



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:24 PM UTC

PDB ID : 5LP6 / pdb_00005lp6
Title : Crystal structure of Tubulin-Stathmin-TTL-Thiocolchicine Complex
Authors : Marangon, J.; Christodoulou, M.; Casagrande, F.; Tiana, G.; Dalla Via, L.; Aliverti, A.; Passarella, D.; Cappelletti, G.; Ricagno, S.
Deposited on : 2016-08-11
Resolution : 2.90 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

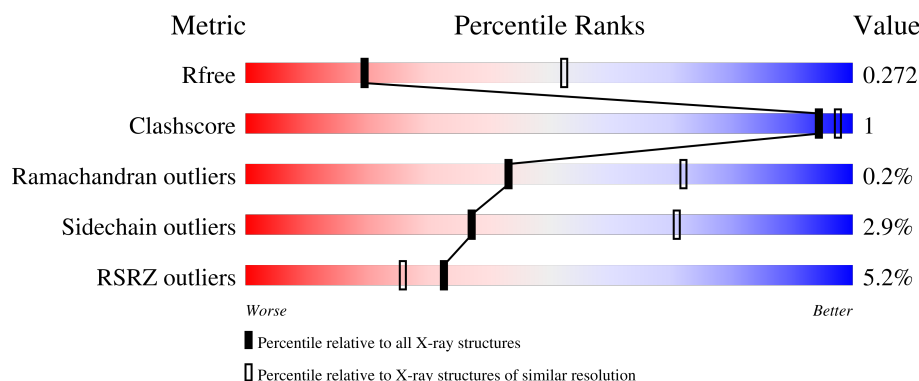
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



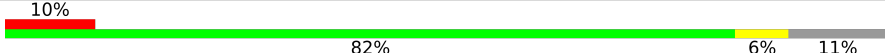
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	440	3% 95% 5%
1	C	440	6% 95% 5%
2	B	445	3% 92% 5%
2	D	445	4% 91% 5%
3	E	143	3% 78% 6% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	

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
6	MG	B	502	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17547 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	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3318	2085	566	640	27			
2	D	421	Total	C	N	O	S	0	0	0
			3308	2079	562	641	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

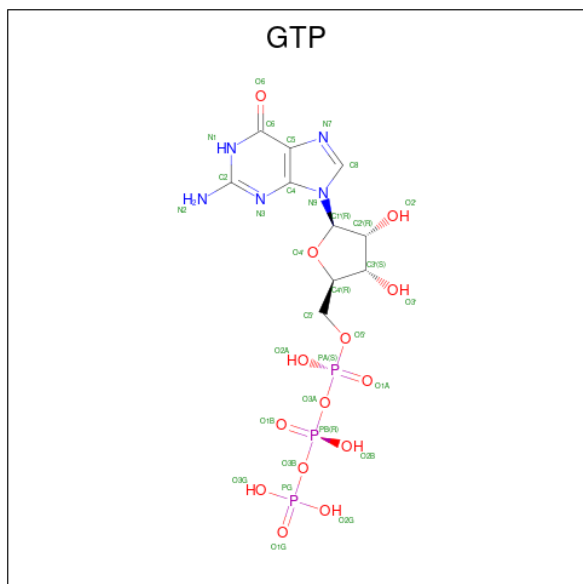
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	340	Total	C	N	O	S	0	0	0
			2794	1795	476	509	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 (CCD ID: 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		

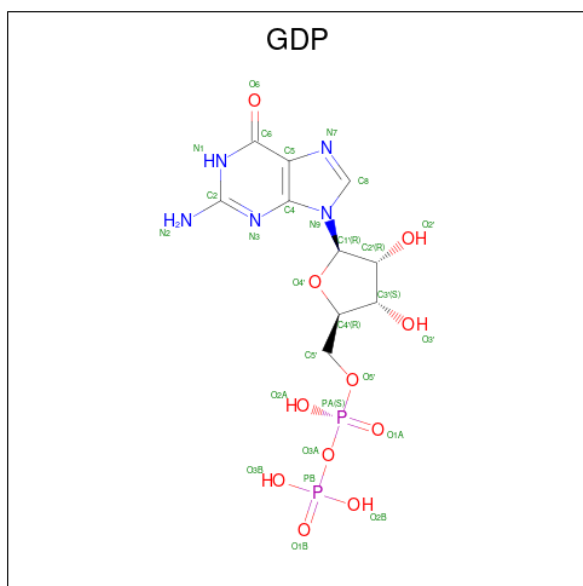
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Mg	0	0
			4	4		
6	B	3	Total	Mg	0	0
			3	3		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

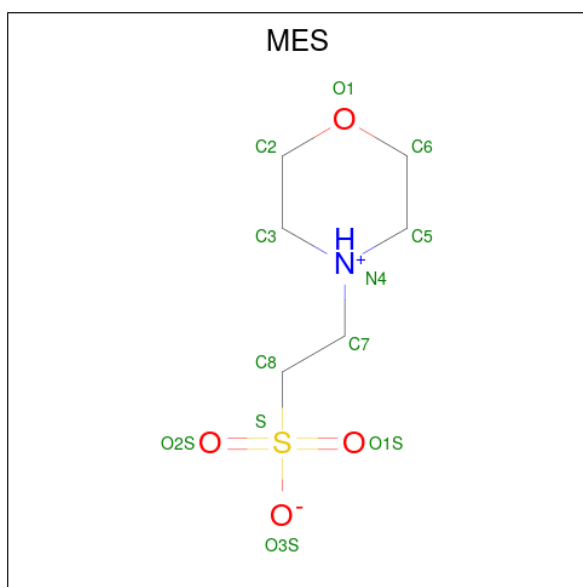
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

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



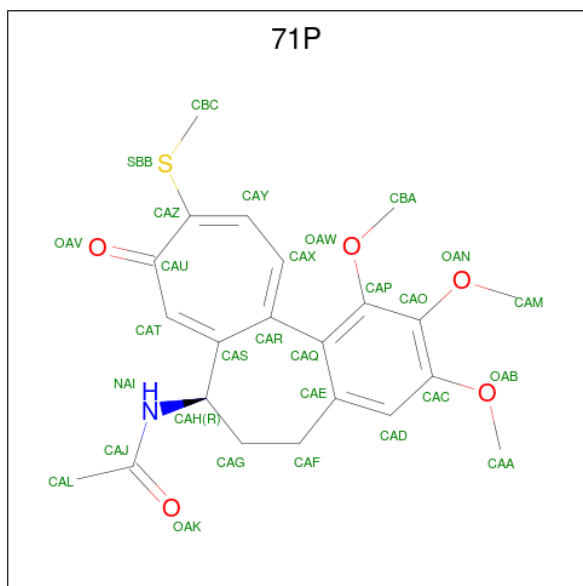
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

- Molecule 10 is {N}-[(7 {R})-1,2,3-trimethoxy-10-methylsulfonyl-9-oxidanylidene-6,7-dihydro-5 {H}-benzo[a]heptalen-7-yl]ethanamide (CCD ID: 71P) (formula: C₂₂H₂₅NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

