



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:16 PM UTC

PDB ID : 7TTD / pdb_00007ttd
Title : Tubulin-RB3_SLD in complex with compound 12e
Authors : White, S.W.; Yun, M.
Deposited on : 2022-02-01
Resolution : 2.27 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

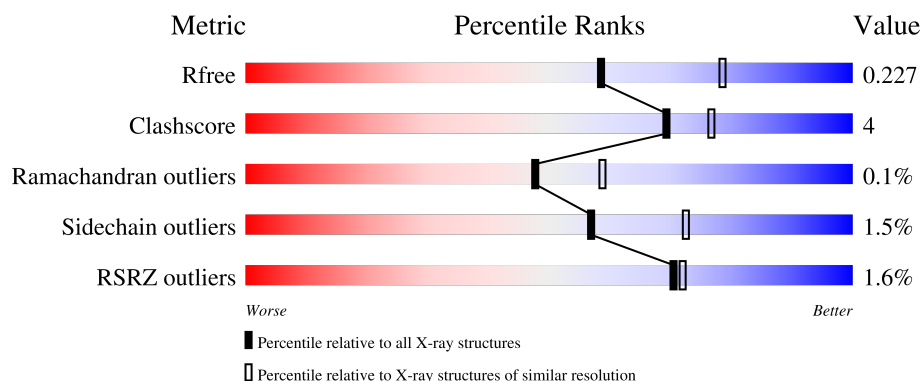
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	438	0% 87% 10% .
1	C	438	0% 87% 10% .
2	B	433	0% 89% 9% .
2	D	433	2% 89% 10%
3	E	143	4% 75% 12% 13%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14686 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	425	Total	C	N	O	S	0	0	0
			3320	2105	562	631	22			
1	C	426	Total	C	N	O	S	0	0	0
			3338	2115	567	634	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
			3312	2081	564	640	27			
2	D	431	Total	C	N	O	S	0	0	0
			3367	2112	576	652	27			

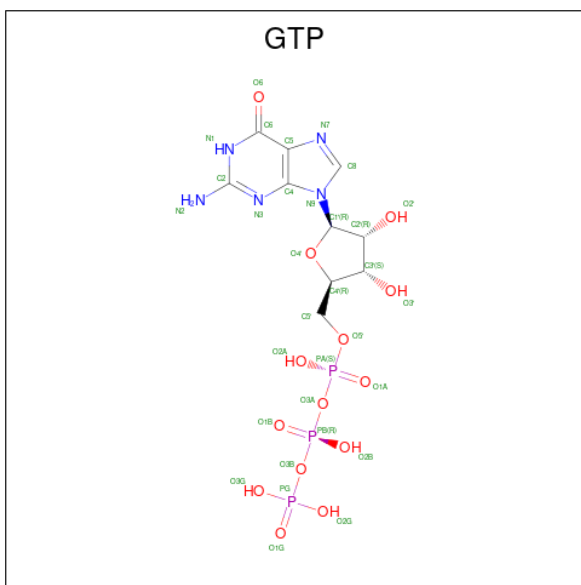
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			1014	628	185	198	3			

There are 4 discrepancies between the modelled and reference sequences:

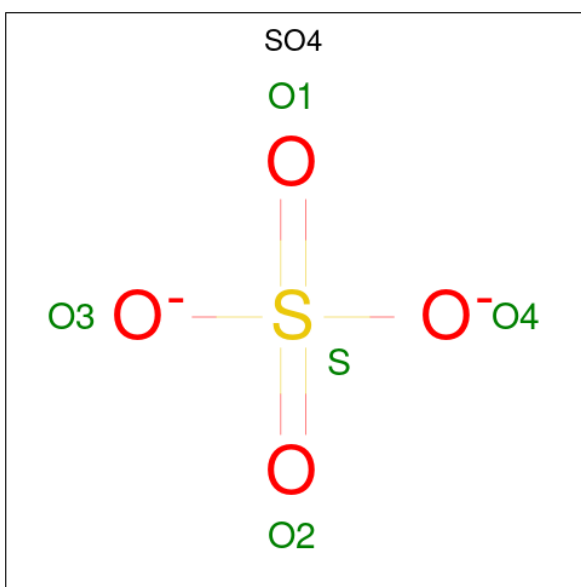
Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



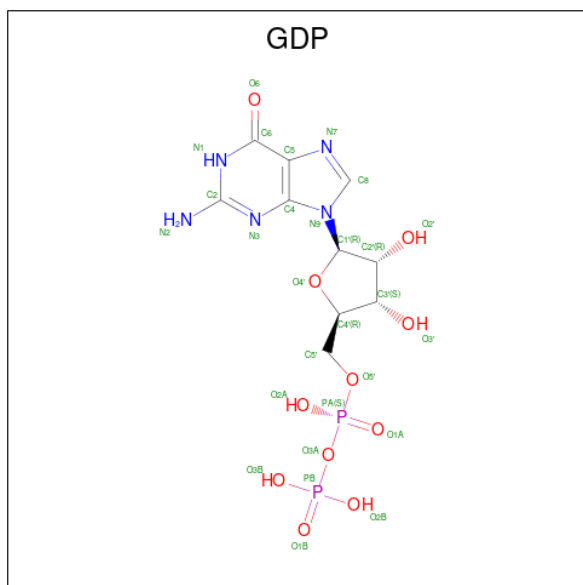
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

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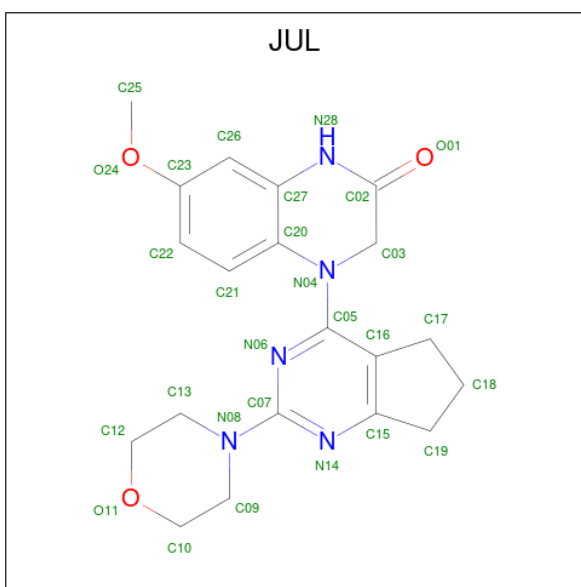
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 7 is 7-methoxy-4-[2-(morpholin-4-yl)-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl]-3,4-dihydroquinoxalin-2(1H)-one (CCD ID: JUL) (formula: $C_{20}H_{23}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			28	20	5	3		
7	D	1	Total	C	N	O	0	0
			28	20	5	3		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg	0	0
			1	1		

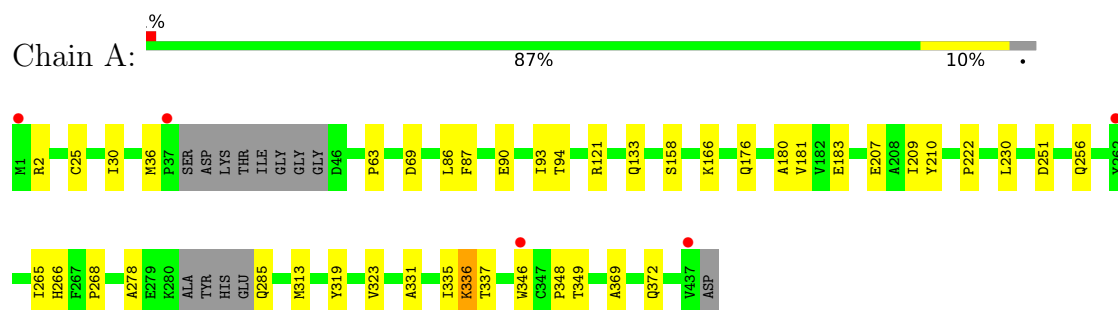
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	40	Total	O	0	0
			40	40		
9	B	26	Total	O	0	0
			26	26		
9	C	28	Total	O	0	0
			28	28		
9	D	36	Total	O	0	0
			36	36		
9	E	4	Total	O	0	0
			4	4		

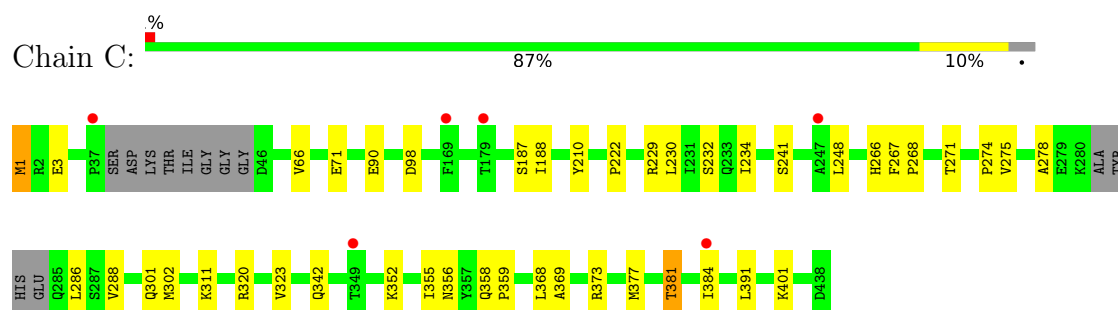
3 Residue-property plots

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.

