



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 10:20 am GMT

PDB ID : 6GJ4  
Title : Tubulin-6j complex  
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Deposited on : 2018-05-16  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, 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)

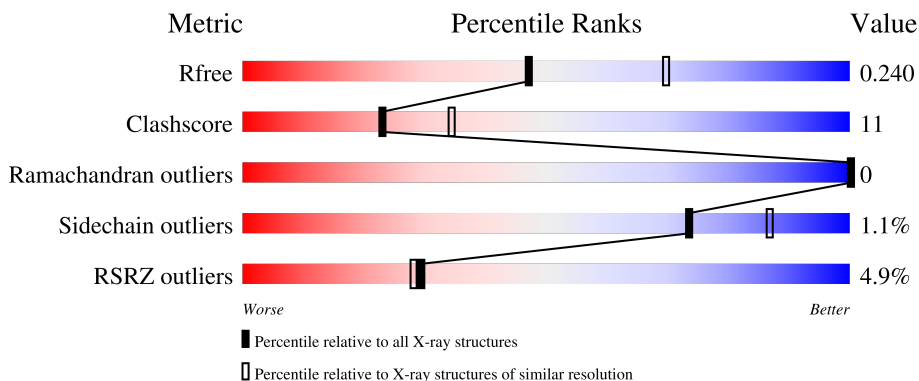
# 1 Overall quality at a glance

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))
$R_{free}$	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)

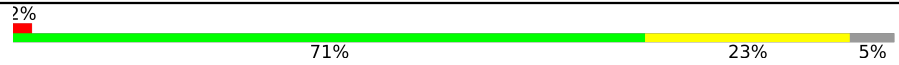

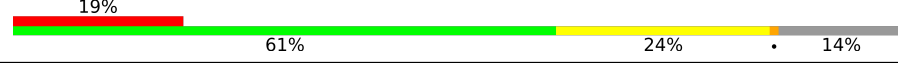
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	 75% 21%
1	C	451	 78% 19%
2	B	445	 74% 22%

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Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	D	445	
3	E	143	
4	F	384	

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 17708 atoms, of which 63 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	435	Total	C	N	O	S	0	0	0
			3394	2148	577	647	22			
1	C	440	Total	C	N	O	S	0	1	0
			3441	2178	584	657	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	428	Total	C	N	O	S	0	0	0
			3357	2110	573	647	27			
2	D	422	Total	C	N	O	S	0	0	0
			3316	2084	563	642	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	330	Total	C	N	O	S	0	0	0
			2707	1743	459	491	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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		

- 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		
6	D	1	Total	Mg	0	0
			1	1		

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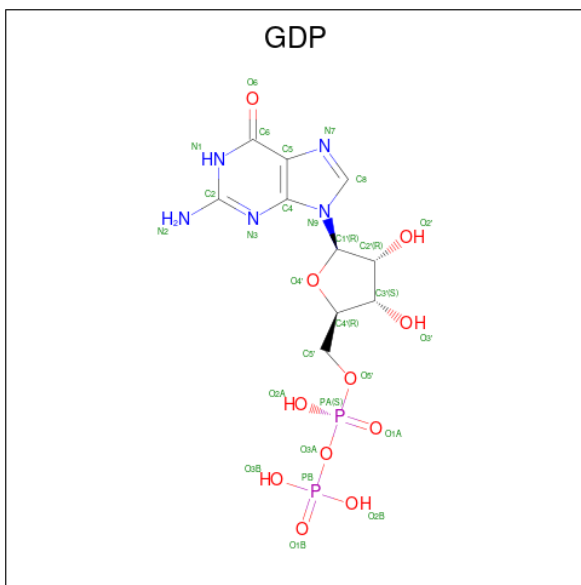
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

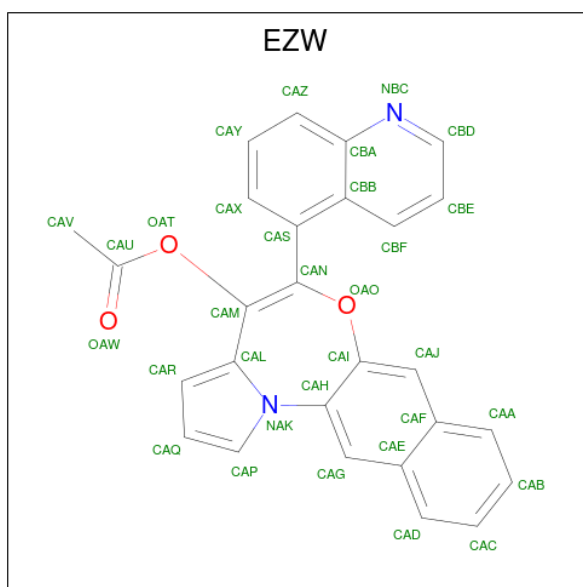
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



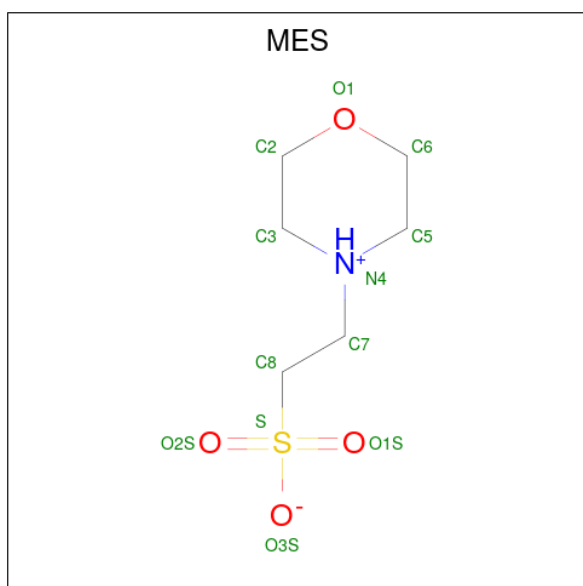
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 5-(quinolin-5-yl)naphtho[2,3-b]pyrrolo[1,2-d][1,4]oxazepin-4-yl acetate (three-letter code: EZW) (formula: C<sub>27</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>).