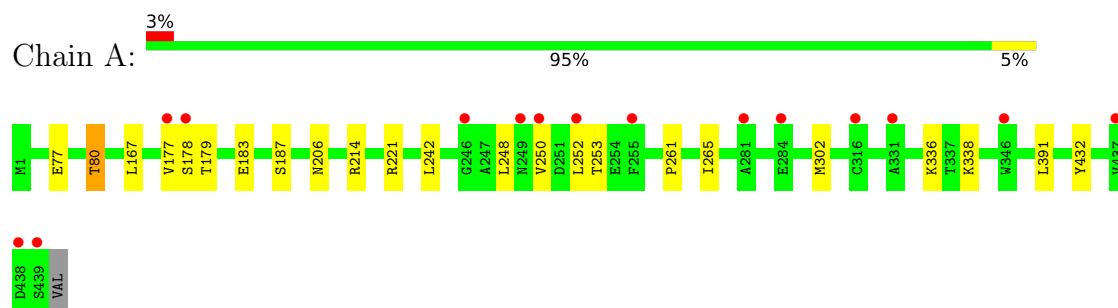
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	21	Total	O	0	0
			21	21		
12	B	16	Total	O	0	0
			16	16		
12	C	35	Total	O	0	0
			35	35		
12	D	11	Total	O	0	0
			11	11		
12	E	1	Total	O	0	0
			1	1		
12	F	5	Total	O	0	0
			5	5		

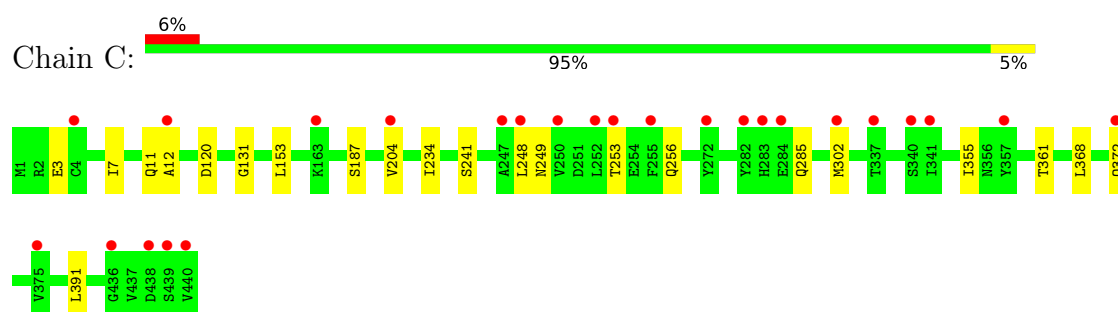
3 Residue-property plots [i](#)

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.

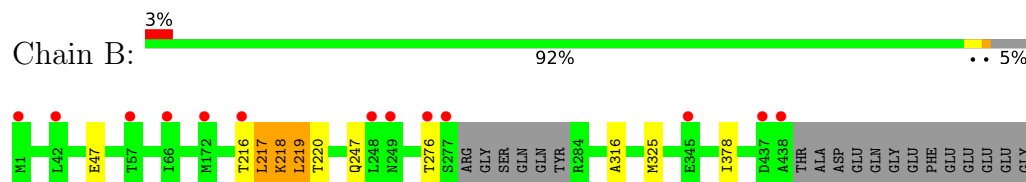
- Molecule 1: Tubulin alpha-1B chain



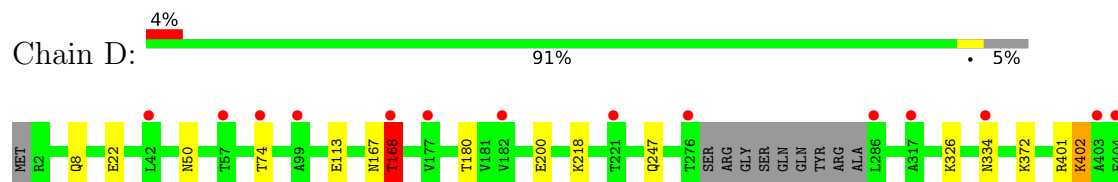
- Molecule 1: Tubulin alpha-1B chain

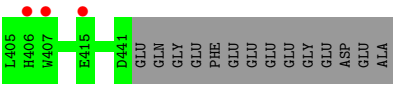


- Molecule 2: Tubulin beta-2B chain

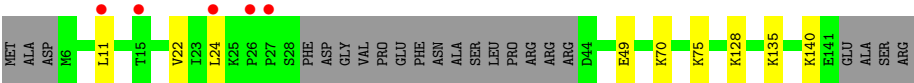
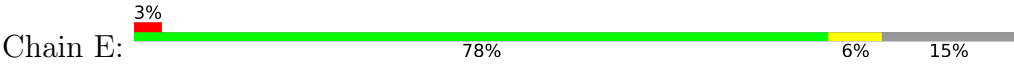


- Molecule 2: Tubulin beta-2B chain

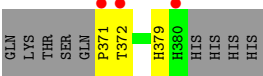
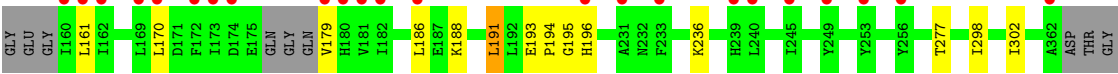
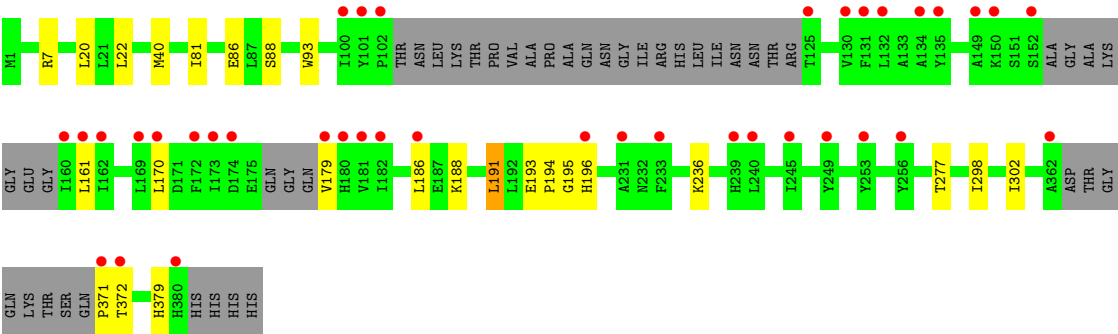
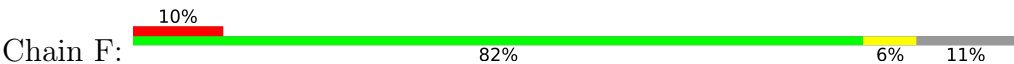




● Molecule 3: Stathmin-4



● Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.62Å 155.28Å 180.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.85 – 2.90 58.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.85-2.90) 99.8 (58.85-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.273 , 0.305 (Not available) , 0.272	Depositor DCC
R_{free} test set	3307 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.8	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	0.91	EDS
Total number of atoms	17547	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CL, GDP, MG, CA, 71P, MES

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	0.56	0/3508	0.84	0/4762
1	C	0.53	0/3515	0.84	0/4772
2	B	0.53	0/3389	0.81	0/4586
2	D	0.56	0/3379	0.80	0/4575
3	E	0.53	0/1008	0.82	0/1337
4	F	0.57	0/2858	0.78	2/3860 (0.1%)
All	All	0.55	0/17657	0.82	2/23892 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	195	GLY	N-CA-C	6.62	122.36	114.48
4	F	93	TRP	N-CA-C	5.04	118.89	112.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3340	14	0
1	C	3437	0	3348	11	0
2	B	3318	0	3201	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3308	0	3182	3	0
3	E	1000	0	1018	0	0
4	F	2794	0	2765	9	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	12	0	13	0	0
10	B	29	0	0	2	0
11	C	1	0	0	0	0
12	A	21	0	0	0	0
12	B	16	0	0	0	0
12	C	35	0	0	1	0
12	D	11	0	0	0	0
12	E	1	0	0	0	0
12	F	5	0	0	0	0
All	All	17547	0	16915	46	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 1.