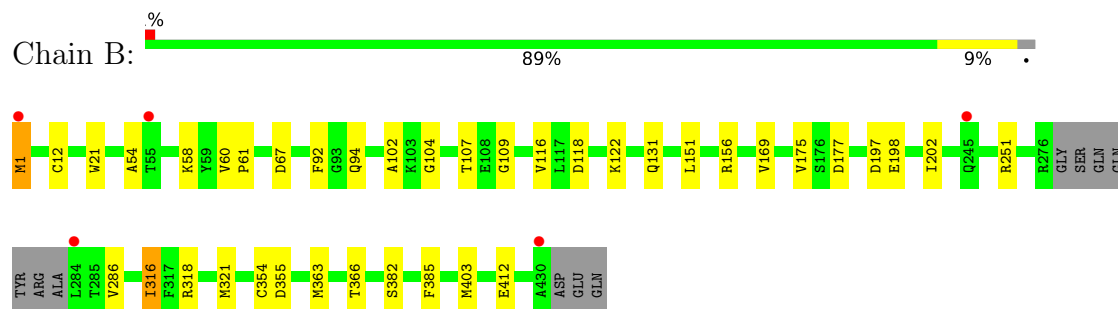
- Molecule 1: Tubulin alpha-1B chain



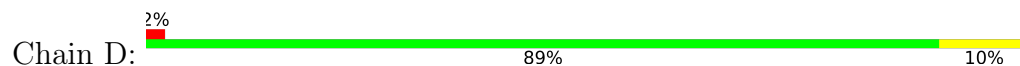
- Molecule 1: Tubulin alpha-1B chain

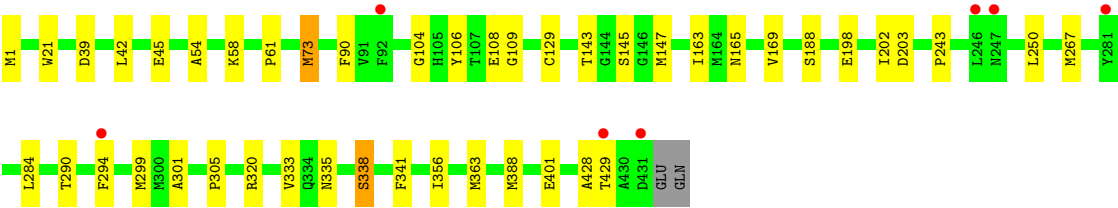


- Molecule 2: Tubulin beta chain

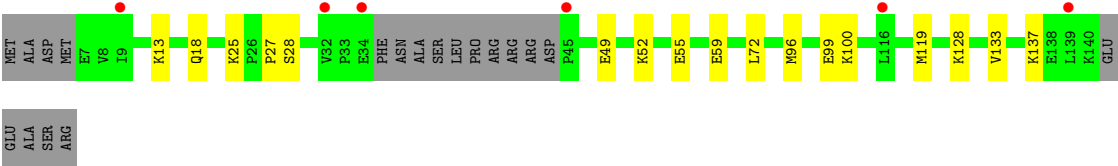


- Molecule 2: Tubulin beta chain





● 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	65.80Å 127.21Å 250.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.96 – 2.27 42.96 – 2.27	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.96-2.27) 92.0 (42.96-2.27)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.173 , 0.224 0.176 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14686	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: JUL, GDP, SO4, GTP, 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	0.33	0/3394	0.50	0/4608
1	C	0.32	0/3412	0.51	0/4630
2	B	0.33	0/3384	0.51	0/4583
2	D	0.35	0/3441	0.55	0/4663
3	E	0.26	0/1025	0.42	0/1363
All	All	0.33	0/14656	0.51	0/19847

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3320	0	3231	26	0
1	C	3338	0	3257	25	0
2	B	3312	0	3187	23	0
2	D	3367	0	3230	24	0
3	E	1014	0	1019	10	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	D	10	0	0	0	0
6	B	28	0	12	1	0
7	B	28	0	0	0	0
7	D	28	0	0	0	0
8	C	1	0	0	0	0
9	A	40	0	0	0	0
9	B	26	0	0	0	0
9	C	28	0	0	0	0
9	D	36	0	0	0	0
9	E	4	0	0	0	0
All	All	14686	0	13972	100	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 4.

