



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:05 PM UTC

PDB ID : 6TIU / pdb_00006tiu
Title : DROSOPHILA GTP-TUBULIN Y222F MUTANT
Authors : Gigant, B.
Deposited on : 2019-11-22
Resolution : 3.57 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

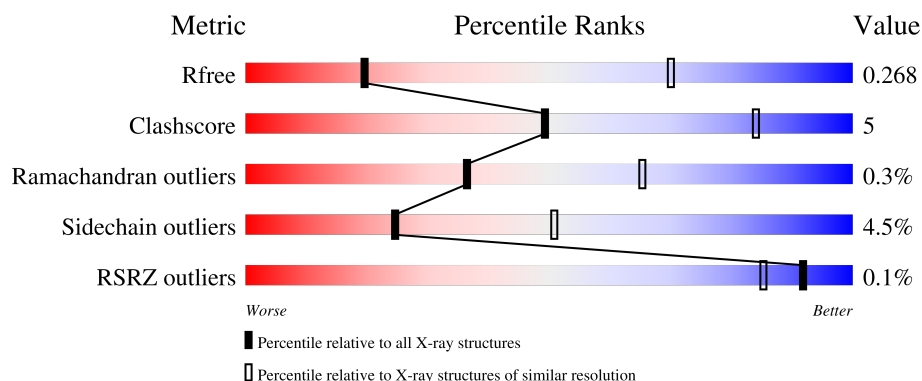
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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	450	 78% 16% . .
1	C	450	 82% 13% . .
2	B	447	 80% 15% . .
2	D	447	 80% 15% .
3	E	143	 73% 12% . 11%

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
5	MG	B	502[A]	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14668 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-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3384	2144	575	642	23			
1	C	432	Total	C	N	O	S	0	0	0
			3368	2133	573	639	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ARG	LYS	engineered mutation	UNP P06603
C	40	ARG	LYS	engineered mutation	UNP P06603

- Molecule 2 is a protein called Tubulin beta-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3348	2105	571	646	26			
2	D	427	Total	C	N	O	S	0	0	0
			3342	2101	570	645	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	PHE	TYR	engineered mutation	UNP Q24560
D	222	PHE	TYR	engineered mutation	UNP Q24560

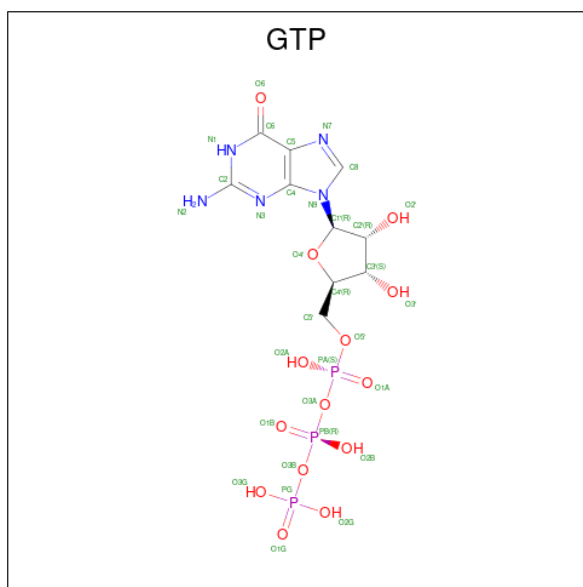
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	127	Total	C	N	O	S	0	0	0
			1041	644	188	205	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	SER	engineered mutation	UNP P63043
E	14	ALA	CYS	conflict	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

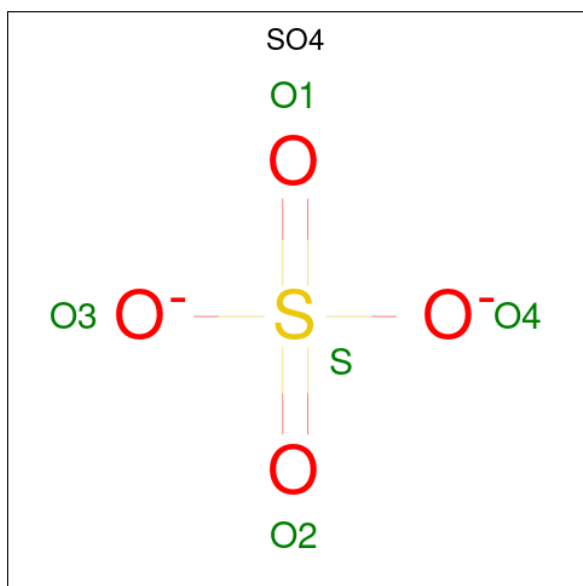
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	1
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

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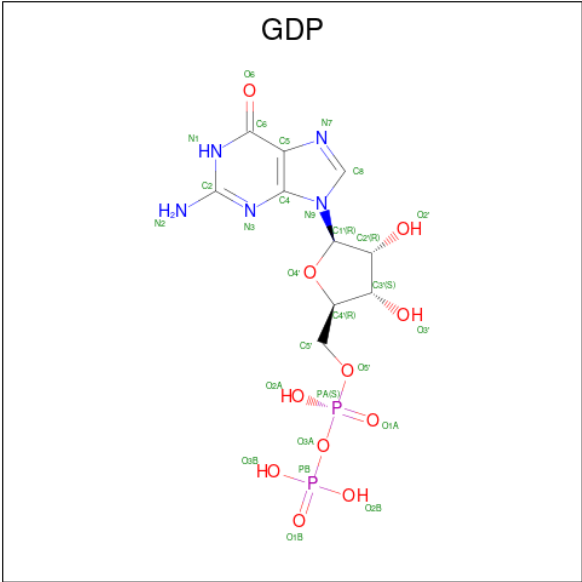
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

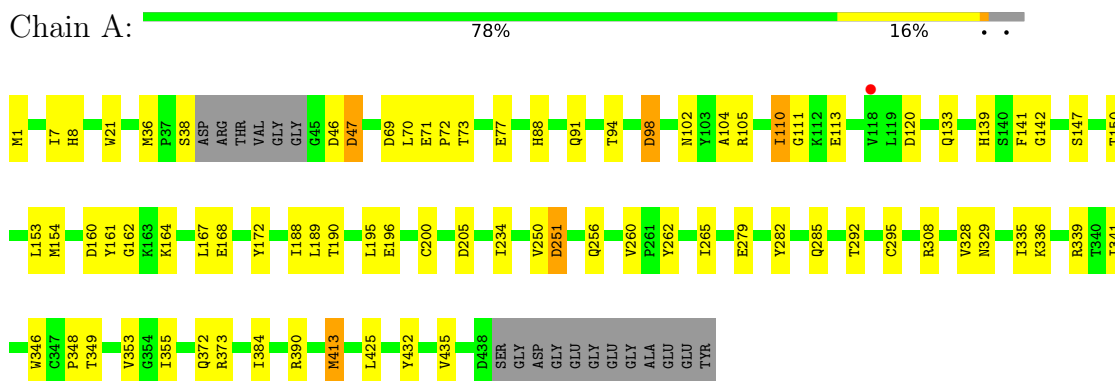


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	1
			28	10	5	11	2		

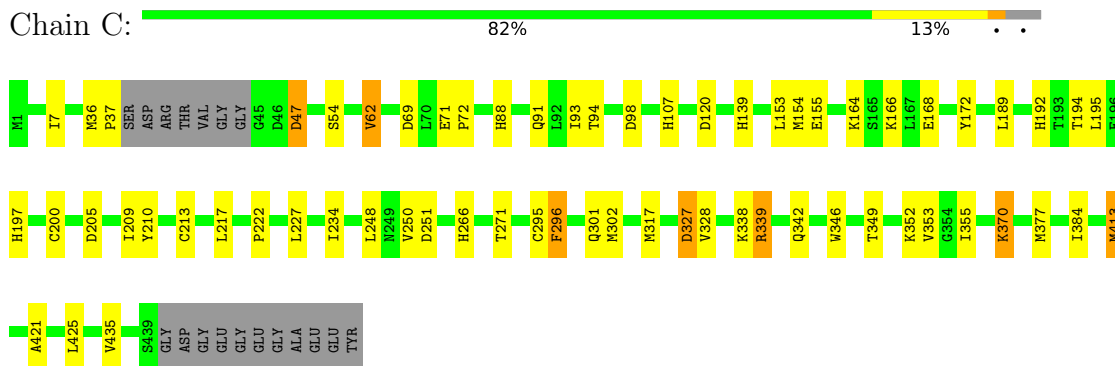
3 Residue-property plots

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.