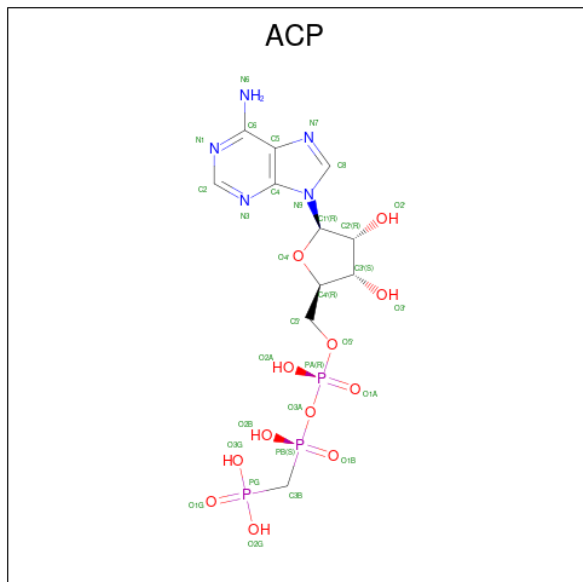
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	B	1	Total	C	H	N	O	0	0
			50	27	18	2	3		
9	D	1	Total	C	H	N	O	0	0
			50	27	18	2	3		

- 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	H	N	O	S		
10	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- 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	
			Total	C	H	N	O			P
11	F	1	45	11	14	5	12	3	0	0

- Molecule 12 is water.

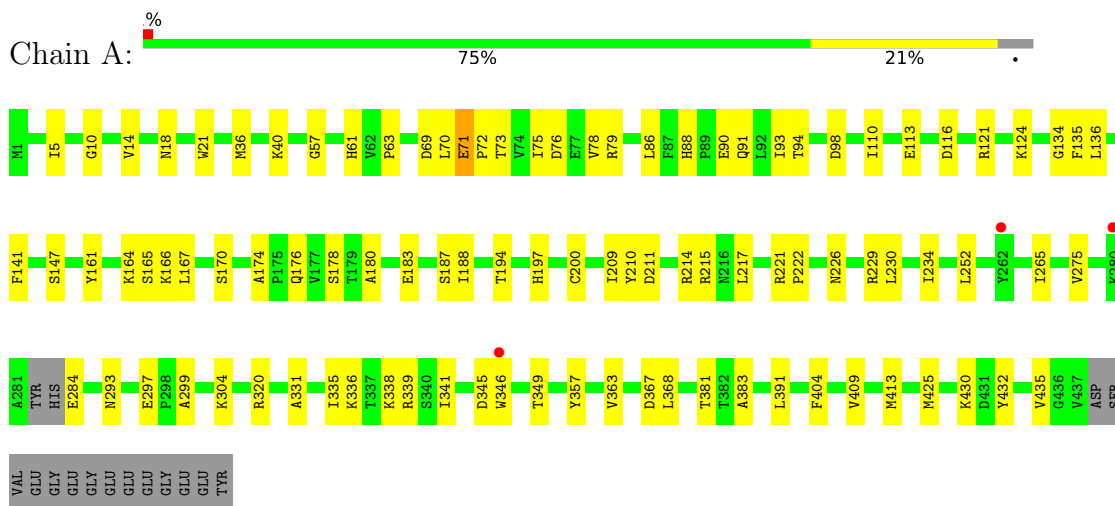
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	35	Total	O	0	0
			35	35		
12	B	44	Total	O	0	0
			44	44		
12	C	85	Total	O	0	0
			85	85		
12	D	17	Total	O	0	0
			17	17		
12	E	8	Total	O	0	0
			8	8		
12	F	16	Total	O	0	0
			16	16		



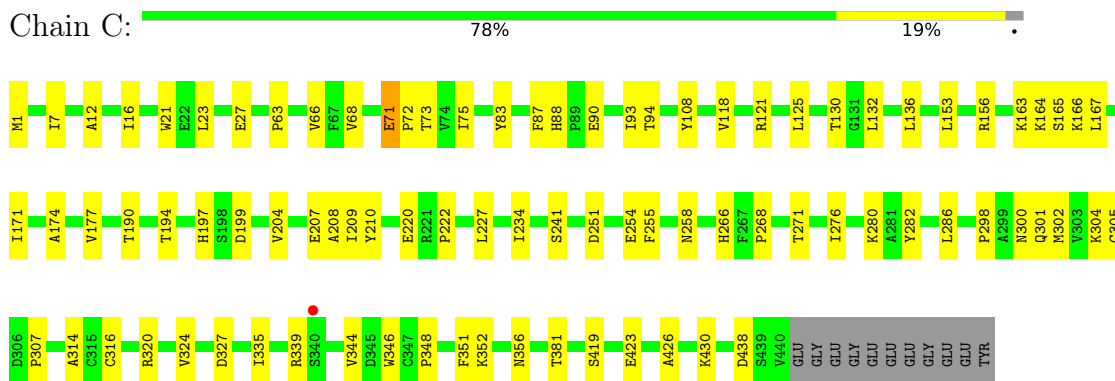
### 3 Residue-property plots

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.

