



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2022 – 06:18 PM JST

PDB ID : 7EN3
Title : Crystal structure of tubulin in complex with Tubulysin analogue TGL
Authors : Wang, Y.; Li, W.
Deposited on : 2021-04-15
Resolution : 2.64 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

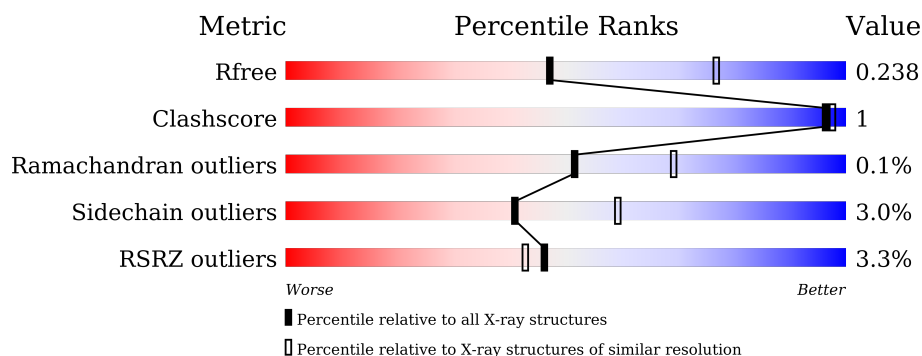
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>%</div> <div>93%</div> <div>• •</div> </div>
1	C	451	<div> <div>93%</div> <div>• •</div> </div>
2	B	445	<div> <div>%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
2	D	445	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
3	E	136	<div> <div>5%</div> <div>85%</div> <div>•</div> <div>11%</div> </div>
4	F	384	<div> <div>9%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17798 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	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	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	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	424	Total	C	N	O	S	0	0	0
			3333	2093	568	645	27			

- 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			

- Molecule 4 is a protein called tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	338	Total	C	N	O	S	0	0	0
			2784	1785	482	503	14			

There are 6 discrepancies between the modelled and reference sequences:

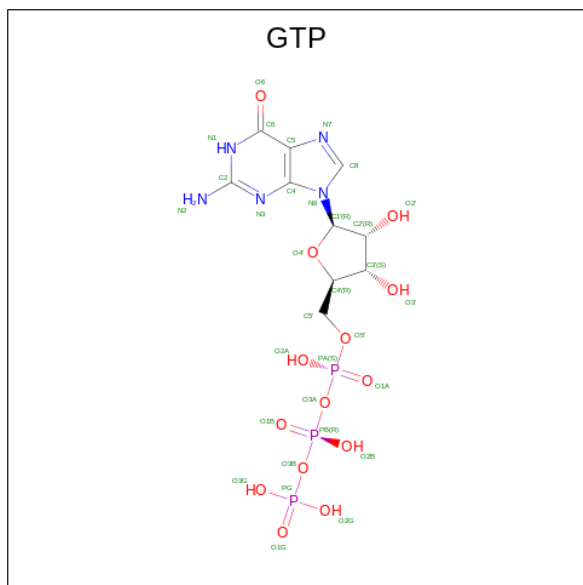
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

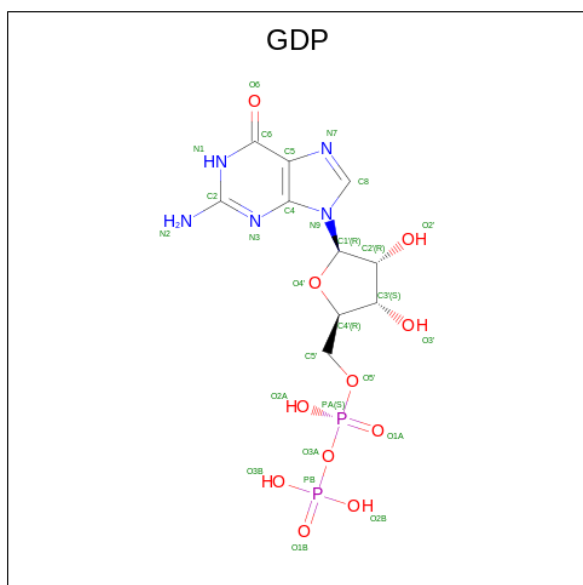
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

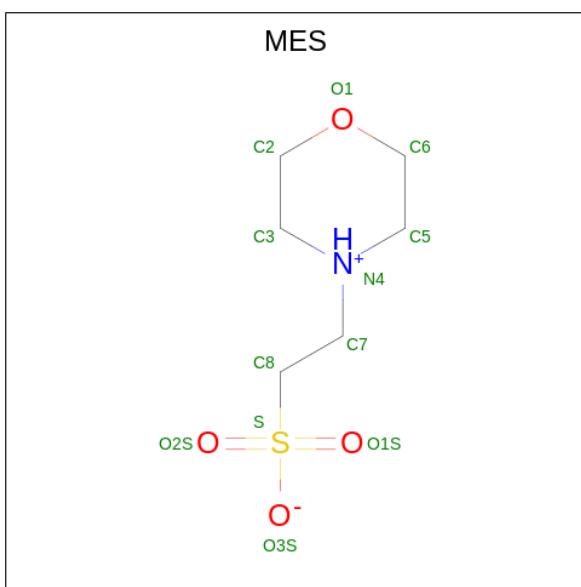
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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

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

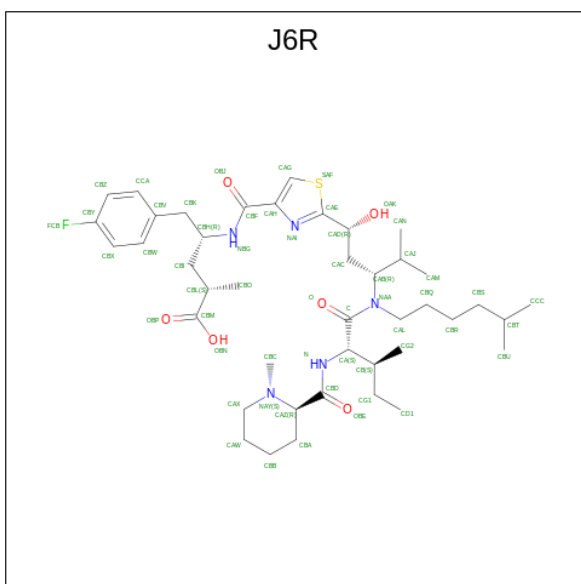
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





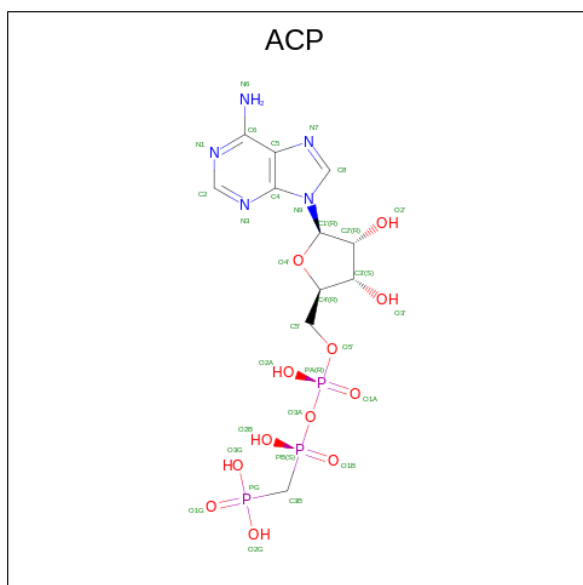
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (2S,4R)-5-(4-fluorophenyl)-2-methyl-4-[[2-[(1R,3R)-4-methyl-3-[5-methylhexyl-[(2S,3S)-3-methyl-2-[[[(2R)-1-methylpiperidin-2-yl]carbonylamino]pentanoyl]amino]-1-oxidanyl-pentyl]-1,3-thiazol-4-yl]carbonylamino]pentanoic acid (three-letter code: J6R) (formula: C₄₂H₆₆FN₅O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	F	N	O	S	
			55	42	1	5	6	1	0
10	D	1	Total	C	F	N	O	S	
			55	42	1	5	6	1	0