All (46) 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:216:THR:O	2:B:218:LYS:N	1.75	1.17
1:A:177:VAL:O	1:A:178:SER:OG	1.59	1.17
1:A:177:VAL:C	1:A:178:SER:HG	1.83	0.82
4:F:191:LEU:HG	4:F:196:HIS:CE1	2.13	0.82
1:A:177:VAL:O	1:A:178:SER:CB	2.42	0.68
2:B:218:LYS:C	2:B:219:LEU:HD23	2.21	0.65
1:A:179:THR:HB	1:A:183:GLU:CD	2.25	0.61
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.82	0.61
1:C:3:GLU:OE1	1:C:131:GLY:O	2.24	0.56
1:C:12:ALA:N	12:C:601:HOH:O	2.40	0.54
2:B:216:THR:O	2:B:217:LEU:C	2.48	0.54
1:C:234:ILE:HD13	1:C:302:MET:HE3	1.90	0.52
2:B:216:THR:O	2:B:218:LYS:CA	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ARG:C	2:D:402:LYS:HG2	2.36	0.51
1:A:179:THR:HB	1:A:183:GLU:OE2	2.12	0.51
1:A:177:VAL:CG2	1:A:206:ASN:HB3	2.41	0.50
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.94	0.50
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.93	0.50
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.94	0.49
2:B:216:THR:C	2:B:218:LYS:N	2.61	0.49
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.95	0.49
10:B:504:71P:OAW	10:B:504:71P:CAX	2.60	0.49
1:A:177:VAL:HG21	1:A:206:ASN:CB	2.41	0.49
4:F:193:GLU:HA	4:F:194:PRO:C	2.39	0.48
1:A:177:VAL:HG11	5:A:501:GTP:O2'	2.14	0.47
4:F:161:LEU:HA	4:F:236:LYS:HE2	1.97	0.47
4:F:191:LEU:HG	4:F:196:HIS:ND1	2.29	0.47
2:D:167:ASN:O	2:D:168:THR:HG22	2.15	0.47
1:A:242:LEU:HD11	1:A:252:LEU:HD21	1.97	0.46
2:B:219:LEU:HD23	2:B:219:LEU:N	2.30	0.46
1:C:204:VAL:HG13	1:C:302:MET:HE2	1.98	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.99	0.45
1:C:234:ILE:HG21	1:C:302:MET:SD	2.57	0.45
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.00	0.44
1:C:11:GLN:O	1:C:12:ALA:HB3	2.18	0.44
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.99	0.44
1:C:11:GLN:HE22	2:D:247:GLN:HE22	1.66	0.43
4:F:371:PRO:HA	4:F:372:THR:HB	1.99	0.43
2:B:216:THR:HG22	2:B:217:LEU:H	1.83	0.43
2:B:316:ALA:HB1	10:B:504:71P:CBA	2.49	0.43
1:C:241:SER:HA	1:C:249:ASN:HD21	1.83	0.43
4:F:81:ILE:O	4:F:88:SER:HB3	2.18	0.42
4:F:191:LEU:HB3	4:F:196:HIS:HA	2.02	0.41
1:A:77:GLU:HA	1:A:80:THR:HG22	2.02	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41
4:F:7:ARG:CD	4:F:40:MET:HE2	2.52	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	437/440 (99%)	423 (97%)	13 (3%)	1 (0%)	43	72
1	C	438/440 (100%)	428 (98%)	10 (2%)	0	100	100
2	B	414/445 (93%)	400 (97%)	12 (3%)	2 (0%)	24	54
2	D	413/445 (93%)	400 (97%)	12 (3%)	1 (0%)	43	72
3	E	117/143 (82%)	114 (97%)	3 (3%)	0	100	100
4	F	330/384 (86%)	310 (94%)	20 (6%)	0	100	100
All	All	2149/2297 (94%)	2075 (97%)	70 (3%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	217	LEU
2	B	218	LYS
2	D	168	THR
1	A	261	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	370/371 (100%)	361 (98%)	9 (2%)	43	75
1	C	371/371 (100%)	364 (98%)	7 (2%)	50	79
2	B	365/383 (95%)	359 (98%)	6 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	364/383 (95%)	351 (96%)	13 (4%)	31	65
3	E	109/127 (86%)	100 (92%)	9 (8%)	10	32
4	F	308/342 (90%)	298 (97%)	10 (3%)	34	68
All	All	1887/1977 (95%)	1833 (97%)	54 (3%)	37	71

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	214	ARG
1	A	221	ARG
1	A	248	LEU
1	A	250	VAL
1	A	253	THR
1	A	302	MET
1	A	336	LYS
1	A	338	LYS
2	B	47	GLU
2	B	219	LEU
2	B	220	THR
2	B	247	GLN
2	B	276	THR
2	B	325	MET
1	C	120	ASP
1	C	253	THR
1	C	256	GLN
1	C	285	GLN
1	C	361	THR
1	C	368	LEU
1	C	372	GLN
2	D	8	GLN
2	D	22	GLU
2	D	50	ASN
2	D	74	THR
2	D	113	GLU
2	D	168	THR
2	D	180	THR
2	D	200	GLU
2	D	218	LYS
2	D	326	LYS
2	D	334	ASN

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Mol	Chain	Res	Type
2	D	372	LYS
2	D	402	LYS
3	E	11	LEU
3	E	22	VAL
3	E	24	LEU
3	E	49	GLU
3	E	70	LYS
3	E	75	LYS
3	E	128	LYS
3	E	135	LYS
3	E	140	LYS
4	F	20	LEU
4	F	22	LEU
4	F	86	GLU
4	F	170	LEU
4	F	179	VAL
4	F	186	LEU
4	F	188	LYS
4	F	191	LEU
4	F	277	THR
4	F	379	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	356	ASN
2	B	50	ASN
2	B	247	GLN
2	B	331	GLN
2	B	339	ASN
2	B	349	ASN
2	B	385	GLN
2	B	436	GLN
1	C	380	ASN
1	C	393	HIS
2	D	15	GLN
2	D	45	GLN
2	D	247	GLN
3	E	18	GLN
3	E	92	ASN
3	E	108	ASN

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Mol	Chain	Res	Type
4	F	242	ASN
4	F	269	GLN
4	F	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	$\# Z > 2$
5	GTP	C	501	6	33,34,34	1.20	3 (9%)	50,54,54	1.68	6 (12%)
5	GTP	A	501	6	33,34,34	1.18	3 (9%)	50,54,54	1.68	5 (10%)
8	GDP	D	600	-	29,30,30	1.18	2 (6%)	45,47,47	1.73	6 (13%)
8	GDP	B	501	6	29,30,30	1.20	4 (13%)	45,47,47	1.76	6 (13%)
10	71P	B	504	-	31,31,31	2.25	10 (32%)	39,44,44	5.08	21 (53%)
9	MES	B	503	-	12,12,12	2.36	1 (8%)	15,16,16	1.26	1 (6%)

