



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:08 AM UTC

PDB ID : 6GF3 / pdb_00006gf3
Title : Tubulin-Jerantinine B acetate complex
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Deposited on : 2018-04-29
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	:	4-5-2 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

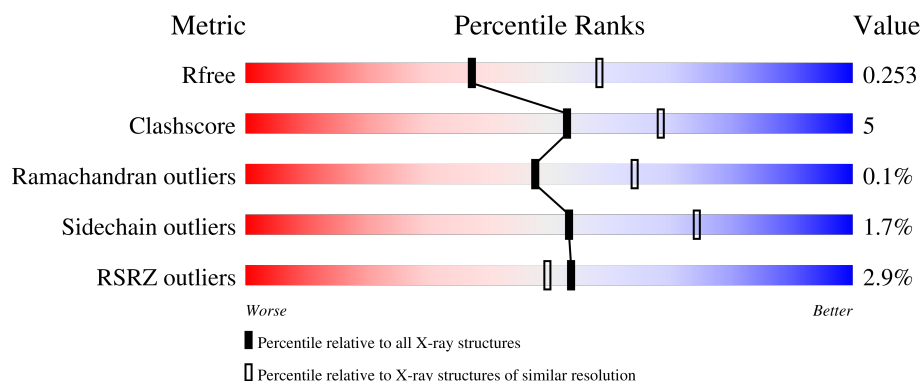
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

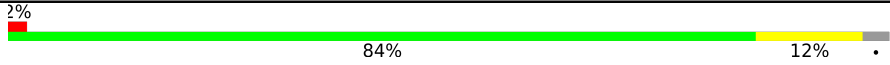
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	451	
1	C	451	
2	B	445	
3	D	445	

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Mol	Chain	Length	Quality of chain
4	E	143	6% 75% 10% 15%
5	F	384	5% 60% 12% 26%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 17309 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	6	0
			3445	2188	583	652	22			
1	C	440	Total	C	N	O	S	0	8	0
			3474	2198	588	664	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	6	0
			3344	2103	569	645	27			

- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	421	Total	C	N	O	S	0	2	0
			3316	2085	562	641	28			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	247	ASN	GLN	conflict	UNP Q6B856

- Molecule 4 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	121	Total	C	N	O	S	0	1	0
			1006	621	182	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043

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

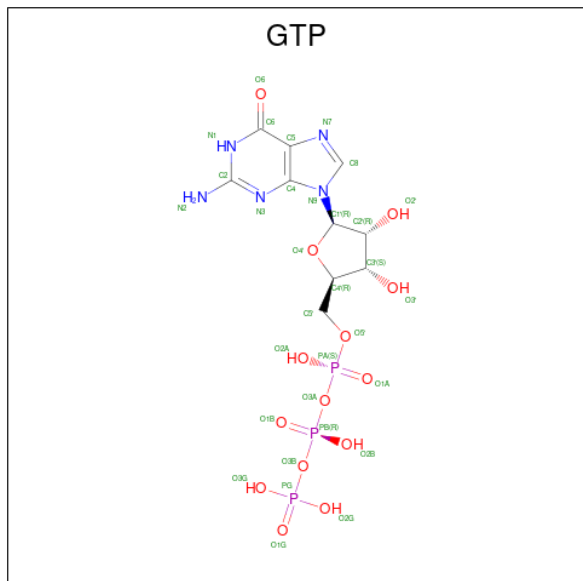
- Molecule 5 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	284	Total	C	N	O	S	0	4	0
			2354	1530	392	420	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 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

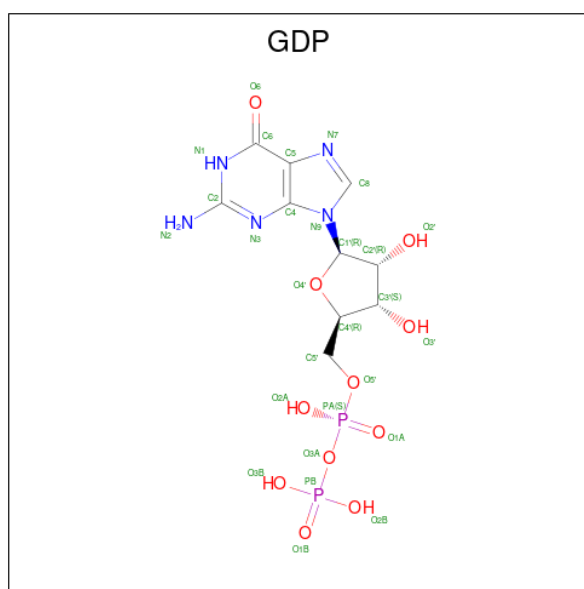
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

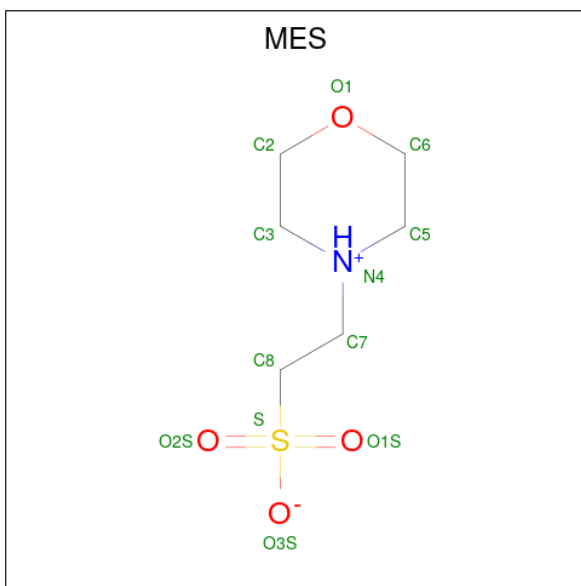
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

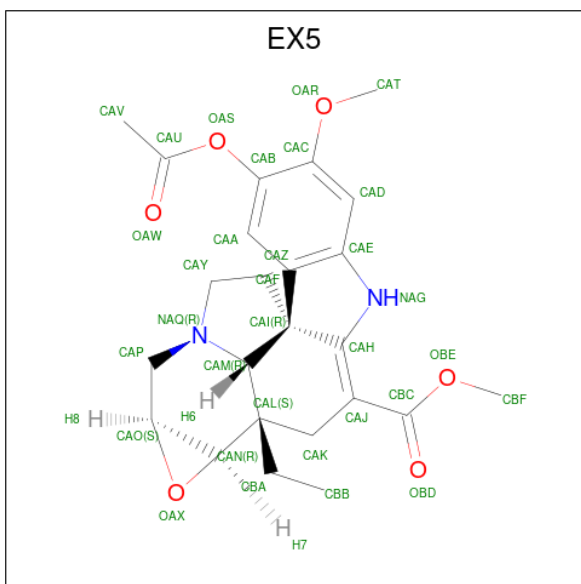
- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES)

(formula: C₆H₁₃NO₄S).



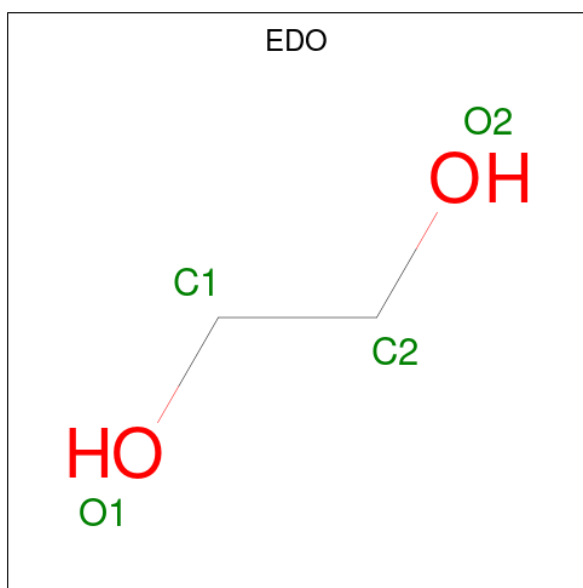
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is Jerantinine B (CCD ID: EX5) (formula: C₂₄H₂₈N₂O₆).



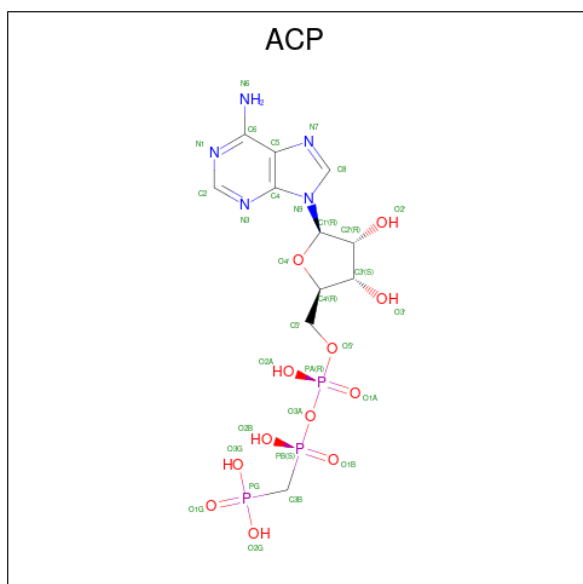
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			32	24	2	6		

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: 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		

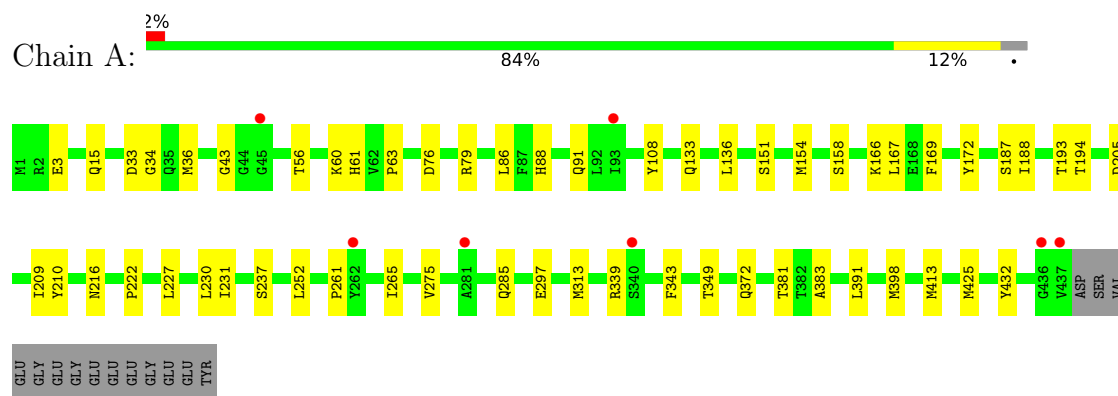
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	30	Total 30	O 30	0	0
14	B	30	Total 30	O 30	0	0
14	C	63	Total 63	O 63	0	0
14	D	9	Total 9	O 9	0	0
14	E	8	Total 8	O 8	0	0
14	F	13	Total 13	O 13	0	0