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



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

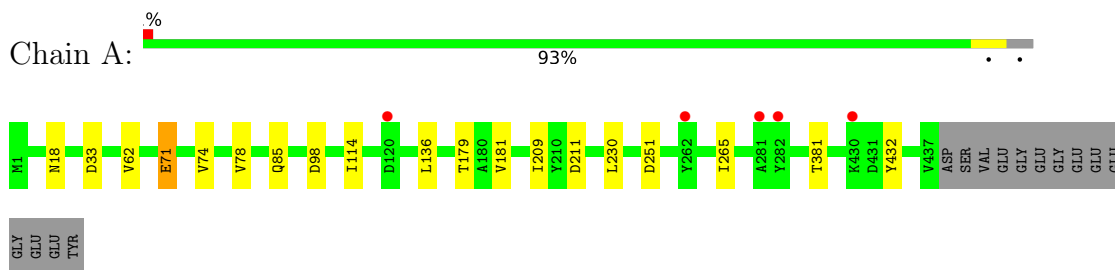
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	39	Total	O		
			39	39	0	0
12	B	45	Total	O		
			45	45	0	0
12	C	50	Total	O		
			50	50	0	0
12	D	15	Total	O		
			15	15	0	0
12	E	2	Total	O		
			2	2	0	0
12	F	6	Total	O		
			6	6	0	0

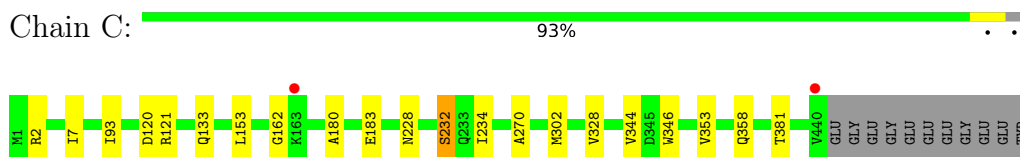
3 Residue-property plots

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.

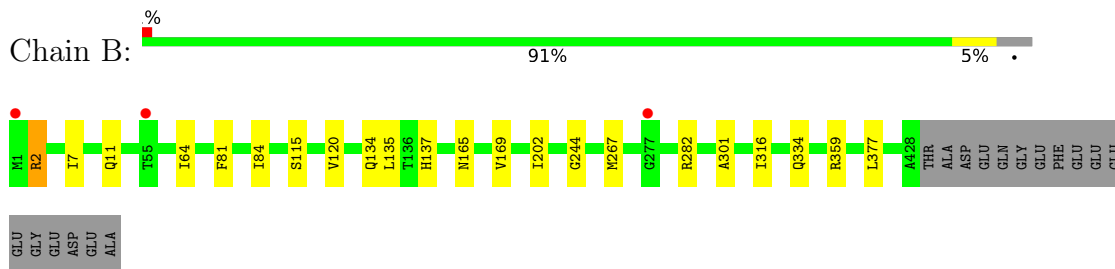
- Molecule 1: Tubulin alpha-1B chain



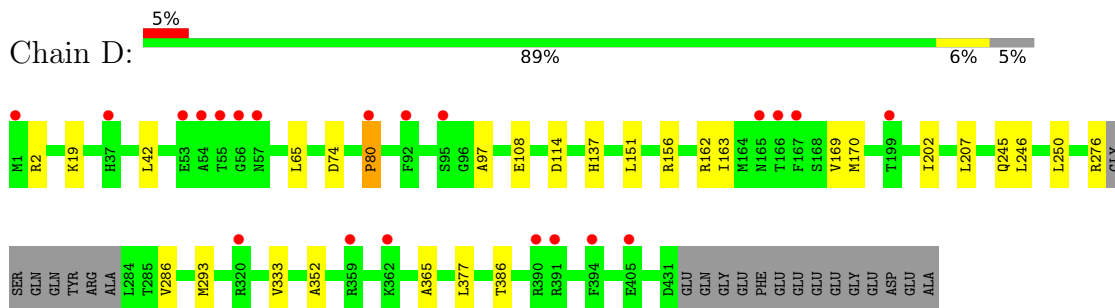
- Molecule 1: Tubulin alpha-1B chain



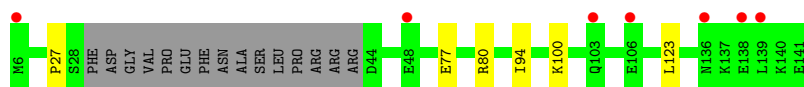
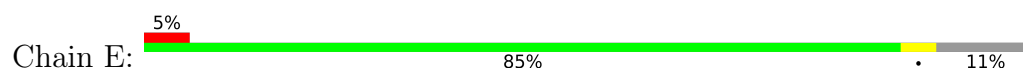
- Molecule 2: Tubulin beta-2B chain



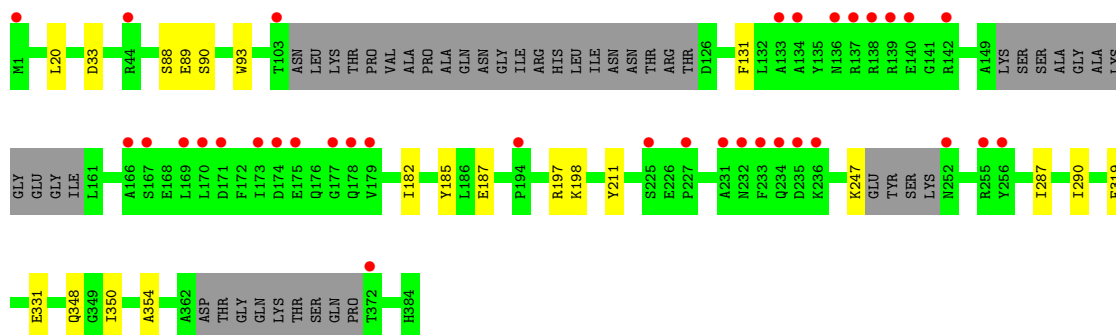
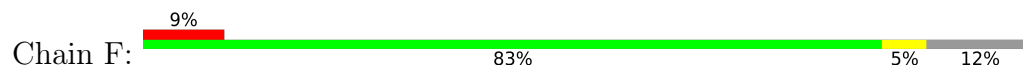
- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Stathmin-4



• Molecule 4: tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.61Å 154.22Å 186.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.05 – 2.64 41.11 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.05-2.64) 98.5 (41.11-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.199 , 0.239 0.201 , 0.238	Depositor DCC
R_{free} test set	4326 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17798	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: GTP, J6R, ACP, CA, MG, MES, GDP

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	0.41	0/3494	0.63	0/4743
1	C	0.41	0/3515	0.64	0/4772
2	B	0.41	0/3444	0.63	1/4664 (0.0%)
2	D	0.40	0/3406	0.61	0/4613
3	E	0.43	0/1008	0.61	0/1337
4	F	0.41	0/2850	0.62	0/3851
All	All	0.41	0/17717	0.63	1/23980 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	ARG	NE-CZ-NH1	5.79	123.19	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	80	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3331	4	0
1	C	3437	0	3348	9	0
2	B	3369	0	3250	7	0
2	D	3333	0	3214	8	0
3	E	1000	0	1018	1	0
4	F	2784	0	2737	5	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	24	0	26	0	0
9	C	12	0	13	0	0
10	B	55	0	0	0	0
10	D	55	0	0	0	0
11	F	31	0	14	0	0
12	A	39	0	0	0	0
12	B	45	0	0	1	0
12	C	50	0	0	0	0
12	D	15	0	0	2	0
12	E	2	0	0	0	0
12	F	6	0	0	0	0
All	All	17798	0	16999	33	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 (33) 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:246:LEU:HD12	2:D:352:ALA:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:NH2	12:D:1101:HOH:O	2.24	0.59
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.71	0.55
2:D:97:ALA:HB3	12:D:1108:HOH:O	2.10	0.51
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.94	0.50
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.93	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.48
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.95	0.48
4:F:350:ILE:O	4:F:354:ALA:HB3	2.15	0.46
1:C:228:ASN:O	1:C:232:SER:OG	2.32	0.46
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.50	0.46
2:B:11:GLN:NE2	12:B:601:HOH:O	2.47	0.46
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.98	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.45
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.44
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.00	0.44
1:C:234:ILE:HG21	1:C:302:MET:SD	2.57	0.44
2:D:202:ILE:HG22	2:D:207:LEU:HD11	2.00	0.43
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.43
2:B:81:PHE:O	2:B:84:ILE:HG22	2.19	0.42
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.53	0.42
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.42
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.51	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.19	0.41
2:D:293:MET:SD	2:D:365:ALA:HB1	2.60	0.41
1:C:270:ALA:HB3	1:C:302:MET:CE	2.51	0.41
2:B:7:ILE:O	2:B:135:LEU:HA	2.20	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.03	0.41
2:B:64:ILE:CD1	2:B:120:VAL:HG22	2.51	0.40
4:F:93:TRP:CD2	4:F:290:ILE:HG12	2.57	0.40
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.40
1:A:71:GLU:HB2	1:A:98:ASP:HB3	2.02	0.40
2:B:267:MET:HG3	2:B:301:ALA:HB3	2.03	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	435/451 (96%)	422 (97%)	13 (3%)	0	100	100
1	C	438/451 (97%)	424 (97%)	14 (3%)	0	100	100
2	B	426/445 (96%)	416 (98%)	9 (2%)	1 (0%)	47	64
2	D	420/445 (94%)	407 (97%)	12 (3%)	1 (0%)	47	64
3	E	117/136 (86%)	114 (97%)	2 (2%)	1 (1%)	17	26
4	F	328/384 (85%)	311 (95%)	17 (5%)	0	100	100
All	All	2164/2312 (94%)	2094 (97%)	67 (3%)	3 (0%)	51	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27	PRO
2	B	244	GLY
2	D	80	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	368/379 (97%)	356 (97%)	12 (3%)	38	55
1	C	371/379 (98%)	365 (98%)	6 (2%)	62	78
2	B	370/383 (97%)	362 (98%)	8 (2%)	52	70
2	D	367/383 (96%)	352 (96%)	15 (4%)	30	47
3	E	109/122 (89%)	105 (96%)	4 (4%)	34	51
4	F	305/342 (89%)	294 (96%)	11 (4%)	35	52
All	All	1890/1988 (95%)	1834 (97%)	56 (3%)	41	59