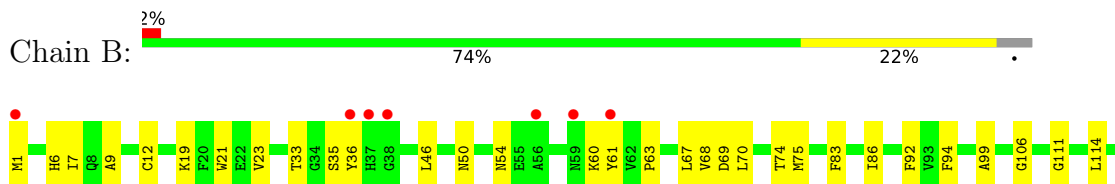
- Molecule 1: Tubulin alpha-1B chain

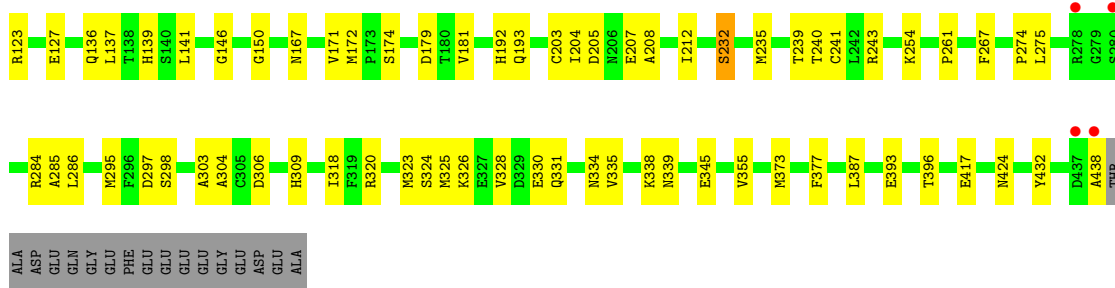


- Molecule 1: Tubulin alpha-1B chain

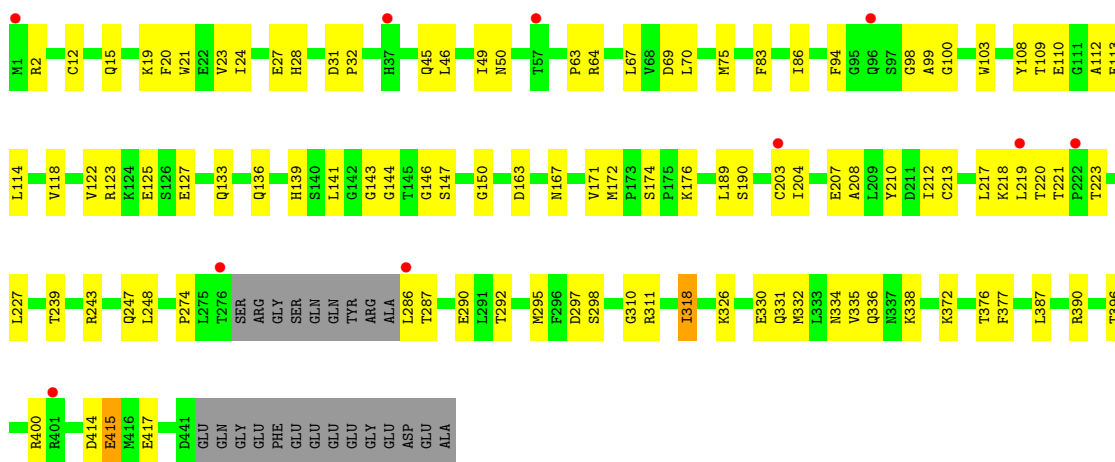


- Molecule 2: Tubulin beta-2B chain

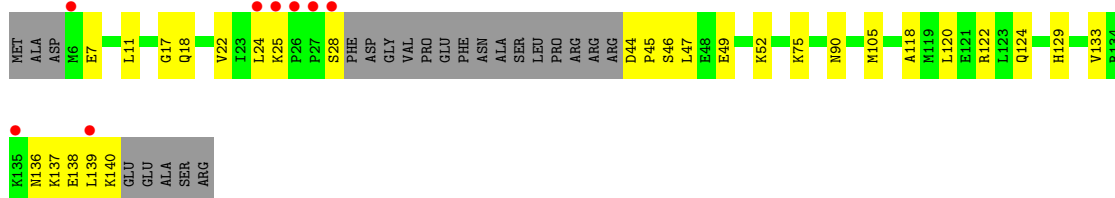




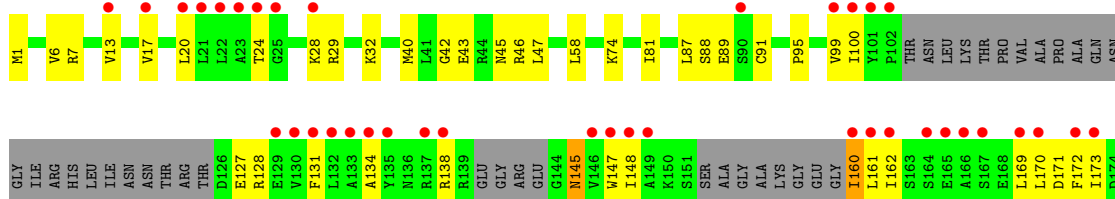
• Molecule 2: Tubulin beta-2B chain

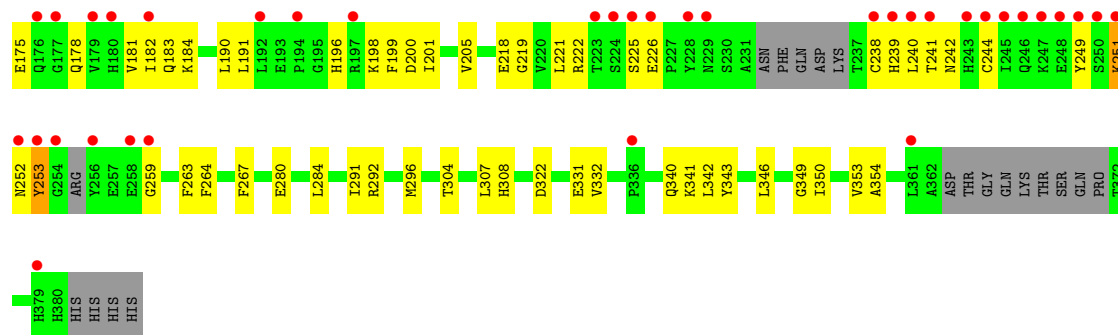


• Molecule 3: Stathmin-4



• 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, $\alpha$ , $\beta$ , $\gamma$	104.97Å 157.81Å 181.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.40 48.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.02-2.40) 100.0 (48.02-2.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.197 , 0.241 0.197 , 0.240	Depositor DCC
$R_{free}$ test set	5776 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, EZW, GDP, ACP, MG, MES, CA

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	0.27	0/3469	0.44	0/4707
1	C	0.29	0/3522	0.46	0/4782
2	B	0.28	0/3432	0.46	0/4650
2	D	0.27	0/3389	0.43	0/4591
3	E	0.25	0/999	0.38	0/1325
4	F	0.25	0/2767	0.41	0/3736
All	All	0.27	0/17578	0.44	0/23791

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	3394	0	3313	78	0
1	C	3441	0	3355	68	0
2	B	3357	0	3227	80	0
2	D	3316	0	3196	79	0
3	E	991	0	1012	24	0
4	F	2707	0	2681	82	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	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	3	0
9	B	32	18	0	0	0
9	D	32	18	0	0	0
10	B	12	13	12	1	0
11	F	31	14	14	2	0
12	A	35	0	0	6	0
12	B	44	0	0	9	0
12	C	85	0	0	10	0
12	D	17	0	0	3	0
12	E	8	0	0	0	0
12	F	16	0	0	0	0
All	All	17645	63	16858	392	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 11.