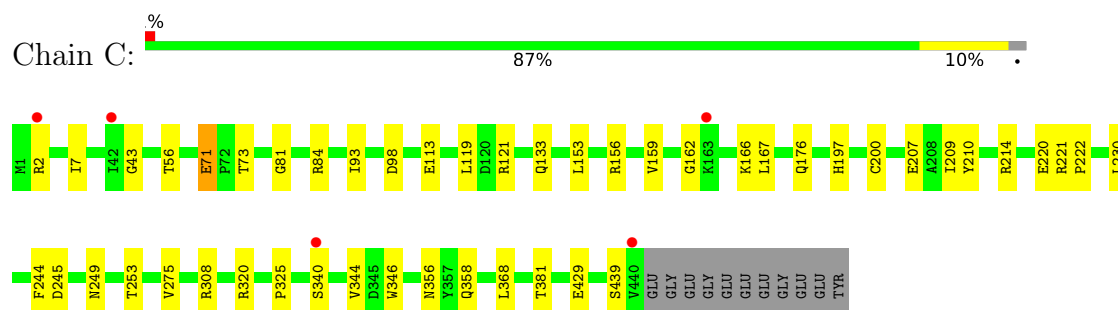
3 Residue-property plots [i](#)

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.

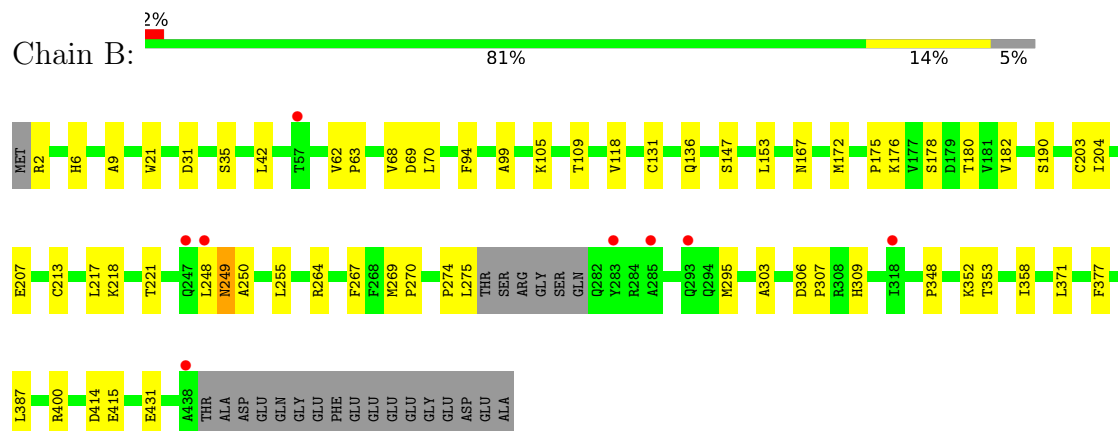
• Molecule 1: Tubulin alpha-1B chain



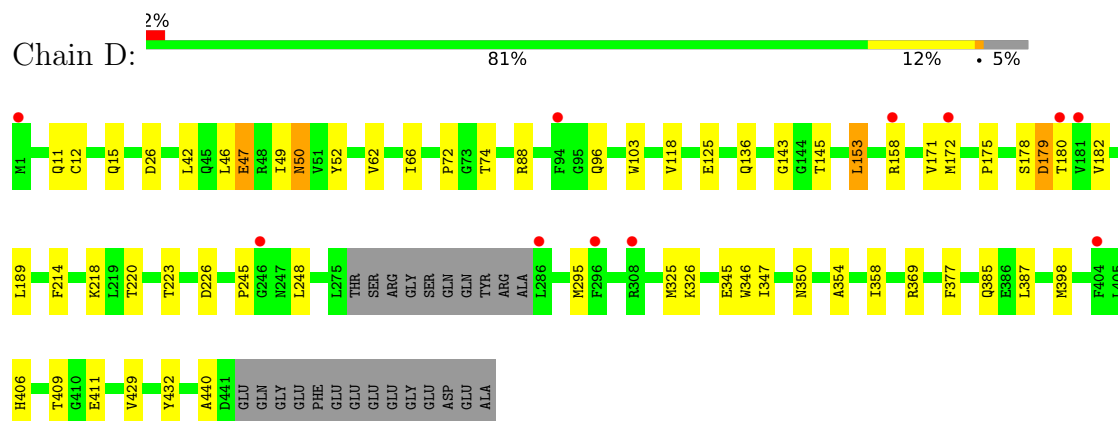
• Molecule 1: Tubulin alpha-1B chain



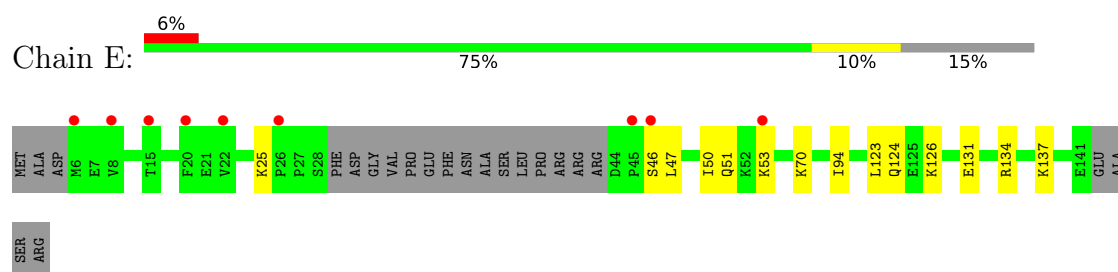
• Molecule 2: Tubulin beta-2B chain



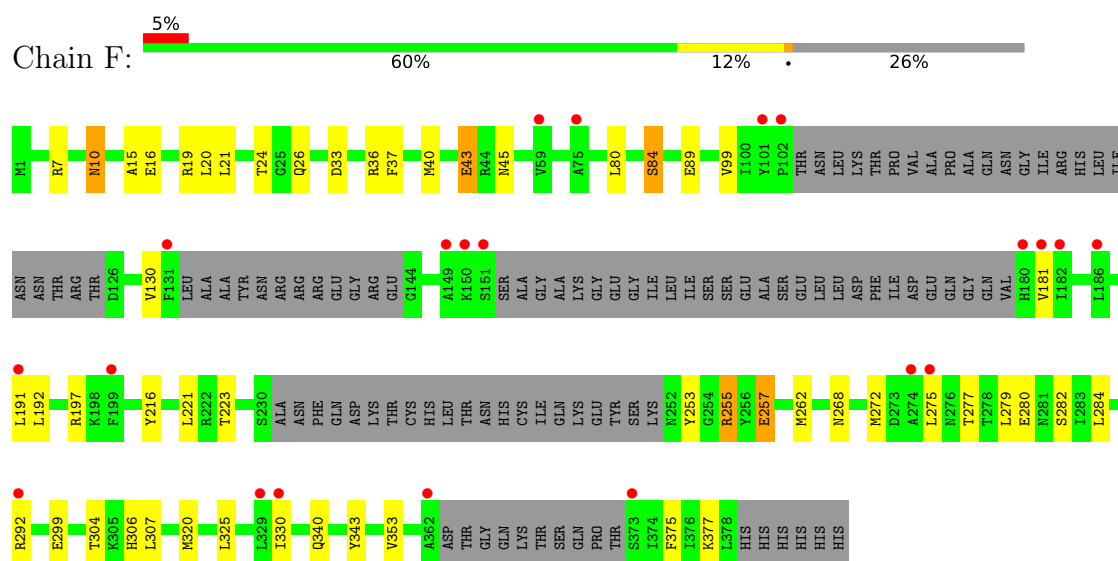
- Molecule 3: Tubulin beta-2B chain



- Molecule 4: Stathmin-4



- Molecule 5: 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	104.72Å 158.15Å 180.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 2.40 47.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.96-2.40) 99.6 (47.96-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.198 , 0.251 0.201 , 0.253	Depositor DCC
R_{free} test set	5877 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17309	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: CA, EX5, ACP, GTP, GDP, MES, MG, EDO

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	0.13	0/3541	0.32	0/4808
1	C	0.15	0/3573	0.33	0/4852
2	B	0.13	0/3430	0.31	0/4646
3	D	0.13	0/3395	0.33	2/4599 (0.0%)
4	E	0.11	0/1017	0.27	0/1349
5	F	0.12	0/2419	0.32	0/3266
All	All	0.13	0/17375	0.32	2/23520 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	440	ALA	CB-CA-C	-7.29	105.82	116.53
3	D	440	ALA	CA-C-O	6.91	122.68	118.33

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	3445	0	3384	33	0
1	C	3474	0	3393	29	0
2	B	3344	0	3224	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	3316	0	3201	38	0
4	E	1006	0	1026	11	0
5	F	2354	0	2361	31	0
6	A	32	0	12	1	0
6	C	32	0	12	1	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
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	5	0
10	B	12	0	12	1	0
10	D	12	0	12	1	0
11	B	32	0	0	0	0
12	C	4	0	6	1	0
13	F	31	0	14	2	0
14	A	30	0	0	1	0
14	B	30	0	0	0	0
14	C	63	0	0	0	0
14	D	9	0	0	2	0
14	E	8	0	0	0	0
14	F	13	0	0	1	0
All	All	17309	0	16681	169	0