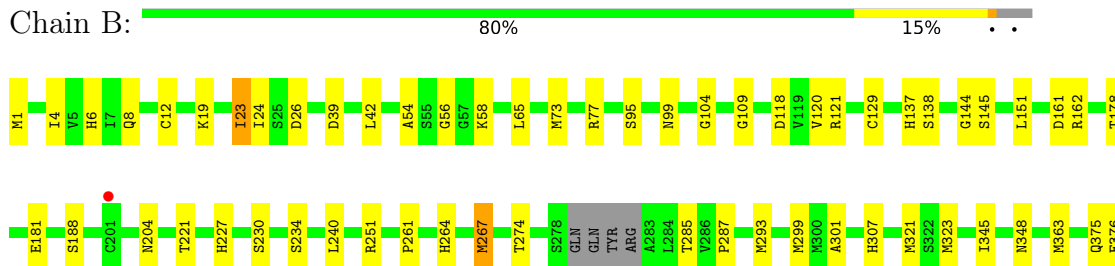
- Molecule 1: Tubulin alpha-1 chain



- Molecule 1: Tubulin alpha-1 chain

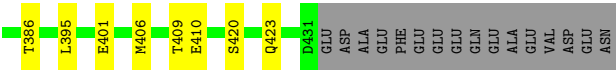
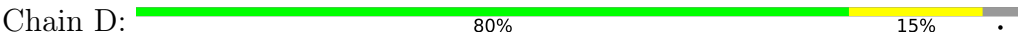


- Molecule 2: Tubulin beta-1 chain





● Molecule 2: Tubulin beta-1 chain



● Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.97Å 126.35Å 249.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 3.57 48.00 – 3.57	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.00-3.57) 98.6 (48.00-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.221 , 0.244 0.239 , 0.268	Depositor DCC
R_{free} test set	1266 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	110.9	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 134.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14668	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: GDP, SO4, MG, GTP

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	0.76	0/3461	1.16	12/4698 (0.3%)
1	C	0.75	0/3443	1.16	7/4674 (0.1%)
2	B	0.72	1/3420 (0.0%)	1.12	1/4631 (0.0%)
2	D	0.74	0/3414	1.15	7/4623 (0.2%)
3	E	0.76	0/1051	1.22	2/1398 (0.1%)
All	All	0.74	1/14789 (0.0%)	1.15	29/20024 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	267	MET	SD-CE	-5.68	1.65	1.79

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	GLY	N-CA-C	7.28	122.09	112.77
1	A	102	ASN	CA-CB-CG	6.48	119.08	112.60
1	C	338	LYS	CA-C-N	6.20	128.59	120.28
1	C	338	LYS	C-N-CA	6.20	128.59	120.28
1	A	260	VAL	N-CA-C	6.18	114.27	108.15
1	C	47	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	251	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	327	ASP	CA-CB-CG	5.77	118.37	112.60
2	B	95	SER	N-CA-C	5.63	117.50	111.36
1	A	47	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	98	ASP	CA-CB-CG	5.57	118.17	112.60
2	D	178	THR	CA-C-N	5.57	131.99	121.97
2	D	178	THR	C-N-CA	5.57	131.99	121.97
2	D	161	ASP	CA-CB-CG	5.52	118.12	112.60
2	D	118	ASP	CA-CB-CG	5.45	118.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	95	SER	N-CA-C	5.44	117.29	111.36
2	D	107	THR	CA-C-N	5.36	127.47	120.28
2	D	107	THR	C-N-CA	5.36	127.47	120.28
1	A	46	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	296	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	111	GLY	CA-C-N	5.21	127.99	120.38
1	A	111	GLY	C-N-CA	5.21	127.99	120.38
1	A	160	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	93	ILE	N-CA-C	5.13	115.70	108.36
3	E	133	VAL	CA-C-N	5.07	127.07	120.28
3	E	133	VAL	C-N-CA	5.07	127.07	120.28
1	A	390	ARG	CA-C-N	5.03	126.98	120.44
1	A	390	ARG	C-N-CA	5.03	126.98	120.44
1	C	251	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3384	0	3295	47	0
1	C	3368	0	3279	35	0
2	B	3348	0	3234	39	0
2	D	3342	0	3230	32	0
3	E	1041	0	1046	13	0
4	A	32	0	12	1	0
4	B	32	0	12	1	0
4	C	32	0	12	1	0
4	D	32	0	12	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	5	0	0	0	0
6	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	10	0	0	0	0
7	B	28	0	12	1	0
All	All	14668	0	14144	156	0