All (392) 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)
3:E:139:LEU:HB3	3:E:140:LYS:HE3	1.33	1.07
4:F:201:ILE:HG12	4:F:221:LEU:HD22	1.42	1.00
1:C:286:LEU:HB2	12:C:612:HOH:O	1.62	0.99
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.28	0.98
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.55	0.88
4:F:81:ILE:HG12	4:F:87:LEU:HD23	1.57	0.86
4:F:99:VAL:HG22	4:F:181:VAL:HG12	1.58	0.86
2:D:372:LYS:NZ	12:D:602:HOH:O	2.10	0.84
4:F:88:SER:HB2	4:F:89:GLU:HA	1.60	0.84
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.63	0.81
1:C:83:TYR:OH	12:C:601:HOH:O	2.00	0.79
2:B:417:GLU:O	12:B:601:HOH:O	2.01	0.79
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:ALA:O	12:D:601:HOH:O	2.02	0.77
1:C:327:ASP:OD2	12:C:602:HOH:O	2.03	0.76
4:F:100:ILE:HD11	4:F:173:ILE:HD13	1.67	0.76
1:A:381:THR:HG22	1:A:383:ALA:H	1.50	0.76
4:F:161:LEU:HD23	4:F:169:LEU:HA	1.69	0.74
1:C:132:LEU:O	1:C:164:LYS:HE2	1.86	0.74
1:A:167:LEU:CD2	1:A:200:CYS:HB3	2.17	0.74
10:B:504:MES:O3S	12:B:602:HOH:O	2.07	0.72
2:B:179:ASP:OD2	12:B:604:HOH:O	2.08	0.72
3:E:120:LEU:O	3:E:124:GLN:HG2	1.90	0.72
2:B:438:ALA:O	12:B:603:HOH:O	2.07	0.71
4:F:1:MET:HG2	4:F:28:LYS:HE2	1.70	0.71
2:B:274:PRO:HB3	2:B:286:LEU:HD21	1.71	0.71
1:A:336:LYS:HD3	1:A:336:LYS:O	1.91	0.71
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.71	0.71
2:B:181:VAL:HG23	1:C:348:PRO:CG	2.21	0.70
4:F:134:ALA:O	4:F:138:ARG:HG3	1.92	0.70
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.70
2:D:318:ILE:HG23	2:D:376:THR:HB	1.73	0.69
1:A:167:LEU:HD12	1:A:252:LEU:HD22	1.75	0.68
1:A:349:THR:N	12:A:602:HOH:O	2.26	0.68
3:E:139:LEU:HB3	3:E:140:LYS:CE	2.20	0.68
1:A:167:LEU:HD23	1:A:200:CYS:HB3	1.75	0.68
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.29	0.68
2:D:2:ARG:HB3	2:D:133:GLN:HG3	1.76	0.67
1:C:438:ASP:OD1	12:C:603:HOH:O	2.12	0.67
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.76	0.67
2:B:325:MET:SD	2:B:355:VAL:HG11	2.34	0.67
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.29	0.67
2:D:70:LEU:HB3	2:D:98:GLY:HA2	1.77	0.67
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.08	0.66
2:B:285:ALA:O	12:B:605:HOH:O	2.12	0.66
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.78	0.66
1:C:426:ALA:O	1:C:430:LYS:HG2	1.96	0.65
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.78	0.65
1:C:220:GLU:OE2	2:D:326:LYS:HD2	1.97	0.65
1:C:1:MET:HG2	1:C:130:THR:OG1	1.97	0.65
2:D:70:LEU:HB3	2:D:98:GLY:CA	2.27	0.65
4:F:201:ILE:HG12	4:F:221:LEU:CD2	2.23	0.65
4:F:88:SER:CB	4:F:89:GLU:HA	2.26	0.64
4:F:331:GLU:HG2	4:F:332:VAL:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:GLN:HA	2:D:167:ASN:O	1.98	0.64
3:E:24:LEU:O	3:E:25:LYS:HG3	1.99	0.63
1:C:163:LYS:HE2	3:E:90:ASN:HB2	1.80	0.63
2:B:33:THR:O	2:B:60:LYS:HE3	1.99	0.63
2:B:432:TYR:OH	12:B:606:HOH:O	2.14	0.62
1:C:71:GLU:HG2	1:C:72:PRO:N	2.13	0.62
3:E:46:SER:OG	3:E:49:GLU:HG3	2.00	0.62
4:F:6:VAL:O	4:F:32:LYS:HG3	2.00	0.61
2:D:396:THR:O	2:D:400:ARG:HG2	2.00	0.61
1:A:57:GLY:O	12:A:601:HOH:O	2.16	0.60
4:F:13:VAL:O	4:F:17:VAL:HG23	2.02	0.60
2:D:147:SER:HG	2:D:190:SER:HG	1.49	0.60
2:D:23:VAL:O	2:D:27:GLU:HG3	2.01	0.60
2:D:15:GLN:NE2	8:D:501:GDP:O6	2.34	0.60
2:B:141:LEU:HD12	2:B:172:MET:SD	2.42	0.59
2:B:345:GLU:OE1	2:B:345:GLU:N	2.29	0.59
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.37	0.59
2:B:19:LYS:HG3	2:B:232:SER:OG	2.02	0.59
4:F:253:TYR:CE2	4:F:259:GLY:HA2	2.37	0.59
4:F:222:ARG:O	4:F:241:THR:HG21	2.01	0.59
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.85	0.59
4:F:190:LEU:HB2	4:F:322:ASP:O	2.02	0.59
2:B:75:MET:N	12:B:608:HOH:O	2.28	0.59
4:F:6:VAL:O	4:F:32:LYS:HE3	2.03	0.59
2:B:323:MET:HB3	2:B:373:MET:HE1	1.84	0.58
2:D:217:LEU:HB3	2:D:219:LEU:HD13	1.84	0.58
1:C:156:ARG:NH1	12:C:608:HOH:O	2.34	0.58
1:C:320:ARG:HA	1:C:356:ASN:O	2.02	0.58
2:B:193:GLN:OE1	3:E:75:LYS:NZ	2.36	0.58
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.32	0.58
4:F:100:ILE:HD11	4:F:173:ILE:CD1	2.33	0.58
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.84	0.58
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.34	0.58
2:B:240:THR:HB	2:B:318:ILE:CD1	2.34	0.58
2:D:98:GLY:O	2:D:100:GLY:N	2.35	0.58
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.69	0.58
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.34	0.57
1:C:209:ILE:HD11	1:C:302:MET:SD	2.45	0.57
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.24	0.57
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.87	0.57
2:D:326:LYS:O	2:D:330:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:NH2	12:A:605:HOH:O	2.37	0.57
4:F:29:ARG:HH21	4:F:32:LYS:NZ	2.03	0.57
4:F:138:ARG:HD3	4:F:145:ASN:HD21	1.68	0.57
2:D:318:ILE:CG2	2:D:376:THR:HB	2.34	0.56
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.87	0.56
1:C:258:ASN:O	12:C:605:HOH:O	2.18	0.56
2:B:1:MET:HG3	2:B:50:ASN:HD22	1.70	0.56
2:B:240:THR:HB	2:B:318:ILE:HD13	1.88	0.56
1:C:220:GLU:CD	2:D:326:LYS:HD2	2.25	0.56
4:F:43:GLU:OE1	4:F:43:GLU:N	2.38	0.56
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.88	0.56
1:C:108:TYR:CE2	3:E:105:MET:HE1	2.41	0.55
2:D:332:MET:O	2:D:336:GLN:HG3	2.07	0.55
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.29	0.55
1:A:141:PHE:O	1:A:147:SER:HB3	2.06	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.40	0.55
3:E:118:ALA:O	3:E:122:ARG:HG2	2.05	0.55
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.33	0.55
2:B:240:THR:CG2	2:B:318:ILE:HD11	2.36	0.55
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.41	0.55
2:B:331:GLN:HA	2:B:334:ASN:ND2	2.23	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.24	0.54
1:C:204:VAL:HG13	1:C:302:MET:HG3	1.90	0.54
3:E:129:HIS:O	3:E:133:VAL:HG23	2.06	0.54
1:A:71:GLU:OE1	1:A:73:THR:HB	2.06	0.54
4:F:88:SER:HA	4:F:91:CYS:H	1.73	0.54
4:F:349:GLY:O	4:F:353:VAL:HG22	2.07	0.54
4:F:128:ARG:NH1	4:F:170:LEU:HD13	2.23	0.54
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.37	0.54
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.23	0.54
4:F:40:MET:HE2	4:F:47:LEU:HG	1.89	0.54
2:B:239:THR:O	2:B:243:ARG:HG2	2.08	0.54
2:D:174:SER:HB2	2:D:207:GLU:HB2	1.90	0.54
2:D:204:ILE:HD12	2:D:204:ILE:N	2.23	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.43	0.53
1:A:349:THR:HB	3:E:25:LYS:HB2	1.89	0.53
2:B:240:THR:HG21	2:B:318:ILE:HD11	1.90	0.53
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.08	0.53
4:F:45:ASN:C	4:F:46:ARG:HG2	2.29	0.53
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.41	0.53
1:A:180:ALA:O	1:A:183:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:251:LYS:O	4:F:251:LYS:HD3	2.08	0.53