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
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
8	GDP	D	600	-	-	5/16/32/32	0/3/3/3
8	GDP	B	501	6	-	5/16/32/32	0/3/3/3
10	71P	B	504	-	-	4/12/25/25	1/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.86	1.66	1.77
10	B	504	71P	CAH-CAS	-6.99	1.43	1.53
10	B	504	71P	CAF-CAE	-4.38	1.41	1.51
10	B	504	71P	CAZ-CAU	-4.30	1.38	1.47
10	B	504	71P	CAG-CAF	-3.87	1.43	1.53
8	B	501	GDP	C5-C4	3.25	1.47	1.38
5	A	501	GTP	C5-C4	3.24	1.47	1.38
8	D	600	GDP	C5-C4	3.22	1.47	1.38
5	C	501	GTP	C5-C4	3.21	1.47	1.38
10	B	504	71P	CAQ-CAR	-2.96	1.46	1.50
10	B	504	71P	CAT-CAS	2.58	1.41	1.36
10	B	504	71P	CAH-NAI	2.48	1.51	1.45
10	B	504	71P	CAX-CAR	2.48	1.41	1.37
8	B	501	GDP	PA-O3A	2.22	1.61	1.59
10	B	504	71P	CAQ-CAP	2.17	1.45	1.40
5	A	501	GTP	C6-N1	-2.17	1.34	1.38
5	C	501	GTP	C5-N7	-2.14	1.34	1.39
5	A	501	GTP	C5-N7	-2.11	1.34	1.39
8	B	501	GDP	C5-N7	-2.08	1.34	1.39
5	C	501	GTP	C6-N1	-2.06	1.35	1.38
8	B	501	GDP	C6-N1	-2.06	1.35	1.38
10	B	504	71P	OAW-CBA	2.05	1.48	1.42
8	D	600	GDP	C6-N1	-2.01	1.35	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	71P	CAH-CAS-CAT	-19.46	99.90	117.06
10	B	504	71P	CAH-CAS-CAR	16.11	130.08	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	71P	CAQ-CAR-CAS	10.26	127.03	118.62
10	B	504	71P	CAF-CAE-CAQ	6.31	130.25	119.88
8	B	501	GDP	C5-C4-N3	-5.92	118.97	128.39
5	C	501	GTP	C5-C4-N3	-5.75	119.24	128.39
5	A	501	GTP	C5-C4-N3	-5.75	119.25	128.39
8	D	600	GDP	C5-C4-N3	-5.66	119.38	128.39
10	B	504	71P	CAF-CAE-CAD	-5.55	107.31	119.35
10	B	504	71P	CAG-CAH-NAI	5.26	119.39	109.76
8	B	501	GDP	C2-N3-C4	5.13	121.14	112.30
5	C	501	GTP	C2-N3-C4	5.02	120.94	112.30
8	D	600	GDP	C2-N3-C4	5.01	120.92	112.30
5	A	501	GTP	C2-N3-C4	4.99	120.90	112.30
10	B	504	71P	CAP-CAQ-CAE	-4.62	112.58	118.41
10	B	504	71P	CAX-CAR-CAS	-4.60	120.00	124.67
8	B	501	GDP	N9-C4-N3	4.42	134.79	125.95
5	C	501	GTP	N9-C4-N3	4.27	134.50	125.95
8	D	600	GDP	N9-C4-N3	4.26	134.47	125.95
5	A	501	GTP	N9-C4-N3	4.14	134.24	125.95
5	A	501	GTP	C6-C5-N7	3.65	136.93	130.29
10	B	504	71P	CBA-OAW-CAP	-3.64	104.87	114.74
10	B	504	71P	CAA-OAB-CAC	-3.62	112.20	117.51
8	D	600	GDP	C6-C5-N7	3.60	136.84	130.29
8	B	501	GDP	C6-C5-N7	3.54	136.73	130.29
5	C	501	GTP	C6-C5-N7	3.51	136.68	130.29
10	B	504	71P	OAW-CAP-CAO	-3.43	112.53	120.35
10	B	504	71P	CAE-CAQ-CAR	3.08	123.62	120.20
10	B	504	71P	CAT-CAS-CAR	2.90	130.03	127.56
5	A	501	GTP	C4-C5-N7	-2.72	106.36	110.67
10	B	504	71P	CAQ-CAR-CAX	-2.67	112.62	116.95
8	B	501	GDP	C4-C5-N7	-2.66	106.45	110.67
8	D	600	GDP	C4-C5-N7	-2.60	106.54	110.67
5	C	501	GTP	C4-C5-N7	-2.54	106.65	110.67
10	B	504	71P	OAK-CAJ-NAI	2.40	126.23	121.98
10	B	504	71P	CAP-CAQ-CAR	2.34	123.79	121.33
5	C	501	GTP	O6-C6-C5	-2.21	120.69	126.53
10	B	504	71P	OAK-CAJ-CAL	-2.20	118.13	122.05
10	B	504	71P	CAD-CAE-CAQ	2.16	122.30	119.54
9	B	503	MES	C5-N4-C3	2.11	113.39	108.84
8	B	501	GDP	O6-C6-C5	-2.09	121.02	126.53
8	D	600	GDP	O6-C6-C5	-2.09	121.02	126.53
10	B	504	71P	CAM-OAN-CAO	2.07	120.35	114.74
10	B	504	71P	CAF-CAG-CAH	-2.06	109.63	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	71P	OAV-CAU-CAT	-2.03	113.58	119.02

There are no chirality outliers.

All (26) 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	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	600	GDP	C5'-O5'-PA-O3A
8	D	600	GDP	C5'-O5'-PA-O1A
10	B	504	71P	CAS-CAH-NAI-CAJ
10	B	504	71P	CAO-CAC-OAB-CAA
10	B	504	71P	CAD-CAC-OAB-CAA
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	600	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
9	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O1A
8	D	600	GDP	PB-O3A-PA-O1A
8	D	600	GDP	PB-O3A-PA-O2A
10	B	504	71P	CAY-CAZ-SBB-CBC
8	B	501	GDP	PB-O3A-PA-O2A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	504	71P	CAE-CAF-CAG-CAH-CAQ-CAR-CAS

2 monomers are involved in 3 short contacts:

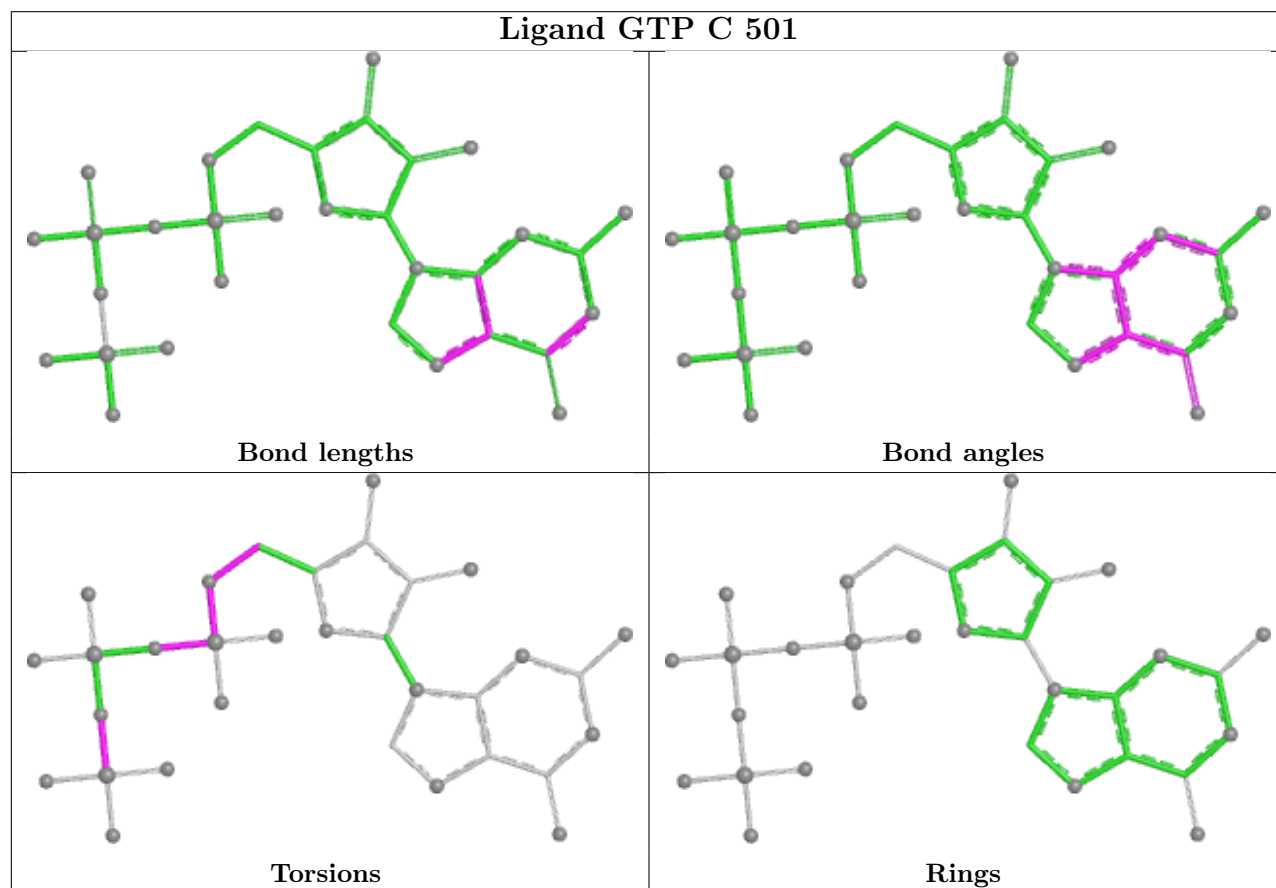
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0