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

All (169) 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)
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.24	0.71
13:F:401:ACP:H8	13:F:401:ACP:H5'1	1.75	0.69
3:D:11:GLN:HA	3:D:74:THR:HG21	1.75	0.67
3:D:66:ILE:HD11	3:D:125:GLU:HG3	1.77	0.67
1:A:381:THR:HG22	1:A:383:ALA:H	1.61	0.66
4:E:131:GLU:OE1	4:E:134:ARG:NH1	2.28	0.66
3:D:62:VAL:HG11	3:D:88:ARG:HG3	1.79	0.64
5:F:292:ARG:NH2	14:F:502:HOH:O	2.30	0.64
5:F:280:GLU:HA	5:F:284[B]:LEU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.79	0.63
2:B:118:VAL:HG11	2:B:153:LEU:HD21	1.80	0.62
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.80	0.62
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.81	0.61
5:F:24:THR:HG23	5:F:26:GLN:H	1.65	0.61
3:D:11:GLN:NE2	14:D:602:HOH:O	2.34	0.60
3:D:385:GLN:HB2	3:D:429:VAL:HG13	1.82	0.59
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.84	0.59
5:F:275:LEU:HD23	5:F:325:LEU:HD12	1.84	0.59
5:F:197:ARG:NH1	5:F:257:GLU:OE2	2.31	0.58
5:F:7:ARG:HG3	5:F:40:MET:HE3	1.84	0.58
3:D:179:ASP:HB2	9:D:501:GDP:H3'	1.85	0.58
2:B:180:THR:HG22	2:B:182:VAL:H	1.69	0.57
3:D:118:VAL:HG11	3:D:153:LEU:HD11	1.86	0.57
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.23	0.57
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.23	0.57
1:C:162:GLY:HA2	4:E:94:ILE:HD11	1.88	0.56
3:D:47:GLU:HG2	3:D:245:PRO:HG3	1.87	0.55
5:F:192:LEU:HD11	5:F:262:MET:HE1	1.89	0.55
5:F:279:LEU:HG	5:F:284[B]:LEU:HG	1.88	0.55
3:D:411:GLU:HA	4:E:137:LYS:HD2	1.89	0.55
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.89	0.55
3:D:46:LEU:HA	3:D:49:ILE:HB	1.91	0.53
5:F:255:ARG:CZ	5:F:255:ARG:HA	2.39	0.53
2:B:175:PRO:HA	2:B:178:SER:HB2	1.89	0.53
3:D:145:THR:N	9:D:501:GDP:O2B	2.39	0.53
3:D:158:ARG:HH21	10:D:503:MES:H52	1.73	0.52
3:D:406:HIS:HA	3:D:409:THR:HG22	1.90	0.52
3:D:26:ASP:CG	3:D:369:ARG:HE	2.18	0.52
3:D:347:ILE:HG22	3:D:350:ASN:HB3	1.92	0.52
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.92	0.51
3:D:175:PRO:HA	3:D:178:SER:HB3	1.92	0.51
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.43	0.50
5:F:223:THR:OG1	5:F:257:GLU:OE2	2.24	0.50
2:B:249:ASN:H	2:B:249:ASN:HD22	1.58	0.50
3:D:182:VAL:HA	3:D:398:MET:HE1	1.94	0.50
1:C:71:GLU:HG2	1:C:73:THR:H	1.76	0.50
1:A:3:GLU:O	1:A:133:GLN:HG2	2.12	0.50
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.94	0.50
5:F:216:TYR:HA	5:F:375:PHE:HD1	1.76	0.50
1:A:154:MET:HG3	1:A:194:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.94	0.50
5:F:221:LEU:HD22	5:F:262:MET:HE3	1.94	0.50
5:F:99:VAL:HG12	5:F:181:VAL:HG12	1.93	0.49
5:F:340:GLN:HA	5:F:343:TYR:HD2	1.77	0.49
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.93	0.49
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.95	0.49
3:D:172:MET:HG2	3:D:387:LEU:HD11	1.95	0.48
5:F:282:SER:HB2	5:F:325:LEU:HD13	1.95	0.48
5:F:80:LEU:O	5:F:84:SER:HB2	2.13	0.48
1:A:158:SER:OG	1:A:166:LYS:NZ	2.46	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.28	0.48
1:A:34:GLY:HA3	1:A:60:LYS:HD3	1.95	0.48
5:F:320:MET:HE2	5:F:330:ILE:HD11	1.94	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.48
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.49	0.48
3:D:248:LEU:HD23	3:D:354:ALA:HB2	1.95	0.48
1:A:151:SER:HB2	1:A:193:THR:HB	1.95	0.48
5:F:320:MET:HB2	5:F:330:ILE:HD11	1.95	0.48
5:F:21:LEU:O	5:F:24:THR:HG22	2.13	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.96	0.47
3:D:72:PRO:HG3	3:D:96:GLN:HE22	1.79	0.47
3:D:158:ARG:HD3	4:E:123:LEU:HD11	1.95	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.47
5:F:43:GLU:HG3	5:F:45:ASN:O	2.15	0.47
1:C:159:VAL:HA	4:E:94:ILE:HG23	1.97	0.47
4:E:126:LYS:HE3	4:E:126:LYS:HB3	1.73	0.47
1:C:221:ARG:NH1	3:D:325:MET:HB3	2.30	0.47
1:A:136[B]:LEU:HD23	1:A:169:PHE:HE2	1.80	0.47
2:B:69:ASP:O	2:B:94:PHE:HA	2.15	0.46
1:C:245:ASP:N	1:C:245:ASP:OD1	2.48	0.46
2:B:136:GLN:HA	2:B:167:ASN:O	2.15	0.46
1:C:244:PHE:CD1	1:C:358[B]:GLN:HG2	2.51	0.46
1:A:349:THR:HB	4:E:25:LYS:HB3	1.97	0.46
5:F:268:ASN:HD21	5:F:272:MET:HE2	1.80	0.46
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.97	0.46
1:C:166:LYS:HE2	1:C:197:HIS:O	2.16	0.46
2:B:274:PRO:HD2	2:B:371:LEU:HD13	1.97	0.46
3:D:346:TRP:CD1	3:D:346:TRP:H	2.33	0.46
1:C:244:PHE:HB2	1:C:356[B]:ASN:HD21	1.80	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.45
3:D:214:PHE:CE2	3:D:220:THR:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASP:HB2	6:C:501:GTP:O3G	2.17	0.45
1:C:220:GLU:HB3	3:D:326:LYS:HD2	1.99	0.45
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.82	0.44
3:D:11:GLN:N	9:D:501:GDP:O3B	2.46	0.44
2:B:221:THR:HG21	1:C:325:PRO:HB2	1.98	0.44
2:B:180:THR:CG2	2:B:182:VAL:HG22	2.48	0.44
2:B:250:ALA:HB1	2:B:255:LEU:HD21	2.00	0.44
2:B:269:MET:HG2	2:B:303:ALA:HB3	1.99	0.44
2:B:400:ARG:HE	1:C:439:SER:HB3	1.83	0.44
1:C:81:GLY:O	1:C:84:ARG:NH1	2.47	0.44
5:F:10:ASN:OD1	5:F:10:ASN:N	2.50	0.44
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.43
1:A:209[B]:ILE:HG13	1:A:227:LEU:HD22	2.00	0.43
4:E:46:SER:OG	4:E:47:LEU:N	2.51	0.43
13:F:401:ACP:O2G	13:F:401:ACP:O1A	2.36	0.43
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	2.00	0.43
2:B:180:THR:HG22	2:B:182:VAL:HG22	1.99	0.43
4:E:50:ILE:HA	4:E:53:LYS:HD3	2.00	0.43
1:A:15:GLN:NE2	6:A:501:GTP:O6	2.51	0.43
1:A:63:PRO:HD3	1:A:86:LEU:HD12	2.01	0.43
3:D:295:MET:HG2	3:D:377:PHE:HB2	2.01	0.43
3:D:143:GLY:HA3	9:D:501:GDP:O3A	2.18	0.43
3:D:52:TYR:OH	3:D:136:GLN:NE2	2.49	0.43
1:A:237:SER:HB2	14:A:614:HOH:O	2.19	0.42
2:B:9:ALA:HA	2:B:68:VAL:O	2.20	0.42
3:D:50:ASN:ND2	3:D:50:ASN:H	2.17	0.42
5:F:340:GLN:N	5:F:340:GLN:OE1	2.52	0.42
1:A:285:GLN:HG3	1:A:372[B]:GLN:OE1	2.20	0.42
2:B:264[A]:ARG:NE	2:B:431:GLU:OE1	2.38	0.42
3:D:12:CYS:SG	3:D:171:VAL:HG21	2.59	0.42
5:F:15:ALA:O	5:F:19:ARG:HG3	2.19	0.42
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.01	0.42
2:B:70:LEU:HD12	2:B:99:ALA:HB2	2.01	0.42
3:D:223:THR:HG22	3:D:226:ASP:OD1	2.20	0.42
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.36	0.42
2:B:2:ARG:HA	2:B:131:CYS:O	2.20	0.42
2:B:42:LEU:HB3	2:B:358:ILE:HD11	2.01	0.42
3:D:214:PHE:O	3:D:218:LYS:HD2	2.19	0.42
3:D:218:LYS:HB3	3:D:218:LYS:HE3	1.86	0.42
10:B:502:MES:H81	10:B:502:MES:H51	1.78	0.42
3:D:42:LEU:HB2	3:D:358:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
4:E:70:LYS:HB2	4:E:70:LYS:HE3	1.72	0.41
5:F:37:PHE:CE1	5:F:40:MET:HB2	2.54	0.41
5:F:216:TYR:HA	5:F:375:PHE:CD1	2.55	0.41
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.01	0.41
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.55	0.41
2:B:414:ASP:OD1	2:B:415:GLU:N	2.52	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41
5:F:33:ASP:OD1	5:F:33:ASP:N	2.53	0.41
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.56	0.41
2:B:31:ASP:OD2	2:B:35:SER:OG	2.38	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.55	0.41
1:C:244:PHE:CZ	1:C:358[A]:GLN:HG2	2.55	0.41
5:F:16:GLU:OE1	5:F:19:ARG:NH2	2.38	0.41
1:A:43:GLY:HA2	1:A:56:THR:O	2.21	0.41
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.56	0.41
1:A:398:MET:HG3	2:B:348:PRO:HD2	2.03	0.41
2:B:204:ILE:HD13	2:B:270:PRO:HG2	2.02	0.41
1:C:2:ARG:HH21	1:C:133:GLN:NE2	2.19	0.41
1:C:43:GLY:HA2	1:C:56:THR:O	2.21	0.41
2:B:352:LYS:HD3	2:B:353:THR:N	2.35	0.41
1:C:253:THR:HB	12:C:504:EDO:H11	2.03	0.41
3:D:11:GLN:HB2	9:D:501:GDP:O2A	2.21	0.41
3:D:432:TYR:OH	14:D:601:HOH:O	2.22	0.41
2:B:295:MET:CG	2:B:377:PHE:HB2	2.51	0.40
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.86	0.40
1:A:297:GLU:OE1	5:F:306:HIS:ND1	2.43	0.40
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.61	0.40
1:C:210:TYR:HE2	1:C:214:ARG:HH11	1.70	0.40
4:E:47:LEU:O	4:E:51:GLN:HG2	2.22	0.40
5:F:268:ASN:ND2	5:F:272:MET:HE2	2.36	0.40
5:F:304:THR:HG22	5:F:307:LEU:HD12	2.02	0.40
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.56	0.40
2:B:218:LYS:HD3	2:B:218:LYS:HA	1.94	0.40
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.04	0.40
3:D:103:TRP:CE3	3:D:189:LEU:HD13	2.56	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	441/451 (98%)	429 (97%)	12 (3%)	0	100	100
1	C	446/451 (99%)	438 (98%)	8 (2%)	0	100	100
2	B	423/445 (95%)	410 (97%)	12 (3%)	1 (0%)	43	58
3	D	419/445 (94%)	404 (96%)	15 (4%)	0	100	100
4	E	118/143 (82%)	115 (98%)	3 (2%)	0	100	100
5	F	275/384 (72%)	257 (94%)	17 (6%)	1 (0%)	30	43
All	All	2122/2319 (92%)	2053 (97%)	67 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	253	TYR
2	B	248	LEU