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

All (156) 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:B:6:HIS:HE1	2:B:8:GLN:HE21	1.07	1.02
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.04	0.99
1:A:133:GLN:HE22	1:A:251:ASP:HB2	1.30	0.96
2:D:204:ASN:HD21	4:D:501:GTP:HN22	1.16	0.93
2:D:6:HIS:CE1	2:D:8:GLN:HE21	1.90	0.90
2:B:204:ASN:HD21	4:B:501[A]:GTP:HN22	1.24	0.85
2:B:6:HIS:CE1	2:B:8:GLN:HE21	1.95	0.83
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.27	0.82
1:A:308:ARG:NH1	1:A:339:ARG:HH12	1.79	0.79
1:C:339:ARG:H	1:C:339:ARG:HD3	1.51	0.75
1:A:71:GLU:OE2	1:A:73:THR:HB	1.90	0.71
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.72	0.71
1:C:296:PHE:CE2	1:C:377:MET:HE1	2.25	0.70
1:A:133:GLN:NE2	1:A:251:ASP:HB2	2.08	0.66
2:B:307:HIS:HD2	2:B:376:GLU:OE1	1.78	0.66
2:B:261:PRO:O	2:B:264:HIS:HD2	1.78	0.66
1:A:292:THR:O	1:A:295:CYS:HB2	1.97	0.65
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.78	0.64
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.80	0.63
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.80	0.63
2:D:261:PRO:O	2:D:264:HIS:HD2	1.82	0.61
2:B:162:ARG:HA	2:B:162:ARG:HE	1.65	0.61
1:A:36:MET:HE2	1:A:38:SER:HB3	1.81	0.61
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.49	0.60
2:B:99:ASN:HD21	1:C:352:LYS:NZ	2.00	0.60
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.84	0.59
2:B:406:MET:HA	2:B:409:THR:HG23	1.86	0.58
1:A:329:ASN:HD21	3:E:20:TRP:NE1	1.97	0.58
2:D:6:HIS:HE1	2:D:8:GLN:NE2	1.88	0.58
1:A:110:ILE:O	1:A:113:GLU:HG2	2.04	0.57
1:A:139:HIS:HE1	1:A:168:GLU:OE1	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.87	0.57
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.86	0.57
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.87	0.56
2:D:73:MET:HE2	2:D:92:PHE:HB3	1.86	0.56
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.23	0.56
2:B:221:THR:OG1	6:B:504:SO4:O4	2.23	0.56
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.87	0.56
2:B:104:GLY:O	2:B:109:GLY:HA3	2.07	0.55
2:D:137:HIS:HD2	2:D:144:GLY:O	1.90	0.55
1:A:308:ARG:HH11	1:A:339:ARG:HH12	1.56	0.54
2:D:54:ALA:HB3	2:D:58:LYS:HG3	1.90	0.54
2:B:267:MET:HE2	2:B:299:MET:HG3	1.90	0.54
1:C:166:LYS:HE2	1:C:197:HIS:O	2.08	0.54
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.90	0.54
2:B:99:ASN:HD21	1:C:352:LYS:HZ1	1.56	0.54
1:A:308:ARG:HH11	1:A:339:ARG:NH1	2.06	0.53
2:B:54:ALA:HB3	2:B:58:LYS:HG3	1.89	0.53
2:D:131:GLN:NE2	2:D:250:LEU:H	2.07	0.53
2:B:12:CYS:HB3	2:B:138:SER:HB3	1.90	0.53
2:D:1:MET:N	2:D:129:CYS:SG	2.73	0.53
2:D:104:GLY:O	2:D:109:GLY:HA3	2.08	0.52
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.91	0.52
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.28	0.52
1:A:308:ARG:NH1	1:A:339:ARG:NH1	2.53	0.52
1:C:107:HIS:CE1	1:C:155:GLU:OE2	2.61	0.52
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.91	0.52
2:B:345:ILE:HG22	2:B:348:ASN:HB3	1.91	0.52
1:C:88:HIS:O	1:C:91:GLN:HG2	2.10	0.52
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.10	0.51
2:B:23:ILE:HG12	2:B:230:SER:HB2	1.92	0.51
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.93	0.50
1:C:154:MET:HE2	1:C:194:THR:HG23	1.93	0.50
1:C:317:MET:SD	1:C:377:MET:HE2	2.51	0.50
1:A:285:GLN:NE2	1:A:372:GLN:H	2.10	0.50
1:A:88:HIS:O	1:A:91:GLN:HG2	2.11	0.50
2:D:48:ASN:O	2:D:62:ARG:NH2	2.44	0.50
1:C:295:CYS:HB3	1:C:377:MET:HE3	1.94	0.49
2:B:227:HIS:HE1	2:B:274:THR:HG23	1.78	0.49
2:D:145:SER:HB2	2:D:188:SER:OG	2.12	0.49
1:A:88:HIS:H	1:A:91:GLN:NE2	2.11	0.49
1:A:189:LEU:HD13	1:A:413:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:HB2	1:A:190:THR:HB	1.94	0.48
2:D:4:ILE:HD11	2:D:240:LEU:HD22	1.95	0.48
2:B:144:GLY:H	7:B:503[B]:GDP:PB	2.36	0.48
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.79	0.48
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.95	0.48
2:D:204:ASN:HD21	4:D:501:GTP:N2	1.98	0.48
3:E:92:ASN:O	3:E:96:MET:SD	2.72	0.48
1:A:71:GLU:OE2	1:A:73:THR:CB	2.61	0.47
2:B:1:MET:N	2:B:129:CYS:SG	2.75	0.47
2:B:23:ILE:HD13	2:B:234:SER:HB2	1.96	0.47
1:C:139:HIS:HE1	1:C:168:GLU:OE1	1.96	0.47
2:D:375:GLN:HE21	2:D:379:LYS:HE3	1.79	0.47
2:B:4:ILE:HD11	2:B:240:LEU:HD22	1.95	0.47
2:B:395:LEU:HD21	2:B:405:GLU:HG3	1.95	0.47
1:C:213:CYS:HA	1:C:217:LEU:HD12	1.96	0.47
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.44	0.47
2:B:137:HIS:HD2	2:B:144:GLY:O	1.98	0.47
1:C:271:THR:OG1	1:C:377:MET:HB3	2.14	0.47
1:C:200:CYS:HA	1:C:266:HIS:HB2	1.97	0.47
2:D:406:MET:HE3	2:D:410:GLU:HG3	1.97	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.50	0.46
1:A:139:HIS:CE1	1:A:168:GLU:OE1	2.69	0.46
3:E:125:GLU:HA	3:E:128:LYS:HD2	1.97	0.46
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.97	0.46
2:D:375:GLN:HE22	2:D:423:GLN:HE21	1.64	0.46
1:A:141:PHE:O	1:A:147:SER:HB3	2.16	0.46
2:B:375:GLN:HE21	2:B:379:LYS:HE3	1.81	0.46
1:C:54:SER:OG	1:C:62:VAL:HG13	2.16	0.45
1:C:271:THR:HG22	1:C:301:GLN:HA	1.97	0.45
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.98	0.45
2:B:145:SER:HB2	2:B:188:SER:OG	2.16	0.45
2:D:176:SER:HB3	2:D:181:GLU:OE2	2.16	0.45
2:D:321:MET:HE3	2:D:363:MET:HE3	1.98	0.45
2:B:118:ASP:OD1	2:B:121:ARG:NH1	2.49	0.45
2:B:321:MET:HE3	2:B:363:MET:HE3	1.98	0.45
2:B:375:GLN:HE22	2:B:423:GLN:HE21	1.64	0.45
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.51	0.45
2:B:307:HIS:CD2	2:B:376:GLU:OE1	2.66	0.45
3:E:132:GLU:HG3	3:E:135:LYS:HZ1	1.82	0.45
1:C:88:HIS:H	1:C:91:GLN:NE2	2.15	0.44
1:A:355:ILE:O	3:E:17:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:MET:HE3	2:B:410:GLU:HG3	1.97	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.00	0.44
1:C:209:ILE:HD11	1:C:302:MET:HG3	1.99	0.44
2:D:80:PRO:O	2:D:81:PHE:HB2	2.17	0.44
1:C:189:LEU:HD13	1:C:413:MET:HE1	1.98	0.44
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.44
1:A:150:THR:O	1:A:154:MET:HG2	2.17	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.44
2:B:23:ILE:HD12	2:B:24:ILE:HG23	2.00	0.43
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.84	0.43
2:B:178:THR:HG23	2:B:181:GLU:HG3	2.00	0.43
3:E:132:GLU:HG3	3:E:135:LYS:NZ	2.34	0.43
2:D:204:ASN:ND2	4:D:501:GTP:HN22	1.99	0.43
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.99	0.43
1:A:346:TRP:CZ2	1:A:435:VAL:HG13	2.55	0.42
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.01	0.42
2:B:161:ASP:O	2:B:251:ARG:NH2	2.52	0.42
1:C:370:LYS:HD3	1:C:370:LYS:H	1.85	0.42
1:A:329:ASN:ND2	3:E:20:TRP:HE1	2.07	0.42
2:D:117:LEU:O	2:D:121:ARG:HG3	2.20	0.42
2:B:19:LYS:O	2:B:23:ILE:HG13	2.20	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
1:A:349:THR:HB	3:E:25:LYS:HB2	2.00	0.42
2:B:65:LEU:O	2:B:73:MET:HE1	2.20	0.42
1:A:336:LYS:HD3	3:E:24:LEU:HD13	2.02	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HG3	2.02	0.41
2:D:204:ASN:HD22	2:D:207:LEU:HD12	1.85	0.41
1:C:36:MET:HA	1:C:37:PRO:HD3	1.93	0.41
2:D:52:ASN:HB2	2:D:60:VAL:HG13	2.02	0.41
2:D:337:ASN:HB3	2:D:340:TYR:HD2	1.85	0.41
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.84	0.41
1:C:295:CYS:CB	1:C:377:MET:HE3	2.50	0.41
2:D:401:GLU:O	3:E:137:LYS:HB2	2.21	0.41
2:D:47:ILE:HD12	2:D:47:ILE:HA	1.96	0.41
2:B:12:CYS:CB	2:B:138:SER:HB3	2.51	0.40
1:C:98:ASP:HB2	4:C:600:GTP:O2G	2.21	0.40
1:A:105:ARG:HG2	1:A:110:ILE:HD13	2.02	0.40
1:C:72:PRO:HA	1:C:94:THR:HG21	2.04	0.40
2:D:136:THR:HG22	2:D:167:TYR:HB2	2.03	0.40
1:A:98:ASP:HB2	4:A:501:GTP:O2G	2.21	0.40
1:C:69:ASP:O	1:C:94:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.86	0.40
3:E:101:LEU:O	3:E:105:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/450 (95%)	412 (96%)	14 (3%)	2 (0%)	24	57
1	C	428/450 (95%)	410 (96%)	18 (4%)	0	100	100
2	B	424/447 (95%)	412 (97%)	11 (3%)	1 (0%)	43	72
2	D	423/447 (95%)	413 (98%)	9 (2%)	1 (0%)	43	72
3	E	123/143 (86%)	120 (98%)	2 (2%)	1 (1%)	16	49
All	All	1826/1937 (94%)	1767 (97%)	54 (3%)	5 (0%)	36	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
2	D	179	VAL
1	A	162	GLY
3	E	142	GLU
2	B	56	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	364/375 (97%)	347 (95%)	17 (5%)	23	50
1	C	361/375 (96%)	345 (96%)	16 (4%)	25	51
2	B	364/382 (95%)	352 (97%)	12 (3%)	33	58
2	D	364/382 (95%)	349 (96%)	15 (4%)	27	53
3	E	110/126 (87%)	99 (90%)	11 (10%)	7	30
All	All	1563/1640 (95%)	1492 (96%)	71 (4%)	24	51

