



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:04 AM EDT

PDB ID : 8DIQ
Title : Tubulin-RB3_SLD-TTL in complex with SB226
Authors : White, S.W.; Yun, M.
Deposited on : 2022-06-29
Resolution : 2.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

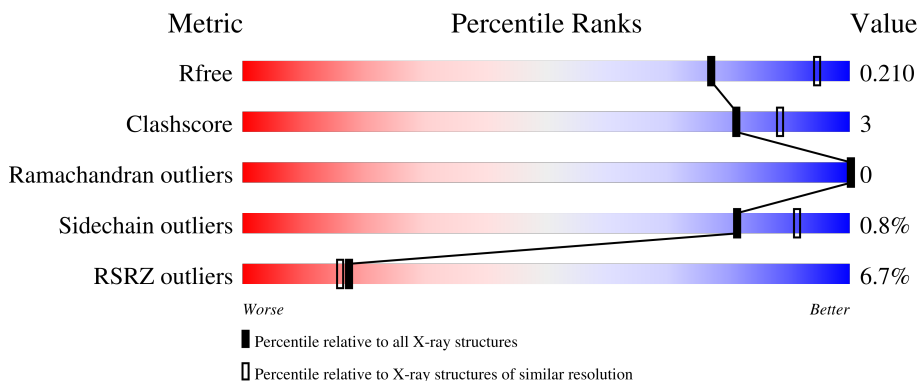
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



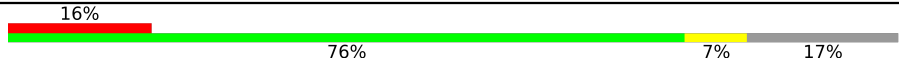
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	450	 2% 90% 7%
1	C	450	 0% 90% 8%
2	B	445	 5% 89% 7%
2	D	445	 7% 84% 10% 6%
3	E	143	 10% 83% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '16%', a large green segment labeled '76%', a small yellow segment labeled '7%', and a grey segment on the right labeled '17%'.</p>

2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 17666 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
2	B	427	Total	C	N	O	S	0	0	0
			3356	2108	575	647	26			
2	D	420	Total	C	N	O	S	0	0	0
			3286	2069	557	634	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	0	0
			993	612	181	195	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	320	Total	C	N	O	S	0	0	0
			2580	1660	437	471	12			

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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

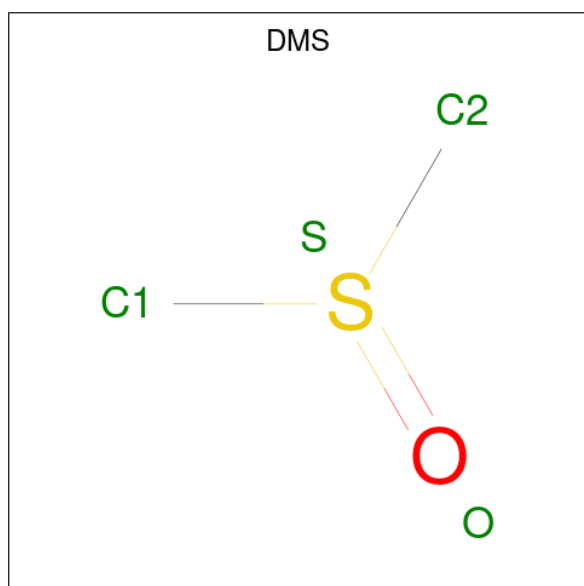
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

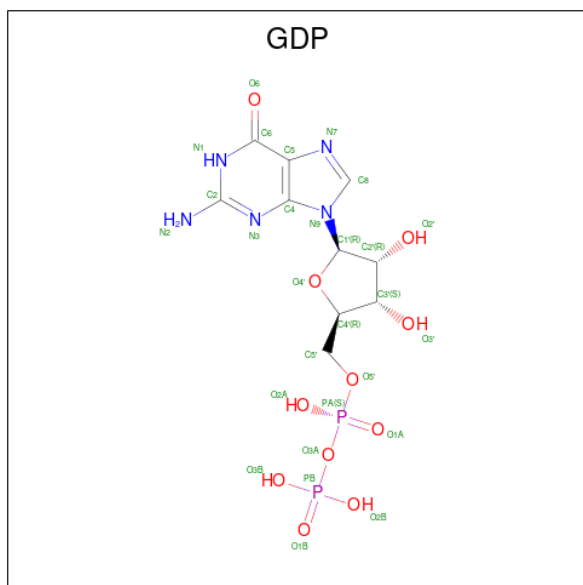
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



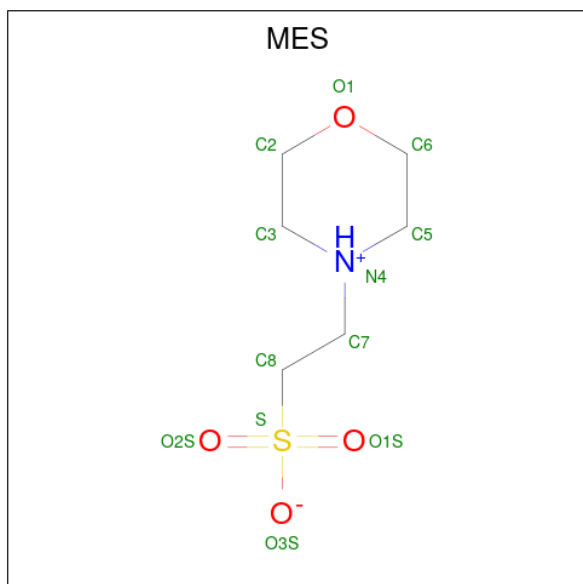
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O S 4 2 1 1	0	0
8	C	1	Total C O S 4 2 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



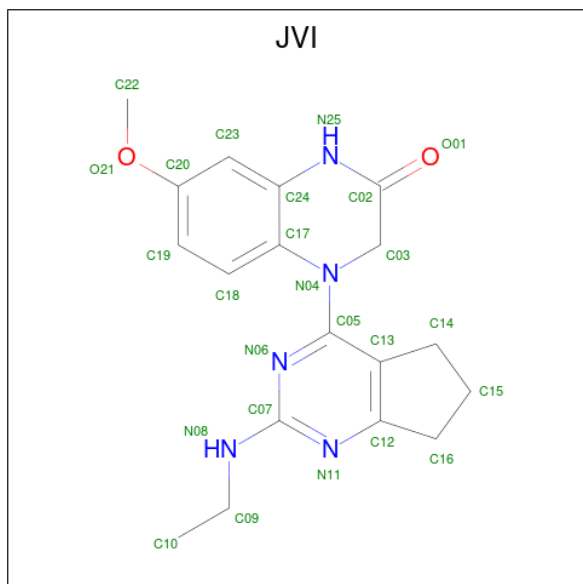
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



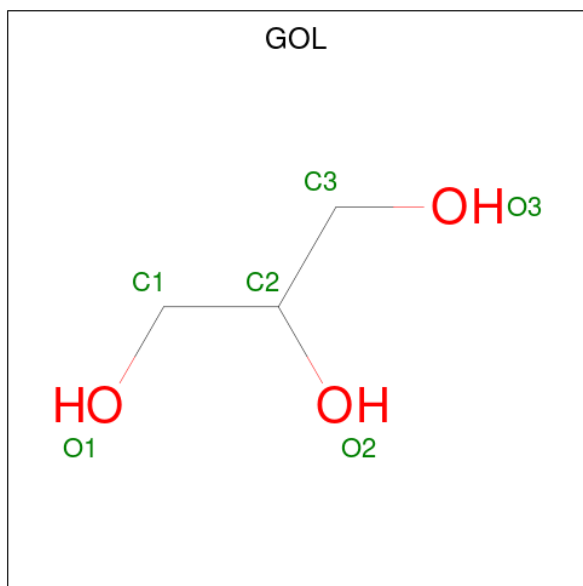
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is 4-[2-(ethylamino)-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl]-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (three-letter code: JVI) (formula: $C_{18}H_{21}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



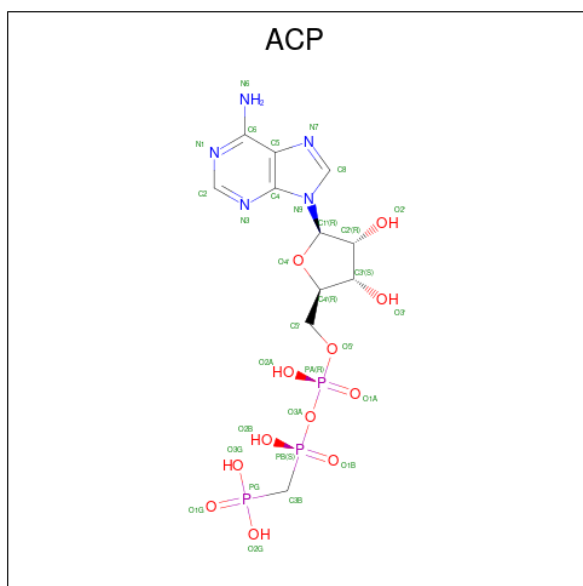
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	B	1	Total	C	N	O	0	0
			25	18	5	2		
11	D	1	Total	C	N	O	0	0
			25	18	5	2		

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 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
13	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