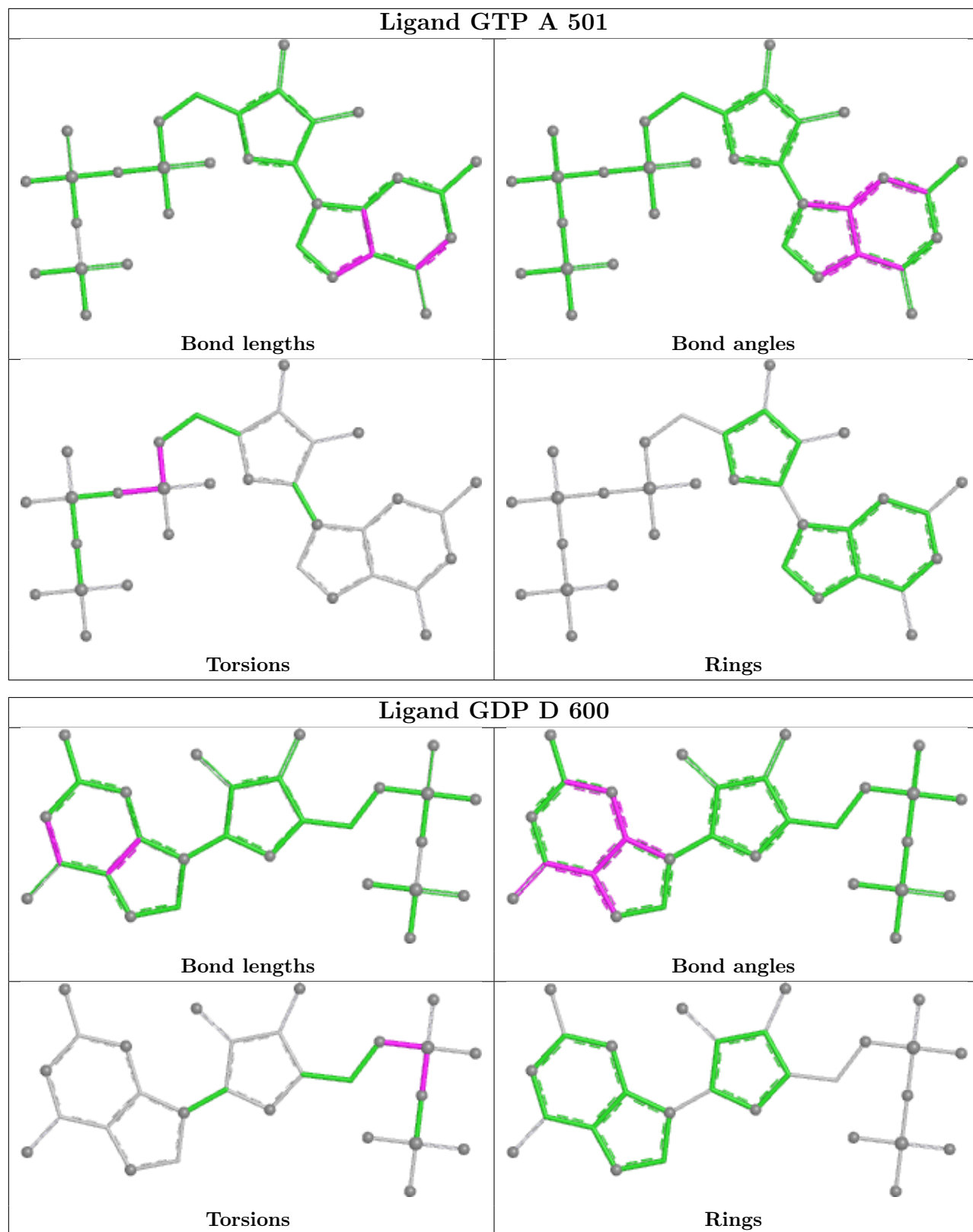
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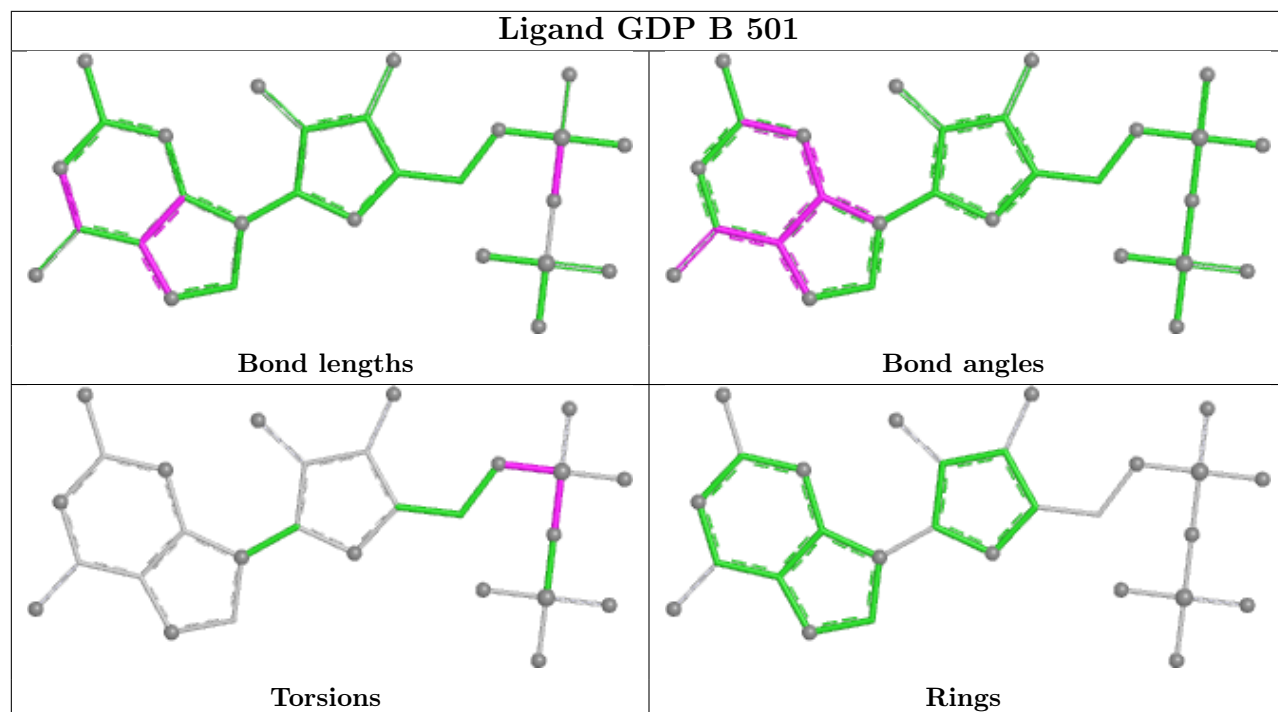
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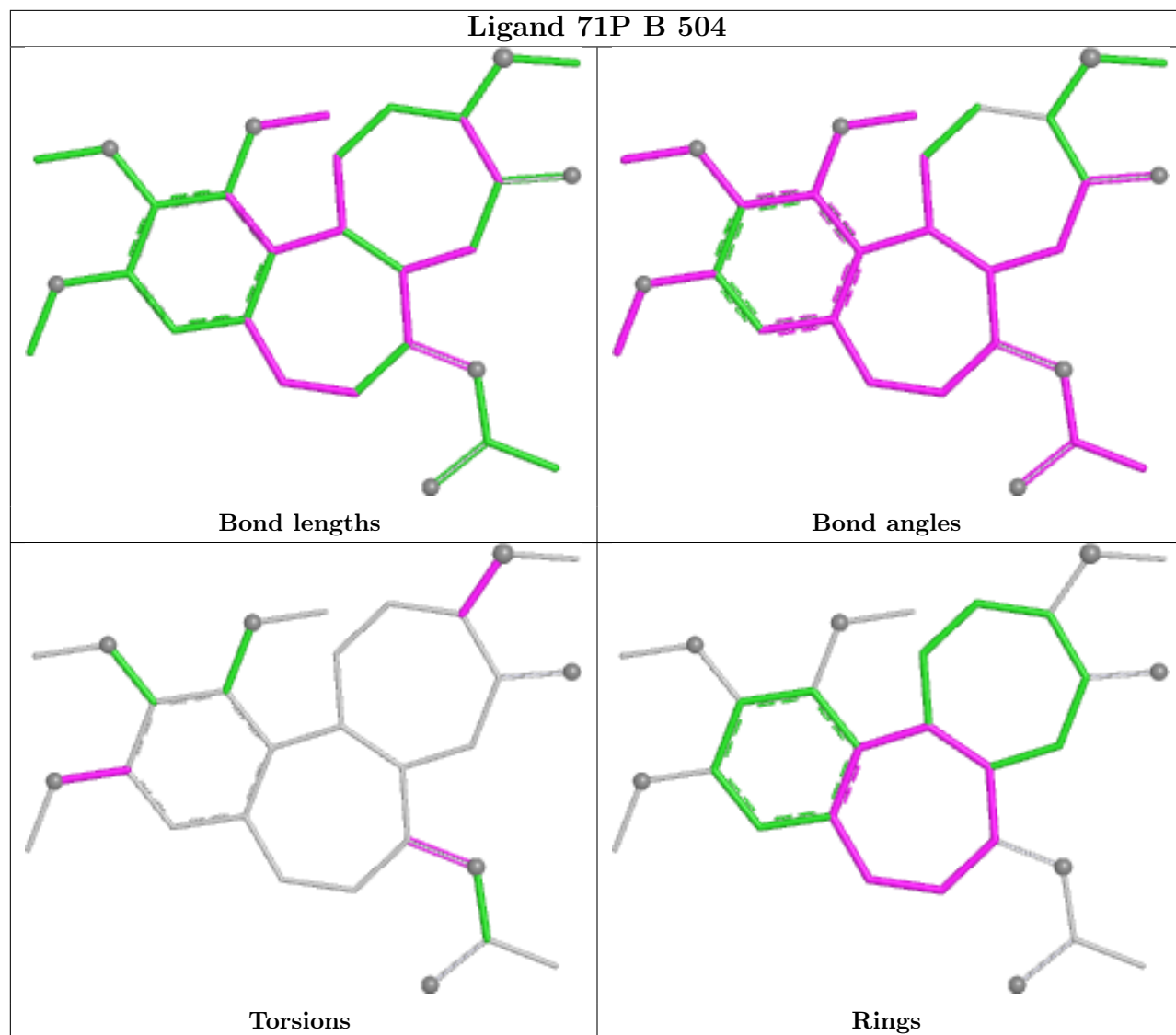
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	71P	2	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	360:PRO	C	369:ARG	N	3.14
1	B	42:LEU	C	45:GLN	N	3.11
1	D	42:LEU	C	45:GLN	N	3.03
1	D	360:PRO	C	369:ARG	N	2.87