All (100) 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:1:MET:N	2:D:129:CYS:SG	2.53	0.81
1:C:271:THR:HG22	1:C:301:GLN:HA	1.63	0.79
2:B:54:ALA:HB3	2:B:58:LYS:HB2	1.70	0.73
1:A:176:GLN:HE22	1:A:207:GLU:HG3	1.55	0.70
1:C:234:ILE:HD11	1:C:302:MET:HE3	1.73	0.70
1:A:349:THR:HB	3:E:25:LYS:HG2	1.74	0.68
1:A:158:SER:OG	1:A:166:LYS:NZ	2.24	0.67
2:B:1:MET:HG2	2:B:131:GLN:HA	1.77	0.67
2:B:316:ILE:HG23	2:B:366:THR:HB	1.80	0.63
1:C:267:PHE:O	1:C:384:ILE:HD13	2.00	0.62
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.82	0.61
1:A:346:TRP:CD1	1:A:346:TRP:H	2.19	0.60
3:E:55:GLU:O	3:E:59:GLU:HG2	2.00	0.60
2:B:385:PHE:CD1	2:B:412:GLU:HG3	2.37	0.60
2:D:73:MET:HE3	2:D:90:PHE:HB3	1.84	0.60
2:B:156:ARG:HG2	3:E:72:LEU:HD11	1.88	0.56
2:D:145:SER:HB2	2:D:188:SER:OG	2.07	0.55
2:B:1:MET:HE1	2:B:251:ARG:HB2	1.89	0.54
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.90	0.53
1:A:30:ILE:HG12	1:A:36:MET:HE2	1.90	0.53
2:D:169:VAL:HA	2:D:202:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HA	1:C:356:ASN:O	2.10	0.52
2:D:42:LEU:HD13	2:D:243:PRO:HG2	1.92	0.52
2:D:143:THR:HG23	2:D:147:MET:HE2	1.92	0.51
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.91	0.51
2:D:290:THR:HG22	2:D:333:VAL:HG11	1.92	0.50
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.52	0.50
2:D:267:MET:HE3	2:D:299:MET:SD	2.51	0.50
1:C:381:THR:O	1:C:384:ILE:HD12	2.11	0.49
1:A:69:ASP:O	1:A:94:THR:HA	2.12	0.49
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.94	0.49
1:A:2:ARG:HB3	1:A:133:GLN:CD	2.38	0.48
1:A:90:GLU:H	1:A:90:GLU:CD	2.21	0.48
1:A:176:GLN:NE2	1:A:207:GLU:HG3	2.27	0.47
1:A:133:GLN:HE22	1:A:251:ASP:HA	1.79	0.47
2:B:94:GLN:CD	1:C:1:MET:HE3	2.39	0.47
2:D:106:TYR:CG	3:E:133:VAL:HG11	2.49	0.47
2:B:286:VAL:HG23	2:B:363:MET:HE1	1.96	0.47
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.95	0.47
1:C:286:LEU:O	1:C:373:ARG:NH1	2.45	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
2:B:169:VAL:HA	2:B:202:ILE:O	2.15	0.47
2:D:401:GLU:OE1	3:E:137:LYS:NZ	2.45	0.46
3:E:96:MET:HA	3:E:99:GLU:HG2	1.98	0.46
2:B:382:SER:OG	2:B:412:GLU:OE2	2.33	0.46
2:D:104:GLY:O	2:D:109:GLY:HA3	2.16	0.46
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.96	0.46
1:C:288:VAL:HG22	1:C:323:VAL:HG22	1.97	0.45
2:B:197:ASP:C	2:B:198:GLU:HG3	2.40	0.45
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.98	0.45
2:B:67:ASP:O	2:B:92:PHE:HA	2.16	0.45
2:D:45:GLU:HB3	2:D:243:PRO:HG3	1.99	0.45
1:C:266:HIS:O	1:C:268:PRO:HD3	2.18	0.44
1:C:358:GLN:HG3	1:C:359:PRO:HD2	1.99	0.44
1:A:336:LYS:HG3	1:A:337:THR:N	2.32	0.44
2:D:388:MET:HB3	2:D:388:MET:HE2	1.64	0.44
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.52	0.44
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.52	0.44
1:A:266:HIS:O	1:A:268:PRO:HD3	2.16	0.44
2:D:294:PHE:HZ	2:D:341:PHE:CE1	2.36	0.44
1:C:248:LEU:HD13	1:C:355:ILE:HD12	2.00	0.44
1:C:274:PRO:HB3	1:C:286:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:100:LYS:HE2	3:E:100:LYS:HB3	1.85	0.44
2:B:321:MET:HE2	2:B:363:MET:HG2	1.99	0.43
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.00	0.43
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.52	0.43
1:C:229:ARG:O	1:C:232:SER:OG	2.29	0.43
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.00	0.43
1:C:401:LYS:HE3	2:D:428:ALA:HB1	2.00	0.43
3:E:13:LYS:HG2	3:E:18:GLN:HB3	1.99	0.43
2:B:318:ARG:HA	2:B:354:CYS:O	2.19	0.43
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.00	0.43
1:A:63:PRO:HG2	1:A:87:PHE:CE1	2.54	0.42
3:E:49:GLU:HA	3:E:52:LYS:HG2	2.01	0.42
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.19	0.42
1:A:285:GLN:OE1	1:A:372:GLN:HG2	2.18	0.42
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.55	0.42
2:D:335:ASN:O	2:D:338:SER:OG	2.37	0.42
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.02	0.42
2:D:54:ALA:HB3	2:D:58:LYS:HB2	2.01	0.42
1:C:271:THR:OG1	1:C:377:MET:HB3	2.20	0.42
2:B:102:ALA:HB2	2:B:403:MET:SD	2.60	0.41
1:A:2:ARG:HB3	1:A:133:GLN:NE2	2.35	0.41
2:D:284:LEU:O	2:D:363:MET:HE2	2.20	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.41
2:B:156:ARG:NH2	2:B:197:ASP:OD2	2.51	0.41
2:B:104:GLY:O	2:B:109:GLY:HA3	2.20	0.41
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.03	0.41
2:B:118:ASP:O	2:B:122:LYS:HE3	2.21	0.41
2:D:267:MET:HE1	2:D:305:PRO:HB3	2.03	0.41
2:B:177:ASP:O	1:C:352:LYS:HD2	2.21	0.41
1:C:90:GLU:H	1:C:90:GLU:CD	2.29	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
1:C:311:LYS:HE2	1:C:342:GLN:OE1	2.21	0.41
2:D:203:ASP:HB3	2:D:301:ALA:HA	2.03	0.41
2:D:108:GLU:H	2:D:108:GLU:HG2	1.75	0.40
2:B:1:MET:HE2	2:B:131:GLN:HG3	2.03	0.40
1:C:3:GLU:OE1	1:C:3:GLU:N	2.41	0.40
2:D:165:ASN:HA	2:D:198:GLU:O	2.21	0.40
1:A:331:ALA:O	1:A:335:ILE:HG13	2.21	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	419/438 (96%)	410 (98%)	9 (2%)	0	100	100
1	C	420/438 (96%)	411 (98%)	9 (2%)	0	100	100
2	B	419/433 (97%)	412 (98%)	6 (1%)	1 (0%)	43	53
2	D	429/433 (99%)	419 (98%)	10 (2%)	0	100	100
3	E	120/143 (84%)	120 (100%)	0	0	100	100
All	All	1807/1885 (96%)	1772 (98%)	34 (2%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	175	VAL

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	358/369 (97%)	355 (99%)	3 (1%)	73	84
1	C	361/369 (98%)	355 (98%)	6 (2%)	53	70
2	B	362/374 (97%)	357 (99%)	5 (1%)	59	74
2	D	367/374 (98%)	361 (98%)	6 (2%)	55	71
3	E	107/126 (85%)	104 (97%)	3 (3%)	38	53
All	All	1555/1612 (96%)	1532 (98%)	23 (2%)	57	72

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	A	256	GLN
1	A	336	LYS
2	B	1	MET
2	B	60	VAL
2	B	107	THR
2	B	316	ILE
2	B	355	ASP
1	C	1	MET
1	C	66	VAL
1	C	188	ILE
1	C	230	LEU
1	C	241	SER
1	C	381	THR
2	D	39	ASP
2	D	73	MET
2	D	320	ARG
2	D	338	SER
2	D	356	ILE
2	D	429	THR
3	E	28	SER
3	E	119	MET
3	E	128	LYS

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	83	GLN
2	B	134	GLN
2	B	335	ASN
1	C	61	HIS
1	C	258	ASN
2	D	11	GLN
2	D	191	GLN
2	D	195	ASN
2	D	280	GLN
2	D	375	GLN