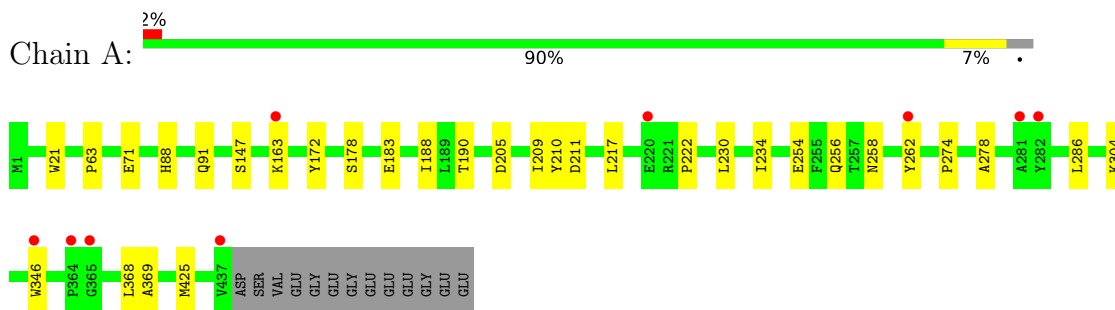
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	85	Total	O	0	0
			85	85		
14	B	61	Total	O	0	0
			61	61		
14	C	147	Total	O	0	0
			147	147		
14	D	30	Total	O	0	0
			30	30		
14	E	9	Total	O	0	0
			9	9		
14	F	16	Total	O	0	0
			16	16		

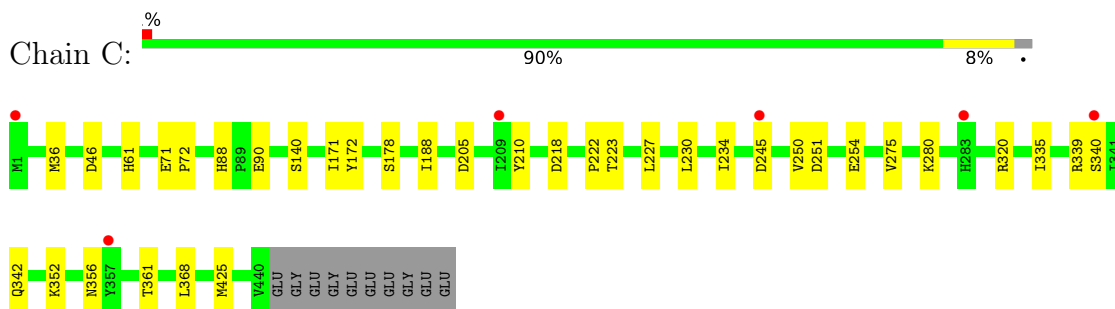
3 Residue-property plots [i](#)

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.

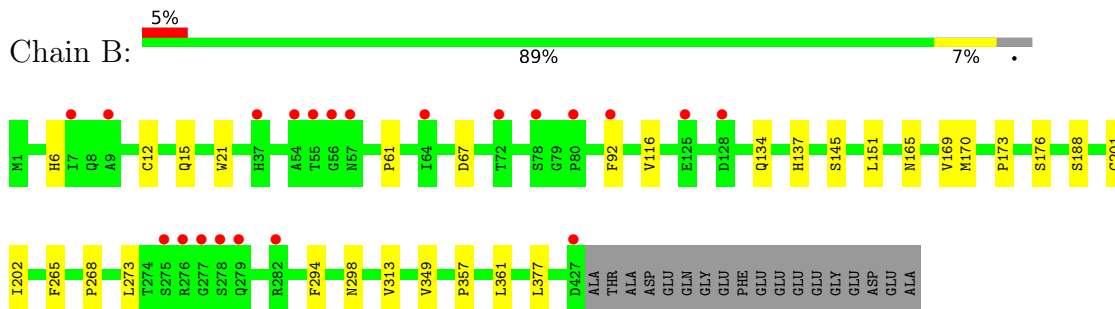
- Molecule 1: Tubulin alpha-1B chain



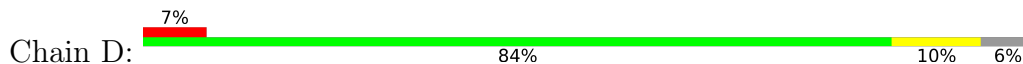
- Molecule 1: Tubulin alpha-1B chain

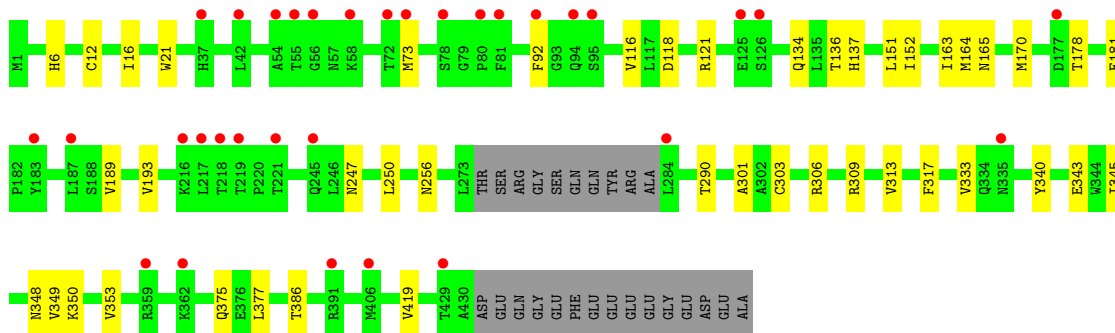


- Molecule 2: Tubulin beta-2B chain

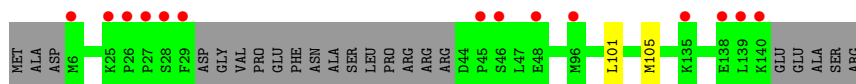
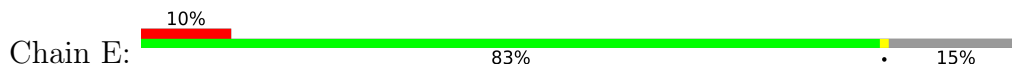


- Molecule 2: Tubulin beta-2B chain

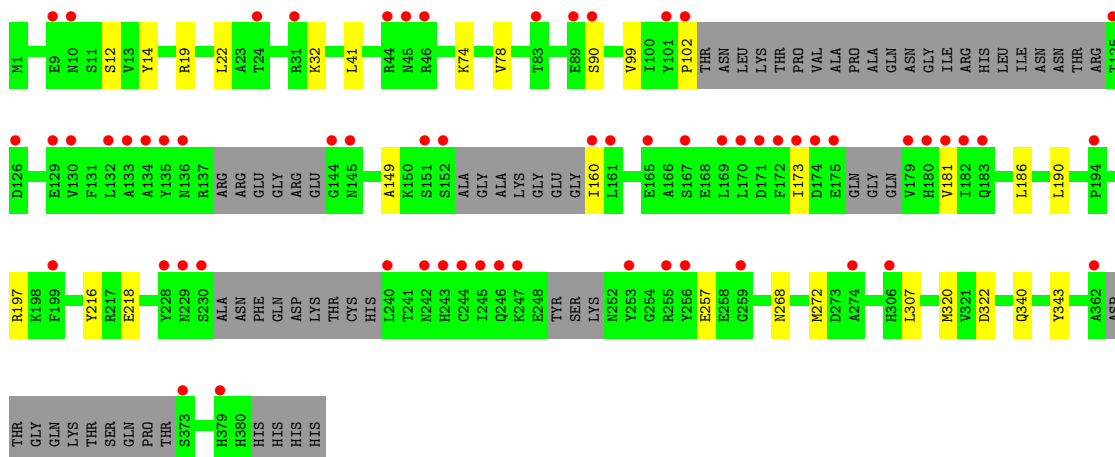
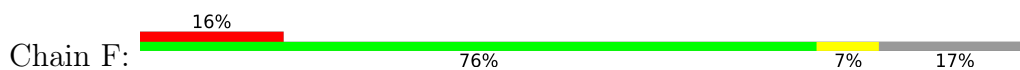




- Molecule 3: Stathmin-4



- Molecule 4: 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	105.49Å 158.41Å 181.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.40 19.92 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.92-2.40) 94.5 (19.92-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.41Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.182 , 0.209 0.182 , 0.210	Depositor DCC
R_{free} test set	2000 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17666	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, GDP, ACP, DMS, MES, CA, JVI, GOL

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	0.25	0/3494	0.41	0/4743
1	C	0.25	0/3515	0.42	0/4772
2	B	0.25	0/3431	0.42	0/4647
2	D	0.25	0/3359	0.41	0/4552
3	E	0.23	0/1001	0.34	0/1328
4	F	0.24	0/2635	0.41	0/3561
All	All	0.25	0/17435	0.41	0/23603

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3330	16	0
1	C	3437	0	3348	18	0
2	B	3356	0	3229	17	0
2	D	3286	0	3155	22	0
3	E	993	0	1005	1	0
4	F	2580	0	2519	14	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	4	0	6	0	0
8	C	4	0	6	0	0
9	B	28	0	12	2	0
10	B	24	0	24	1	0
11	B	25	0	0	0	0
11	D	25	0	0	1	0
12	B	6	0	8	0	0
13	F	31	0	13	1	0
14	A	85	0	0	0	0
14	B	61	0	0	0	0
14	C	147	0	0	0	0
14	D	30	0	0	0	0
14	E	9	0	0	0	0
14	F	16	0	0	0	0
All	All	17666	0	16691	87	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 3.