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(Å ²)	Q<0.9
1	A	439/440 (99%)	0.61	15 (3%)	48	39	64, 76, 84, 94	0
1	C	440/440 (100%)	0.82	25 (5%)	29	23	64, 75, 83, 88	0
2	B	422/445 (94%)	0.68	13 (3%)	51	42	64, 76, 84, 92	1 (0%)
2	D	421/445 (94%)	0.57	17 (4%)	42	34	66, 77, 86, 93	5 (1%)
3	E	121/143 (84%)	0.65	5 (4%)	41	33	71, 80, 86, 91	0
4	F	340/384 (88%)	0.90	38 (11%)	10	9	72, 79, 91, 99	0
All	All	2183/2297 (95%)	0.71	113 (5%)	33	26	64, 77, 87, 99	6 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	LEU	5.0
1	A	255	PHE	4.5
3	E	27	PRO	4.5
1	C	302	MET	4.3
4	F	179	VAL	4.2
1	A	439	SER	4.2
1	C	252	LEU	4.1
4	F	173	ILE	3.9
4	F	160	ILE	3.9
4	F	181	VAL	3.8
1	A	178	SER	3.7
1	C	248	LEU	3.6
1	A	438	ASP	3.6
1	C	247	ALA	3.5
4	F	240	LEU	3.5
2	B	42	LEU	3.4
4	F	100	ILE	3.4
4	F	180	HIS	3.3
1	C	340	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	216	THR	3.3
1	C	439	SER	3.3
4	F	130	VAL	3.2
4	F	245	ILE	3.2
4	F	196	HIS	3.2
2	B	172	MET	3.2
4	F	102	PRO	3.2
4	F	149	ALA	3.1
4	F	182	ILE	3.1
2	B	276	THR	2.9
4	F	249	TYR	2.9
4	F	231	ALA	2.9
1	A	281	ALA	2.9
4	F	172	PHE	2.8
2	D	168	THR	2.8
1	C	372	GLN	2.8
2	B	249	ASN	2.8
2	D	403	ALA	2.7
4	F	170	LEU	2.7
4	F	233	PHE	2.7
1	C	283	HIS	2.7
4	F	380	HIS	2.7
1	C	337	THR	2.7
2	D	276	THR	2.7
4	F	371	PRO	2.7
2	D	334	ASN	2.7
3	E	26	PRO	2.7
1	C	4	CYS	2.6
1	C	440	VAL	2.6
1	A	177	VAL	2.6
4	F	174	ASP	2.6
1	C	272	TYR	2.6
1	C	375	VAL	2.6
4	F	169	LEU	2.6
2	B	1	MET	2.6
2	D	99	ALA	2.6
4	F	161	LEU	2.5
4	F	150	LYS	2.5
2	D	286	LEU	2.5
4	F	135	TYR	2.5
1	C	438	ASP	2.5
1	C	255	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	317	ALA	2.5
4	F	134	ALA	2.5
2	D	407	TRP	2.4
4	F	132	LEU	2.4
1	A	249	ASN	2.3
2	D	177	VAL	2.3
2	B	438	ALA	2.3
1	C	357	TYR	2.3
4	F	372	THR	2.3
1	A	284	GLU	2.3
2	B	277	SER	2.3
2	D	406	HIS	2.3
4	F	101	TYR	2.3
3	E	11	LEU	2.3
1	C	282	TYR	2.3
1	A	437	VAL	2.3
2	B	248	LEU	2.3
1	C	341	ILE	2.3
2	D	221	THR	2.3
1	C	250	VAL	2.3
4	F	131	PHE	2.2
4	F	162	ILE	2.2
4	F	239	HIS	2.2
2	D	182	VAL	2.2
4	F	256	TYR	2.2
2	D	42	LEU	2.2
2	D	415	GLU	2.2
2	B	437	ASP	2.2
1	A	331	ALA	2.2
1	A	346	TRP	2.2
4	F	253	TYR	2.2
1	C	284	GLU	2.2
4	F	152	SER	2.2
2	B	66	ILE	2.1
1	C	204	VAL	2.1
1	C	436	GLY	2.1
1	C	253	THR	2.1
2	D	74	THR	2.1
4	F	125	THR	2.1
1	C	12	ALA	2.1
4	F	362	ALA	2.1
1	C	163	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	404	PHE	2.1
2	B	57	THR	2.1
2	D	57	THR	2.1
3	E	15	THR	2.1
2	B	345	GLU	2.1
1	A	316	CYS	2.0
1	A	250	VAL	2.0
4	F	186	LEU	2.0
3	E	24	LEU	2.0
1	A	246	GLY	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 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(Å ²)	Q<0.9
6	MG	B	506	1/1	0.62	0.35	87,87,87,87	0
6	MG	A	506	1/1	0.69	0.35	84,84,84,84	0
6	MG	B	502	1/1	0.70	0.41	88,88,88,88	0
10	71P	B	504	29/29	0.80	0.32	96,97,99,100	29
6	MG	A	502	1/1	0.82	0.35	68,68,68,68	0
11	CA	C	503	1/1	0.82	0.12	123,123,123,123	0
6	MG	C	502	1/1	0.83	0.31	55,55,55,55	0
8	GDP	D	600	28/28	0.84	0.15	101,102,107,109	0
7	CL	A	503	1/1	0.87	0.17	98,98,98,98	0
6	MG	B	505	1/1	0.87	0.17	71,71,71,71	0
9	MES	B	503	12/12	0.92	0.20	94,95,97,99	0
6	MG	A	505	1/1	0.92	0.41	79,79,79,79	0
6	MG	A	504	1/1	0.92	0.13	95,95,95,95	0

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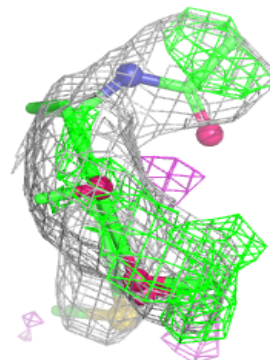
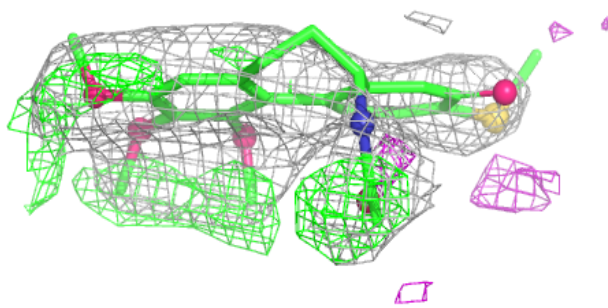
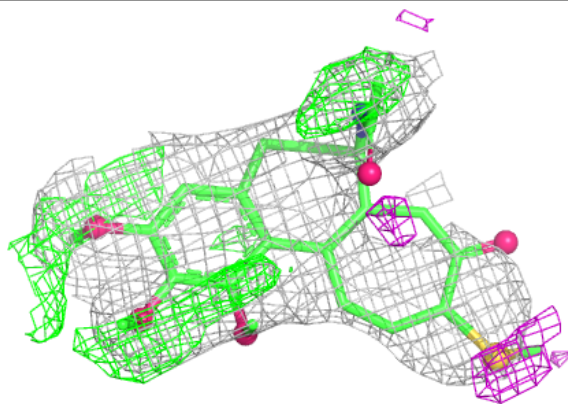
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	0.93	0.12	81,83,84,85	0
8	GDP	B	501	28/28	0.93	0.13	77,77,78,79	0
5	GTP	C	501	32/32	0.93	0.14	77,79,80,81	0

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.