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	62	VAL
1	A	71	GLU
1	A	74	VAL
1	A	85	GLN
1	A	114	ILE
1	A	136	LEU
1	A	179	THR
1	A	181	VAL
1	A	211	ASP
1	A	251	ASP
1	A	381	THR
2	B	2	ARG
2	B	115	SER
2	B	137	HIS
2	B	282	ARG
2	B	316	ILE
2	B	334	GLN
2	B	359	ARG
2	B	377	LEU
1	C	2	ARG
1	C	120	ASP
1	C	133	GLN
1	C	232	SER
1	C	358	GLN
1	C	381	THR
2	D	19	LYS
2	D	42	LEU
2	D	65	LEU
2	D	74	ASP
2	D	108	GLU
2	D	114	ASP
2	D	137	HIS
2	D	151	LEU
2	D	156	ARG
2	D	162	ARG
2	D	245	GLN
2	D	276	ARG
2	D	286	VAL
2	D	333	VAL
2	D	386	THR
3	E	77	GLU
3	E	80	ARG

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Mol	Chain	Res	Type
3	E	100	LYS
3	E	123	LEU
4	F	20	LEU
4	F	33	ASP
4	F	88	SER
4	F	89	GLU
4	F	90	SER
4	F	187	GLU
4	F	197	ARG
4	F	211	TYR
4	F	247	LYS
4	F	331	GLU
4	F	348	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	ASN
1	A	300	ASN
1	A	301	GLN
2	B	11	GLN
2	B	245	GLN
2	B	334	GLN
1	C	11	GLN
1	C	356	ASN
1	C	358	GLN
2	D	8	GLN
2	D	134	GLN
4	F	252	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 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
5	GTP	A	501	6	26,34,34	1.16	2 (7%)	33,54,54	1.99	8 (24%)
8	GDP	D	501	-	24,30,30	1.21	2 (8%)	31,47,47	1.92	6 (19%)
5	GTP	C	502	6	26,34,34	1.07	2 (7%)	33,54,54	1.98	7 (21%)
9	MES	C	501	-	12,12,12	2.00	1 (8%)	14,16,16	1.64	2 (14%)
8	GDP	B	501	6	24,30,30	1.11	2 (8%)	31,47,47	1.96	5 (16%)
9	MES	B	504	-	12,12,12	2.29	1 (8%)	14,16,16	1.35	1 (7%)
11	ACP	F	401	-	27,33,33	1.45	6 (22%)	32,52,52	1.46	4 (12%)
10	J6R	B	505	-	52,57,57	1.65	8 (15%)	60,78,78	1.87	12 (20%)
9	MES	B	503	-	12,12,12	1.99	1 (8%)	14,16,16	6.81	7 (50%)
10	J6R	D	502	-	52,57,57	1.60	7 (13%)	60,78,78	1.48	9 (15%)

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	A	501	6	-	4/18/38/38	0/3/3/3
8	GDP	D	501	-	-	4/12/32/32	0/3/3/3
5	GTP	C	502	6	-	5/18/38/38	0/3/3/3
9	MES	C	501	-	-	1/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	9/15/38/38	0/3/3/3
10	J6R	B	505	-	-	5/53/76/76	0/3/3/3
9	MES	B	503	-	-	5/6/14/14	0/1/1/1
10	J6R	D	502	-	-	2/53/76/76	1/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.65	1.66	1.77
9	C	501	MES	C8-S	-6.55	1.68	1.77
10	D	502	J6R	CAH-CBF	-6.27	1.35	1.50
9	B	503	MES	C8-S	-6.21	1.68	1.77
10	B	505	J6R	CAH-CBF	-6.08	1.35	1.50
10	B	505	J6R	CAE-SAF	-5.27	1.57	1.73
10	D	502	J6R	CBK-CBV	-4.36	1.40	1.51
10	B	505	J6R	CBK-CBV	-4.34	1.40	1.51
5	A	501	GTP	C5-C6	4.00	1.48	1.41
8	D	501	GDP	C5-C6	3.69	1.47	1.41
8	B	501	GDP	C5-C6	3.54	1.47	1.41
5	C	502	GTP	C5-C6	3.41	1.47	1.41
10	D	502	J6R	CAE-SAF	-3.19	1.63	1.73
11	F	401	ACP	PG-O3G	3.00	1.61	1.54
11	F	401	ACP	PG-O2G	2.96	1.61	1.54
11	F	401	ACP	PB-O3A	2.96	1.61	1.58
10	B	505	J6R	CBI-CBL	2.79	1.56	1.53
10	D	502	J6R	CBA-CAZ	2.69	1.59	1.53
11	F	401	ACP	C5-C4	2.53	1.47	1.40
10	D	502	J6R	FCB-CBY	2.47	1.42	1.36
10	D	502	J6R	CAJ-CAB	2.36	1.57	1.53
8	D	501	GDP	C5-C4	2.36	1.47	1.40
8	B	501	GDP	C5-C4	2.35	1.47	1.40
10	B	505	J6R	C-NAA	2.34	1.39	1.34
5	A	501	GTP	C5-C4	2.34	1.47	1.40
11	F	401	ACP	PB-O2B	2.30	1.61	1.56
11	F	401	ACP	C2-N3	2.24	1.35	1.32
10	B	505	J6R	CAB-NAA	2.17	1.51	1.47
5	C	502	GTP	C5-C4	2.16	1.46	1.40
10	D	502	J6R	CAB-NAA	2.13	1.51	1.47
10	B	505	J6R	CAC-CAB	2.08	1.56	1.53
10	B	505	J6R	CBA-CAZ	2.02	1.57	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O2S-S-C8	-16.37	87.20	106.92
9	B	503	MES	O1S-S-C8	11.82	121.15	106.92
9	B	503	MES	O3S-S-O2S	-10.35	85.98	111.27
9	B	503	MES	O2S-S-O1S	-9.05	82.63	113.95
10	B	505	J6R	CBQ-CAL-NAA	8.95	127.14	113.31
9	B	503	MES	O3S-S-O1S	5.17	123.91	111.27
8	B	501	GDP	C4-C5-C6	-4.92	116.10	120.80
5	C	502	GTP	C2-N3-C4	4.83	120.87	115.36
8	B	501	GDP	C2-N1-C6	4.82	123.60	115.93
5	C	502	GTP	C4-C5-C6	-4.82	116.19	120.80
5	A	501	GTP	C4-C5-C6	-4.80	116.21	120.80
8	D	501	GDP	C2-N1-C6	4.60	123.23	115.93
8	D	501	GDP	C2-N3-C4	4.57	120.58	115.36
5	A	501	GTP	C2-N1-C6	4.52	123.12	115.93
10	D	502	J6R	CBI-CBH-CBK	-4.46	106.80	112.42
8	D	501	GDP	C4-C5-C6	-4.38	116.62	120.80
5	C	502	GTP	C2-N1-C6	4.38	122.89	115.93
9	B	503	MES	O3S-S-C8	4.36	112.83	105.77
5	A	501	GTP	C2-N3-C4	4.30	120.27	115.36
8	B	501	GDP	C2-N3-C4	4.21	120.16	115.36
8	B	501	GDP	N3-C2-N1	-4.12	121.72	127.22
8	B	501	GDP	C5-C6-N1	-4.07	117.86	123.43
5	C	502	GTP	N3-C2-N1	-4.04	121.84	127.22
5	A	501	GTP	C5-C6-N1	-4.02	117.93	123.43
10	B	505	J6R	CAW-CBB-CBA	4.02	119.61	111.42
8	D	501	GDP	N3-C2-N1	-4.02	121.86	127.22
10	D	502	J6R	CBQ-CAL-NAA	-4.00	107.14	113.31
8	D	501	GDP	C5-C6-N1	-3.99	117.98	123.43
10	B	505	J6R	CAH-CAG-SAF	-3.94	106.95	111.79
9	C	501	MES	O1S-S-C8	3.84	111.53	106.92
5	C	502	GTP	C5-C6-N1	-3.83	118.19	123.43
5	A	501	GTP	N3-C2-N1	-3.80	122.16	127.22
10	D	502	J6R	CAH-CAG-SAF	-3.73	107.22	111.79
11	F	401	ACP	N3-C2-N1	-3.58	123.08	128.68
11	F	401	ACP	C3'-C2'-C1'	3.29	105.94	100.98
9	B	504	MES	O3S-S-C8	3.19	110.93	105.77
10	B	505	J6R	CBQ-CBR-CBS	-3.17	102.42	113.62
10	B	505	J6R	CAL-NAA-C	3.16	130.83	122.36
11	F	401	ACP	PB-O3A-PA	-3.13	122.65	132.56
10	D	502	J6R	CBI-CBH-NBG	2.91	117.45	110.49
10	B	505	J6R	CBB-CAW-CAX	2.84	116.67	111.19
10	D	502	J6R	CBD-CAZ-NAY	-2.77	107.40	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	J6R	CBQ-CBR-CBS	-2.74	103.92	113.62
9	C	501	MES	O2S-S-C8	2.71	110.17	106.92
5	A	501	GTP	PA-O3A-PB	-2.63	123.81	132.83
10	D	502	J6R	CAH-CBF-NBG	2.62	120.08	115.20
10	B	505	J6R	CBZ-CBY-CBX	-2.61	119.36	122.83
10	D	502	J6R	CAW-CBB-CBA	-2.43	106.45	111.42
5	A	501	GTP	C4-C5-N7	-2.43	106.86	109.40
8	D	501	GDP	C4-C5-N7	-2.40	106.89	109.40
5	A	501	GTP	C1'-N9-C4	-2.39	122.44	126.64
10	D	502	J6R	CBZ-CBY-CBX	-2.38	119.66	122.83
10	B	505	J6R	CAX-NAY-CAZ	-2.29	107.90	112.39
11	F	401	ACP	C4-C5-N7	-2.27	107.04	109.40
10	B	505	J6R	CAH-CBF-NBG	2.19	119.27	115.20
9	B	503	MES	C6-O1-C2	2.15	117.06	109.89
5	C	502	GTP	C4-C5-N7	-2.13	107.17	109.40
10	B	505	J6R	CD1-CG1-CB	-2.11	105.42	113.84
10	B	505	J6R	CBW-CBX-CBY	2.11	120.55	118.36
5	C	502	GTP	PB-O3B-PG	-2.04	125.83	132.83
10	B	505	J6R	CBB-CBA-CAZ	2.02	114.99	111.23