All (87) 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:145:SER:HG	2:B:188:SER:HG	1.40	0.69
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.75	0.66
2:D:118:ASP:OD1	2:D:121:ARG:NH1	2.28	0.66
2:B:173:PRO:HA	2:B:176:SER:HB2	1.81	0.61
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.84	0.60
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.85	0.58
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.87	0.57
2:D:116:VAL:HG11	2:D:151:LEU:HD21	1.88	0.56
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.88	0.56
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:CYS:HB2	5:D:501:GTP:C8	2.44	0.53
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.92	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.50
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.94	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.49
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.52	0.49
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.93	0.49
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.48	0.49
4:F:102:PRO:HB3	4:F:173:ILE:HG22	1.93	0.49
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.95	0.49
1:C:178:SER:OG	2:D:350:LYS:NZ	2.45	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.49
2:B:134:GLN:HA	2:B:165:ASN:O	2.12	0.48
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.95	0.48
1:C:230:LEU:O	1:C:234:ILE:HD12	2.13	0.48
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.95	0.48
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.48	0.48
2:D:134:GLN:HA	2:D:165:ASN:O	2.13	0.48
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.96	0.47
2:D:178:THR:O	2:D:181:GLU:HG3	2.15	0.47
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.97	0.47
2:B:15:GLN:NE2	9:B:501:GDP:O6	2.47	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.97	0.47
4:F:268:ASN:O	4:F:272:MET:HG3	2.15	0.47
1:A:88:HIS:O	1:A:91:GLN:HG2	2.14	0.47
1:C:46:ASP:OD1	1:C:46:ASP:N	2.46	0.46
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.98	0.46
2:D:313:VAL:HB	2:D:349:VAL:HG22	1.98	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.45
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.99	0.45
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.51	0.45
4:F:74:LYS:HE3	13:F:402:ACP:O1A	2.17	0.44
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.99	0.44
1:A:230:LEU:O	1:A:234:ILE:HD12	2.18	0.44
1:A:262:TYR:HE2	1:A:346:TRP:CZ2	2.36	0.44
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.39	0.44
1:C:218:ASP:OD2	1:C:280:LYS:NZ	2.50	0.44
1:A:178:SER:HB2	1:A:183:GLU:OE1	2.18	0.43
2:B:357:PRO:HB2	2:B:361:LEU:O	2.19	0.43
1:C:245:ASP:OD1	1:C:245:ASP:N	2.46	0.43
3:E:101:LEU:O	3:E:105:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.83	0.43
2:D:309:ARG:NH2	2:D:343:GLU:OE1	2.44	0.43
2:B:170:MET:HG3	2:B:377:LEU:HD11	2.00	0.42
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.84	0.42
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.42
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.00	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.42
2:B:294:PHE:O	10:B:503:MES:H82	2.20	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.42
2:D:290:THR:HG22	2:D:333:VAL:HG21	2.01	0.42
2:D:317:PHE:HB2	2:D:353:VAL:HG22	2.01	0.42
4:F:19:ARG:CZ	4:F:19:ARG:HB3	2.50	0.42
4:F:149:ALA:O	4:F:160:ILE:HA	2.19	0.42
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.55	0.42
2:D:152:ILE:HG23	2:D:164:MET:HG2	2.02	0.42
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.01	0.42
1:A:163:LYS:HE2	1:A:163:LYS:HB3	1.89	0.41
2:B:116:VAL:HG11	2:B:151:LEU:HD11	2.01	0.41
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.02	0.41
4:F:32:LYS:HB3	4:F:32:LYS:HE2	1.70	0.41
2:D:301:ALA:O	2:D:303:CYS:N	2.53	0.41
2:D:16:ILE:HD11	2:D:136:THR:HB	2.02	0.41
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.41
2:D:256:ASN:HB3	11:D:503:JVI:C20	2.50	0.41
4:F:78:VAL:HG21	4:F:181:VAL:HG11	2.01	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.35	0.41
1:C:223:THR:O	1:C:227:LEU:HG	2.21	0.41
2:D:189:VAL:O	2:D:193:VAL:HG23	2.21	0.41
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.56	0.41
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.56	0.41
4:F:190:LEU:HB2	4:F:322:ASP:O	2.21	0.41
2:B:169:VAL:HA	2:B:202:ILE:O	2.21	0.40
2:D:375:GLN:HB2	2:D:419:VAL:HG13	2.02	0.40
2:B:273:LEU:HD11	2:B:298:ASN:HA	2.04	0.40
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	427 (98%)	8 (2%)	0	100	100
1	C	438/450 (97%)	432 (99%)	6 (1%)	0	100	100
2	B	425/445 (96%)	417 (98%)	8 (2%)	0	100	100
2	D	416/445 (94%)	406 (98%)	10 (2%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	304/384 (79%)	294 (97%)	10 (3%)	0	100	100
All	All	2135/2317 (92%)	2093 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/378 (97%)	366 (100%)	2 (0%)	88	95
1	C	371/378 (98%)	367 (99%)	4 (1%)	73	87
2	B	367/383 (96%)	365 (100%)	2 (0%)	88	95
2	D	358/383 (94%)	355 (99%)	3 (1%)	81	91
3	E	107/127 (84%)	107 (100%)	0	100	100
4	F	279/342 (82%)	275 (99%)	4 (1%)	67	82
All	All	1850/1991 (93%)	1835 (99%)	15 (1%)	81	91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	256	GLN
2	B	137	HIS
2	B	268	PRO
1	C	251	ASP
1	C	340	SER
1	C	342	GLN
1	C	361	THR
2	D	137	HIS
2	D	247	ASN
2	D	386	THR
4	F	12	SER
4	F	22	LEU
4	F	90	SER
4	F	99	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	301	GLN
2	B	15	GLN
2	B	165	ASN
2	B	414	ASN
1	C	372	GLN
1	C	406	HIS
2	D	99	ASN
2	D	165	ASN
4	F	260	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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
11	JVI	D	503	-	28,28,28	2.97	12 (42%)	34,40,40	2.27	10 (29%)
5	GTP	D	501	7	26,34,34	1.14	2 (7%)	32,54,54	1.57	7 (21%)
8	DMS	A	504	-	3,3,3	0.66	0	3,3,3	0.50	0
5	GTP	C	501	7	26,34,34	1.10	2 (7%)	32,54,54	1.49	6 (18%)
5	GTP	A	501	7	26,34,34	1.13	2 (7%)	32,54,54	1.49	6 (18%)
11	JVI	B	505	-	28,28,28	3.00	12 (42%)	34,40,40	2.20	11 (32%)
8	DMS	C	504	-	3,3,3	0.66	0	3,3,3	0.51	0
9	GDP	B	501	7	24,30,30	0.95	1 (4%)	30,47,47	1.12	3 (10%)
12	GOL	B	506	-	5,5,5	0.89	0	5,5,5	1.03	0
13	ACP	F	402	7	27,33,33	2.04	8 (29%)	32,52,52	1.39	2 (6%)
10	MES	B	503	-	12,12,12	2.29	1 (8%)	14,16,16	1.88	5 (35%)
10	MES	B	502	-	12,12,12	2.28	1 (8%)	14,16,16	1.89	4 (28%)