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	47	ASP
1	A	77	GLU
1	A	110	ILE
1	A	120	ASP
1	A	188	ILE
1	A	195	LEU
1	A	196	GLU
1	A	234	ILE
1	A	250	VAL
1	A	256	GLN
1	A	279	GLU
1	A	341	ILE
1	A	373	ARG
1	A	384	ILE
1	A	413	MET
1	A	425	LEU
2	B	23	ILE
2	B	26	ASP
2	B	39	ASP
2	B	42	LEU
2	B	77	ARG
2	B	120	VAL
2	B	151	LEU
2	B	293	MET
2	B	323	MET
2	B	409	THR
2	B	420	SER

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Mol	Chain	Res	Type
2	B	431	ASP
1	C	47	ASP
1	C	62	VAL
1	C	71	GLU
1	C	120	ASP
1	C	164	LYS
1	C	195	LEU
1	C	234	ILE
1	C	250	VAL
1	C	327	ASP
1	C	339	ARG
1	C	342	GLN
1	C	349	THR
1	C	370	LYS
1	C	384	ILE
1	C	413	MET
1	C	425	LEU
2	D	42	LEU
2	D	75	SER
2	D	77	ARG
2	D	99	ASN
2	D	120	VAL
2	D	176	SER
2	D	178	THR
2	D	198	GLU
2	D	278	SER
2	D	293	MET
2	D	323	MET
2	D	386	THR
2	D	395	LEU
2	D	409	THR
2	D	420	SER
3	E	25	LYS
3	E	70	LYS
3	E	82	VAL
3	E	87	ILE
3	E	96	MET
3	E	122	ARG
3	E	125	GLU
3	E	134	ARG
3	E	135	LYS
3	E	139	LEU

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Mol	Chain	Res	Type
3	E	142	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	88	HIS
1	A	91	GLN
1	A	139	HIS
1	A	249	ASN
1	A	256	GLN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	342	GLN
1	A	356	ASN
2	B	6	HIS
2	B	11	GLN
2	B	37	HIS
2	B	48	ASN
2	B	99	ASN
2	B	137	HIS
2	B	204	ASN
2	B	227	HIS
2	B	264	HIS
2	B	307	HIS
2	B	375	GLN
2	B	423	GLN
1	C	8	HIS
1	C	35	GLN
1	C	50	ASN
1	C	91	GLN
1	C	107	HIS
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	301	GLN
1	C	329	ASN
1	C	380	ASN
2	D	6	HIS
2	D	37	HIS
2	D	94	GLN

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Mol	Chain	Res	Type
2	D	131	GLN
2	D	137	HIS
2	D	204	ASN
2	D	227	HIS
2	D	264	HIS
2	D	347	ASN
2	D	375	GLN
2	D	414	ASN
2	D	423	GLN
3	E	18	GLN
3	E	78	HIS
3	E	111	ASN
3	E	129	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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z > 2$
6	SO4	D	503	-	4,4,4	0.38	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	D	501	5	33,34,34	0.60	1 (3%)	50,54,54	0.94	3 (6%)
4	GTP	B	501[A]	5	33,34,34	0.35	0	50,54,54	0.41	0
6	SO4	B	504	-	4,4,4	0.56	0	6,6,6	0.33	0
6	SO4	A	503	-	4,4,4	0.78	0	6,6,6	0.19	0
6	SO4	B	505	-	4,4,4	0.20	0	6,6,6	0.28	0
7	GDP	B	503[B]	-	29,30,30	0.44	0	45,47,47	0.73	1 (2%)
4	GTP	C	600	5	33,34,34	0.38	0	50,54,54	0.53	0
4	GTP	A	501	5	33,34,34	0.42	0	50,54,54	0.52	0
6	SO4	D	504	-	4,4,4	0.39	0	6,6,6	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	D	501	5	-	5/22/38/38	0/3/3/3
4	GTP	B	501[A]	5	-	4/22/38/38	0/3/3/3
7	GDP	B	503[B]	-	-	4/16/32/32	0/3/3/3
4	GTP	C	600	5	-	8/22/38/38	0/3/3/3
4	GTP	A	501	5	-	8/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	GTP	PG-O1G	2.09	1.57	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	GTP	O2B-PB-O3B	4.40	119.18	107.27
4	D	501	GTP	O5'-PA-O1A	2.62	119.30	108.94
4	D	501	GTP	O3B-PB-O1B	-2.24	103.97	110.70
7	B	503[B]	GDP	O2B-PB-O3A	2.12	111.73	104.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O1A
7	B	503[B]	GDP	PA-O3A-PB-O2B
4	A	501	GTP	PB-O3B-PG-O3G
4	B	501[A]	GTP	C5'-O5'-PA-O3A
4	B	501[A]	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	C5'-O5'-PA-O2A
7	B	503[B]	GDP	C5'-O5'-PA-O1A
4	A	501	GTP	PB-O3A-PA-O2A
4	D	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	PB-O3B-PG-O1G
4	C	600	GTP	PB-O3B-PG-O1G
4	B	501[A]	GTP	PG-O3B-PB-O1B
4	A	501	GTP	PB-O3B-PG-O2G
4	C	600	GTP	PB-O3B-PG-O2G
4	C	600	GTP	PB-O3B-PG-O3G
7	B	503[B]	GDP	PA-O3A-PB-O3B
4	A	501	GTP	PB-O3A-PA-O1A
4	C	600	GTP	PB-O3A-PA-O1A
4	C	600	GTP	PB-O3A-PA-O2A
4	D	501	GTP	PB-O3A-PA-O1A
4	B	501[A]	GTP	PG-O3B-PB-O2B
7	B	503[B]	GDP	PB-O3A-PA-O2A