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	374/379 (99%)	373 (100%)	1 (0%)	86	93
1	C	379/379 (100%)	373 (98%)	6 (2%)	55	76
2	B	369/383 (96%)	366 (99%)	3 (1%)	73	86
3	D	366/383 (96%)	359 (98%)	7 (2%)	50	71
4	E	110/127 (87%)	109 (99%)	1 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	261/342 (76%)	246 (94%)	15 (6%)	18	33
All	All	1859/1993 (93%)	1826 (98%)	33 (2%)	53	73

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
2	B	62	VAL
2	B	249	ASN
2	B	275	LEU
1	C	71	GLU
1	C	113	GLU
1	C	308	ARG
1	C	340	SER
1	C	381	THR
1	C	429	GLU
3	D	15	GLN
3	D	47	GLU
3	D	50	ASN
3	D	153	LEU
3	D	179	ASP
3	D	180	THR
3	D	345	GLU
4	E	124	GLN
5	F	10	ASN
5	F	20	LEU
5	F	36	ARG
5	F	43	GLU
5	F	84	SER
5	F	89	GLU
5	F	130	VAL
5	F	191	LEU
5	F	255	ARG
5	F	257	GLU
5	F	277	THR
5	F	299	GLU
5	F	353[A]	VAL
5	F	353[B]	VAL
5	F	377	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	216	ASN
1	A	393	HIS
2	B	6	HIS
2	B	11	GLN
2	B	15	GLN
2	B	101	ASN
2	B	247	GLN
2	B	249	ASN
2	B	293	GLN
2	B	331	GLN
2	B	436	GLN
1	C	11	GLN
1	C	101	ASN
1	C	133	GLN
1	C	285	GLN
1	C	372	GLN
3	D	14	ASN
3	D	96	GLN
3	D	247	ASN
3	D	349	ASN
4	E	124	GLN
5	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	$\# Z > 2$
9	GDP	D	501	7	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
12	EDO	C	504	-	3,3,3	0.44	0	2,2,2	0.37	0
9	GDP	B	501	7	29,30,30	1.18	2 (6%)	45,47,47	1.72	6 (13%)
6	GTP	C	501	7	33,34,34	0.98	2 (6%)	50,54,54	1.55	10 (20%)
10	MES	B	502	-	12,12,12	2.26	1 (8%)	15,16,16	1.74	2 (13%)
11	EX5	B	503	-	37,37,37	3.14	13 (35%)	50,60,60	2.27	18 (36%)
13	ACP	F	401	-	31,33,33	2.06	10 (32%)	47,52,52	1.75	8 (17%)
6	GTP	A	501	7	33,34,34	1.02	3 (9%)	50,54,54	1.53	9 (18%)
10	MES	D	503	-	12,12,12	2.32	1 (8%)	15,16,16	1.81	2 (13%)

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
9	GDP	D	501	7	-	2/16/32/32	0/3/3/3
12	EDO	C	504	-	-	0/1/1/1	-
9	GDP	B	501	7	-	3/16/32/32	0/3/3/3
6	GTP	C	501	7	-	6/22/38/38	0/3/3/3
10	MES	B	502	-	-	0/6/14/14	0/1/1/1
11	EX5	B	503	-	-	6/15/77/77	0/6/6/6
13	ACP	F	401	-	-	3/19/38/38	0/3/3/3
6	GTP	A	501	7	-	7/22/38/38	0/3/3/3
10	MES	D	503	-	-	1/6/14/14	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	503	EX5	CAI-CAF	-9.55	1.38	1.51
11	B	503	EX5	CAK-CAL	8.62	1.67	1.54
10	D	503	MES	C8-S	-7.75	1.66	1.77
10	B	502	MES	C8-S	-7.55	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	503	EX5	CAI-CAH	-6.94	1.40	1.51
13	F	401	ACP	PG-O1G	5.58	1.61	1.50
11	B	503	EX5	CAZ-CAY	4.81	1.61	1.52
11	B	503	EX5	CAE-NAG	-4.71	1.30	1.38
11	B	503	EX5	CAH-NAG	-4.20	1.31	1.38
13	F	401	ACP	C5-C4	4.14	1.46	1.39
13	F	401	ACP	PB-O3A	4.11	1.63	1.58
11	B	503	EX5	CAK-CAJ	-3.97	1.44	1.50
11	B	503	EX5	CAD-CAC	3.61	1.45	1.38
13	F	401	ACP	PA-O3A	3.58	1.63	1.59
11	B	503	EX5	CBC-CAJ	-3.50	1.39	1.47
11	B	503	EX5	CAA-CAB	3.21	1.44	1.38
9	D	501	GDP	C5-C4	3.20	1.47	1.38
13	F	401	ACP	C5-N7	-3.07	1.33	1.39
9	B	501	GDP	C5-C4	3.04	1.47	1.38
13	F	401	ACP	PG-O3G	-2.73	1.48	1.55
11	B	503	EX5	CAI-CAM	2.58	1.61	1.56
13	F	401	ACP	PG-O2G	2.58	1.60	1.55
6	A	501	GTP	PB-O3A	2.38	1.62	1.59
9	D	501	GDP	C6-N1	-2.36	1.34	1.38
6	A	501	GTP	PA-O3A	2.35	1.62	1.59
9	B	501	GDP	C6-N1	-2.34	1.34	1.38
11	B	503	EX5	CAZ-CAI	2.32	1.59	1.55
13	F	401	ACP	C4-N9	-2.31	1.32	1.37
13	F	401	ACP	C5-C6	2.26	1.47	1.41
6	C	501	GTP	PA-O3A	2.18	1.61	1.59
6	C	501	GTP	C2-N3	2.17	1.38	1.33
11	B	503	EX5	CAL-CAN	2.15	1.56	1.52
6	A	501	GTP	C2-N3	2.13	1.38	1.33
9	D	501	GDP	C5-N7	-2.12	1.34	1.39
13	F	401	ACP	C8-N9	-2.10	1.34	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	503	EX5	CAF-CAI-CAH	6.47	106.91	101.26
11	B	503	EX5	CAI-CAM-NAQ	6.09	111.18	104.43
9	D	501	GDP	C5-C4-N3	-5.96	118.90	128.39
13	F	401	ACP	C5-C4-N3	-5.95	118.53	126.72
9	B	501	GDP	C5-C4-N3	-5.88	119.03	128.39
9	B	501	GDP	C2-N3-C4	4.95	120.83	112.30
9	D	501	GDP	C2-N3-C4	4.85	120.66	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	501	GTP	C5-C4-N3	-4.84	120.69	128.39
6	A	501	GTP	C5-C4-N3	-4.81	120.73	128.39
11	B	503	EX5	CAZ-CAI-CAM	-4.81	97.76	102.80
10	D	503	MES	C5-N4-C3	4.71	118.98	108.84
10	B	502	MES	C5-N4-C3	4.70	118.97	108.84
13	F	401	ACP	N3-C4-N9	4.62	135.03	127.17
6	C	501	GTP	C2-N3-C4	4.59	120.20	112.30
9	D	501	GDP	N9-C4-N3	4.41	134.78	125.95
6	A	501	GTP	C2-N3-C4	4.38	119.84	112.30
9	B	501	GDP	N9-C4-N3	4.30	134.54	125.95
11	B	503	EX5	CAB-OAS-CAU	4.25	126.63	117.66
11	B	503	EX5	CAZ-CAI-CAF	-3.76	98.65	110.72
11	B	503	EX5	CBF-OBE-CBC	-3.75	108.90	115.85
13	F	401	ACP	C2-N3-C4	3.66	120.77	111.83
9	B	501	GDP	C6-C5-N7	3.49	136.64	130.29
13	F	401	ACP	C4-C5-N7	-3.35	106.75	110.58
9	D	501	GDP	C6-C5-N7	3.29	136.28	130.29
11	B	503	EX5	CAF-CAI-CAM	3.12	124.09	118.60
6	C	501	GTP	N9-C4-N3	3.10	132.15	125.95
13	F	401	ACP	N3-C2-N1	-3.07	123.93	128.58
11	B	503	EX5	CBB-CBA-CAL	-2.99	110.81	116.55
6	A	501	GTP	N9-C4-N3	2.93	131.82	125.95
6	C	501	GTP	C2-N1-C6	-2.92	119.81	125.11
6	A	501	GTP	C2-N1-C6	-2.91	119.83	125.11
11	B	503	EX5	CAY-NAQ-CAM	-2.86	98.99	105.78
11	B	503	EX5	CAI-CAF-CAE	-2.81	105.66	108.37
11	B	503	EX5	OBE-CBC-CAJ	2.81	116.83	112.27
11	B	503	EX5	CBA-CAL-CAM	2.80	114.02	109.53
6	C	501	GTP	N9-C8-N7	-2.77	108.27	113.40
6	A	501	GTP	N9-C8-N7	-2.70	108.39	113.40
9	B	501	GDP	C4-C5-N7	-2.66	106.46	110.67
6	C	501	GTP	C5-C6-N1	2.58	119.82	113.25
10	B	502	MES	O1S-S-C8	2.57	110.62	106.73
9	D	501	GDP	C4-C5-N7	-2.57	106.59	110.67
6	A	501	GTP	C8-N7-C5	2.54	108.79	104.26
6	C	501	GTP	O6-C6-C5	-2.49	119.97	126.53
6	C	501	GTP	C8-N7-C5	2.44	108.61	104.26
6	A	501	GTP	O6-C6-C5	-2.43	120.13	126.53
6	A	501	GTP	C5-C6-N1	2.39	119.34	113.25
13	F	401	ACP	C5-N7-C8	2.37	107.18	103.45
11	B	503	EX5	CAK-CAJ-CAH	2.31	121.50	117.36
11	B	503	EX5	OAX-CAO-CAP	-2.22	113.67	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	501	GTP	O2B-PB-O3A	2.22	113.27	107.27
9	B	501	GDP	O6-C6-C5	-2.19	120.75	126.53
11	B	503	EX5	CAO-OAX-CAN	2.18	64.10	60.97
13	F	401	ACP	C4-N9-C8	2.18	108.03	105.74
11	B	503	EX5	CAL-CAM-NAQ	2.15	115.92	111.05
11	B	503	EX5	CAZ-CAY-NAQ	-2.12	99.73	104.38
6	C	501	GTP	O2A-PA-O3A	2.12	113.00	107.27
11	B	503	EX5	OBD-CBC-CAJ	-2.10	120.94	125.13
10	D	503	MES	O3S-S-C8	2.10	110.11	106.00
13	F	401	ACP	O2G-PG-C3B	2.09	111.46	106.40
6	A	501	GTP	O2B-PB-O3A	2.07	112.86	107.27
9	D	501	GDP	O6-C6-C5	-2.04	121.14	126.53