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
11	JVI	D	503	-	-	5/8/27/27	0/4/4/4
5	GTP	D	501	7	-	8/18/38/38	0/3/3/3
5	GTP	C	501	7	-	7/18/38/38	0/3/3/3
5	GTP	A	501	7	-	5/18/38/38	0/3/3/3
11	JVI	B	505	-	-	5/8/27/27	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	501	7	-	4/12/32/32	0/3/3/3
12	GOL	B	506	-	-	0/4/4/4	-
13	ACP	F	402	7	-	3/15/38/38	0/3/3/3
10	MES	B	503	-	-	3/6/14/14	0/1/1/1
10	MES	B	502	-	-	4/6/14/14	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	JVI	C02-N25	8.53	1.44	1.35
11	D	503	JVI	C02-N25	8.34	1.44	1.35
10	B	503	MES	C8-S	-7.67	1.66	1.77
10	B	502	MES	C8-S	-7.63	1.66	1.77
13	F	402	ACP	PB-O3A	6.53	1.65	1.58
11	B	505	JVI	C07-N08	5.84	1.43	1.34
11	D	503	JVI	C07-N08	5.81	1.43	1.34
11	B	505	JVI	C05-N04	5.47	1.45	1.37
11	D	503	JVI	C05-N04	5.46	1.45	1.37
11	D	503	JVI	C16-C12	4.96	1.54	1.50
11	B	505	JVI	C16-C12	4.96	1.54	1.50
11	B	505	JVI	C24-N25	4.86	1.48	1.39
11	D	503	JVI	C24-N25	4.72	1.47	1.39
5	A	501	GTP	C5-C6	-3.98	1.39	1.47
5	D	501	GTP	C5-C6	-3.97	1.39	1.47
11	B	505	JVI	C03-N04	-3.96	1.41	1.46
11	D	503	JVI	C03-N04	-3.92	1.41	1.46
5	C	501	GTP	C5-C6	-3.85	1.39	1.47
13	F	402	ACP	O4'-C1'	3.23	1.45	1.41
11	D	503	JVI	C24-C17	-3.22	1.36	1.40
11	B	505	JVI	C24-C17	-3.16	1.37	1.40
13	F	402	ACP	C6-N6	3.07	1.45	1.34
11	D	503	JVI	C03-C02	3.05	1.55	1.51
11	B	505	JVI	C03-C02	3.04	1.55	1.51
11	B	505	JVI	C17-N04	2.95	1.45	1.40
11	D	503	JVI	C17-N04	2.94	1.45	1.40
13	F	402	ACP	O3'-C3'	-2.86	1.36	1.43
13	F	402	ACP	O2'-C2'	2.86	1.49	1.43
13	F	402	ACP	C5-C4	-2.65	1.33	1.40
11	B	505	JVI	O01-C02	-2.43	1.18	1.23
11	D	503	JVI	O01-C02	-2.42	1.18	1.23
9	B	501	GDP	C6-N1	-2.33	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	JVI	C14-C13	2.32	1.55	1.51
11	B	505	JVI	C14-C13	2.30	1.55	1.51
5	D	501	GTP	C2-N3	2.23	1.38	1.33
5	A	501	GTP	C2-N3	2.20	1.38	1.33
5	C	501	GTP	C2-N3	2.19	1.38	1.33
13	F	402	ACP	C2-N3	2.15	1.35	1.32
11	B	505	JVI	C18-C17	2.12	1.43	1.39
13	F	402	ACP	PB-O2B	-2.07	1.51	1.56
11	D	503	JVI	C18-C17	2.04	1.43	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	503	JVI	C15-C16-C12	6.62	108.75	103.93
11	B	505	JVI	C15-C16-C12	5.93	108.25	103.93
13	F	402	ACP	N3-C2-N1	-5.35	120.32	128.68
11	D	503	JVI	C16-C12-N11	4.72	130.01	123.41
11	B	505	JVI	C16-C12-N11	4.60	129.84	123.41
10	B	502	MES	C5-N4-C3	4.52	119.01	108.83
10	B	503	MES	C5-N4-C3	4.38	118.69	108.83
11	B	505	JVI	C13-C12-N11	-4.07	121.34	125.80
5	D	501	GTP	PB-O3B-PG	-3.90	119.45	132.83
11	D	503	JVI	C16-C12-C13	-3.82	108.34	111.09
11	D	503	JVI	C13-C12-N11	-3.78	121.65	125.80
11	D	503	JVI	C24-N25-C02	-3.49	120.17	124.49
11	B	505	JVI	C24-N25-C02	-3.43	120.25	124.49
5	D	501	GTP	PA-O3A-PB	-3.29	121.53	132.83
5	C	501	GTP	C8-N7-C5	3.26	109.20	102.99
11	D	503	JVI	C15-C14-C13	3.26	107.81	103.52
5	A	501	GTP	C5-C6-N1	3.24	119.67	113.95
5	C	501	GTP	PB-O3B-PG	-3.21	121.82	132.83
11	B	505	JVI	N11-C07-N06	-3.18	121.20	126.23
11	B	505	JVI	C16-C12-C13	-3.16	108.81	111.09
5	D	501	GTP	C8-N7-C5	3.14	108.98	102.99
5	D	501	GTP	C5-C6-N1	3.13	119.48	113.95
11	B	505	JVI	C15-C14-C13	3.11	107.62	103.52
11	D	503	JVI	N11-C07-N06	-3.10	121.33	126.23
5	C	501	GTP	PA-O3A-PB	-3.04	122.41	132.83
5	A	501	GTP	PB-O3B-PG	-3.03	122.42	132.83
5	C	501	GTP	C5-C6-N1	2.97	119.20	113.95
5	A	501	GTP	PA-O3A-PB	-2.97	122.65	132.83
13	F	402	ACP	C5-C6-N6	2.96	124.85	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C8-N7-C5	2.95	108.62	102.99
9	B	501	GDP	PA-O3A-PB	-2.95	122.71	132.83
11	B	505	JVI	C09-N08-C07	-2.92	120.25	123.85
5	A	501	GTP	C2-N1-C6	-2.82	119.91	125.10
5	C	501	GTP	C2-N1-C6	-2.79	119.96	125.10
5	D	501	GTP	C2-N1-C6	-2.77	120.00	125.10
10	B	502	MES	O1S-S-C8	2.59	110.04	106.92
9	B	501	GDP	C8-N7-C5	2.44	107.64	102.99
10	B	503	MES	O3S-S-C8	2.43	109.70	105.77
11	D	503	JVI	C09-N08-C07	-2.41	120.88	123.85
11	D	503	JVI	C13-C05-N06	-2.29	119.07	122.61
9	B	501	GDP	C5-C6-N1	2.25	117.93	113.95
11	D	503	JVI	C07-N06-C05	2.22	122.00	114.34
10	B	502	MES	O3S-S-C8	2.21	109.33	105.77
10	B	503	MES	O2S-S-C8	2.20	109.57	106.92
10	B	503	MES	C6-C5-N4	-2.20	106.76	110.10
5	A	501	GTP	O6-C6-C5	-2.19	120.09	124.37
11	B	505	JVI	C07-N06-C05	2.19	121.90	114.34
5	D	501	GTP	O6-C6-C5	-2.17	120.13	124.37
11	B	505	JVI	C13-C05-N06	-2.16	119.28	122.61
10	B	503	MES	O1S-S-C8	2.08	109.42	106.92
5	D	501	GTP	C3'-C2'-C1'	2.05	104.07	100.98
10	B	502	MES	O2S-S-C8	2.04	109.37	106.92
11	B	505	JVI	C14-C13-C12	-2.02	108.57	110.96
5	C	501	GTP	O6-C6-C5	-2.02	120.43	124.37

There are no chirality outliers.

All (44) 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	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	502	MES	C7-C8-S-O1S
10	B	502	MES	C7-C8-S-O2S

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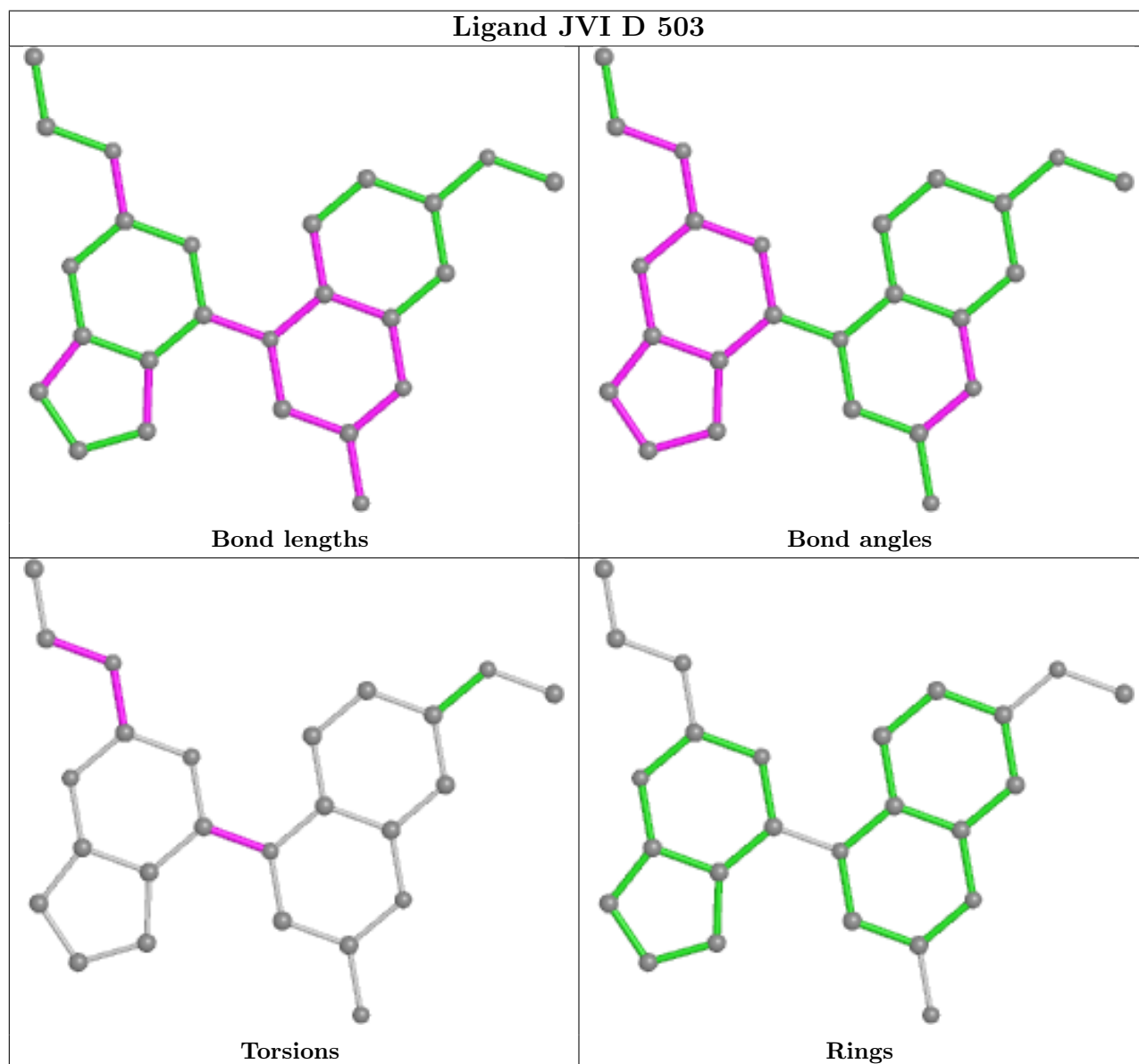
Mol	Chain	Res	Type	Atoms
13	F	402	ACP	PB-C3B-PG-O1G
13	F	402	ACP	PB-C3B-PG-O2G
11	B	505	JVI	N06-C05-N04-C03
11	D	503	JVI	N06-C05-N04-C03
11	B	505	JVI	C13-C05-N04-C03
11	D	503	JVI	C13-C05-N04-C03
10	B	502	MES	C7-C8-S-O3S
10	B	503	MES	C7-C8-S-O3S
11	B	505	JVI	C10-C09-N08-C07
11	D	503	JVI	C10-C09-N08-C07
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
5	D	501	GTP	C3'-C4'-C5'-O5'
13	F	402	ACP	PB-C3B-PG-O3G
5	D	501	GTP	PB-O3A-PA-O1A
10	B	502	MES	C8-C7-N4-C3
11	D	503	JVI	N06-C07-N08-C09
5	D	501	GTP	O4'-C4'-C5'-O5'
11	D	503	JVI	N11-C07-N08-C09
11	B	505	JVI	N11-C07-N08-C09
11	B	505	JVI	N06-C07-N08-C09
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G