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.44	0.53
3:E:139:LEU:CB	3:E:140:LYS:HE3	2.23	0.52
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.09	0.52
1:A:116:ASP:HB2	12:A:622:HOH:O	2.10	0.52
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.09	0.52
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.92	0.52
1:C:165:SER:HA	1:C:199:ASP:OD2	2.09	0.52
2:D:83:PHE:O	2:D:86:ILE:HG22	2.10	0.52
1:A:69:ASP:O	1:A:94:THR:HA	2.10	0.52
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.45	0.52
2:B:123:ARG:O	2:B:127:GLU:HG2	2.09	0.52
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.92	0.52
3:E:44:ASP:N	3:E:45:PRO:HD3	2.25	0.52
1:C:298:PRO:HA	1:C:301:GLN:OE1	2.10	0.52
2:D:217:LEU:CB	2:D:219:LEU:HD13	2.40	0.52
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.44	0.52
1:A:331:ALA:O	1:A:335:ILE:HD13	2.09	0.52
2:B:69:ASP:O	2:B:94:PHE:HA	2.10	0.52
2:D:239:THR:O	2:D:243:ARG:HG2	2.10	0.52
4:F:32:LYS:HD2	4:F:32:LYS:N	2.24	0.52
1:A:221:ARG:HD3	2:B:326:LYS:HA	1.91	0.52
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.92	0.52
1:A:176:GLN:HG2	1:A:210:TYR:CE2	2.45	0.51
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.43	0.51
4:F:242:ASN:O	4:F:244:CYS:N	2.44	0.51
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.46	0.51
4:F:226:GLU:HB3	4:F:238:CYS:HB3	1.91	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.10	0.51
11:F:401:ACP:O2B	11:F:401:ACP:O3G	2.29	0.51
1:A:229:ARG:HD3	1:A:363:VAL:HG21	1.93	0.51
1:C:234:ILE:HD12	1:C:234:ILE:H	1.76	0.51
4:F:225:SER:HB2	4:F:252:ASN:HB3	1.92	0.51
2:B:286:LEU:N	2:B:286:LEU:HD12	2.26	0.51
4:F:218:GLU:HB3	4:F:342:LEU:HD13	1.92	0.51
2:B:338:LYS:HG2	2:B:339:ASN:OD1	2.11	0.51
2:D:46:LEU:HA	2:D:49:ILE:HB	1.93	0.51
2:B:35:SER:HB3	2:B:60:LYS:HZ2	1.76	0.51
2:B:192:HIS:CG	2:B:424:ASN:HD22	2.28	0.51
4:F:292:ARG:HG3	4:F:296:MET:SD	2.51	0.51
1:A:404:PHE:CD1	2:B:261:PRO:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:O	2:B:284:ARG:HG3	2.10	0.50
2:D:28:HIS:HA	2:D:45:GLN:HB3	1.92	0.50
4:F:100:ILE:CD1	4:F:173:ILE:HG21	2.41	0.50
1:A:221:ARG:NH1	2:B:325:MET:HB3	2.26	0.50
4:F:221:LEU:HD11	4:F:267:PHE:CD2	2.46	0.50
1:A:98:ASP:OD2	2:B:254:LYS:HE3	2.11	0.50
4:F:100:ILE:HD11	4:F:173:ILE:HG21	1.93	0.50
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.93	0.50
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.94	0.50
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.46	0.50
4:F:161:LEU:CD2	4:F:169:LEU:HA	2.40	0.50
2:D:207:GLU:HB3	2:D:390:ARG:HH12	1.76	0.50
2:D:221:THR:HG23	2:D:221:THR:O	2.12	0.50
2:D:417:GLU:OE1	12:D:603:HOH:O	2.18	0.50
2:D:108:TYR:CG	3:E:133:VAL:HG11	2.47	0.49
1:A:166:LYS:HE2	1:A:197:HIS:O	2.12	0.49
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.49
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.41	0.49
2:D:208:ALA:O	2:D:212:ILE:HG13	2.13	0.49
2:D:287:THR:OG1	2:D:290:GLU:HG3	2.12	0.49
2:D:19:LYS:O	2:D:23:VAL:HG23	2.11	0.49
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.95	0.49
2:D:176:LYS:HD3	2:D:210:TYR:CD2	2.47	0.49
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.39	0.49
2:D:220:THR:O	2:D:221:THR:HG22	2.13	0.49
1:A:88:HIS:N	1:A:91:GLN:OE1	2.41	0.49
1:A:293:ASN:HD21	1:A:339:ARG:HH21	1.61	0.49
2:B:393:GLU:O	2:B:396:THR:HG22	2.12	0.49
4:F:42:GLY:HA3	4:F:47:LEU:HD12	1.95	0.49
2:B:303:ALA:O	2:B:304:ALA:HB3	2.13	0.49
2:B:331:GLN:HA	2:B:334:ASN:HD21	1.77	0.49
4:F:161:LEU:HG	4:F:169:LEU:HD23	1.95	0.49
2:B:23:VAL:HG21	2:B:232:SER:OG	2.13	0.48
2:B:286:LEU:HD12	2:B:286:LEU:H	1.78	0.48
2:B:114:LEU:O	2:B:114:LEU:HG	2.13	0.48
1:C:163:LYS:HG3	3:E:90:ASN:OD1	2.13	0.48
4:F:171:ASP:O	4:F:175:GLU:HG3	2.13	0.48
1:A:430:LYS:HA	1:A:430:LYS:HD3	1.50	0.48
2:B:67:LEU:N	2:B:67:LEU:HD12	2.29	0.48
1:A:341:ILE:N	1:A:341:ILE:HD12	2.29	0.48
1:C:419:SER:O	1:C:423:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.47
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.95	0.47
2:B:74:THR:N	12:B:608:HOH:O	2.46	0.47
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.48	0.47
4:F:47:LEU:C	4:F:47:LEU:HD23	2.35	0.47
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.79	0.47
2:B:331:GLN:O	2:B:335:VAL:HG23	2.15	0.47
2:D:69:ASP:O	2:D:94:PHE:HA	2.14	0.47
2:D:295:MET:CG	2:D:377:PHE:HB2	2.44	0.47
2:B:334:ASN:OD1	2:B:335:VAL:N	2.47	0.47
4:F:331:GLU:HG2	4:F:332:VAL:H	1.76	0.47
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.15	0.47
1:C:351:PHE:CD1	1:C:351:PHE:N	2.83	0.47
1:A:215:ARG:NH2	1:A:299:ALA:O	2.48	0.47
2:D:146:GLY:O	2:D:150:GLY:HA3	2.15	0.47
1:A:284:GLU:N	12:A:608:HOH:O	2.47	0.47
2:D:310:GLY:O	2:D:311:ARG:HG2	2.15	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.47
4:F:350:ILE:O	4:F:354:ALA:HB3	2.14	0.46
1:A:134:GLY:HA3	1:A:165:SER:O	2.15	0.46
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.96	0.46
2:B:181:VAL:CG2	1:C:348:PRO:HD2	2.46	0.46
1:A:134:GLY:HA2	1:A:164:LYS:HB3	1.98	0.46
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.98	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.51	0.46
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.50	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.50	0.46
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.98	0.46
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.98	0.46
4:F:198:LYS:HG2	4:F:199:PHE:N	2.31	0.46
1:C:305:CYS:O	1:C:307:PRO:HD3	2.15	0.46
4:F:1:MET:HE1	4:F:28:LYS:CG	2.45	0.46
1:A:40:LYS:HA	1:A:40:LYS:HD3	1.83	0.46
2:D:108:TYR:CD2	3:E:133:VAL:HG11	2.51	0.45
2:D:218:LYS:HA	2:D:218:LYS:HD2	1.76	0.45
2:B:9:ALA:HA	2:B:68:VAL:O	2.16	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.45
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.45
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.97	0.45
3:E:11:LEU:HD11	3:E:18:GLN:OE1	2.17	0.45
3:E:47:LEU:HD12	3:E:47:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HD12	1:C:234:ILE:N	2.31	0.45
1:C:255:PHE:HD1	1:C:316:CYS:SG	2.39	0.45
1:A:110:ILE:O	1:A:113:GLU:HG2	2.17	0.45
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.97	0.45
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.52	0.45
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.99	0.45
2:D:414:ASP:OD1	2:D:415:GLU:N	2.50	0.45
4:F:160:ILE:HD12	4:F:160:ILE:N	2.31	0.45
4:F:7:ARG:HD3	4:F:40:MET:CE	2.47	0.45
4:F:100:ILE:HD12	4:F:100:ILE:O	2.17	0.45
4:F:226:GLU:OE2	4:F:249:TYR:HE2	2.00	0.45
1:A:275:VAL:HG13	1:A:368:LEU:HD22	1.98	0.45
1:C:220:GLU:CG	2:D:326:LYS:HD2	2.47	0.45
1:C:271:THR:HG23	1:C:300:ASN:O	2.17	0.45