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Mol	Chain	Res	Type
2	D	426	GLN
3	E	18	GLN
3	E	92	ASN
3	E	115	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 11 ligands modelled in this entry, 1 is 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
4	GTP	A	501	-	33,34,34	0.87	0	50,54,54	1.54	8 (16%)
4	GTP	C	501	8	33,34,34	0.86	1 (3%)	50,54,54	1.70	11 (22%)
7	JUL	B	502	-	32,32,32	2.58	11 (34%)	43,46,46	2.21	11 (25%)
5	SO4	D	504	-	4,4,4	0.27	0	6,6,6	0.19	0
4	GTP	D	501	-	33,34,34	0.88	1 (3%)	50,54,54	1.73	11 (22%)
5	SO4	A	502	-	4,4,4	0.25	0	6,6,6	0.14	0
7	JUL	D	502	-	32,32,32	2.66	11 (34%)	43,46,46	2.09	9 (20%)
6	GDP	B	501	-	29,30,30	1.12	2 (6%)	45,47,47	1.66	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	503	-	4,4,4	0.28	0	6,6,6	0.14	0
5	SO4	D	503	-	4,4,4	0.26	0	6,6,6	0.24	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	A	501	-	-	1/22/38/38	0/3/3/3
4	GTP	C	501	8	-	5/22/38/38	0/3/3/3
4	GTP	D	501	-	-	5/22/38/38	0/3/3/3
7	JUL	D	502	-	-	3/9/36/36	0/5/5/5
6	GDP	B	501	-	-	5/16/32/32	0/3/3/3
7	JUL	B	502	-	-	2/9/36/36	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	502	JUL	C02-N28	9.12	1.45	1.35
7	B	502	JUL	C02-N28	8.76	1.45	1.35
7	D	502	JUL	C05-N04	5.66	1.45	1.37
7	B	502	JUL	C27-N28	4.98	1.48	1.39
7	D	502	JUL	C27-N28	4.81	1.48	1.39
7	B	502	JUL	C05-N04	4.39	1.43	1.37
7	D	502	JUL	C19-C15	4.28	1.54	1.50
7	B	502	JUL	C03-C02	3.77	1.56	1.51
7	D	502	JUL	C03-C02	3.65	1.56	1.51
7	B	502	JUL	C20-N04	3.61	1.46	1.40
7	B	502	JUL	C19-C15	3.60	1.53	1.50
7	B	502	JUL	C17-C16	3.09	1.56	1.51
6	B	501	GDP	PB-O1B	3.05	1.60	1.50
6	B	501	GDP	PA-O1A	3.03	1.61	1.50
7	D	502	JUL	C17-C16	2.89	1.56	1.51
7	D	502	JUL	O01-C02	-2.74	1.17	1.23
7	D	502	JUL	C20-N04	2.70	1.45	1.40
7	B	502	JUL	C05-N06	-2.48	1.31	1.34
7	B	502	JUL	O01-C02	-2.34	1.18	1.23
7	D	502	JUL	O24-C23	2.22	1.41	1.37
7	D	502	JUL	C26-C27	2.20	1.43	1.39
7	B	502	JUL	O24-C23	2.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	GTP	C6-N1	-2.09	1.34	1.38
7	D	502	JUL	C03-N04	-2.08	1.42	1.46
4	D	501	GTP	PG-O2G	2.06	1.62	1.54
7	B	502	JUL	C21-C20	2.04	1.42	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	502	JUL	C19-C15-N14	7.08	132.37	123.41
7	D	502	JUL	C19-C15-N14	6.70	131.90	123.41
7	D	502	JUL	C16-C15-N14	-6.53	118.09	125.50
7	B	502	JUL	C16-C15-N14	-5.62	119.13	125.50
4	C	501	GTP	C5-C4-N3	-5.44	119.73	128.39
4	C	501	GTP	C2-N3-C4	5.34	121.50	112.30
4	D	501	GTP	C2-N3-C4	5.32	121.46	112.30
4	A	501	GTP	C5-C4-N3	-5.30	119.95	128.39
4	D	501	GTP	C5-C4-N3	-5.15	120.20	128.39
7	B	502	JUL	C03-N04-C20	4.64	119.71	114.97
4	A	501	GTP	C2-N3-C4	4.57	120.17	112.30
7	B	502	JUL	C18-C19-C15	4.57	107.09	103.84
6	B	501	GDP	C5-C4-N3	-4.57	121.12	128.39
6	B	501	GDP	C2-N3-C4	4.46	119.98	112.30
7	D	502	JUL	C07-N14-C15	4.18	120.78	116.19
7	D	502	JUL	C27-N28-C02	-4.06	119.59	124.45
4	C	501	GTP	N9-C4-N3	4.00	133.94	125.95
4	D	501	GTP	N9-C4-N3	3.96	133.88	125.95
4	A	501	GTP	N9-C4-N3	3.79	133.54	125.95
7	B	502	JUL	N14-C07-N08	3.64	122.30	117.12
6	B	501	GDP	N9-C4-N3	3.64	133.23	125.95
7	B	502	JUL	C19-C15-C16	-3.40	108.50	111.25
4	A	501	GTP	C8-N7-C5	3.37	110.26	104.26
7	B	502	JUL	C07-N06-C05	3.18	121.32	114.97
4	D	501	GTP	C8-N7-C5	3.16	109.89	104.26
6	B	501	GDP	C8-N7-C5	2.95	109.52	104.26
7	D	502	JUL	C16-C05-N06	-2.95	118.11	122.60
7	D	502	JUL	C20-N04-C05	2.82	124.41	119.21
4	D	501	GTP	C6-C5-N7	2.74	135.28	130.29
7	B	502	JUL	C07-N14-C15	2.74	119.20	116.19
4	A	501	GTP	C4-C5-N7	-2.73	106.34	110.67
4	C	501	GTP	C5'-C4'-C3'	-2.67	105.59	115.21
7	D	502	JUL	C07-N06-C05	2.67	120.31	114.97
4	C	501	GTP	C2-N1-C6	-2.66	120.28	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	GTP	N9-C8-N7	-2.64	108.50	113.40
4	C	501	GTP	C8-N7-C5	2.64	108.95	104.26
6	B	501	GDP	C2-N1-C6	-2.58	120.43	125.11
6	B	501	GDP	N9-C8-N7	-2.55	108.67	113.40
7	B	502	JUL	C16-C05-N06	-2.51	118.78	122.60
4	D	501	GTP	C2-N1-C6	-2.49	120.60	125.11
7	D	502	JUL	C17-C16-C15	-2.40	107.80	110.67
7	D	502	JUL	C03-N04-C20	2.40	117.42	114.97
6	B	501	GDP	C6-C5-N7	2.33	134.52	130.29
4	A	501	GTP	C2-N1-C6	-2.32	120.90	125.11
4	D	501	GTP	C5-C6-N1	2.31	119.14	113.25
7	B	502	JUL	C20-N04-C05	2.30	123.45	119.21
7	B	502	JUL	C27-N28-C02	-2.29	121.71	124.45
6	B	501	GDP	O6-C6-C5	-2.28	120.52	126.53
4	A	501	GTP	C6-C5-N7	2.25	134.38	130.29
4	A	501	GTP	N9-C8-N7	-2.24	109.25	113.40
4	C	501	GTP	C6-C5-N7	2.21	134.31	130.29
4	C	501	GTP	C5-C6-N1	2.17	118.79	113.25
4	D	501	GTP	C4-C5-N7	-2.17	107.23	110.67
4	D	501	GTP	O3'-C3'-C4'	-2.14	104.94	111.08
4	C	501	GTP	O2B-PB-O3B	2.11	112.99	107.27
4	C	501	GTP	C4-C5-N7	-2.09	107.35	110.67
4	C	501	GTP	N9-C8-N7	-2.05	109.60	113.40
4	D	501	GTP	O5'-C5'-C4'	-2.04	102.06	108.99

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
7	B	502	JUL	C16-C05-N04-C03
7	B	502	JUL	N06-C05-N04-C03
7	D	502	JUL	C16-C05-N04-C03