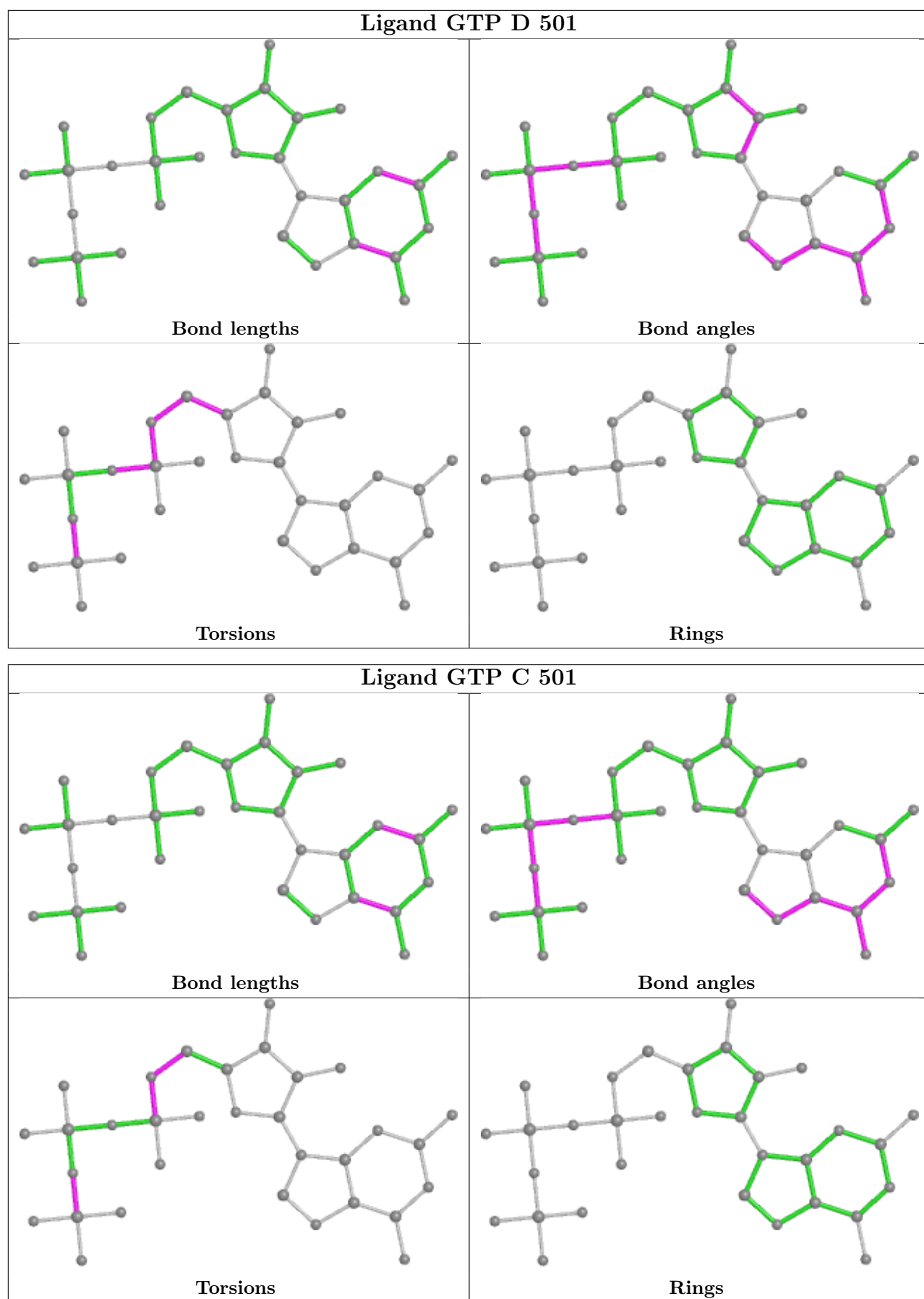
There are no ring outliers.

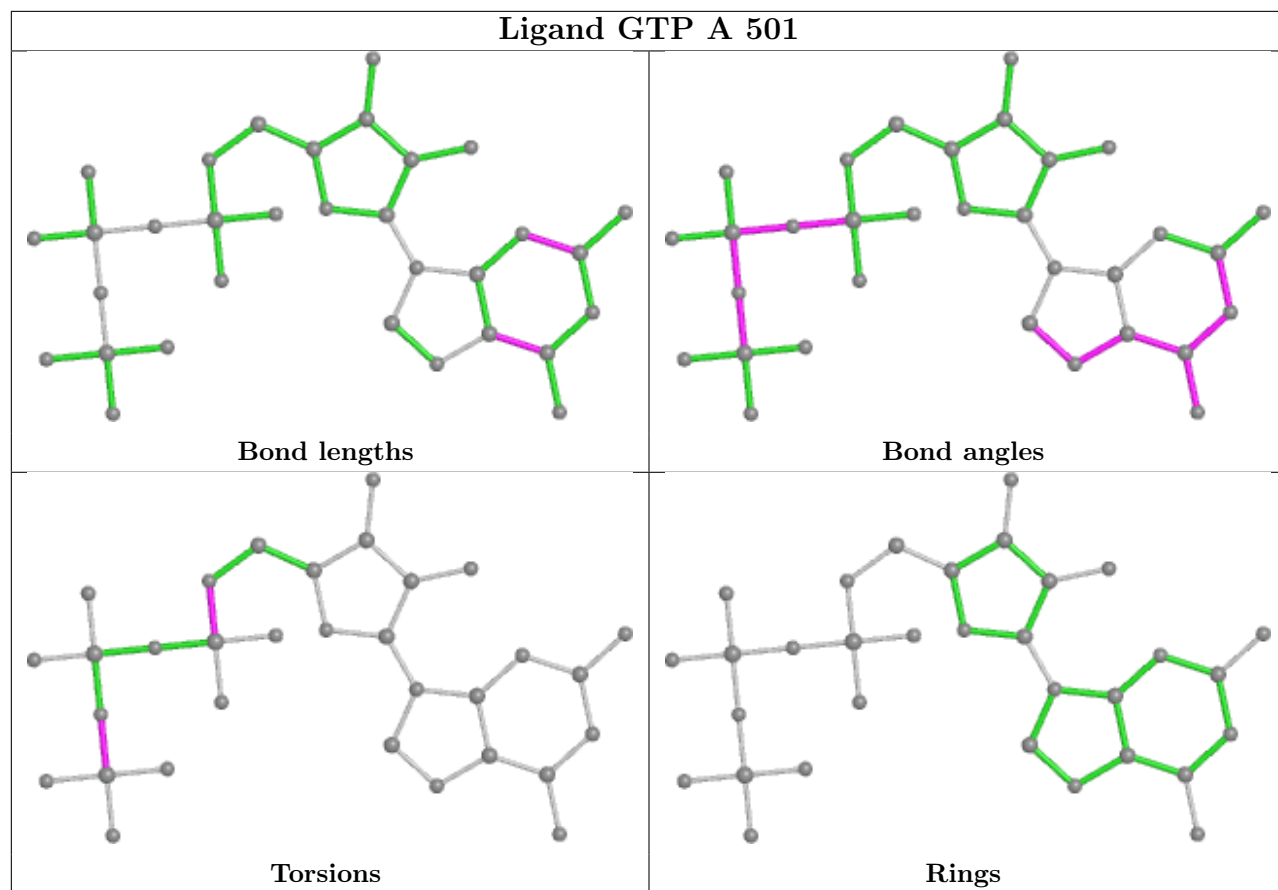
5 monomers are involved in 6 short contacts:

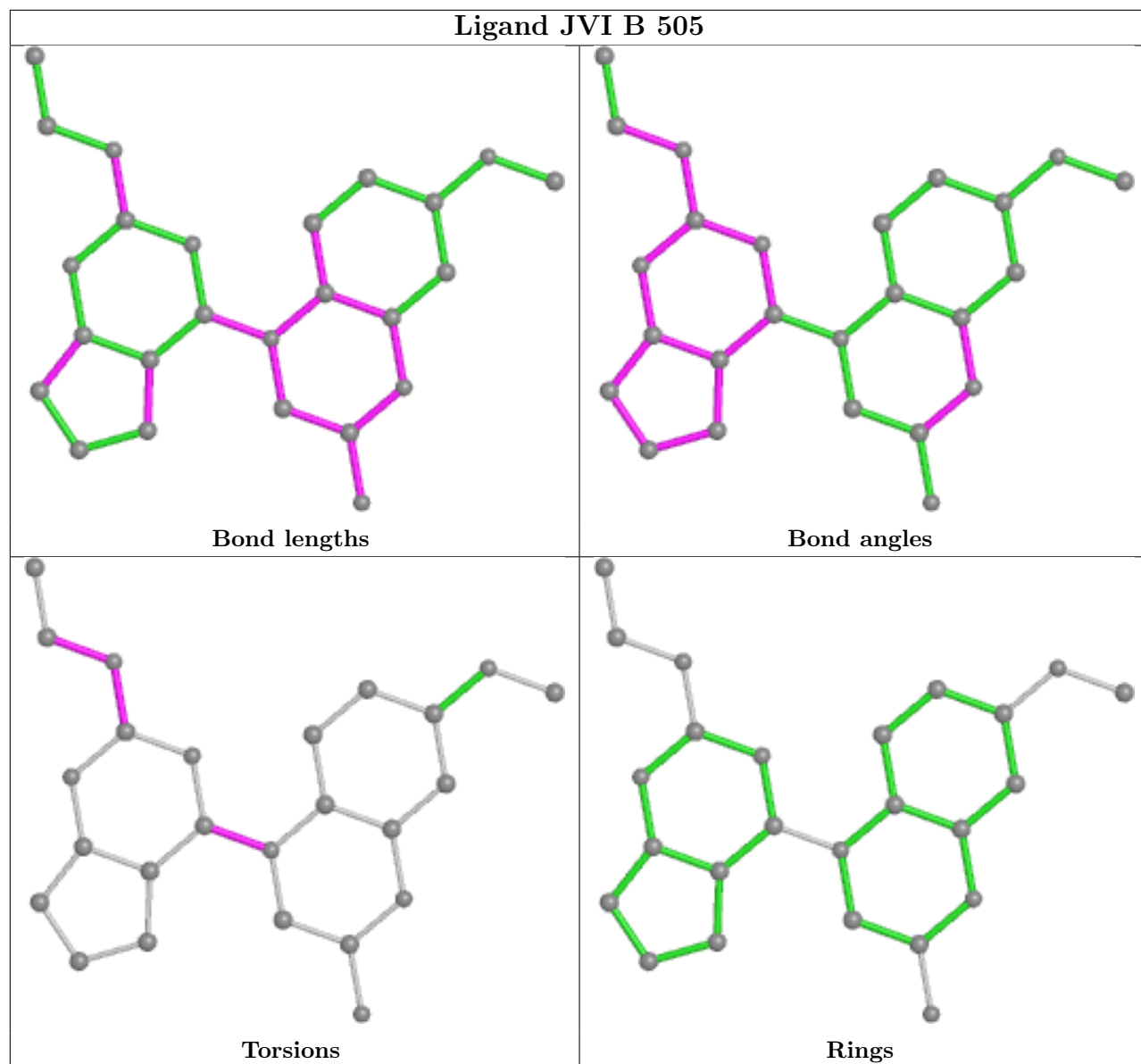
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	503	JVI	1	0
5	D	501	GTP	1	0
9	B	501	GDP	2	0
13	F	402	ACP	1	0
10	B	503	MES	1	0

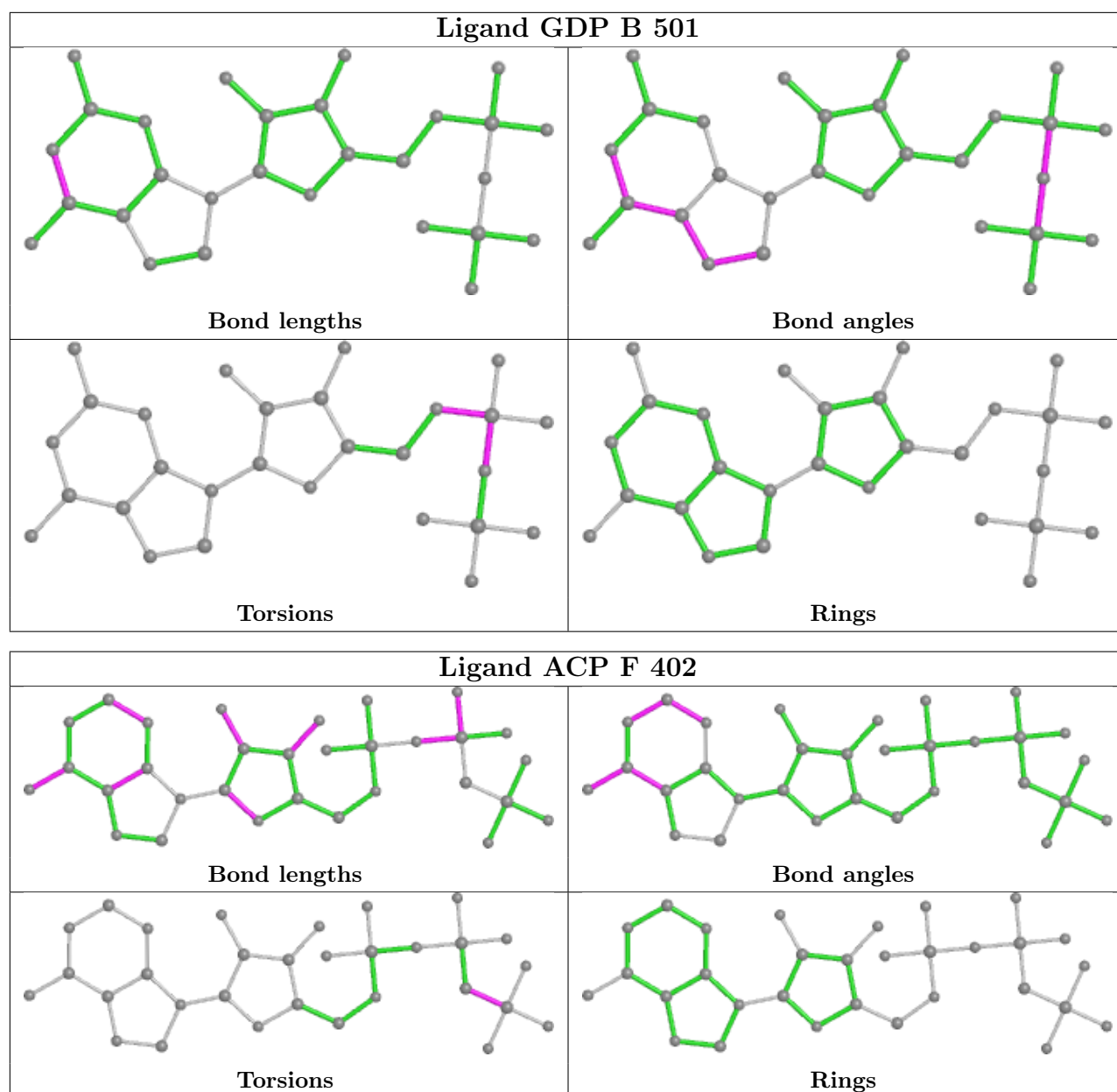
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	437/450 (97%)	-0.01	9 (2%) 63 61	36, 55, 87, 123	0
1	C	440/450 (97%)	-0.15	6 (1%) 75 73	27, 44, 72, 108	0
2	B	427/445 (95%)	0.13	21 (4%) 29 28	33, 53, 93, 133	0
2	D	420/445 (94%)	0.33	32 (7%) 13 12	39, 72, 108, 139	0
3	E	121/143 (84%)	0.54	14 (11%) 4 4	45, 71, 107, 135	0
4	F	320/384 (83%)	0.72	62 (19%) 1 0	45, 80, 137, 168	0
All	All	2165/2317 (93%)	0.19	144 (6%) 17 16	27, 60, 107, 168	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	6.5
4	F	172	PHE	4.8
1	A	282	TYR	4.8
2	B	427	ASP	4.8
4	F	379	HIS	4.8
4	F	125	THR	4.5
4	F	130	VAL	4.5
4	F	136	ASN	4.5
3	E	48	GLU	4.5
4	F	133	ALA	4.5
2	B	55	THR	4.3
4	F	242	ASN	4.3
4	F	182	ILE	4.3
2	D	217	LEU	4.3
4	F	89	GLU	4.2
2	D	37	HIS	4.2
4	F	255	ARG	4.2
3	E	29	PHE	4.2
4	F	181	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
4	F	165	GLU	4.1
4	F	132	LEU	4.1
4	F	152	SER	3.9
2	D	219	THR	3.9
3	E	26	PRO	3.9
2	B	57	ASN	3.9
2	B	72	THR	3.8
2	D	55	THR	3.8
4	F	160	ILE	3.8
1	A	281	ALA	3.8
4	F	167	SER	3.8
2	B	275	SER	3.7
4	F	246	GLN	3.7
4	F	175	GLU	3.6
3	E	45	PRO	3.6
2	D	125	GLU	3.6
4	F	45	ASN	3.5
4	F	102	PRO	3.5
3	E	28	SER	3.5
4	F	243	HIS	3.5
4	F	228	TYR	3.5
4	F	179	VAL	3.4
4	F	46	ARG	3.4
2	B	279	GLN	3.4
2	D	78	SER	3.4
2	D	126	SER	3.4
1	A	437	VAL	3.3
4	F	253	TYR	3.3
3	E	138	GLU	3.3
2	D	58	LYS	3.3
4	F	170	LEU	3.3
2	D	284	LEU	3.2
1	A	346	TRP	3.2
2	B	277	GLY	3.2
4	F	230	SER	3.2
2	D	187	LEU	3.2
4	F	259	GLY	3.1
3	E	25	LYS	3.1
2	B	80	PRO	3.1
4	F	101	TYR	3.1
4	F	10	ASN	3.1
4	F	245	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	362	ALA	3.0
1	A	220	GLU	3.0
4	F	229	ASN	3.0
2	D	80	PRO	3.0
2	D	73	MET	3.0
3	E	135	LYS	3.0
2	D	218	THR	2.9
3	E	46	SER	2.9
4	F	135	TYR	2.9
4	F	180	HIS	2.9
2	D	94	GLN	2.9
1	C	1	MET	2.9
3	E	27	PRO	2.9
4	F	173	ILE	2.8
2	D	406	MET	2.8
4	F	9	GLU	2.8
4	F	134	ALA	2.8
2	D	362	LYS	2.8
3	E	139	LEU	2.8
1	C	340	SER	2.7
1	A	364	PRO	2.7
4	F	144	GLY	2.7
2	D	429	THR	2.7
1	A	262	TYR	2.7
3	E	140	LYS	2.6
4	F	256	TYR	2.6
4	F	151	SER	2.6
4	F	194	PRO	2.6
2	B	54	ALA	2.6
2	B	56	GLY	2.5
2	D	216	LYS	2.5
4	F	169	LEU	2.5
4	F	247	LYS	2.5
4	F	240	LEU	2.5
3	E	6	MET	2.5
1	C	209	ILE	2.5
2	B	7	ILE	2.5
1	C	245	ASP	2.5
4	F	31	ARG	2.4
2	D	42	LEU	2.4
4	F	90	SER	2.4
4	F	145	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	128	ASP	2.4
2	D	81	PHE	2.4
4	F	373	SER	2.4
1	C	357	TYR	2.4
1	C	283	HIS	2.4
2	D	92	PHE	2.3
1	A	163	LYS	2.3
4	F	161	LEU	2.3
4	F	199	PHE	2.3
2	B	282	ARG	2.3
2	D	177	ASP	2.3
2	D	95	SER	2.3
4	F	129	GLU	2.3
4	F	174	ASP	2.3
2	D	54	ALA	2.3
4	F	24	THR	2.2
4	F	306	HIS	2.2
4	F	274	ALA	2.2
2	B	37	HIS	2.2
2	B	64	ILE	2.2
2	D	245	GLN	2.2
3	E	96	MET	2.2
4	F	183	GLN	2.2
4	F	44	ARG	2.2
2	D	183	TYR	2.1
2	B	276	ARG	2.1
2	B	78	SER	2.1
2	B	278	SER	2.1
4	F	83	THR	2.1
2	D	391	ARG	2.1
2	B	92	PHE	2.1
2	B	125	GLU	2.1
4	F	171	ASP	2.1
2	D	359	ARG	2.1
2	D	56	GLY	2.1
2	B	9	ALA	2.0
2	D	335	ASN	2.0
2	D	221	THR	2.0
1	A	365	GLY	2.0
2	D	72	THR	2.0
4	F	126	ASP	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](#)