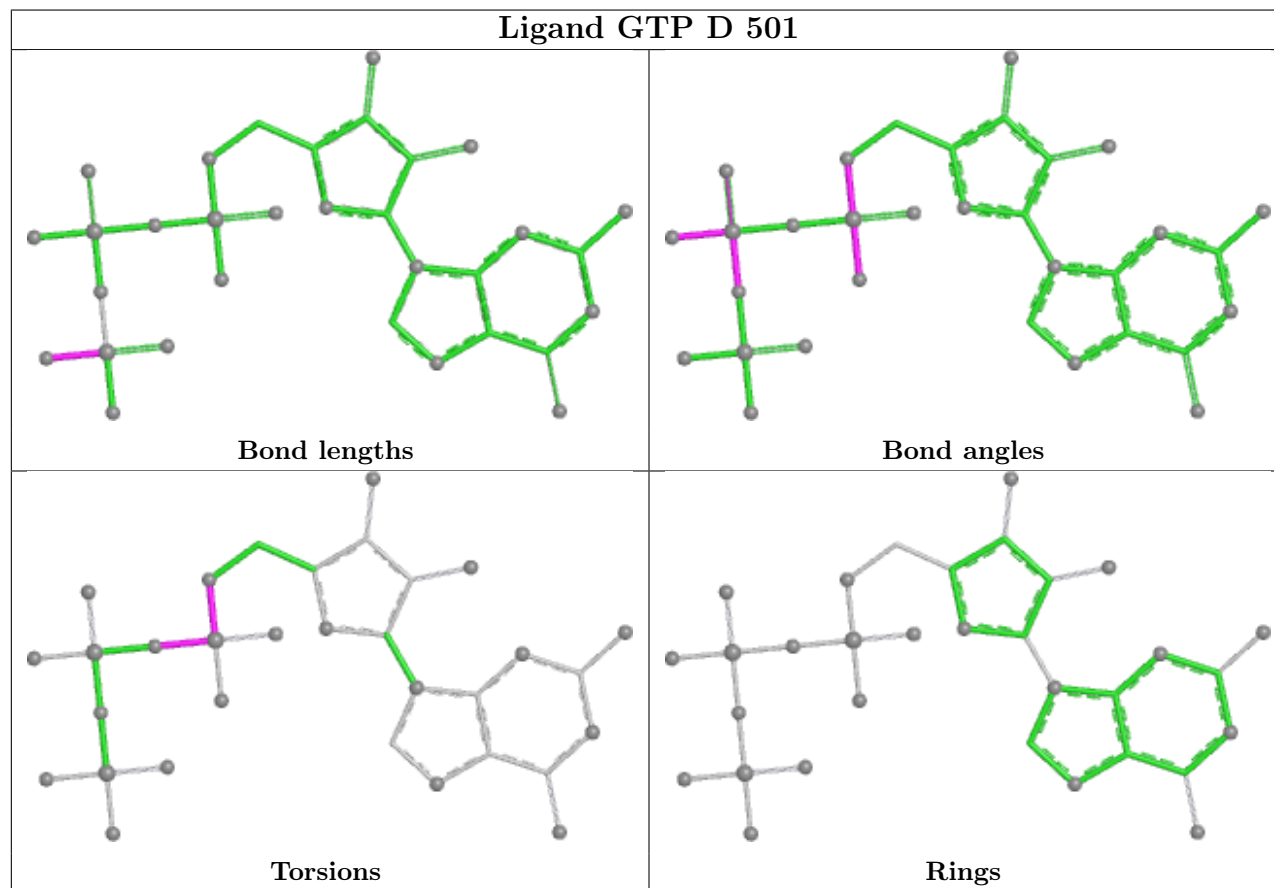
There are no ring outliers.

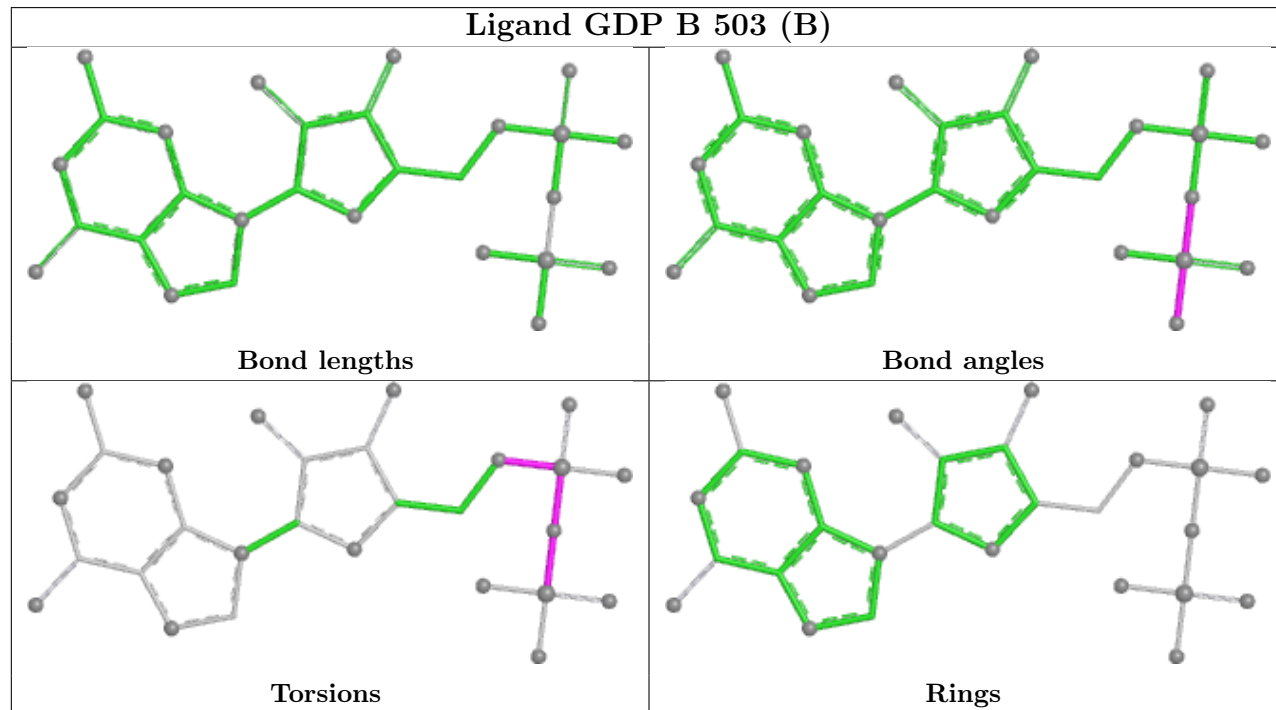
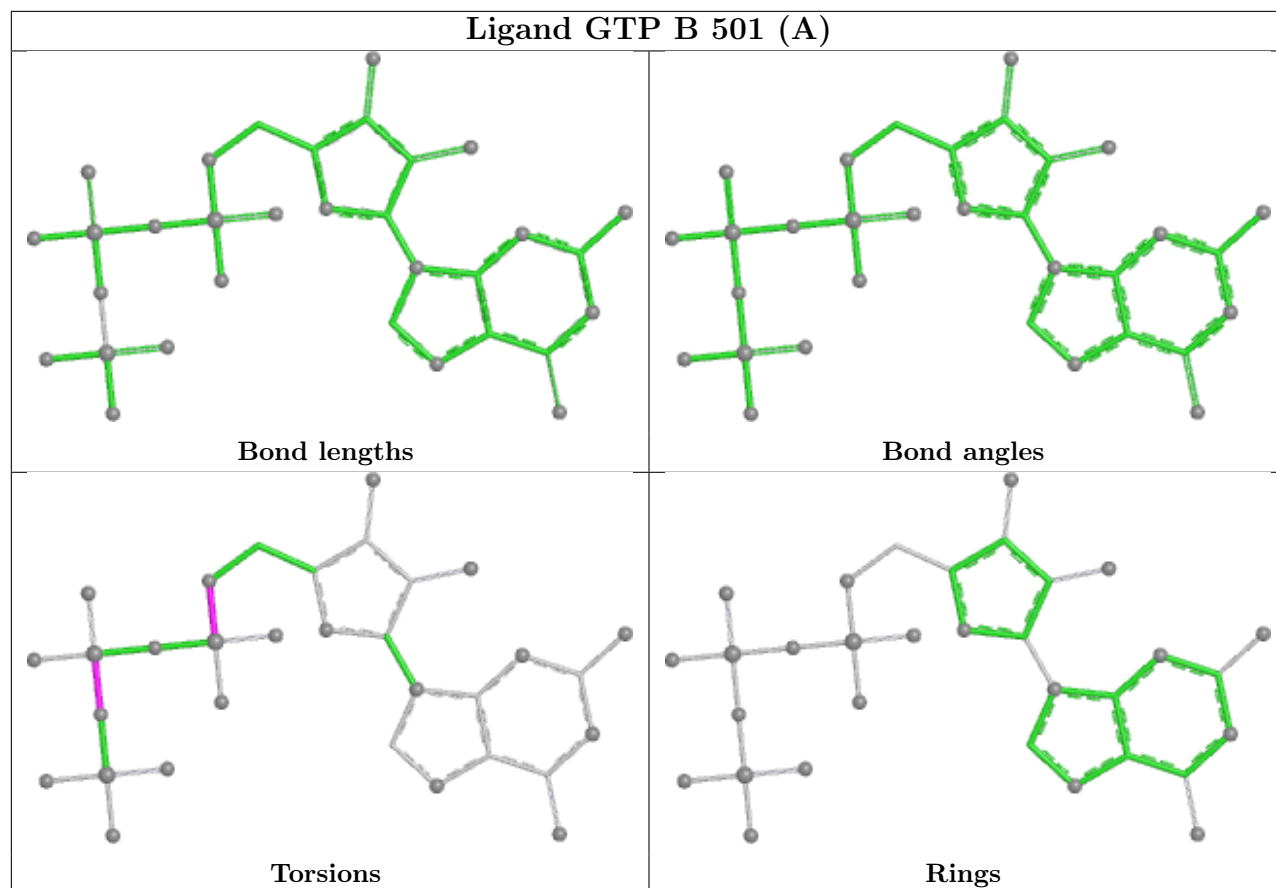
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	GTP	3	0
4	B	501[A]	GTP	1	0
6	B	504	SO4	1	0
7	B	503[B]	GDP	1	0
4	C	600	GTP	1	0
4	A	501	GTP	1	0