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	503	MES	N4-C7-C8-S
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O1S
9	C	501	MES	N4-C7-C8-S
10	B	505	J6R	CBQ-CAL-NAA-C
10	B	505	J6R	CBQ-CAL-NAA-CAB
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A

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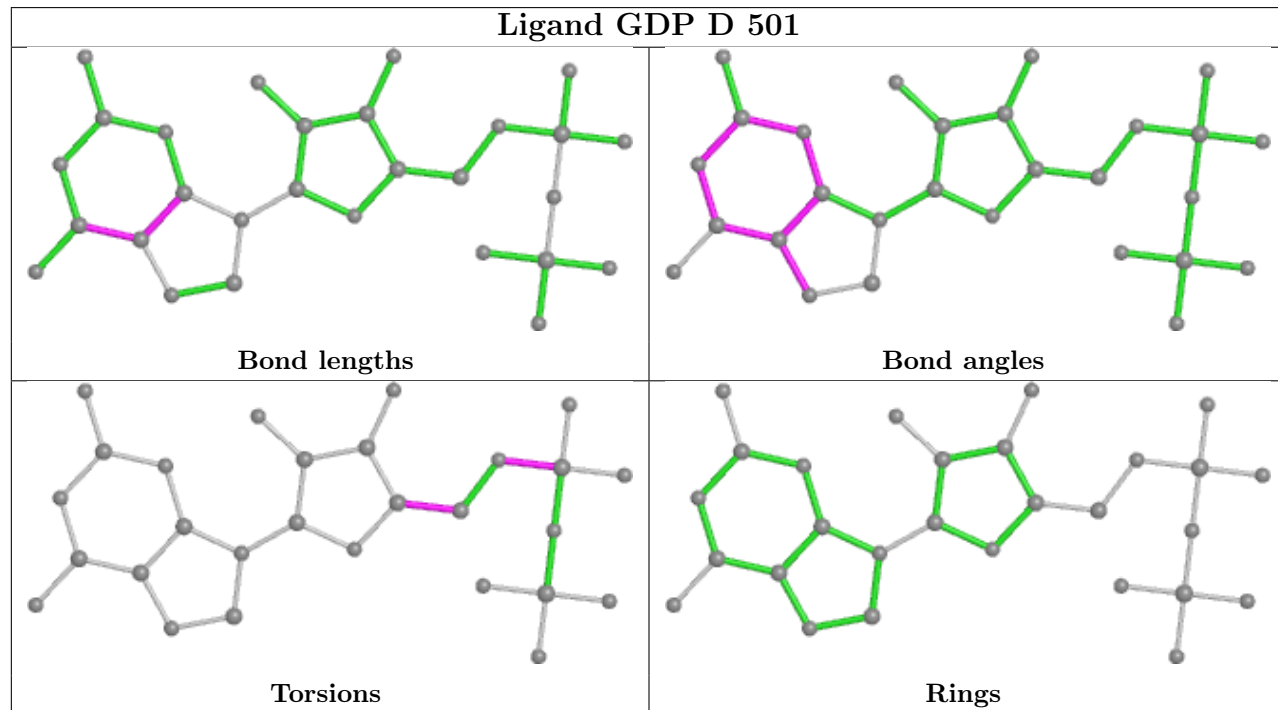
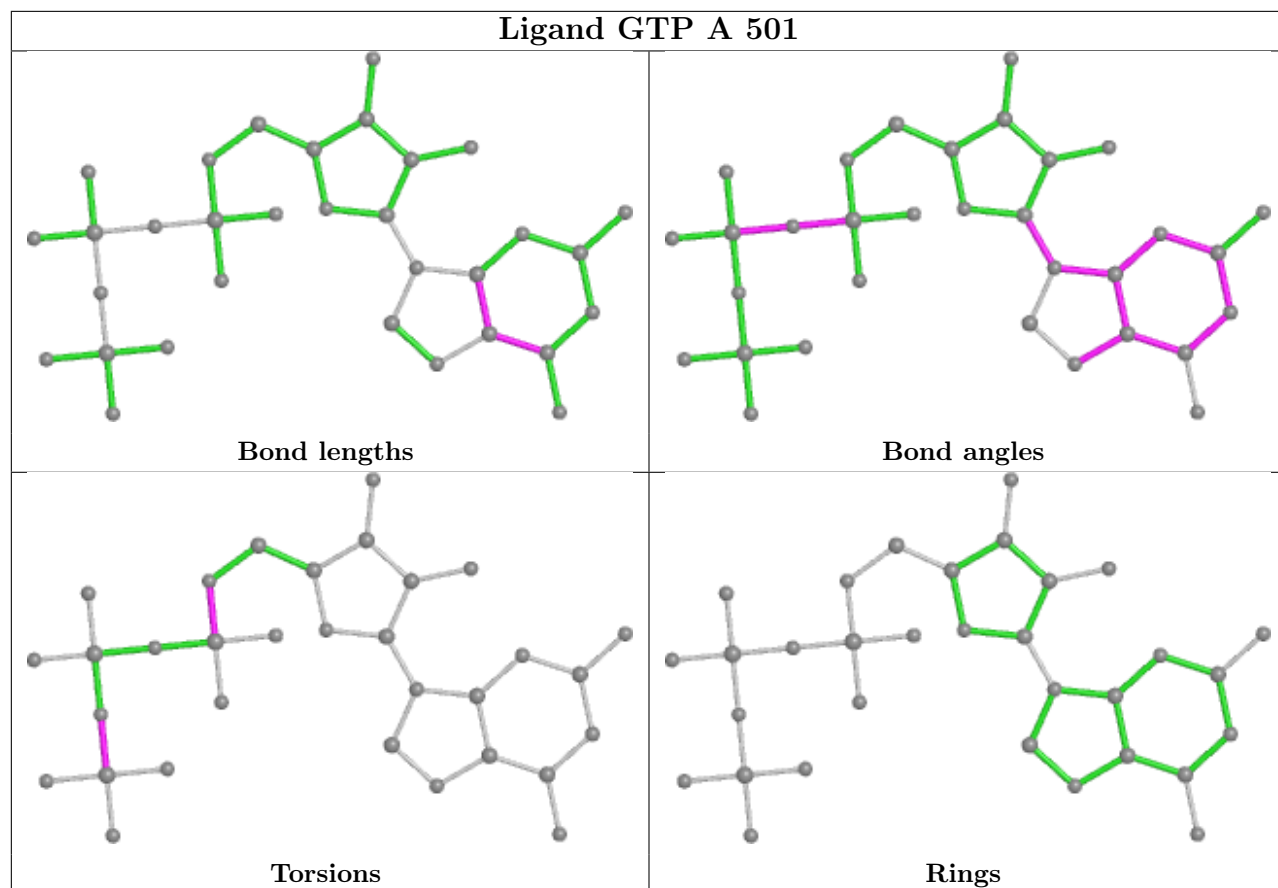
Mol	Chain	Res	Type	Atoms
9	B	504	MES	C7-C8-S-O3S
10	D	502	J6R	CG2-CB-CG1-CD1
10	B	505	J6R	CBQ-CBR-CBS-CBT
10	D	502	J6R	CA-CB-CG1-CD1
5	C	502	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O2S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	O4'-C4'-C5'-O5'
10	B	505	J6R	NAA-CAL-CBQ-CBR
9	B	503	MES	C8-C7-N4-C3
9	B	503	MES	C8-C7-N4-C5
8	D	501	GDP	C3'-C4'-C5'-O5'
10	B	505	J6R	CG2-CB-CG1-CD1
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	502	GTP	PB-O3B-PG-O2G
11	F	401	ACP	PB-O3A-PA-O2A
5	C	502	GTP	C5'-O5'-PA-O3A