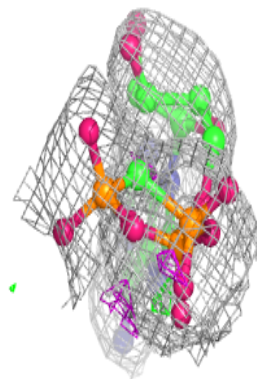
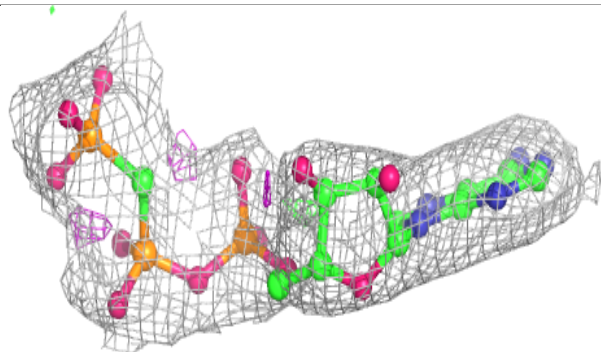
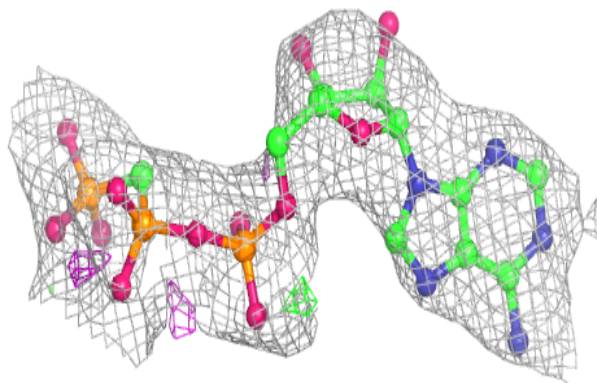
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	D	502	1/1	0.57	0.21	97,97,97,97	0
8	DMS	C	504	4/4	0.68	0.27	110,113,114,115	0
12	GOL	B	506	6/6	0.81	0.22	101,103,104,105	0
10	MES	B	503	12/12	0.82	0.34	85,88,95,100	12
13	ACP	F	402	31/31	0.85	0.19	77,90,120,124	0
8	DMS	A	504	4/4	0.86	0.27	110,112,115,116	0
7	MG	F	401	1/1	0.87	0.13	84,84,84,84	0
5	GTP	D	501	32/32	0.93	0.14	55,67,111,117	0
11	JVI	D	503	25/25	0.94	0.13	53,63,79,83	0
10	MES	B	502	12/12	0.94	0.16	54,70,83,85	0
6	CA	A	502	1/1	0.94	0.03	72,72,72,72	0
6	CA	C	502	1/1	0.96	0.03	53,53,53,53	0
7	MG	A	503	1/1	0.96	0.05	39,39,39,39	0
11	JVI	B	505	25/25	0.96	0.11	38,47,66,78	0
7	MG	B	504	1/1	0.97	0.03	46,46,46,46	0
5	GTP	C	501	32/32	0.98	0.11	27,37,45,46	0
9	GDP	B	501	28/28	0.98	0.10	34,43,47,51	0
5	GTP	A	501	32/32	0.98	0.10	30,42,48,52	0
7	MG	C	503	1/1	0.98	0.07	37,37,37,37	0

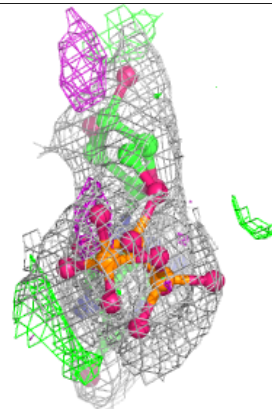
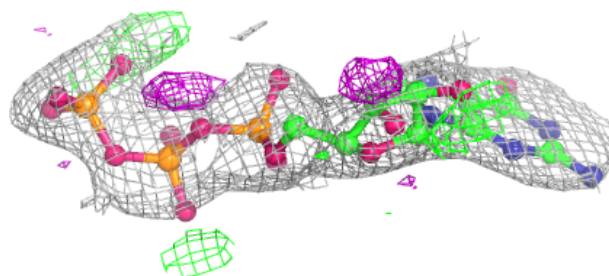
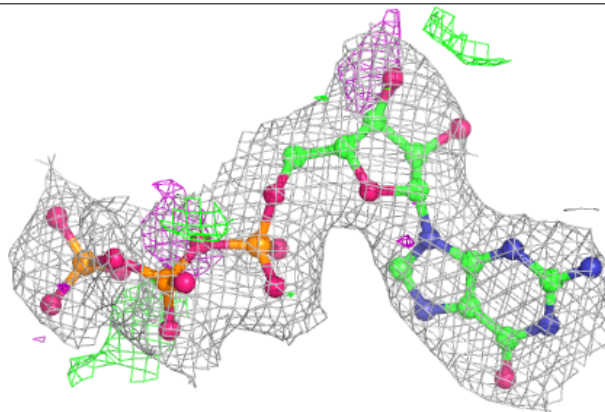
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

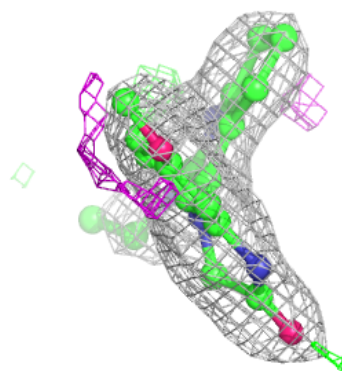
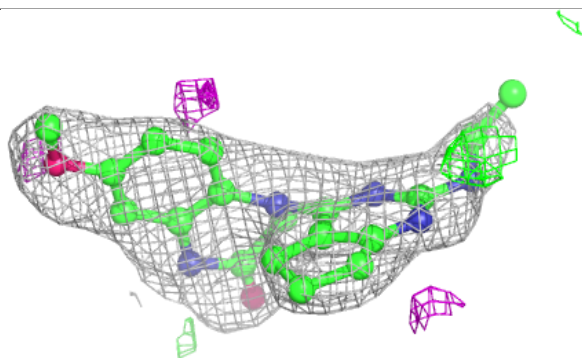
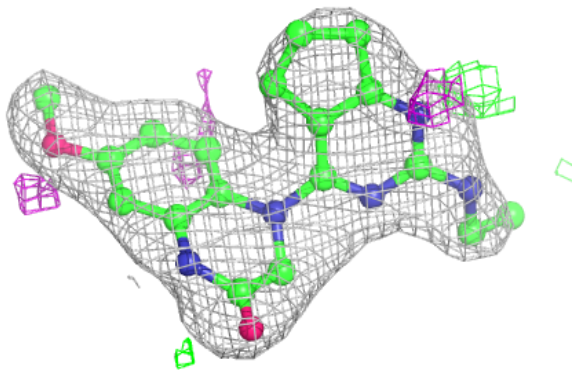
**Electron density around GTP D 501:**