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	GTP	PB-O3B-PG-O3G
6	A	501	GTP	C5'-O5'-PA-O3A
6	A	501	GTP	C5'-O5'-PA-O1A
6	C	501	GTP	PB-O3B-PG-O2G
6	C	501	GTP	C5'-O5'-PA-O3A
6	C	501	GTP	C5'-O5'-PA-O1A
6	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O2A
13	F	401	ACP	PG-C3B-PB-O1B
13	F	401	ACP	PG-C3B-PB-O2B
11	B	503	EX5	CAJ-CBC-OBE-CBF
11	B	503	EX5	OBD-CBC-OBE-CBF
11	B	503	EX5	CAV-CAU-OAS-CAB
11	B	503	EX5	OAW-CAU-OAS-CAB
10	D	503	MES	C8-C7-N4-C3
13	F	401	ACP	O4'-C4'-C5'-O5'
11	B	503	EX5	CAM-CAL-CBA-CBB
11	B	503	EX5	CAN-CAL-CBA-CBB
6	A	501	GTP	PB-O3A-PA-O2A
6	C	501	GTP	PB-O3A-PA-O2A
6	A	501	GTP	C5'-O5'-PA-O2A

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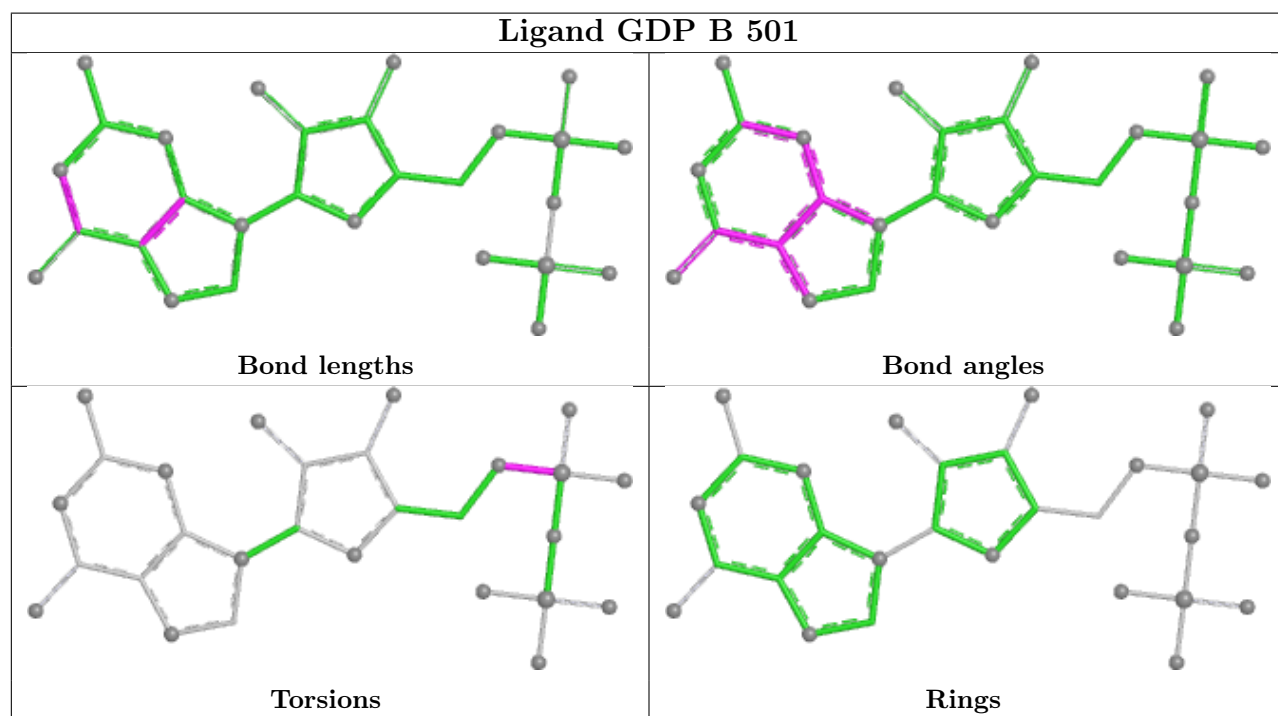
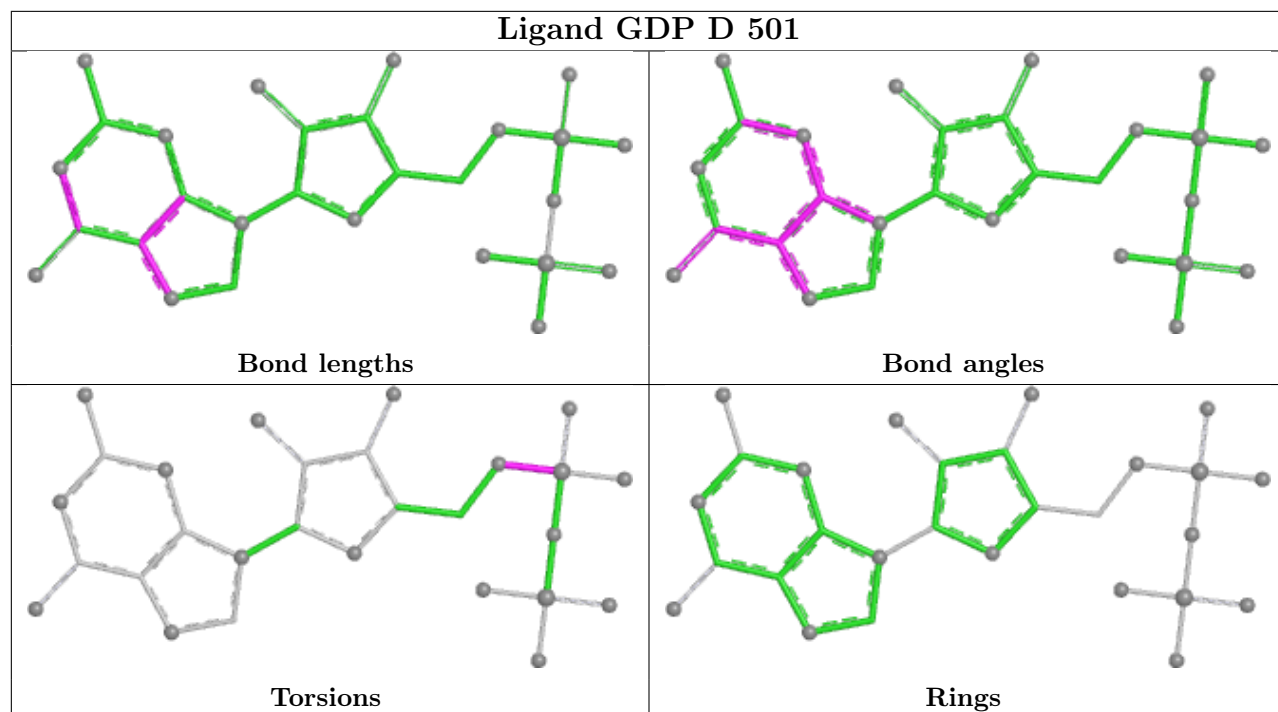
Mol	Chain	Res	Type	Atoms
6	A	501	GTP	PB-O3B-PG-O1G
6	C	501	GTP	C4'-C5'-O5'-PA
6	A	501	GTP	PB-O3B-PG-O2G