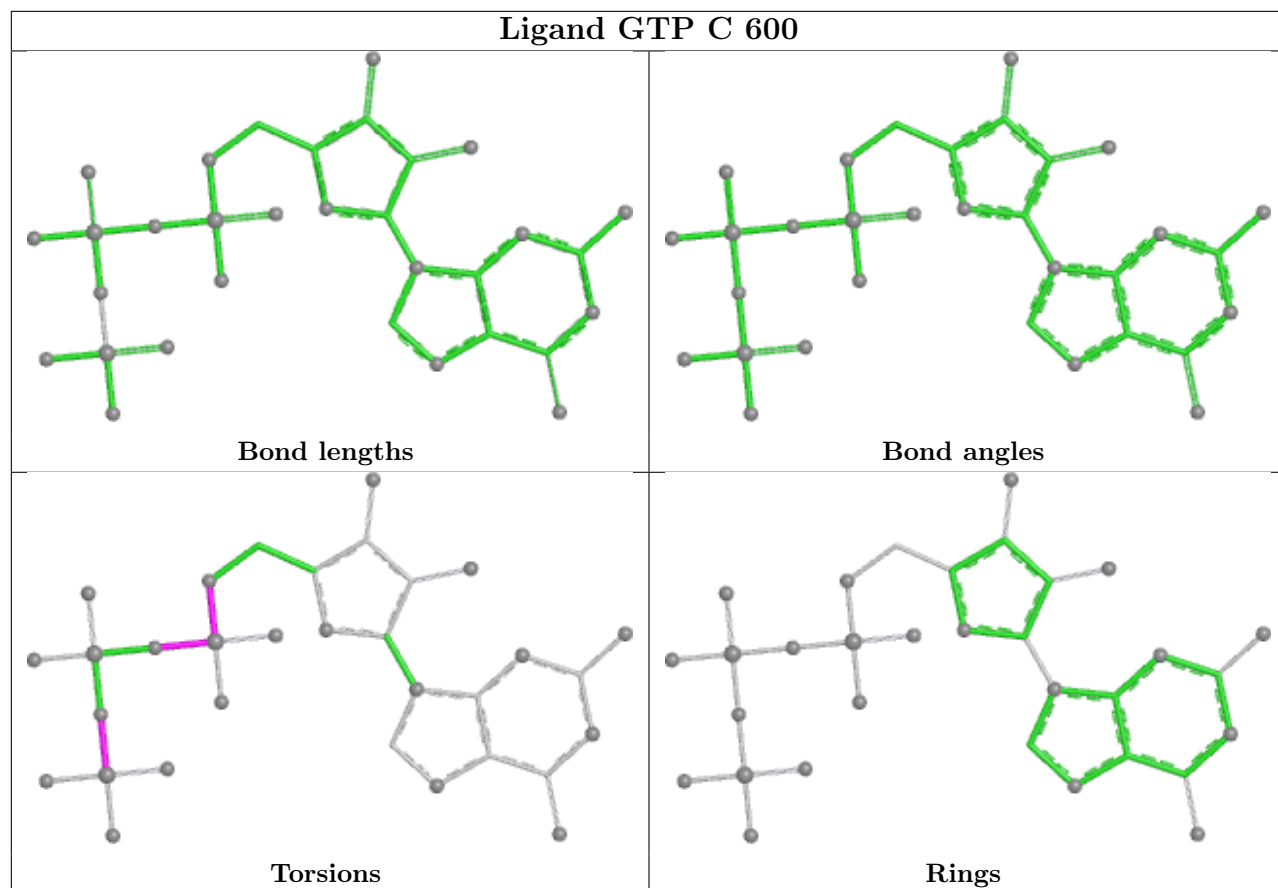
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