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.47	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.53	0.44
1:C:68:VAL:HG21	1:C:118:VAL:HG21	2.00	0.44
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.99	0.44
4:F:252:ASN:OD1	4:F:253:TYR:N	2.50	0.44
1:A:341:ILE:HG22	1:A:341:ILE:O	2.16	0.44
2:B:1:MET:HG3	2:B:50:ASN:ND2	2.32	0.44
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.82	0.44
2:D:147:SER:OG	2:D:190:SER:OG	2.22	0.44
4:F:161:LEU:HG	4:F:169:LEU:CD2	2.48	0.44
4:F:161:LEU:HD12	4:F:162:ILE:H	1.82	0.44
1:C:12:ALA:HB2	5:C:501:GTP:C8	2.52	0.44
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.52	0.44
3:E:7:GLU:O	3:E:22:VAL:HA	2.17	0.44
2:B:146:GLY:O	2:B:150:GLY:HA3	2.17	0.44
2:D:223:THR:O	2:D:227:LEU:HG	2.18	0.44
1:C:174:ALA:HB2	1:C:207:GLU:N	2.32	0.44
2:D:99:ALA:HB1	2:D:144:GLY:HA3	1.99	0.44
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.48	0.44
4:F:145:ASN:HD22	4:F:145:ASN:HA	1.66	0.44
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.52	0.44
1:A:176:GLN:HG2	1:A:210:TYR:CD2	2.53	0.44
2:D:118:VAL:O	2:D:122:VAL:HG23	2.17	0.44
1:C:71:GLU:CG	1:C:72:PRO:HD2	2.47	0.44
1:C:286:LEU:N	12:C:612:HOH:O	2.41	0.44
2:D:172:MET:HE1	2:D:203:CYS:HA	2.00	0.44
2:B:74:THR:HB	12:B:608:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:45:ASN:O	4:F:46:ARG:HG2	2.17	0.43
1:A:194:THR:O	1:A:194:THR:HG22	2.18	0.43
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.58	0.43
1:A:63:PRO:HD3	1:A:86:LEU:HG	2.01	0.43
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.48	0.43
2:B:208:ALA:HB2	2:B:304:ALA:HB2	2.01	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.43
2:D:274:PRO:HB3	2:D:286:LEU:HD12	2.00	0.43
2:D:70:LEU:HB3	2:D:98:GLY:HA3	1.96	0.43
4:F:218:GLU:HB3	4:F:342:LEU:CD1	2.49	0.43
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.32	0.43
2:B:235:MET:HB3	2:B:235:MET:HE2	1.86	0.43
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.18	0.43
2:B:320:ARG:O	2:B:373:MET:HA	2.18	0.43
2:D:247:GLN:O	2:D:248:LEU:HB2	2.18	0.43
4:F:99:VAL:O	4:F:127:GLU:N	2.51	0.43
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.19	0.43
1:A:338:LYS:HG3	1:A:339:ARG:HG3	2.00	0.42
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.54	0.42
2:B:181:VAL:HG23	1:C:348:PRO:CD	2.49	0.42
2:D:141:LEU:HD12	2:D:172:MET:SD	2.59	0.42
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.42
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.54	0.42
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.37	0.42
1:A:234:ILE:HD12	1:A:234:ILE:N	2.34	0.42
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.49	0.42
4:F:29:ARG:HH21	4:F:32:LYS:HZ2	1.68	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.42
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.55	0.42
2:B:241:CYS:SG	2:B:318:ILE:HD12	2.58	0.42
4:F:253:TYR:HE2	4:F:259:GLY:HA2	1.82	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.54	0.42
3:E:52:LYS:HA	3:E:52:LYS:HD2	1.80	0.42
3:E:124:GLN:OE1	3:E:124:GLN:HA	2.19	0.42
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.47	0.42
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.54	0.42
1:C:282:TYR:HE2	12:C:606:HOH:O	1.99	0.42
2:D:174:SER:CB	2:D:207:GLU:HB2	2.50	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.42
2:D:114:LEU:HG	2:D:114:LEU:O	2.19	0.42
1:A:174:ALA:O	1:A:178:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASN:O	2:B:61:TYR:HA	2.19	0.42
2:D:109:THR:HG21	3:E:137:LYS:NZ	2.35	0.42
1:A:211:ASP:HB3	1:A:215:ARG:NH1	2.34	0.42
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.54	0.42
2:D:163:ASP:OD1	2:D:163:ASP:N	2.47	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.41
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.89	0.41
1:A:10:GLY:O	1:A:14:VAL:HG23	2.20	0.41
2:B:326:LYS:O	2:B:330:GLU:HG3	2.20	0.41
2:B:334:ASN:O	2:B:338:LYS:HB3	2.19	0.41
1:C:75:ILE:HB	1:C:94:THR:CG2	2.51	0.41
2:D:310:GLY:C	2:D:311:ARG:HG2	2.40	0.41
4:F:1:MET:HE1	4:F:28:LYS:HG3	2.03	0.41
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.41
1:C:351:PHE:N	1:C:351:PHE:HD1	2.18	0.41
2:B:324:SER:O	2:B:328:VAL:HG23	2.20	0.41
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.50	0.41
1:A:167:LEU:HD21	1:A:200:CYS:HB3	1.99	0.41
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.03	0.41
2:D:75:MET:CE	2:D:94:PHE:HD2	2.33	0.41
1:C:276:ILE:HD11	1:C:280:LYS:C	2.41	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.94	0.41
1:A:5:ILE:O	1:A:135:PHE:HA	2.21	0.41
1:A:75:ILE:HB	1:A:94:THR:HG21	2.03	0.41
1:A:176:GLN:N	12:A:607:HOH:O	2.40	0.41
2:B:181:VAL:HG23	1:C:348:PRO:HG3	2.01	0.41
1:C:23:LEU:O	1:C:27:GLU:HG3	2.20	0.41
2:D:213:CYS:O	2:D:219:LEU:N	2.40	0.41
2:D:220:THR:O	2:D:221:THR:CG2	2.68	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.41
1:A:136:LEU:HD12	1:A:136:LEU:N	2.36	0.41
2:B:323:MET:HB3	2:B:373:MET:CE	2.50	0.41
1:C:314:ALA:HB2	12:C:605:HOH:O	2.21	0.41
1:C:324:VAL:HG22	12:C:602:HOH:O	2.19	0.41
4:F:239:HIS:C	4:F:240:LEU:HD12	2.41	0.41
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.56	0.40
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.03	0.40
1:C:266:HIS:O	1:C:268:PRO:HD3	2.21	0.40
2:D:123:ARG:O	2:D:127:GLU:HG3	2.21	0.40
2:D:297:ASP:OD1	2:D:298:SER:N	2.54	0.40
4:F:148:ILE:HG22	4:F:183:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:72:PRO:N	2.36	0.40
2:B:274:PRO:HG3	2:B:286:LEU:HD11	2.03	0.40
1:C:177:VAL:HG13	1:C:177:VAL:O	2.21	0.40
4:F:346:LEU:O	4:F:350:ILE:HG13	2.21	0.40
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.36	0.40
2:D:331:GLN:O	2:D:335:VAL:HG23	2.20	0.40
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.57	0.40
2:B:106:GLY:O	2:B:111:GLY:HA3	2.22	0.40
2:D:110:GLU:H	2:D:110:GLU:HG2	1.71	0.40
4:F:145:ASN:ND2	4:F:147:TRP:HE1	2.19	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	431/451 (96%)	415 (96%)	16 (4%)	0	100	100
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	426/445 (96%)	415 (97%)	11 (3%)	0	100	100
2	D	418/445 (94%)	402 (96%)	16 (4%)	0	100	100
3	E	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
4	F	316/384 (82%)	306 (97%)	10 (3%)	0	100	100
All	All	2146/2319 (92%)	2079 (97%)	67 (3%)	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	366/379 (97%)	365 (100%)	1 (0%)	92	97
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	87
2	B	366/383 (96%)	364 (100%)	2 (0%)	88	95
2	D	365/383 (95%)	360 (99%)	5 (1%)	67	82
3	E	108/127 (85%)	106 (98%)	2 (2%)	57	75
4	F	298/342 (87%)	291 (98%)	7 (2%)	50	70
All	All	1875/1993 (94%)	1854 (99%)	21 (1%)	73	87