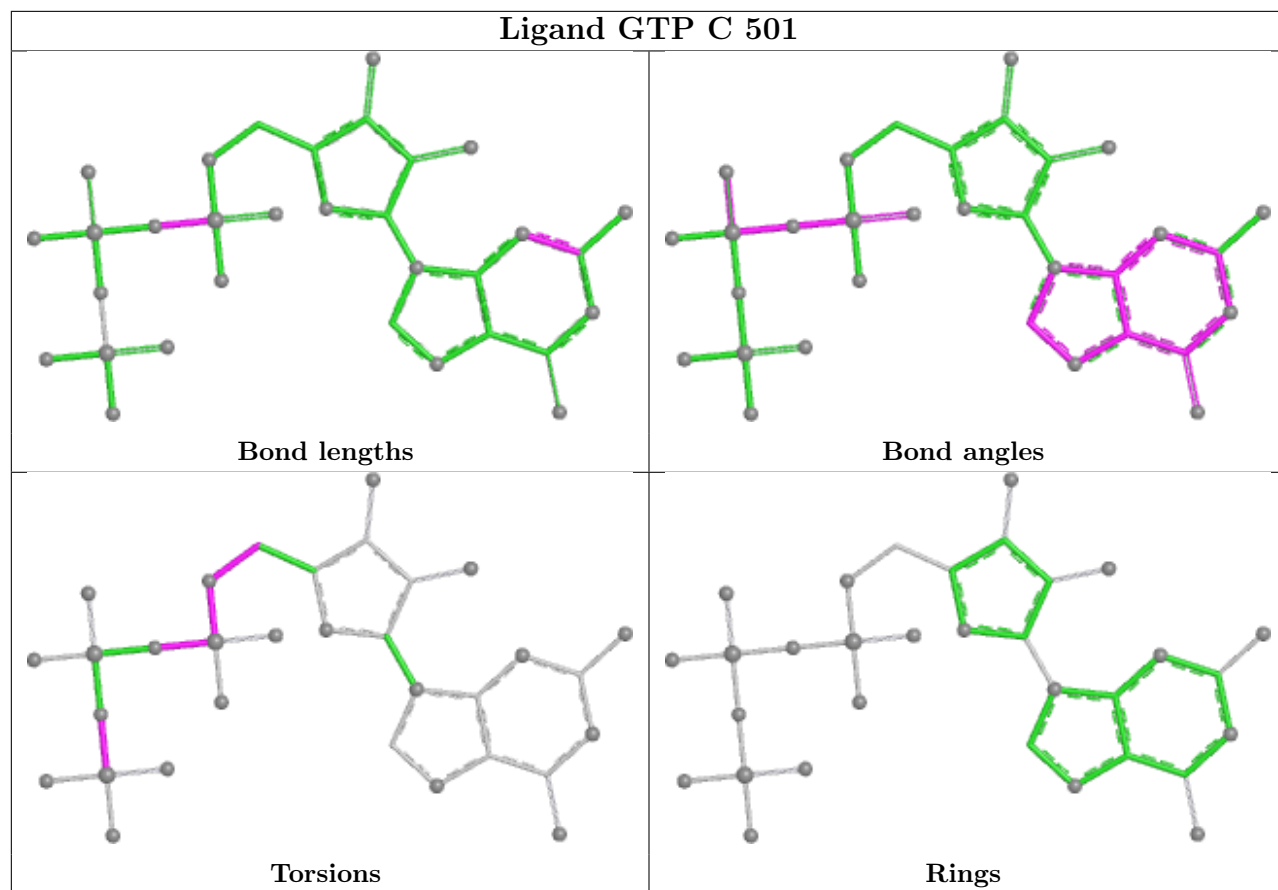
There are no ring outliers.

7 monomers are involved in 12 short contacts:

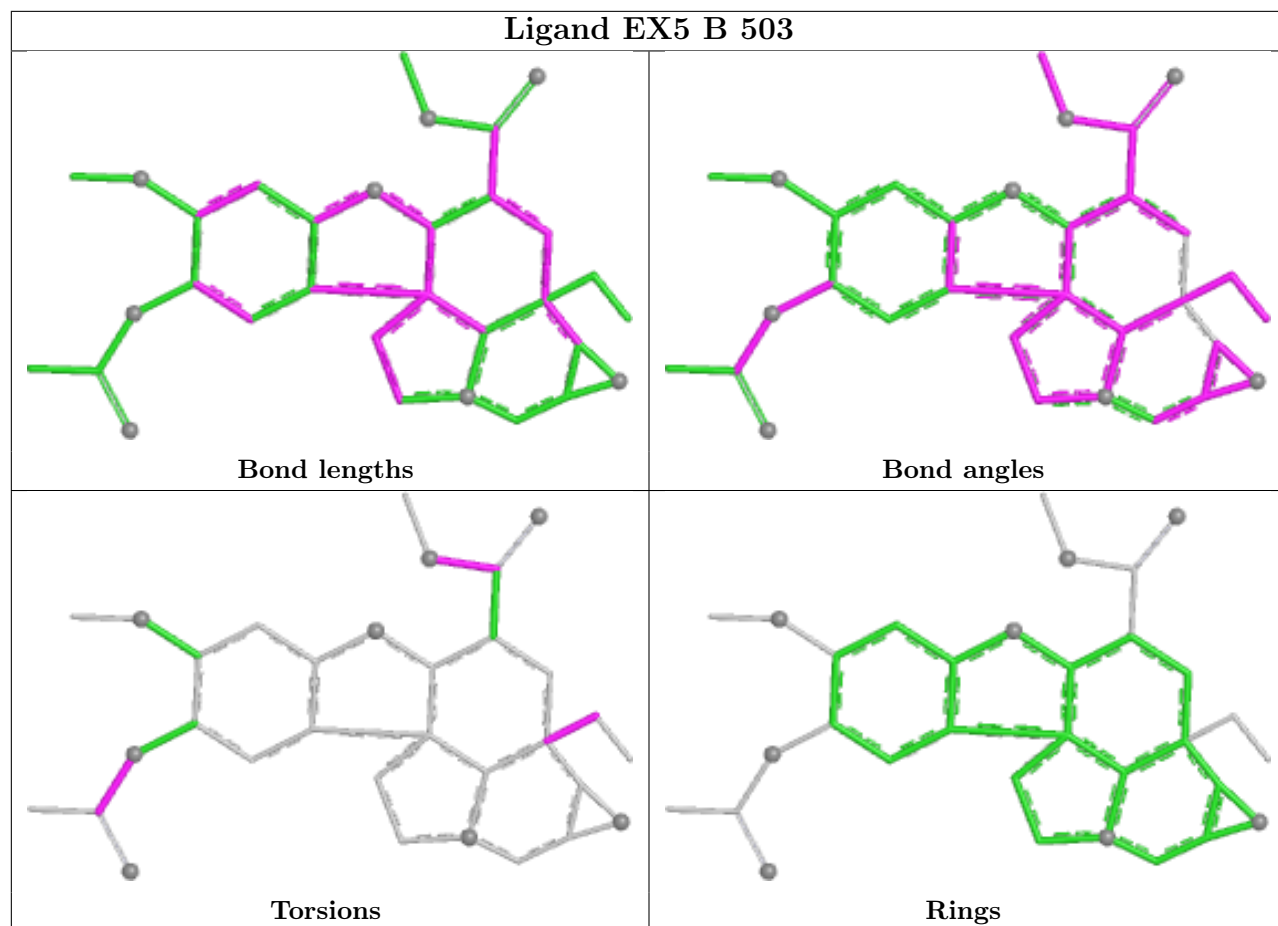
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	5	0
12	C	504	EDO	1	0
6	C	501	GTP	1	0
10	B	502	MES	1	0
13	F	401	ACP	2	0
6	A	501	GTP	1	0
10	D	503	MES	1	0

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.