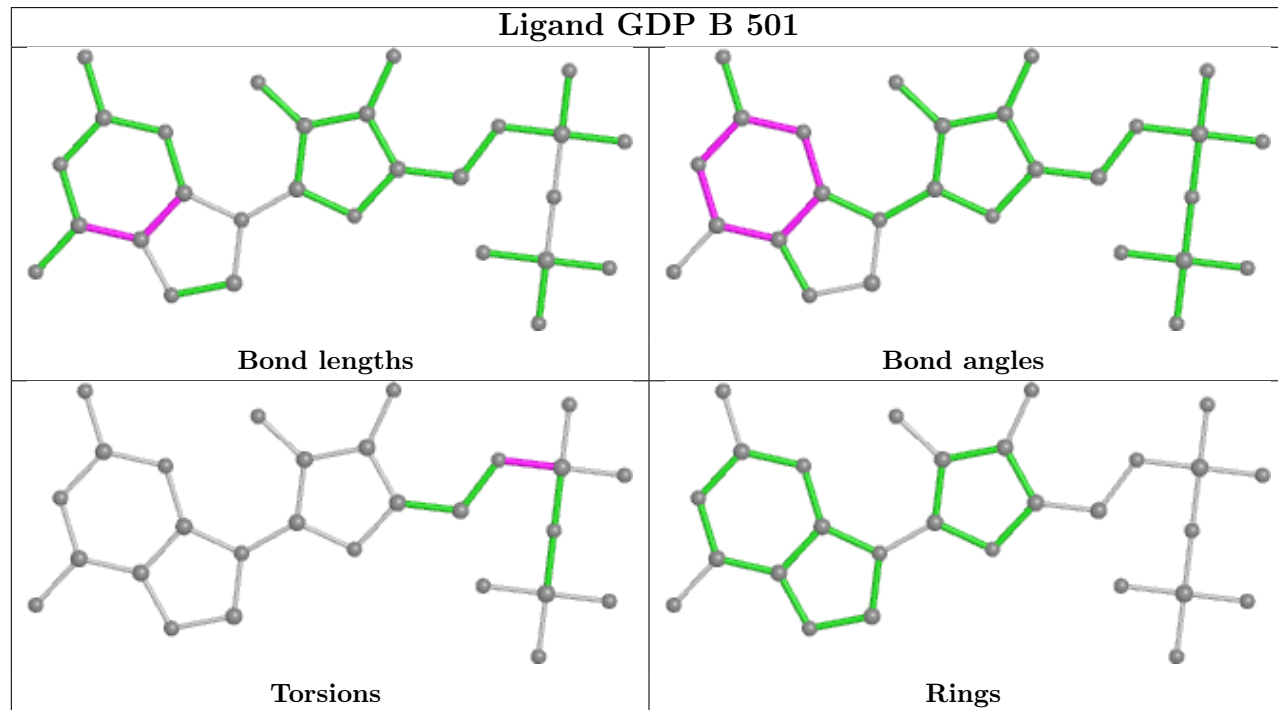
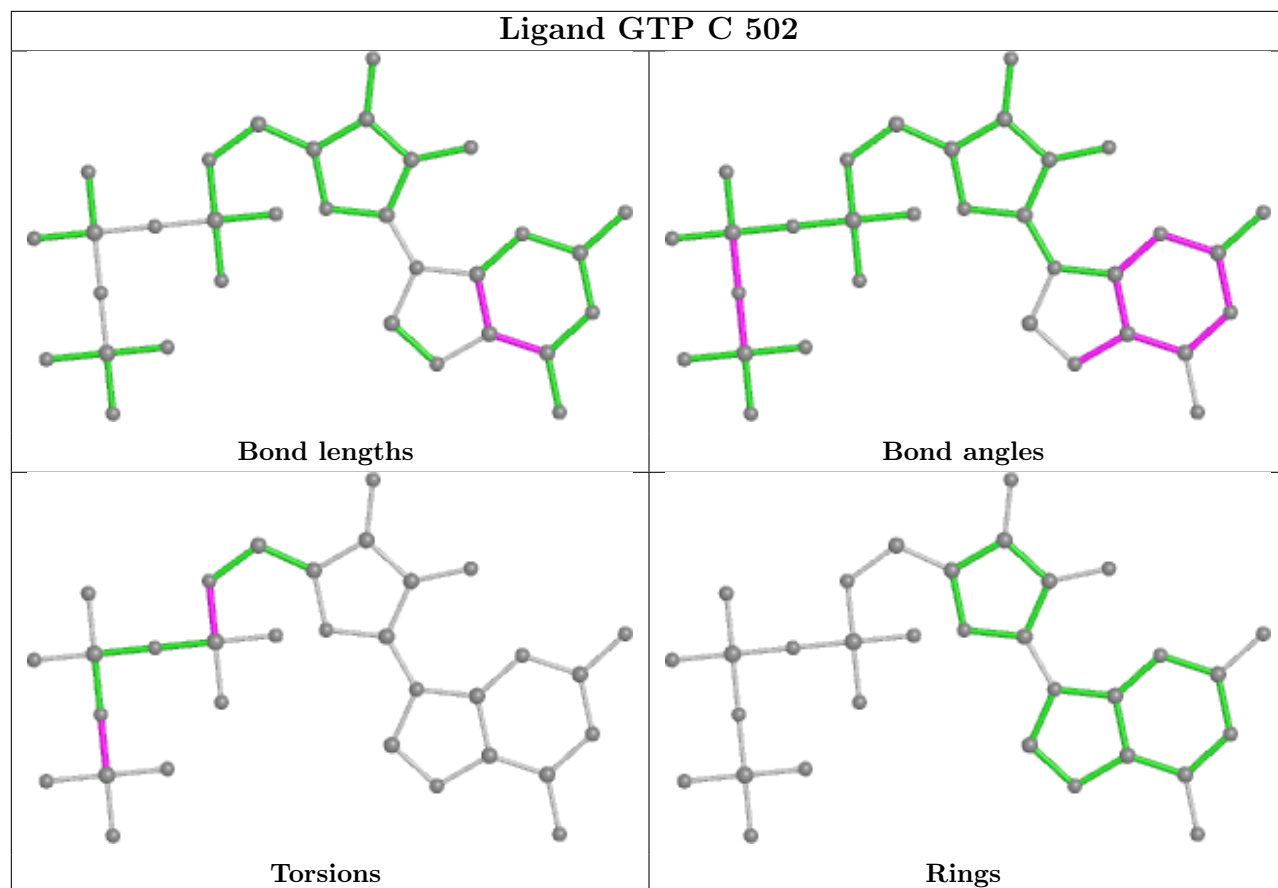
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	502	J6R	CAW-CAX-CAZ-CBA-CBB-NAY