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

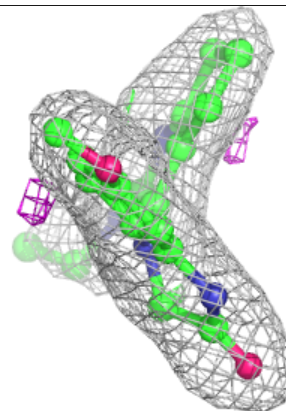
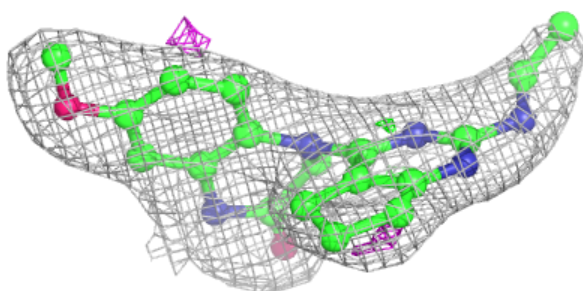
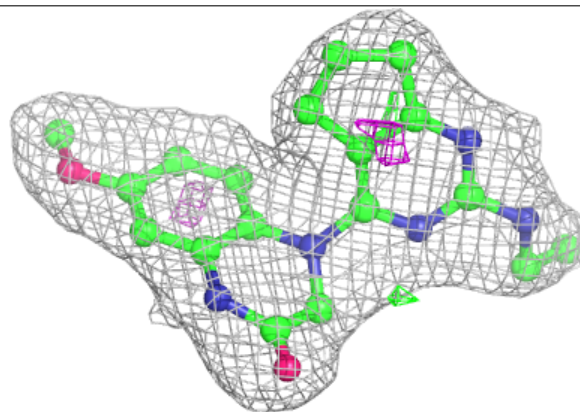


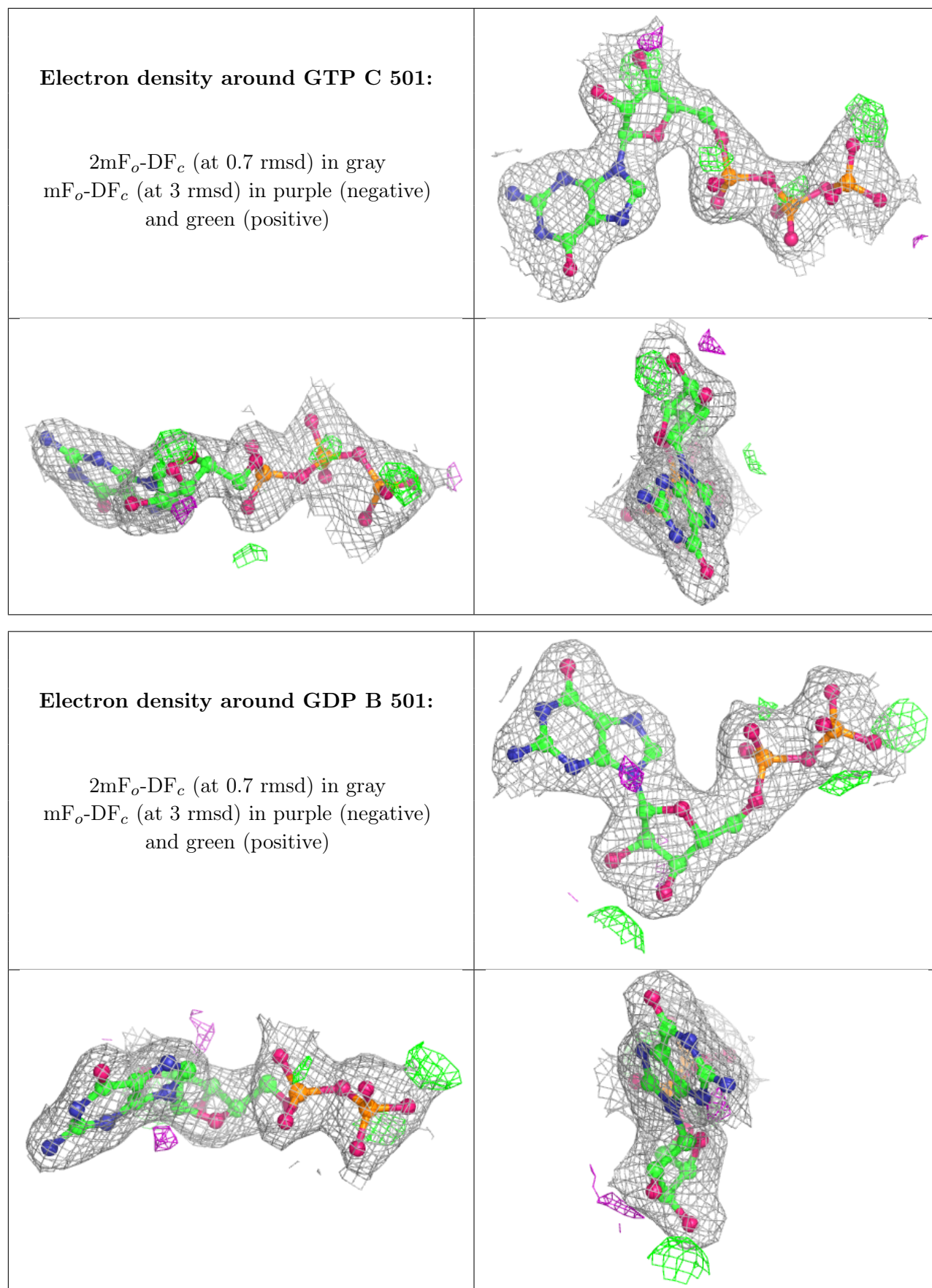
Electron density around JVI D 503:

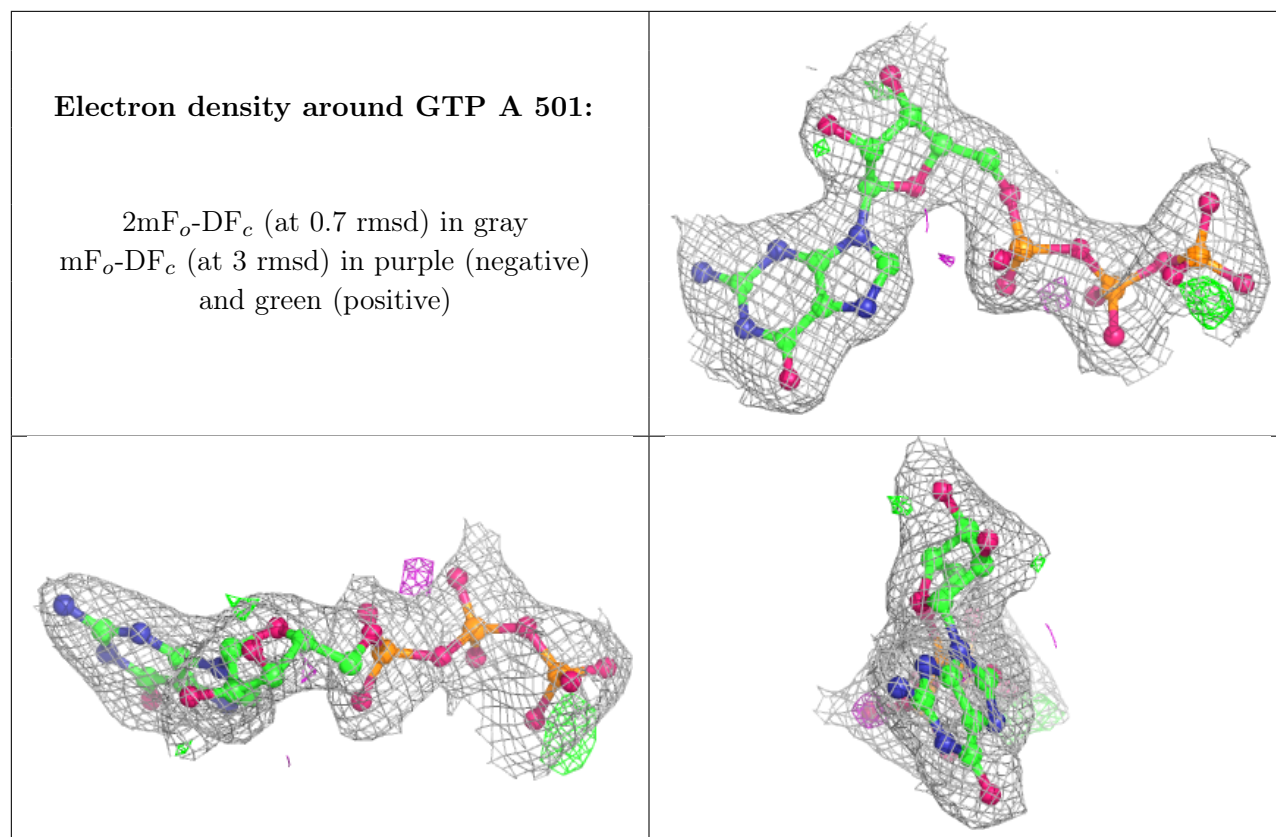
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around JVI 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)







6.5 Other polymers [i](#)

There are no such residues in this entry.