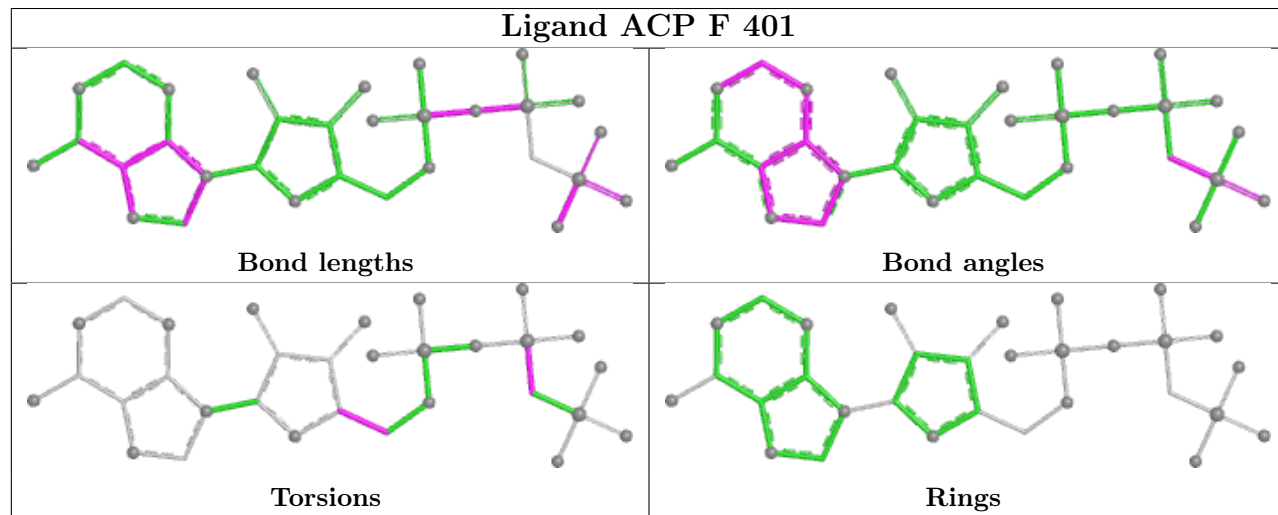


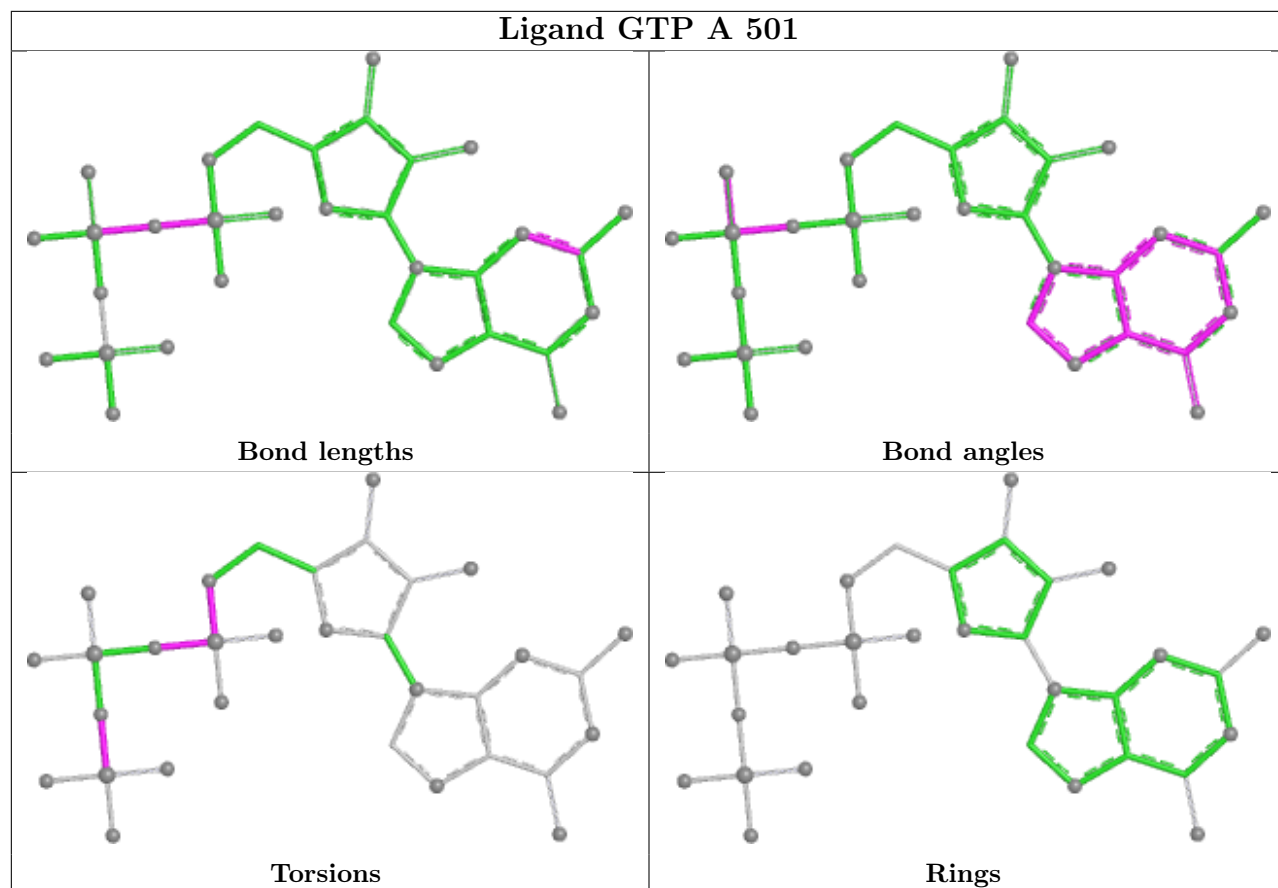


Ligand EX5 B 503



Ligand ACP F 401





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%)	0.09	7 (1%)	70 66	34, 77, 124, 190	6 (1%)
1	C	440/451 (97%)	-0.22	5 (1%)	78 74	30, 60, 96, 130	8 (1%)
2	B	421/445 (94%)	-0.01	8 (1%)	66 62	28, 69, 119, 190	6 (1%)
3	D	421/445 (94%)	0.33	11 (2%)	57 53	48, 94, 133, 170	2 (0%)
4	E	121/143 (84%)	0.33	9 (7%)	20 17	40, 90, 143, 207	1 (0%)
5	F	284/384 (73%)	0.60	21 (7%)	20 17	50, 113, 172, 212	4 (1%)
All	All	2124/2319 (91%)	0.14	61 (2%)	53 50	28, 80, 138, 212	27 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	286	LEU	5.8
5	F	275	LEU	5.0
5	F	292	ARG	4.3
3	D	94	PHE	3.9
3	D	180	THR	3.7
3	D	1	MET	3.5
2	B	248	LEU	3.4
4	E	15	THR	3.3
5	F	181	VAL	3.2
5	F	151	SER	3.1
5	F	131	PHE	3.1
4	E	20	PHE	3.1
1	C	440	VAL	3.1
5	F	330	ILE	3.0
1	C	42	ILE	2.9
3	D	308	ARG	2.9
5	F	191	LEU	2.8
1	A	437	VAL	2.8
5	F	149	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
5	F	274	ALA	2.7
2	B	438	ALA	2.7
3	D	246	GLY	2.7
4	E	26	PRO	2.7
4	E	8	VAL	2.6
4	E	6	MET	2.5
2	B	247	GLN	2.5
5	F	362	ALA	2.5
5	F	373	SER	2.5
1	A	45	GLY	2.5
1	A	340	SER	2.5
5	F	102	PRO	2.5
5	F	186	LEU	2.5
1	A	262	TYR	2.4
4	E	46	SER	2.4
1	A	436	GLY	2.4
4	E	53	LYS	2.4
5	F	182	ILE	2.4
2	B	293	GLN	2.4
3	D	172	MET	2.4
5	F	150	LYS	2.4
2	B	318	ILE	2.3
1	A	281	ALA	2.3
1	C	163	LYS	2.3
5	F	101	TYR	2.3
4	E	45	PRO	2.3
5	F	59	VAL	2.3
2	B	57	THR	2.2
3	D	296	PHE	2.2
3	D	404	PHE	2.2
3	D	181	VAL	2.2
1	A	93	ILE	2.2
2	B	285	ALA	2.2
5	F	75	ALA	2.1
4	E	22	VAL	2.1
5	F	329	LEU	2.1
2	B	283	TYR	2.1
5	F	199	PHE	2.1
1	C	2	ARG	2.1
3	D	158	ARG	2.0
5	F	180	HIS	2.0
1	C	340	SER	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](#)

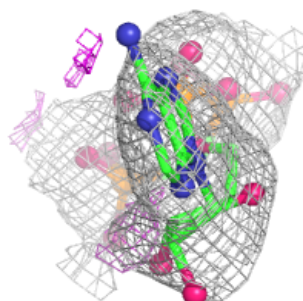
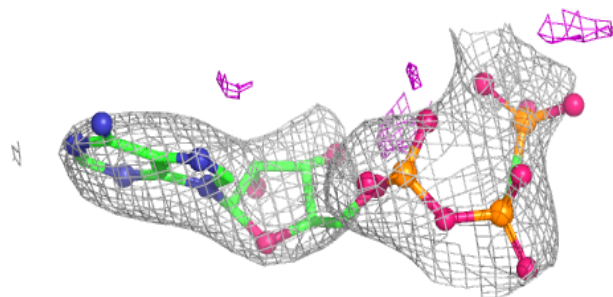
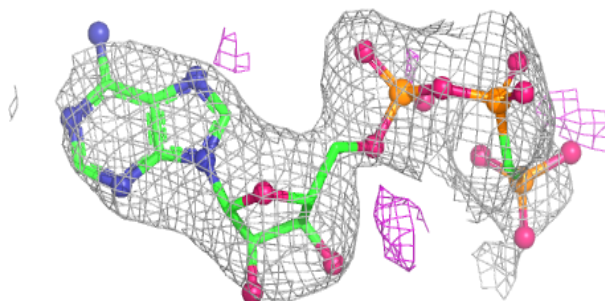
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ACP	F	401	31/31	0.81	0.10	120,132,190,191	0
10	MES	D	503	12/12	0.84	0.17	115,129,133,135	0
12	EDO	C	504	4/4	0.85	0.23	78,79,81,83	0
9	GDP	D	501	28/28	0.90	0.11	69,87,102,118	0
7	MG	D	502	1/1	0.91	0.14	126,126,126,126	0
11	EX5	B	503	32/32	0.94	0.11	58,72,83,86	0
10	MES	B	502	12/12	0.94	0.09	51,66,85,87	0
8	CA	A	503	1/1	0.94	0.08	113,113,113,113	0
7	MG	C	502	1/1	0.96	0.06	52,52,52,52	0
6	GTP	C	501	32/32	0.97	0.07	45,52,62,72	0
8	CA	C	503	1/1	0.97	0.04	81,81,81,81	0
6	GTP	A	501	32/32	0.98	0.05	50,59,67,71	0
9	GDP	B	501	28/28	0.98	0.06	44,54,63,67	0
7	MG	B	504	1/1	0.99	0.05	52,52,52,52	0
7	MG	A	502	1/1	0.99	0.02	57,57,57,57	0

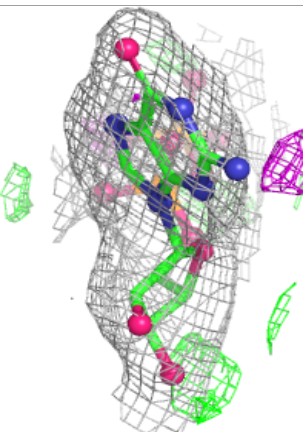
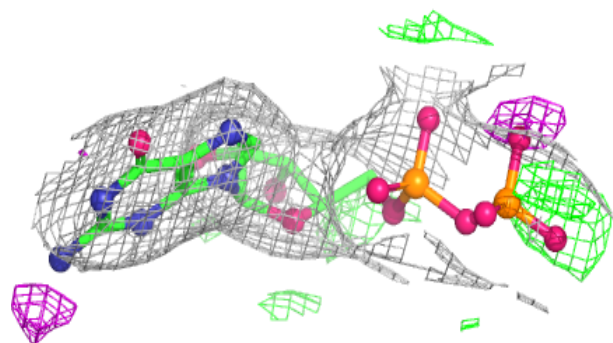
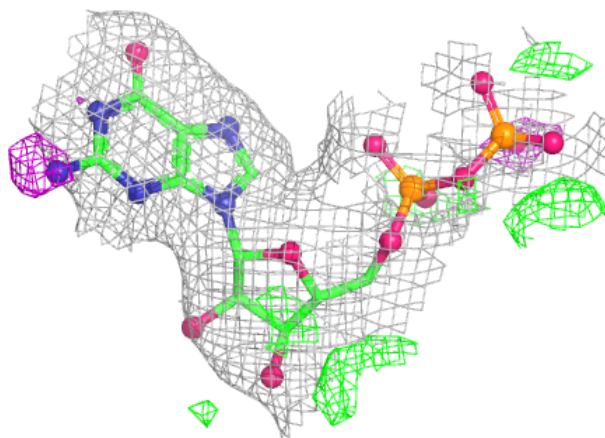
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