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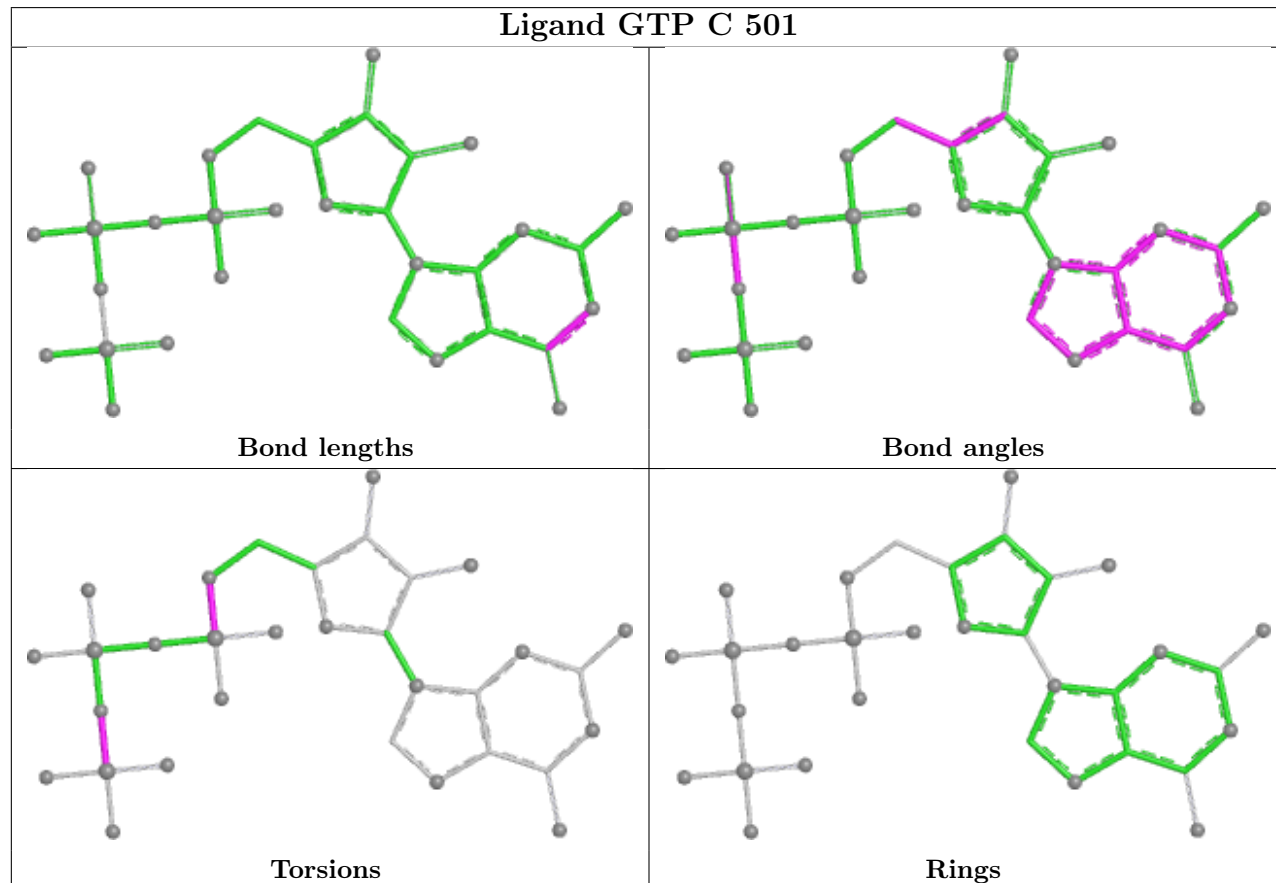
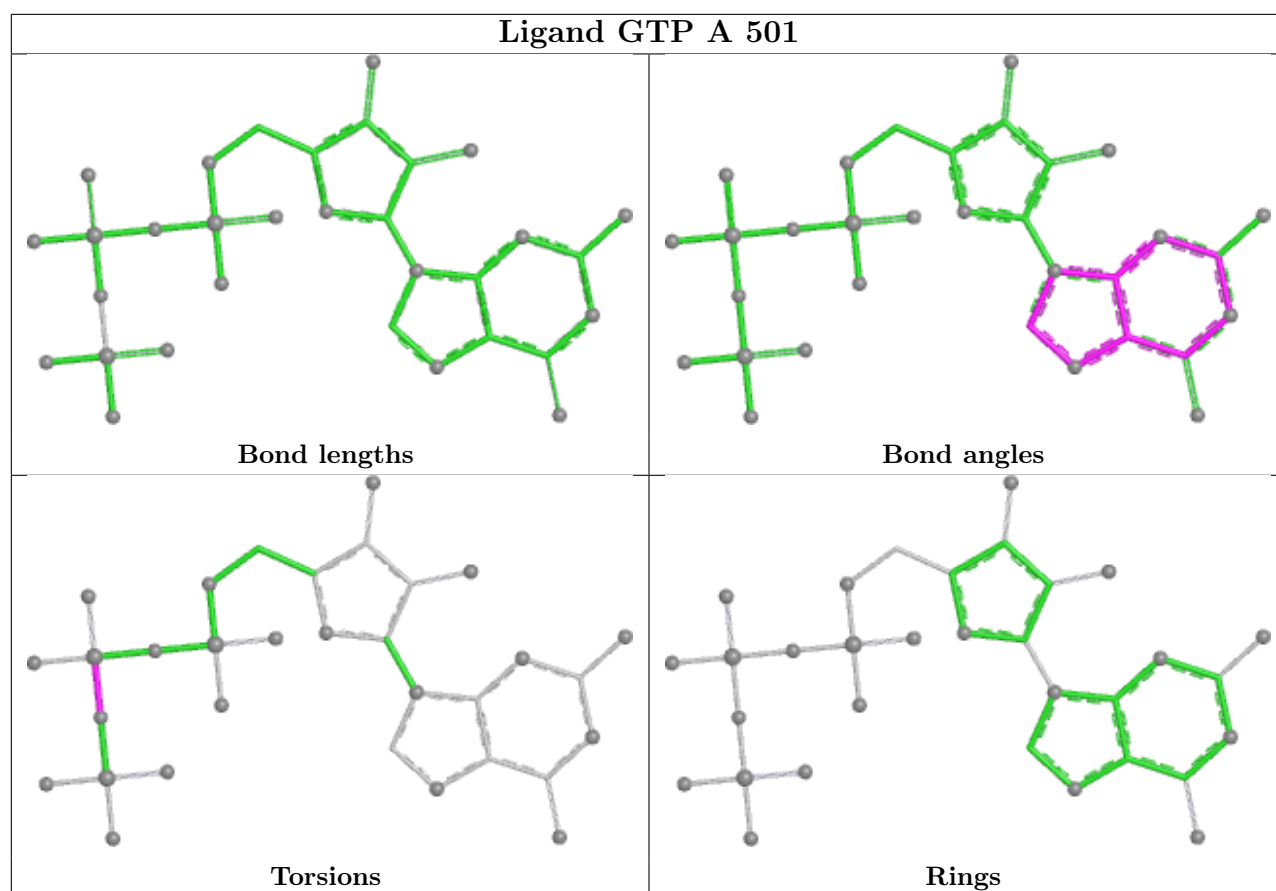
Mol	Chain	Res	Type	Atoms
7	D	502	JUL	N06-C05-N04-C03
4	A	501	GTP	PG-O3B-PB-O1B
6	B	501	GDP	C5'-O5'-PA-O2A
7	D	502	JUL	N06-C05-N04-C20
6	B	501	GDP	PB-O3A-PA-O2A
4	C	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O3G
6	B	501	GDP	PB-O3A-PA-O1A

There are no ring outliers.

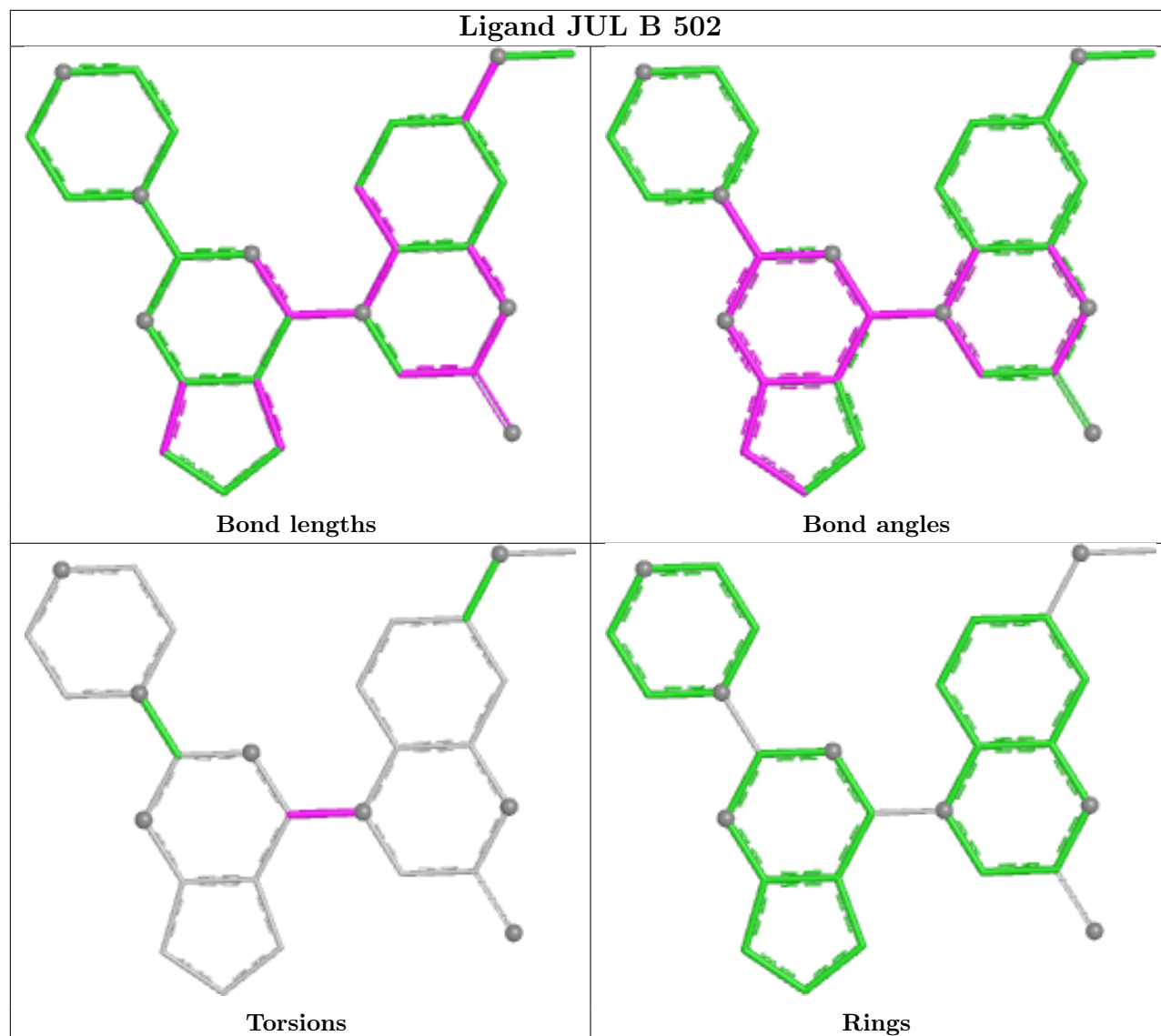
1 monomer is involved in 1 short contact:

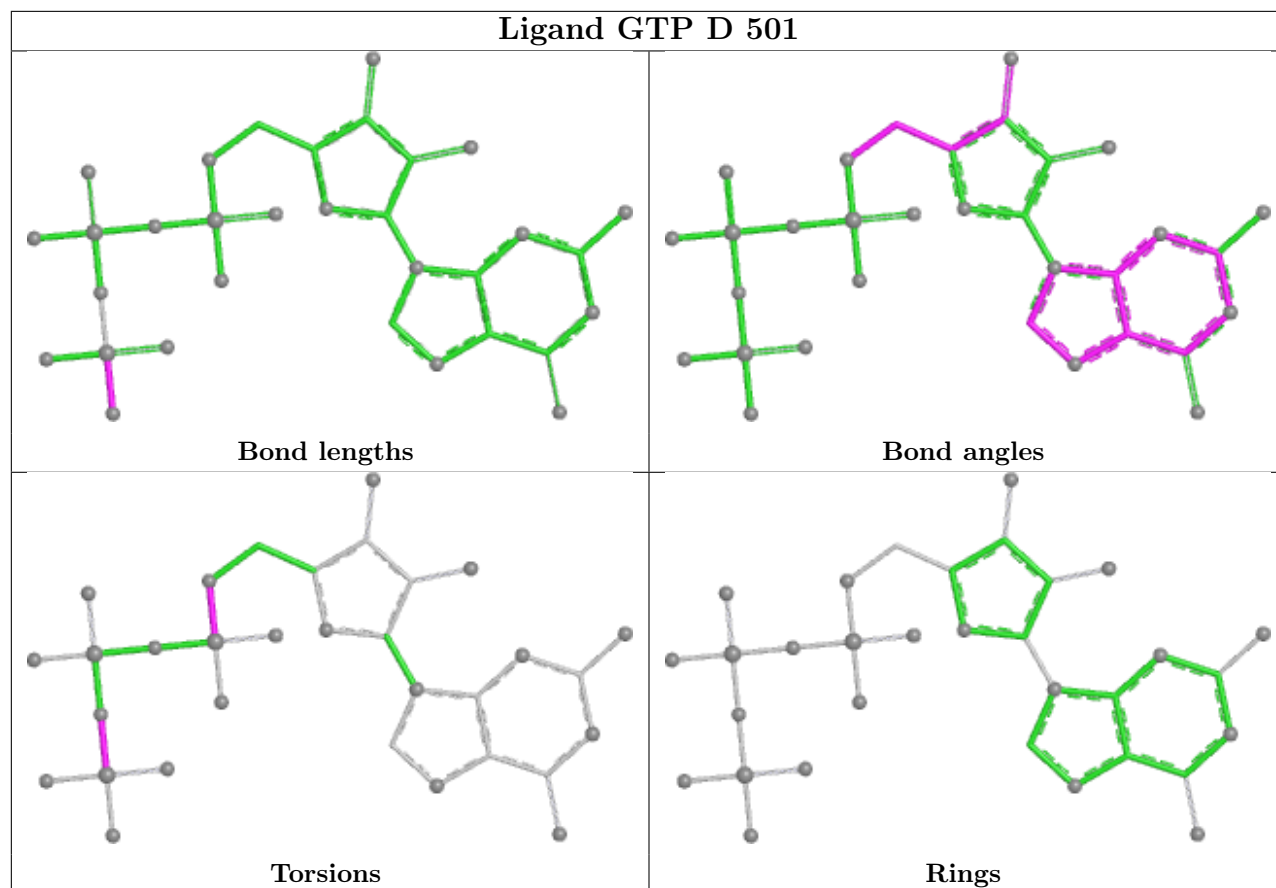
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GDP	1	0

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.