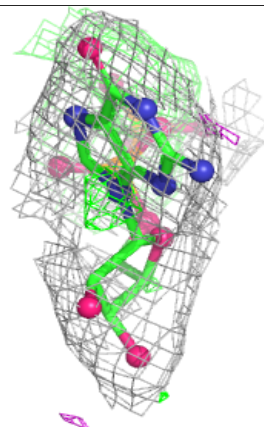
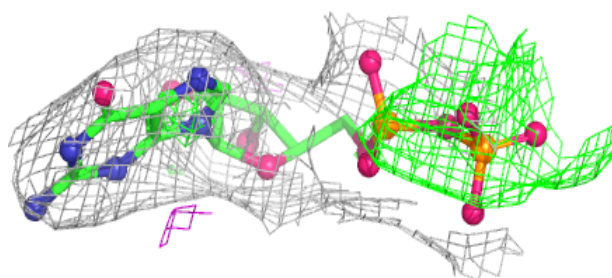
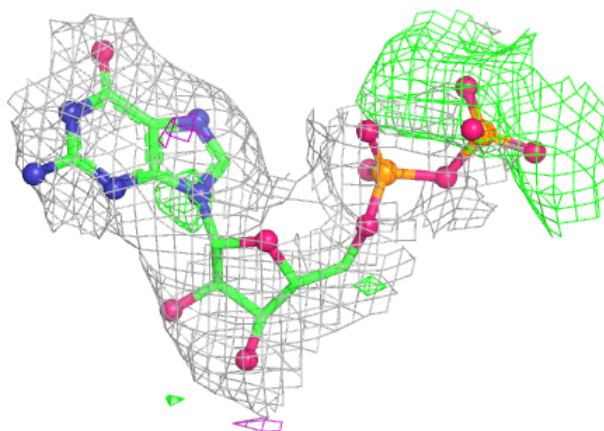
Electron density around 71P B 504:

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



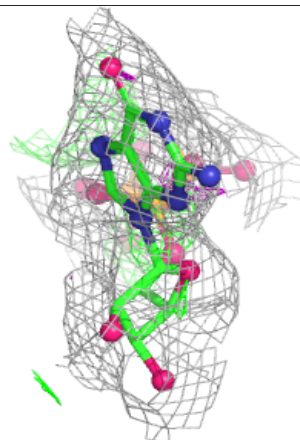
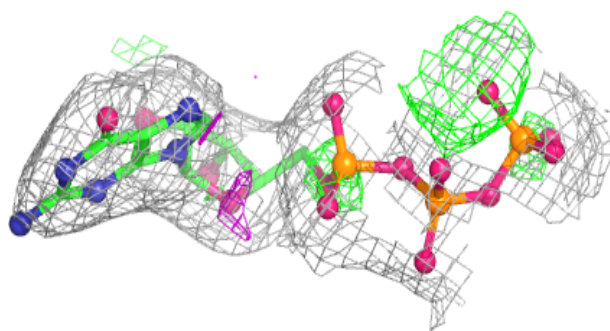
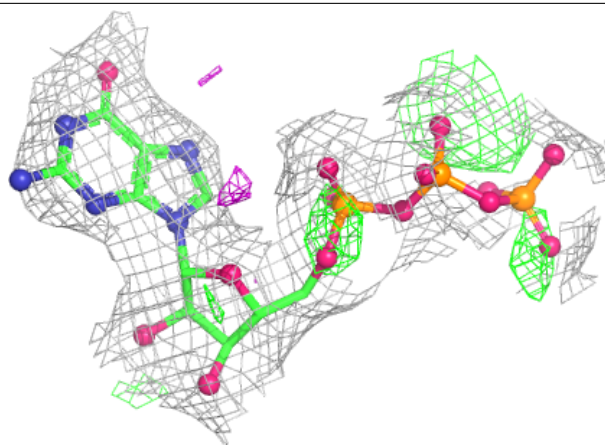
Electron density around GDP D 600:

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



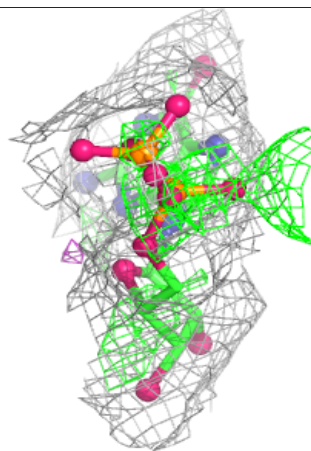
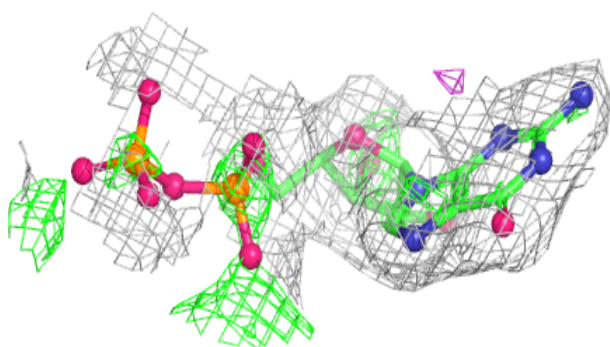
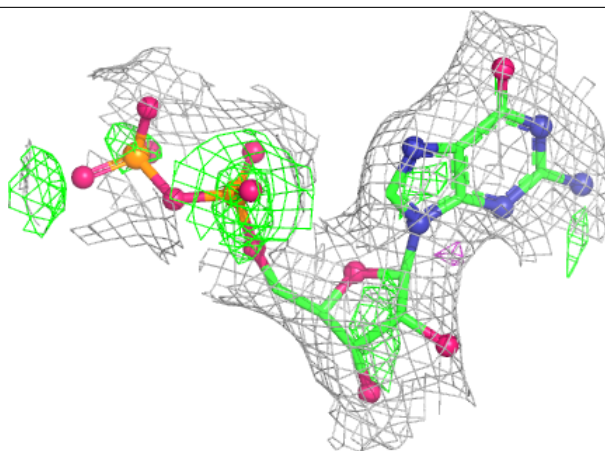
Electron density around GTP A 501:

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

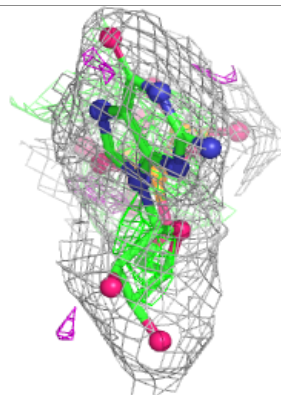
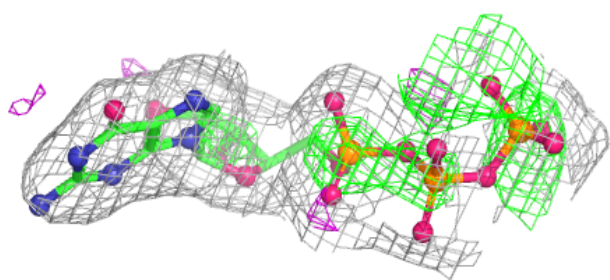
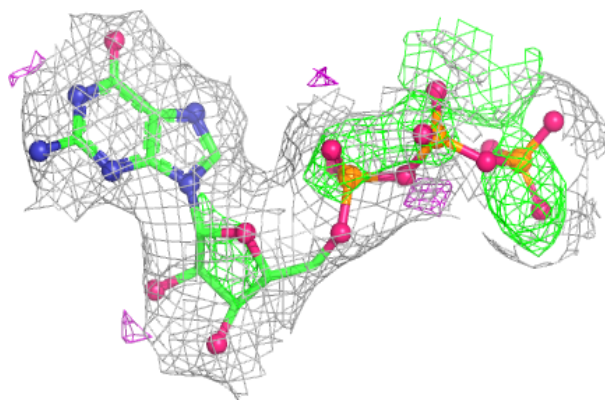


Electron density around GDP B 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.