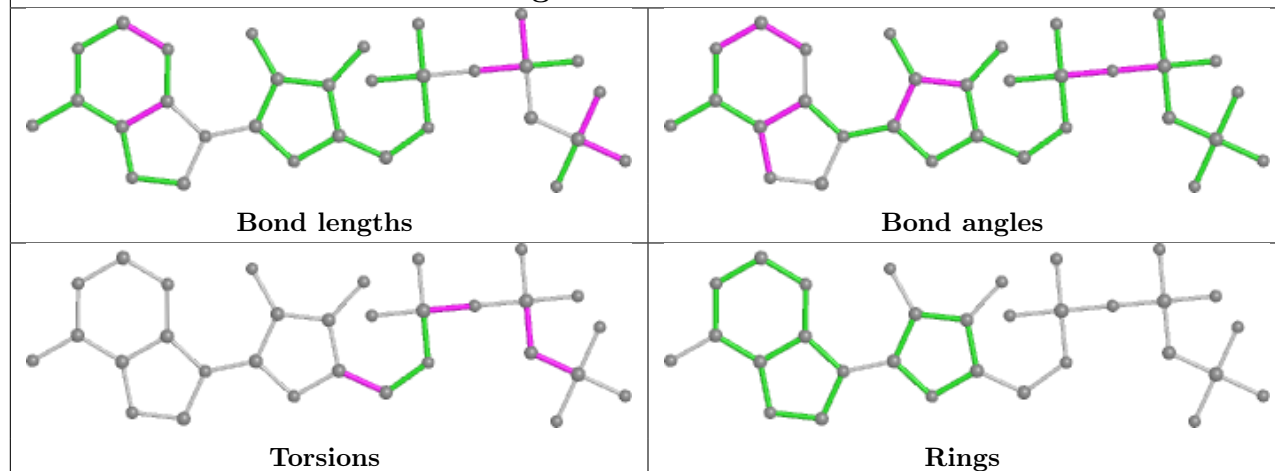
No monomer is involved in short contacts.

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.