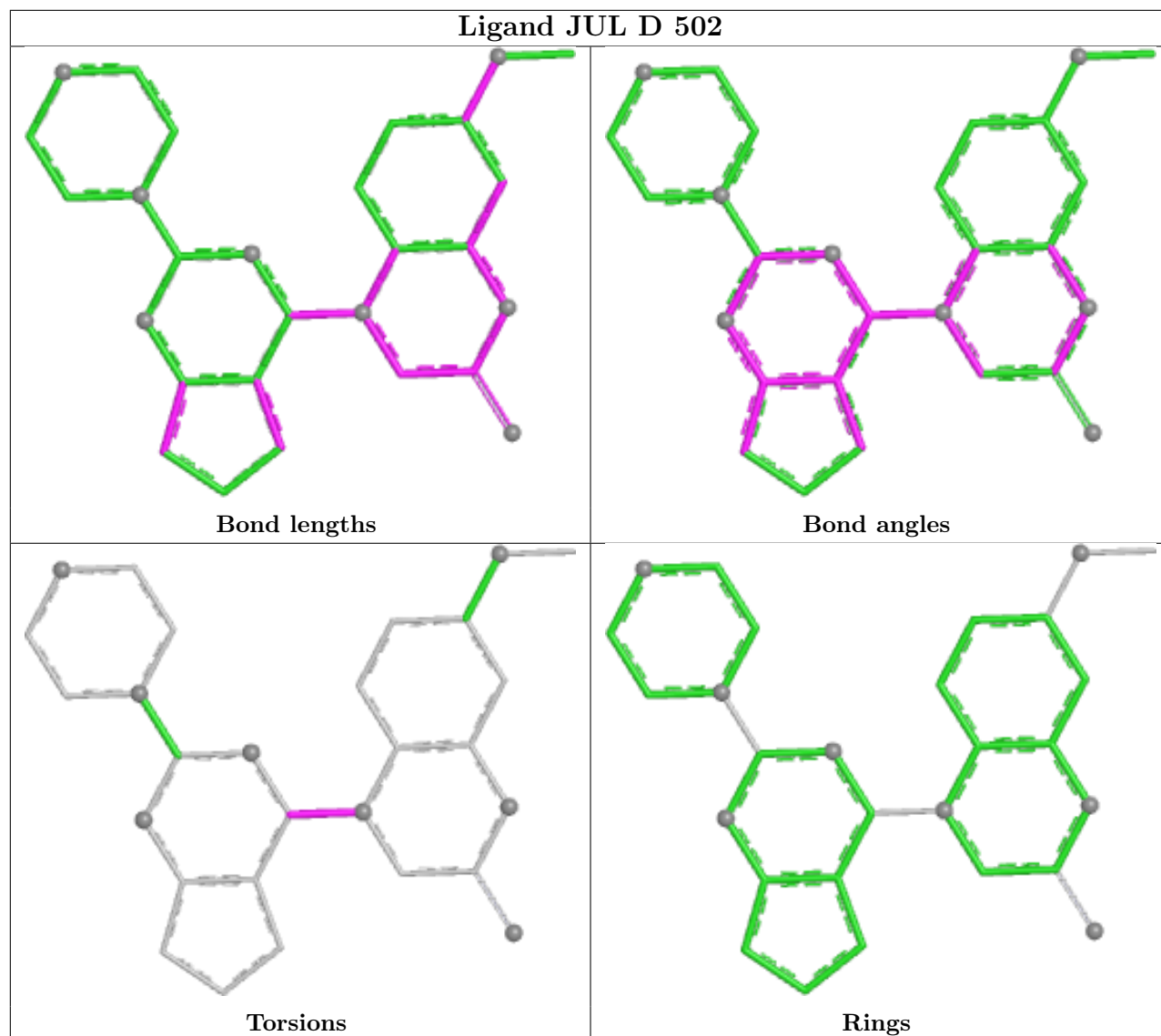


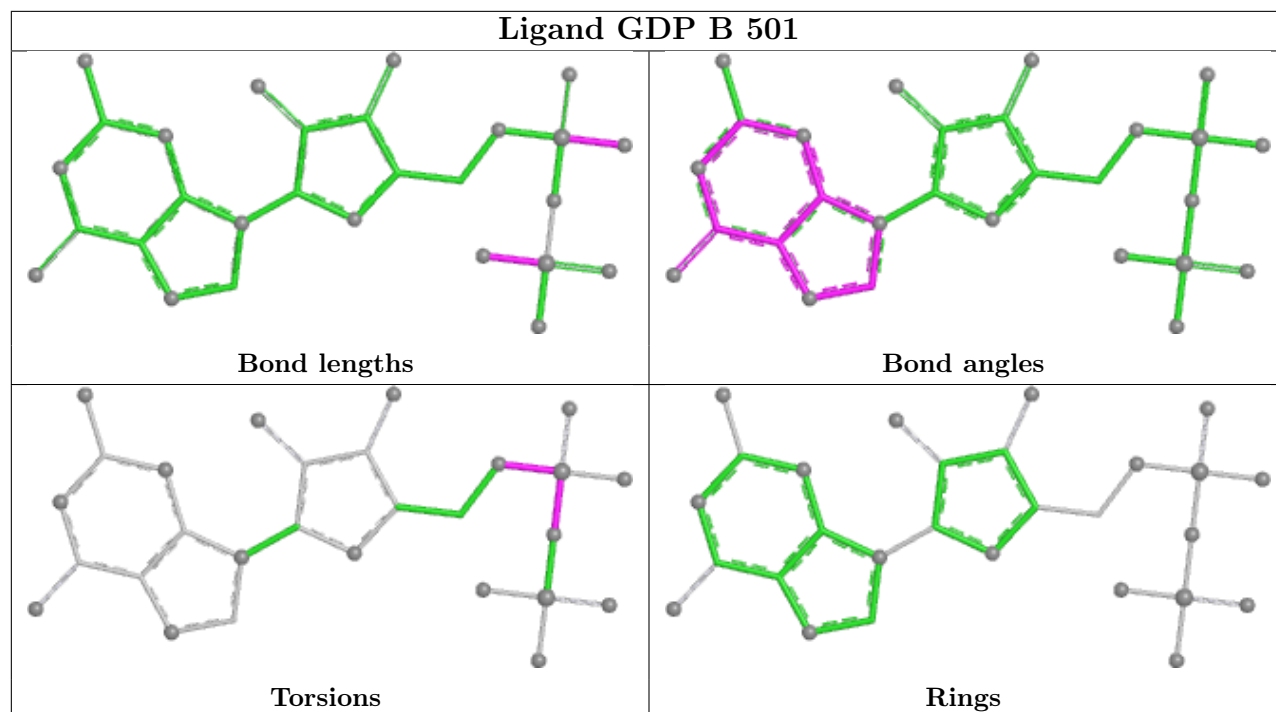
Ligand JUL B 502





Ligand JUL D 502





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

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	425/438 (97%)	-0.10	5 (1%) 76 78	34, 52, 82, 105	0
1	C	426/438 (97%)	-0.00	6 (1%) 73 75	33, 54, 88, 111	0
2	B	423/433 (97%)	-0.03	5 (1%) 76 78	34, 50, 85, 115	0
2	D	431/433 (99%)	-0.07	7 (1%) 70 72	28, 48, 87, 111	0
3	E	124/143 (86%)	0.23	6 (4%) 35 36	49, 67, 97, 103	0
All	All	1829/1885 (97%)	-0.03	29 (1%) 70 72	28, 52, 87, 115	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	PRO	5.3
2	D	92	PHE	5.0
2	B	284	LEU	4.7
3	E	45	PRO	4.1
3	E	9	ILE	4.1
1	C	384	ILE	3.5
2	D	431	ASP	3.4
2	D	294	PHE	3.3
1	A	1	MET	3.2
2	D	246	LEU	2.9
1	A	437	VAL	2.9
2	B	55	THR	2.9
2	D	281	TYR	2.7
1	C	349	THR	2.7
2	B	430	ALA	2.6
1	C	247	ALA	2.5
1	C	169	PHE	2.5
2	D	429	THR	2.5
3	E	34	GLU	2.5
1	A	37	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	245	GLN	2.4
3	E	32	VAL	2.3
3	E	116	LEU	2.2
1	A	346	TRP	2.2
3	E	139	LEU	2.2
1	C	179	THR	2.2
2	B	1	MET	2.1
1	A	262	TYR	2.0
2	D	247	ASN	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.

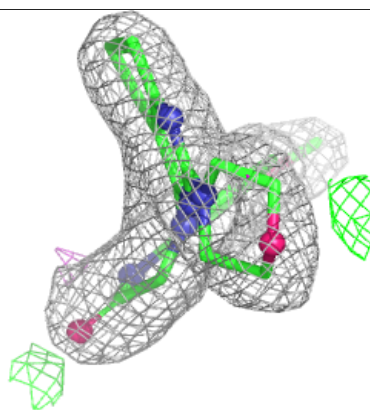
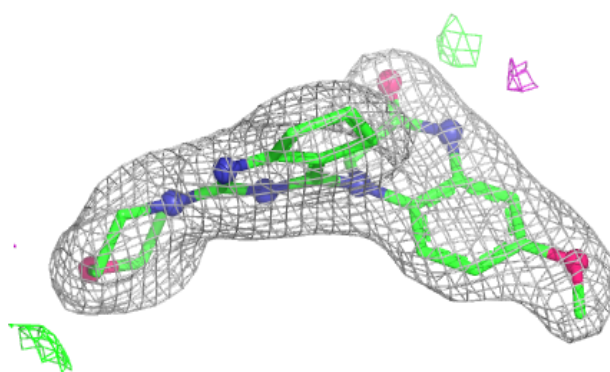
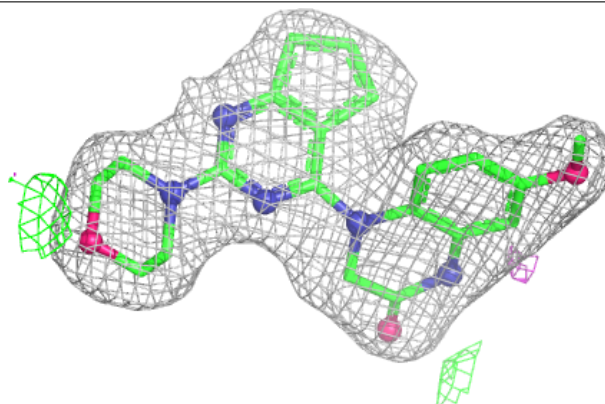
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	D	504	5/5	0.59	0.14	105,110,115,122	0
5	SO4	B	503	5/5	0.79	0.09	97,108,112,114	0
5	SO4	D	503	5/5	0.88	0.11	75,83,90,92	0
5	SO4	A	502	5/5	0.89	0.10	107,112,113,119	0
7	JUL	B	502	28/28	0.95	0.07	37,45,52,53	0
7	JUL	D	502	28/28	0.96	0.06	35,43,52,54	0
4	GTP	D	501	32/32	0.97	0.06	28,38,58,63	0
6	GDP	B	501	28/28	0.97	0.06	33,42,48,66	0
4	GTP	A	501	32/32	0.98	0.05	30,39,47,61	0
4	GTP	C	501	32/32	0.98	0.06	28,45,53,59	0
8	MG	C	502	1/1	0.98	0.04	44,44,44,44	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.

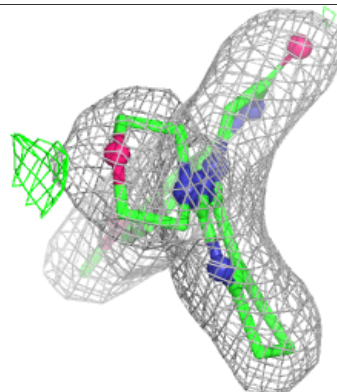
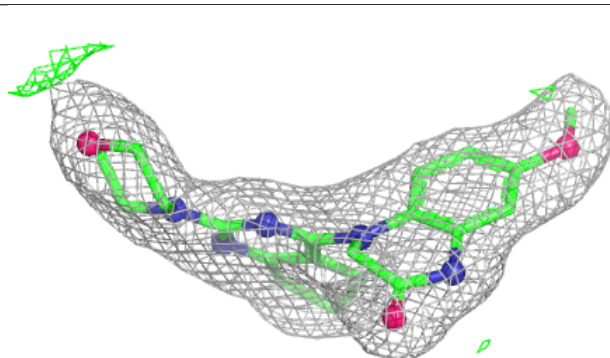
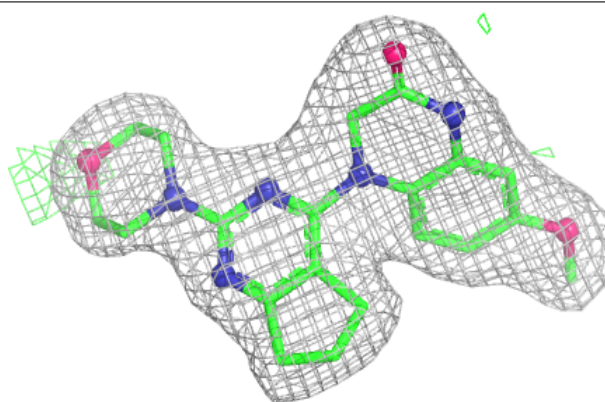
Electron density around JUL B 502:

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



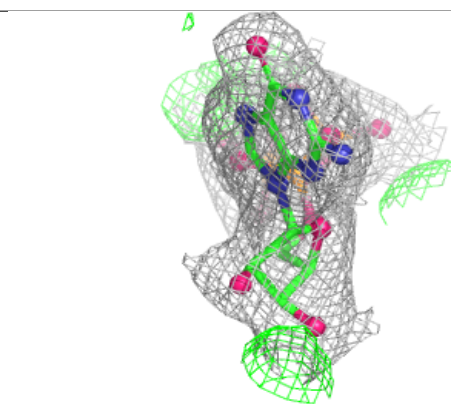
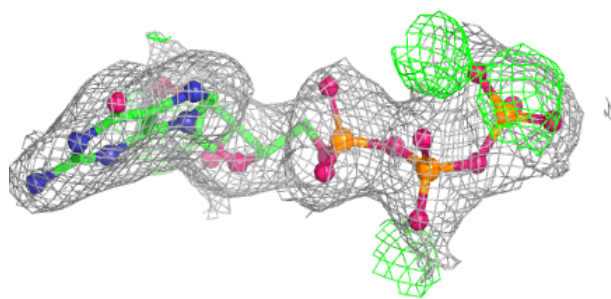
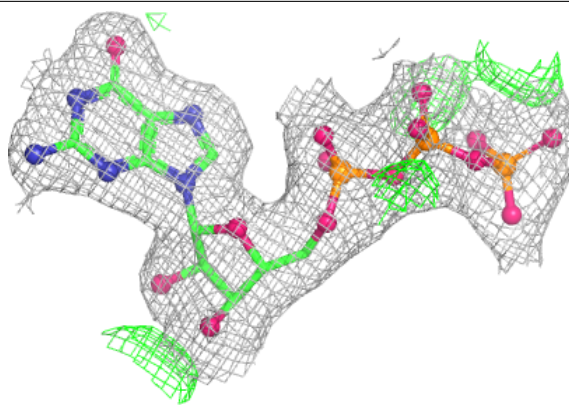
Electron density around JUL D 502:

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

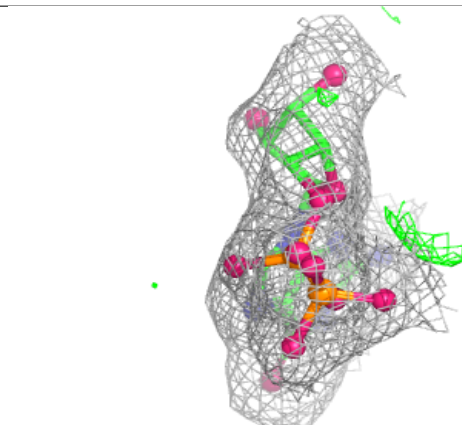
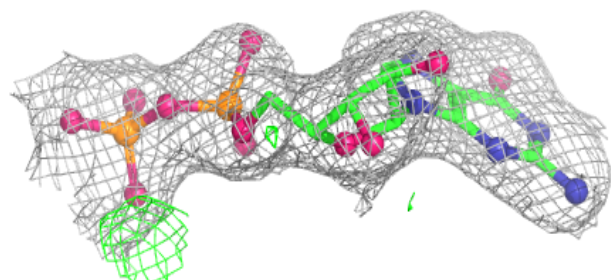
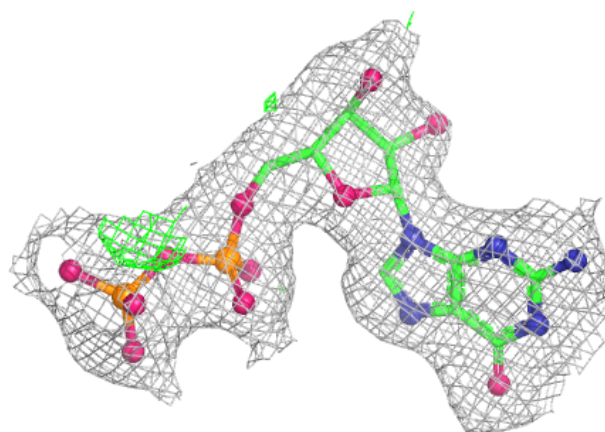


Electron density around GTP D 501:

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

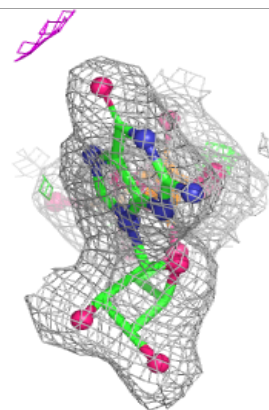
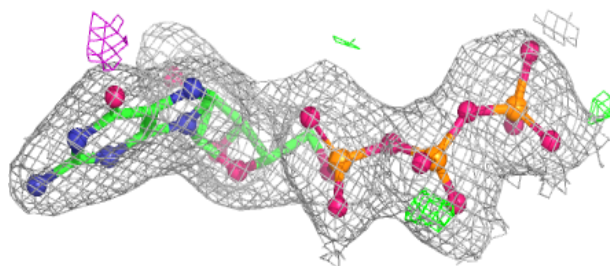
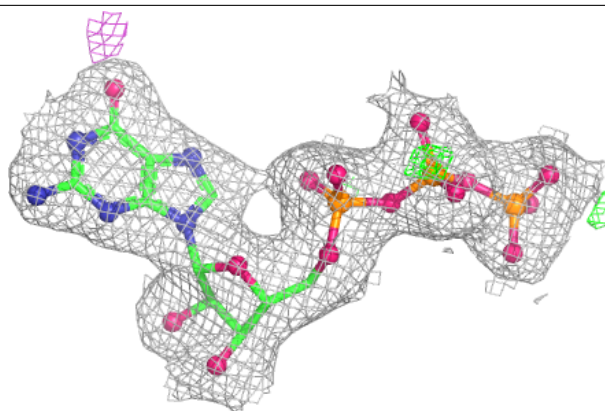
**Electron density around GDP B 501:**

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

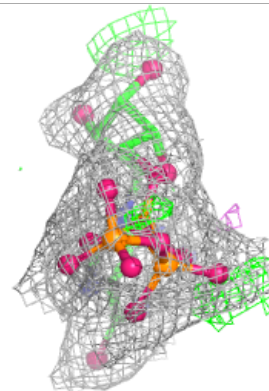
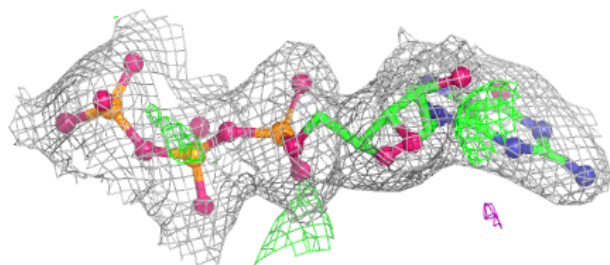
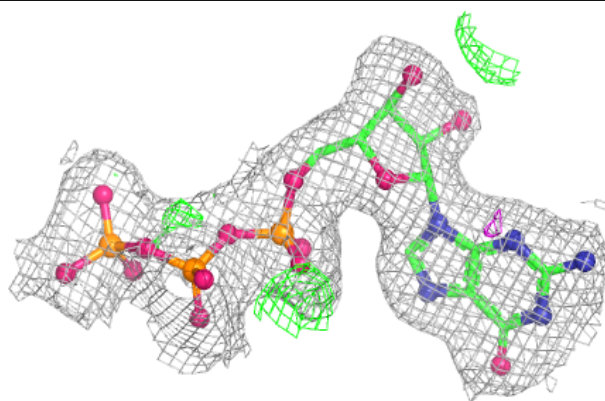


Electron density around GTP A 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.