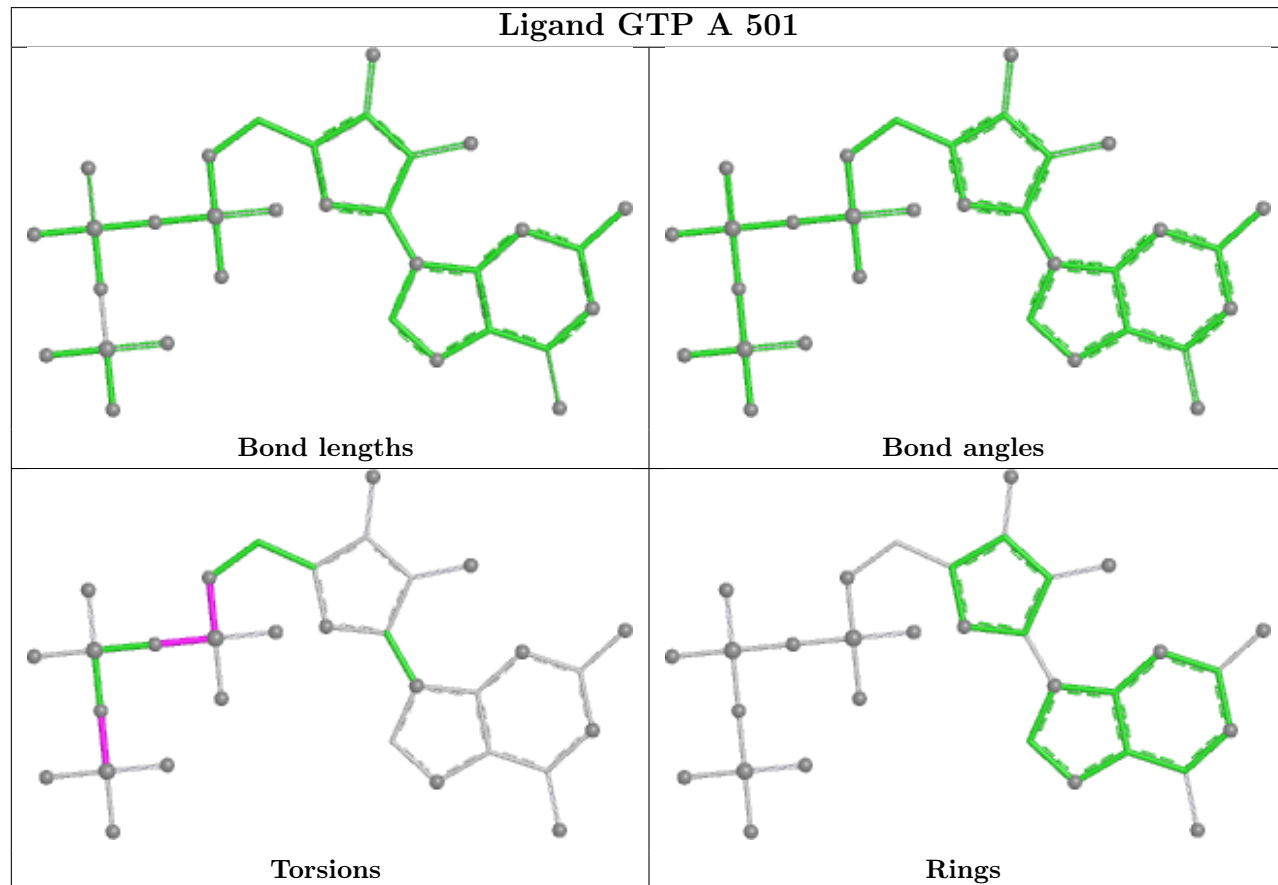




Ligand GTP C 600



Ligand GTP A 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/450 (96%)	-0.52	1 (0%) 91 79	81, 103, 145, 246	0
1	C	432/450 (96%)	-0.49	0 100 100	80, 108, 156, 229	0
2	B	428/447 (95%)	-0.48	1 (0%) 91 79	71, 104, 162, 256	0
2	D	427/447 (95%)	-0.44	0 100 100	55, 100, 148, 234	0
3	E	127/143 (88%)	-0.57	0 100 100	80, 122, 171, 230	0
All	All	1846/1937 (95%)	-0.49	2 (0%) 92 85	55, 105, 156, 256	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	201	CYS	2.7
1	A	118	VAL	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

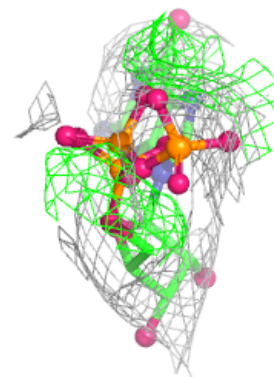
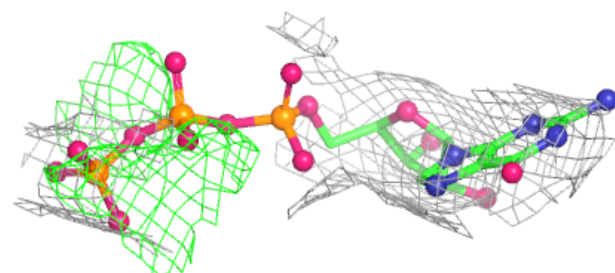
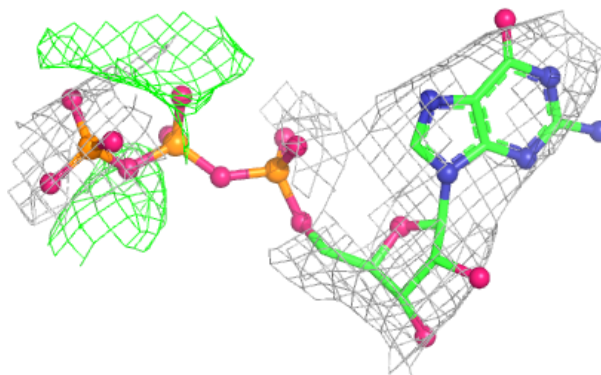
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	502[A]	1/1	0.16	0.41	80,80,80,80	1
5	MG	A	502	1/1	0.57	0.35	95,95,95,95	0
5	MG	C	601	1/1	0.67	0.22	94,94,94,94	0
6	SO4	B	505	5/5	0.71	0.07	156,157,157,158	0
6	SO4	A	503	5/5	0.74	0.17	82,83,84,85	0
6	SO4	B	504	5/5	0.76	0.11	113,114,115,117	0
6	SO4	D	504	5/5	0.81	0.07	127,129,129,130	0
4	GTP	B	501[A]	32/32	0.82	0.11	79,83,88,89	32
5	MG	D	502	1/1	0.84	0.20	80,80,80,80	0
7	GDP	B	503[B]	28/28	0.85	0.07	65,69,73,75	28
6	SO4	D	503	5/5	0.92	0.06	83,88,89,90	0
4	GTP	C	600	32/32	0.93	0.08	85,94,101,104	0
4	GTP	D	501	32/32	0.93	0.07	82,87,92,93	0
4	GTP	A	501	32/32	0.93	0.08	79,84,89,90	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.