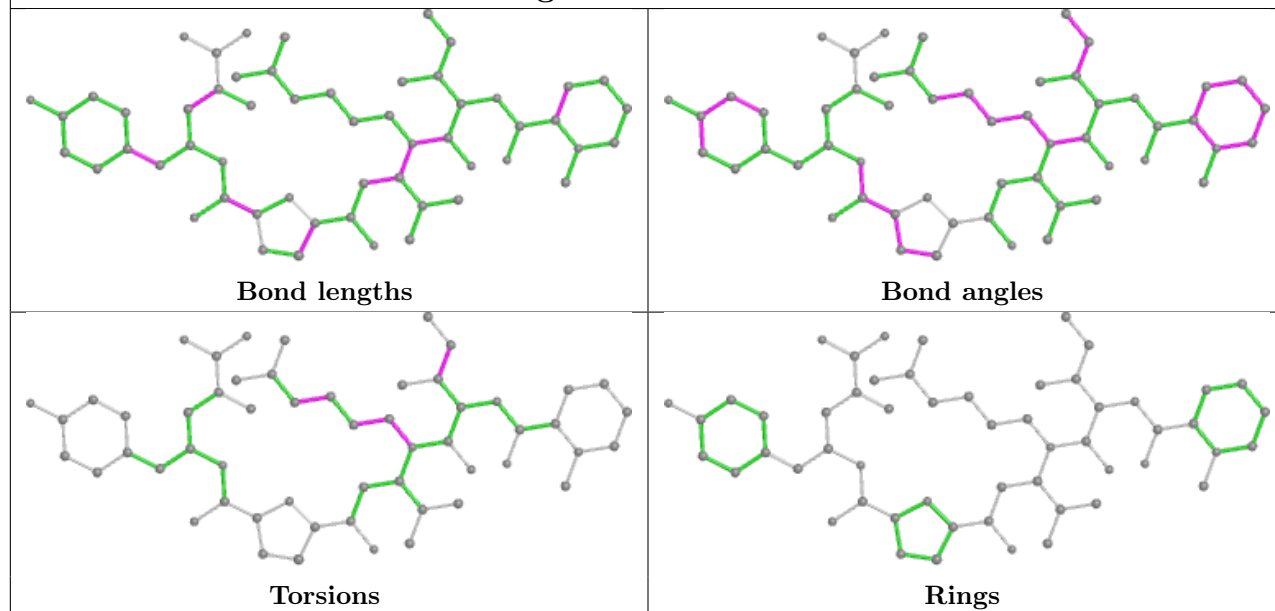


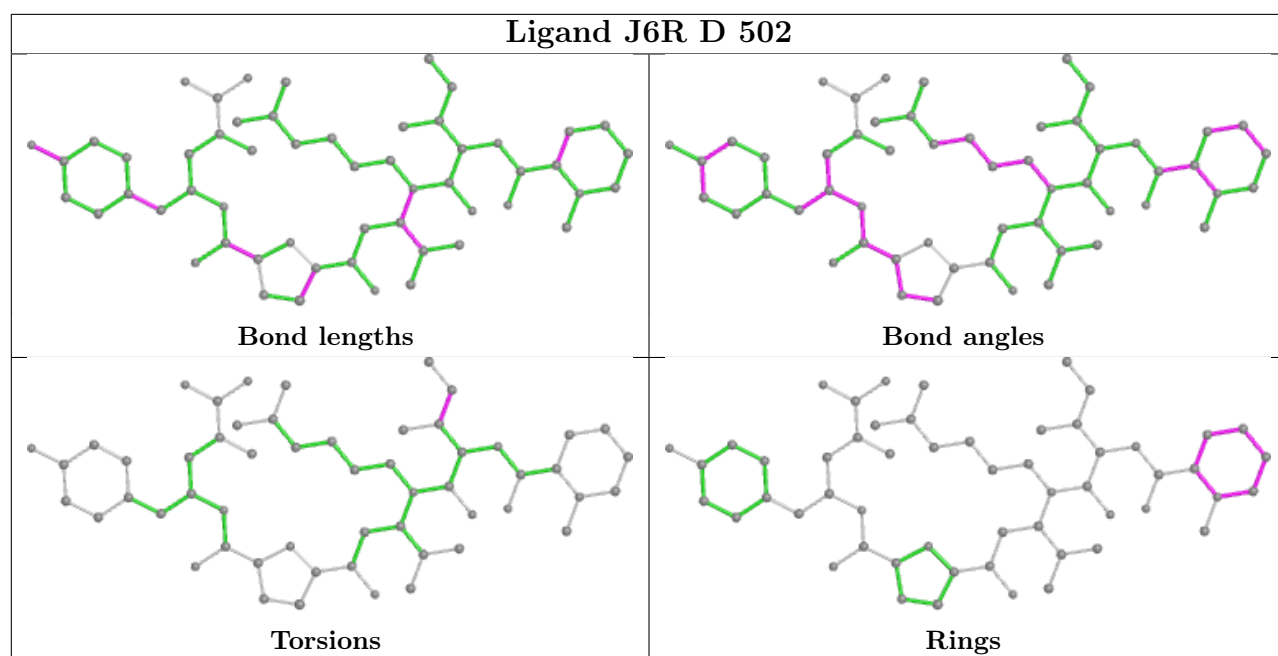


Ligand ACP F 401



Ligand J6R B 505





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	437/451 (96%)	-0.19	5 (1%)	80 78	25, 39, 61, 99	0
1	C	440/451 (97%)	-0.40	2 (0%)	91 90	21, 32, 53, 81	0
2	B	428/445 (96%)	-0.22	3 (0%)	87 86	21, 34, 63, 95	0
2	D	424/445 (95%)	0.18	21 (4%)	28 25	28, 49, 81, 109	0
3	E	121/136 (88%)	0.37	7 (5%)	23 20	32, 54, 80, 97	0
4	F	338/384 (88%)	0.31	35 (10%)	6 4	29, 56, 108, 131	0
All	All	2188/2312 (94%)	-0.06	73 (3%)	46 43	21, 41, 81, 131	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	137	ARG	8.7
2	B	1	MET	7.4
4	F	231	ALA	6.4
2	D	55	THR	5.9
4	F	372	THR	5.5
4	F	175	GLU	4.5
1	A	282	TYR	4.1
2	D	54	ALA	4.0
4	F	234	GLN	4.0
4	F	178	GLN	3.8
2	D	37	HIS	3.8
1	A	281	ALA	3.7
4	F	140	GLU	3.7
4	F	173	ILE	3.7
2	D	57	ASN	3.6
4	F	166	ALA	3.5
2	D	390	ARG	3.5
2	D	391	ARG	3.5
4	F	136	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
3	E	6	MET	3.4
1	C	440	VAL	3.4
2	D	56	GLY	3.4
4	F	256	TYR	3.4
4	F	255	ARG	3.3
4	F	174	ASP	3.3
4	F	170	LEU	3.2
4	F	133	ALA	3.1
2	D	80	PRO	3.1
4	F	171	ASP	3.0
4	F	142	ARG	3.0
4	F	233	PHE	2.9
2	D	1	MET	2.9
2	D	320	ARG	2.9
4	F	167	SER	2.8
2	D	92	PHE	2.8
2	D	95	SER	2.8
2	D	166	THR	2.8
1	A	430	LYS	2.8
4	F	177	GLY	2.8
4	F	232	ASN	2.8
4	F	139	ARG	2.8
2	B	55	THR	2.7
4	F	252	ASN	2.7
4	F	179	VAL	2.7
3	E	103	GLN	2.6
2	D	53	GLU	2.6
2	D	199	THR	2.6
2	D	359	ARG	2.6
2	B	277	GLY	2.6
3	E	136	ASN	2.5
4	F	103	THR	2.5
3	E	106	GLU	2.4
2	D	394	PHE	2.4
4	F	225	SER	2.4
1	A	262	TYR	2.4
4	F	235	ASP	2.4
1	A	120	ASP	2.4
1	C	163	LYS	2.3
3	E	48	GLU	2.3
3	E	138	GLU	2.3
4	F	169	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	362	LYS	2.2
3	E	139	LEU	2.2
4	F	236	LYS	2.2
4	F	194	PRO	2.1
4	F	138	ARG	2.1
2	D	405	GLU	2.1
2	D	165	ASN	2.1
4	F	134	ALA	2.0
4	F	1	MET	2.0
2	D	167	PHE	2.0
4	F	44	ARG	2.0
4	F	227	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MES	C	501	12/12	0.71	0.40	80,84,96,96	0
9	MES	B	503	12/12	0.89	0.21	70,74,76,79	0
11	ACP	F	401	31/31	0.89	0.18	61,73,106,112	0
10	J6R	D	502	55/55	0.90	0.29	60,65,70,72	0
7	CA	A	503	1/1	0.90	0.07	62,62,62,62	0
9	MES	B	504	12/12	0.94	0.17	52,54,55,55	0
10	J6R	B	505	55/55	0.95	0.16	32,35,40,44	0
8	GDP	D	501	28/28	0.95	0.17	37,42,46,50	0
6	MG	A	502	1/1	0.95	0.13	30,30,30,30	0
7	CA	C	504	1/1	0.97	0.04	46,46,46,46	0
6	MG	B	502	1/1	0.97	0.17	44,44,44,44	0

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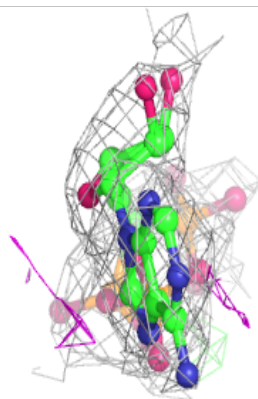
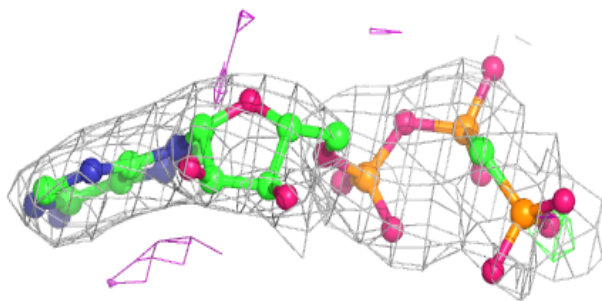
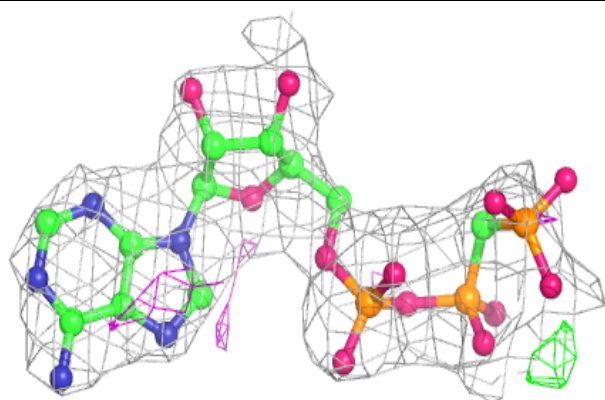
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	503	1/1	0.98	0.10	27,27,27,27	0
8	GDP	B	501	28/28	0.98	0.14	21,23,24,24	0
5	GTP	A	501	32/32	0.98	0.17	21,26,28,29	0
5	GTP	C	502	32/32	0.99	0.11	21,21,22,22	0

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

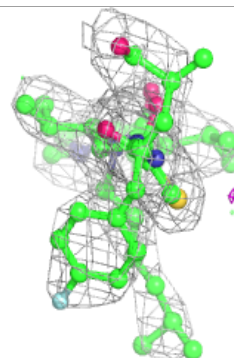
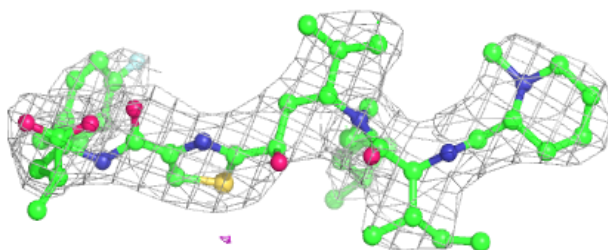
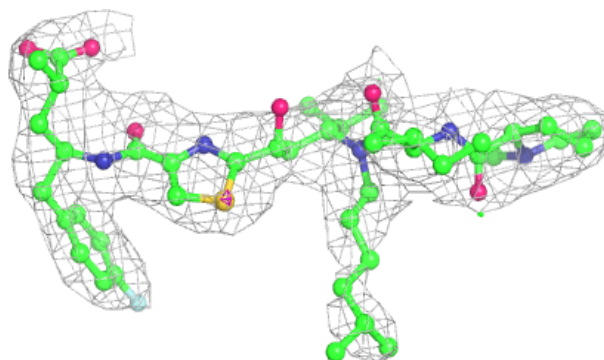
Electron density around ACP F 401:

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

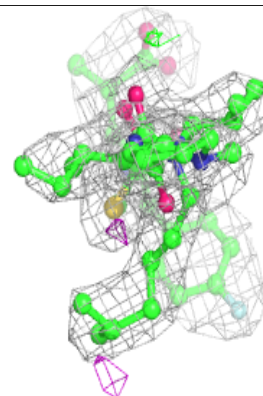
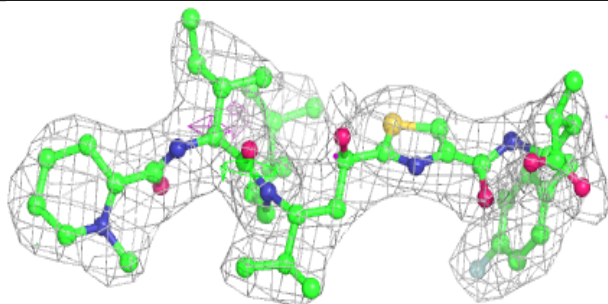
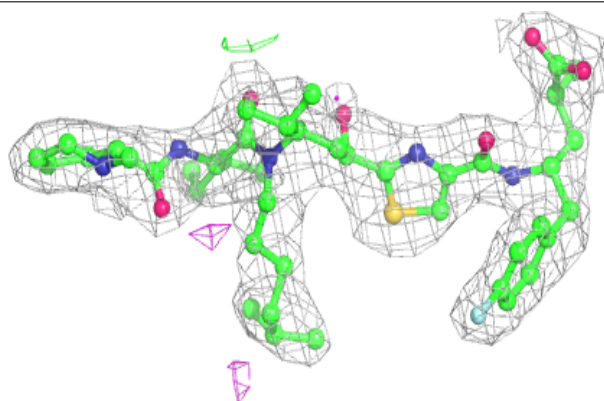


Electron density around J6R D 502:

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

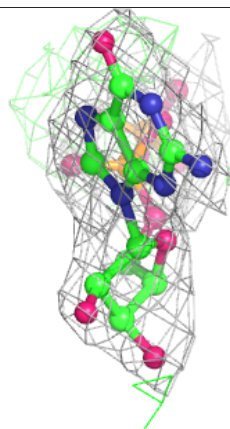
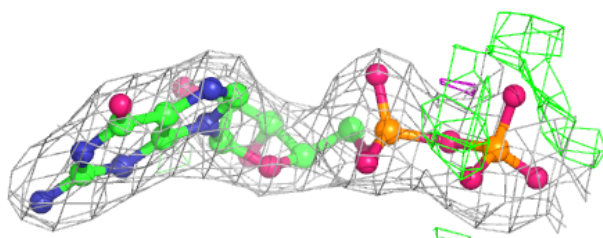
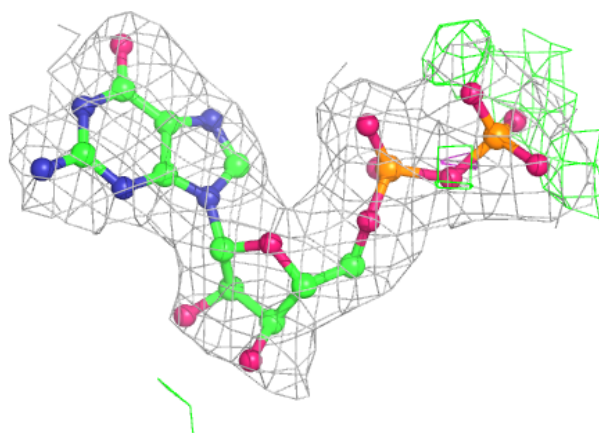
**Electron density around J6R B 505:**

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

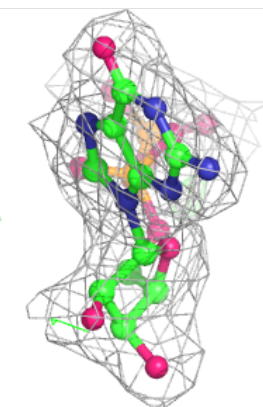
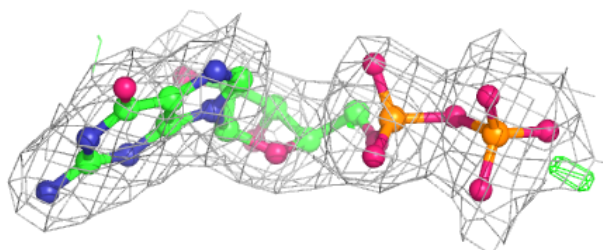
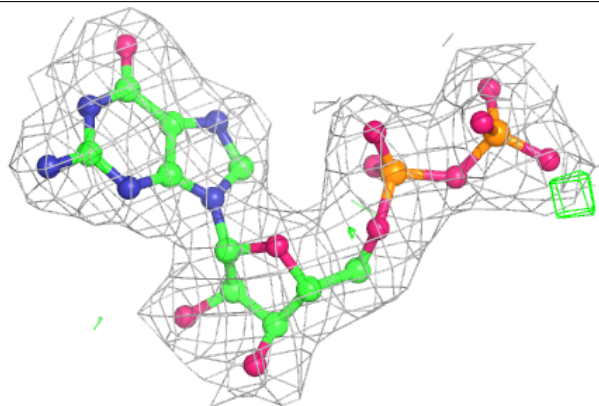


Electron density around GDP D 501:

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

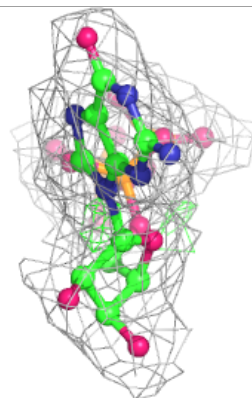
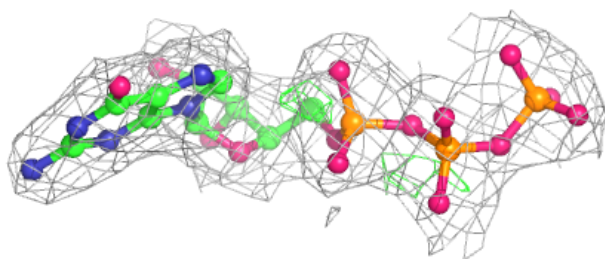
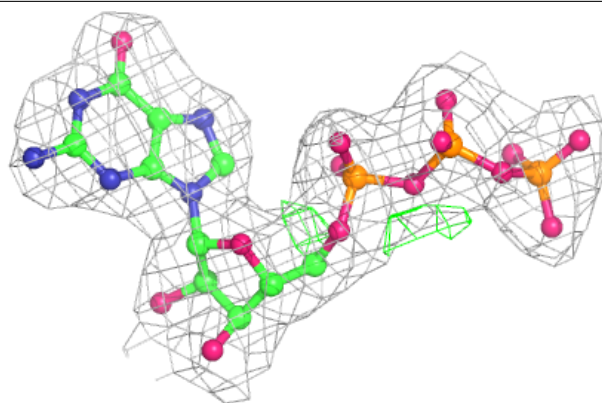
**Electron density around GDP B 501:**

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

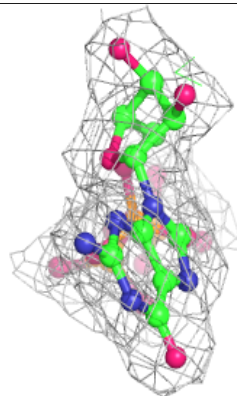
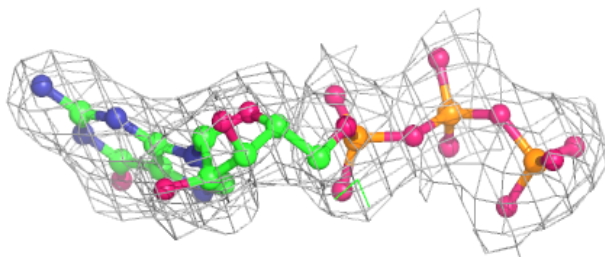
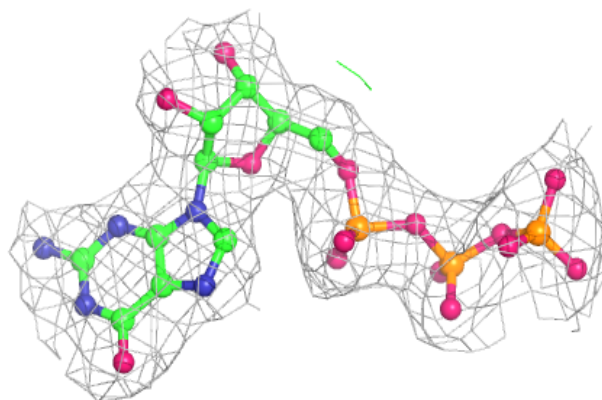


Electron density around GTP A 501:

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

**Electron density around GTP C 502:**

$2mF_o-DF_c$ (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.