501:**

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



Electron density around GDP B 506:

$2mF_o-DF_c$ (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.