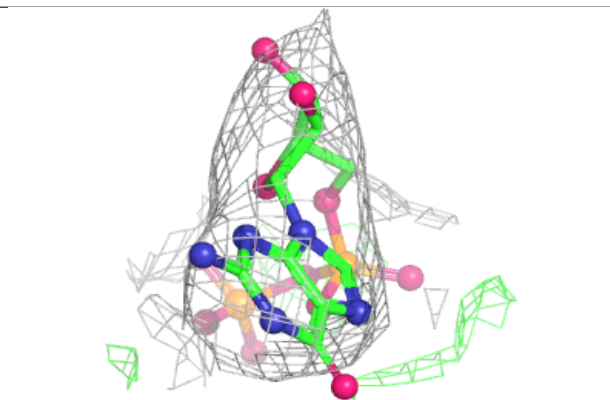
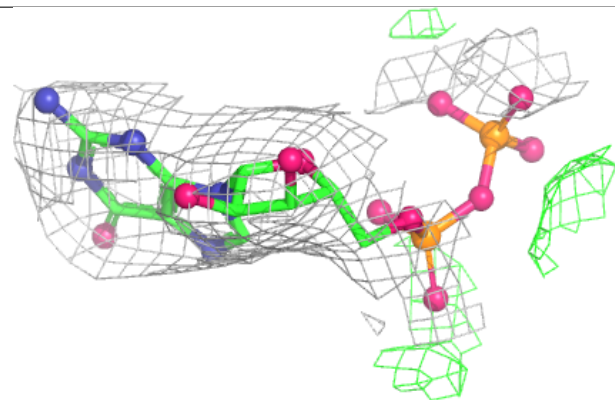
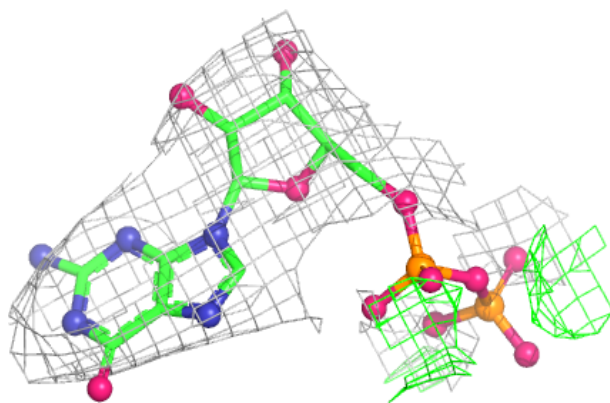
Electron density around GTP B 501 (A):

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

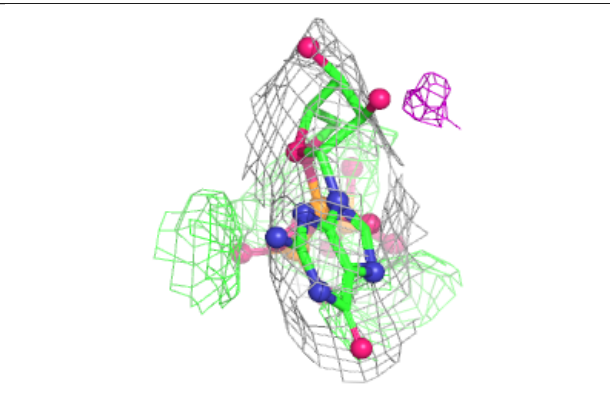
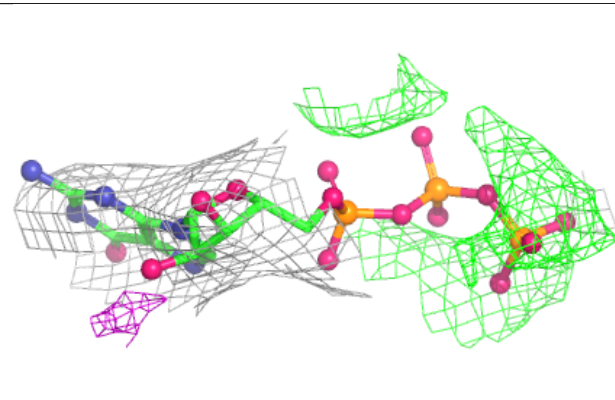
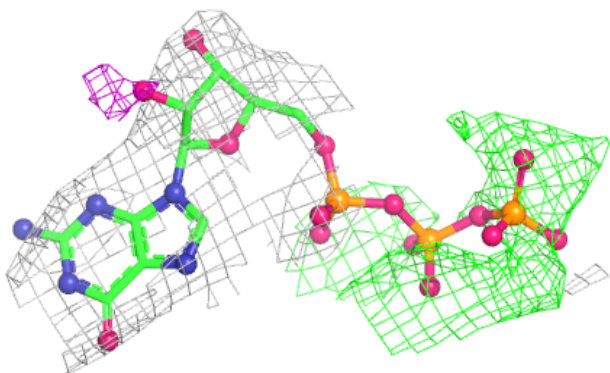


Electron density around GDP B 503 (B):

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

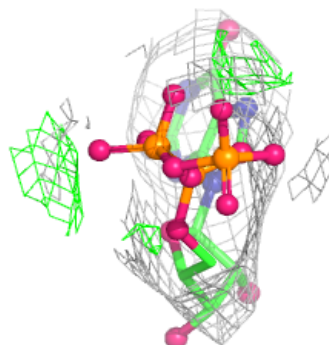
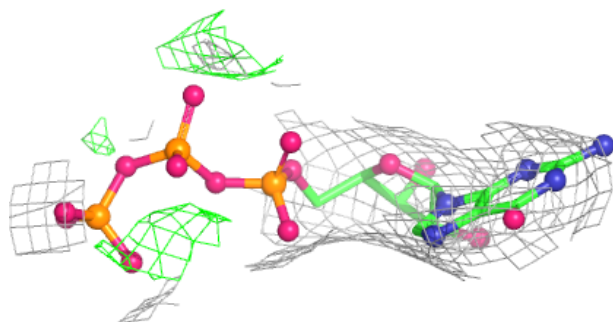
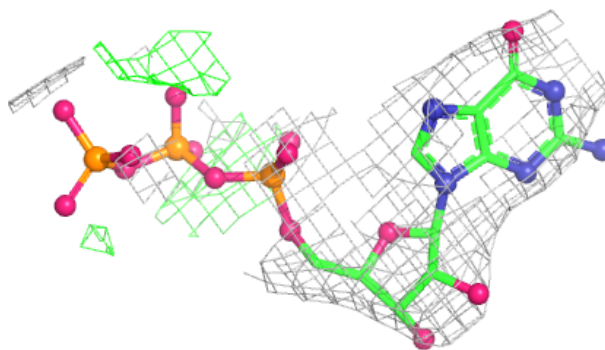
**Electron density around GTP C 600:**

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

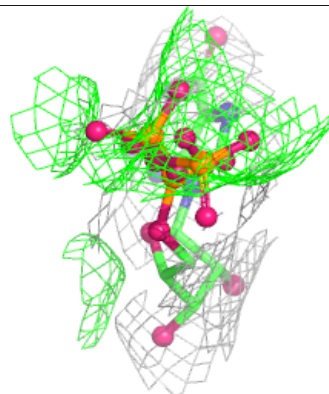
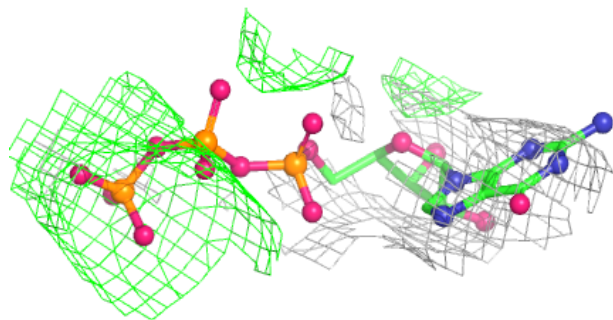
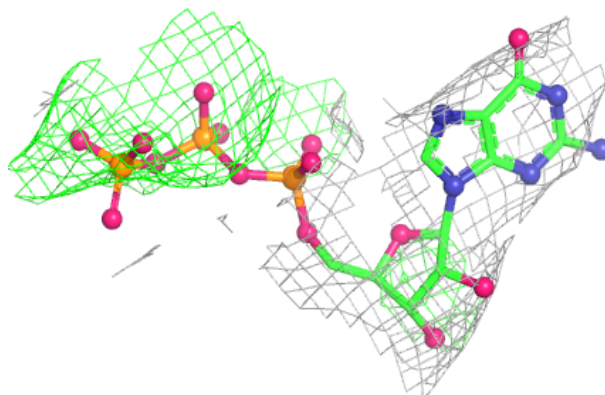


Electron density around GTP D 501:

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

**Electron density around 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.