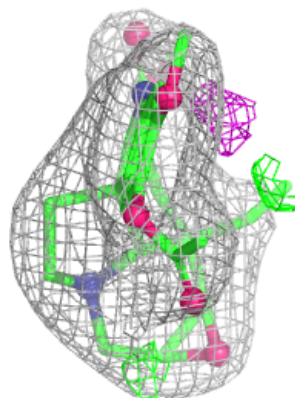
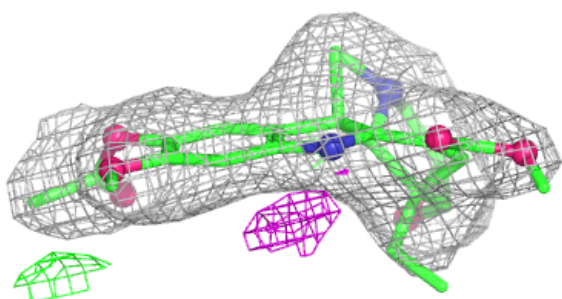
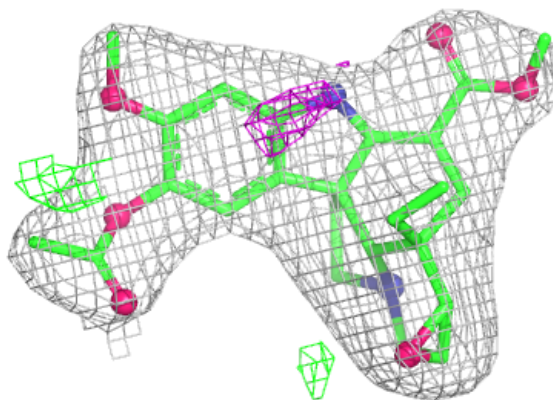
**Electron density around GDP D 501:**

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

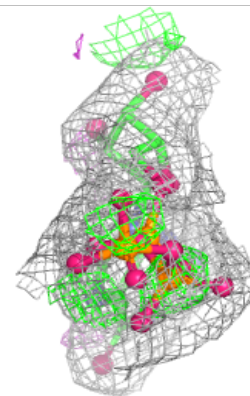
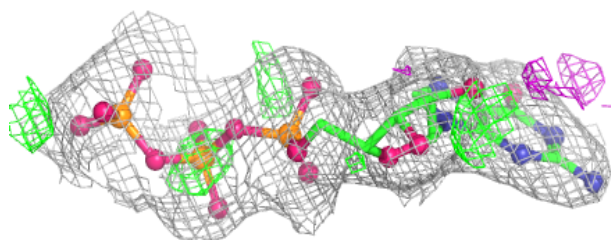
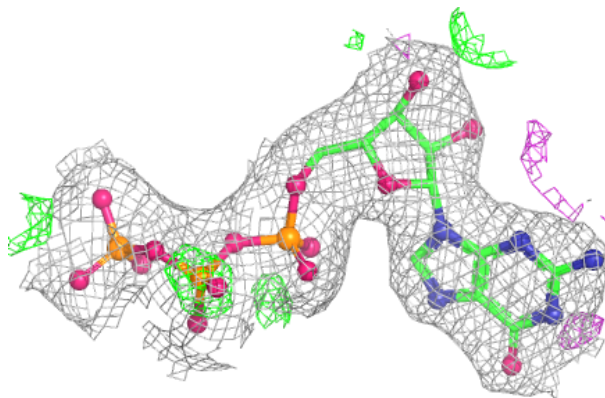


Electron density around EX5 B 503:

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

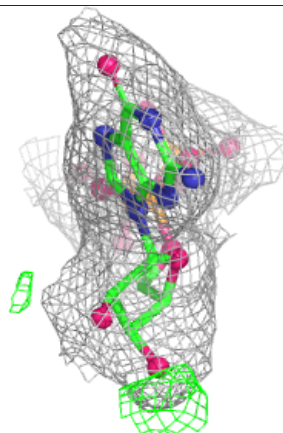
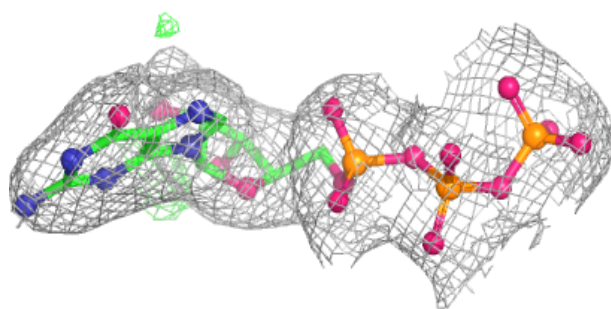
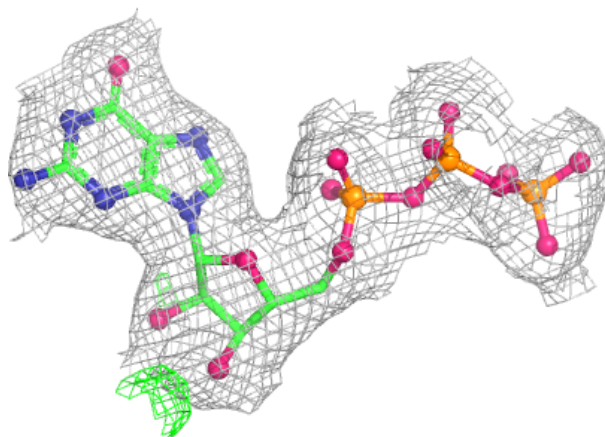
**Electron density around GTP C 501:**

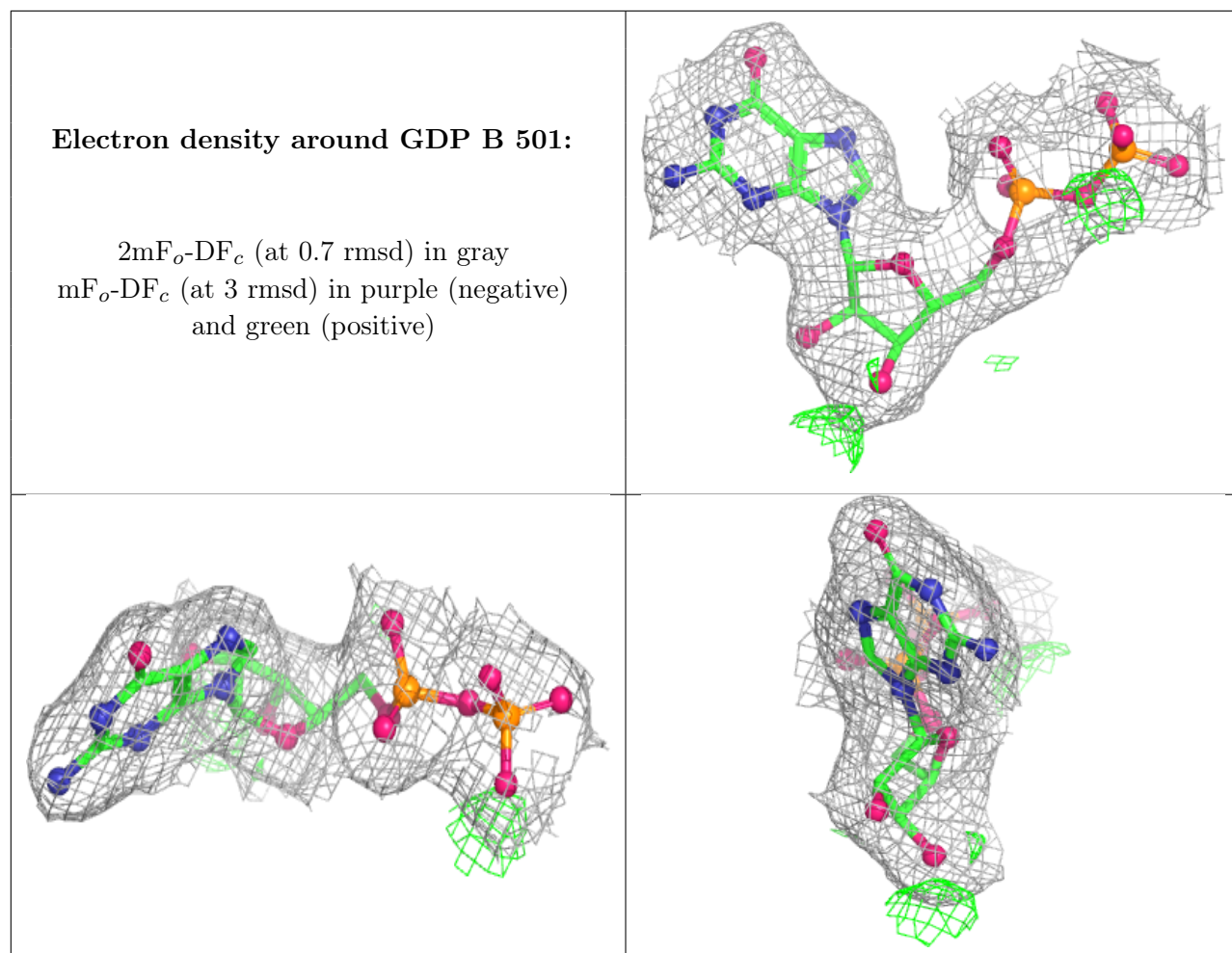
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP A 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.