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
2	B	139	HIS
2	B	232	SER
1	C	71	GLU
1	C	241	SER
1	C	251	ASP
1	C	381	THR
2	D	50	ASN
2	D	113	GLU
2	D	139	HIS
2	D	318	ILE
2	D	415	GLU
3	E	136	ASN
3	E	138	GLU
4	F	145	ASN
4	F	160	ILE
4	F	172	PHE
4	F	178	GLN
4	F	184	LYS
4	F	251	LYS
4	F	253	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
2	B	192	HIS
2	B	247	GLN
2	B	424	ASN
2	D	334	ASN
3	E	136	ASN
4	F	145	ASN
4	F	348	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\# Z  > 2$
8	GDP	D	501	6	24,30,30	0.98	1 (4%)	30,47,47	1.02	3 (10%)
5	GTP	C	501	6	26,34,34	1.11	1 (3%)	32,54,54	1.32	4 (12%)
8	GDP	B	501	6	24,30,30	1.03	2 (8%)	30,47,47	1.11	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	EZW	D	503	-	31,37,37	3.22	17 (54%)	39,54,54	1.87	8 (20%)
5	GTP	A	501	6	26,34,34	1.18	1 (3%)	32,54,54	1.47	6 (18%)
10	MES	B	504	-	12,12,12	2.11	1 (8%)	14,16,16	2.19	5 (35%)
11	ACP	F	401	6	27,33,33	1.85	7 (25%)	32,52,52	1.58	6 (18%)
9	EZW	B	503	-	31,37,37	3.14	16 (51%)	39,54,54	1.66	9 (23%)

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
8	GDP	D	501	6	-	6/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	EZW	D	503	-	-	4/6/24/24	0/5/6/6
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
9	EZW	B	503	-	-	4/6/24/24	0/5/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	EZW	CAP-NAK	8.61	1.47	1.38
9	B	503	EZW	CAP-NAK	8.44	1.46	1.38
10	B	504	MES	C8-S	-7.00	1.67	1.77
9	D	503	EZW	CAS-CAN	4.97	1.55	1.47
9	D	503	EZW	CAQ-CAR	4.75	1.55	1.39
9	D	503	EZW	CBB-CBA	-4.70	1.34	1.42
9	B	503	EZW	CAS-CAN	4.68	1.54	1.47
9	B	503	EZW	CAQ-CAR	4.63	1.54	1.39
9	B	503	EZW	CBB-CBA	-4.59	1.34	1.42
9	D	503	EZW	CAZ-CBA	-4.46	1.34	1.41
9	B	503	EZW	CAZ-CBA	-4.38	1.34	1.41
9	D	503	EZW	CBA-NBC	-4.34	1.29	1.37
5	A	501	GTP	C5-C6	-4.29	1.38	1.47
11	F	401	ACP	PB-O1B	4.20	1.61	1.51
9	D	503	EZW	CAS-CBB	-4.15	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	O4'-C1'	4.07	1.46	1.41
9	B	503	EZW	CBA-NBC	-4.02	1.30	1.37
9	B	503	EZW	CAS-CBB	-3.97	1.35	1.43
9	B	503	EZW	CBF-CBB	-3.87	1.34	1.42
9	D	503	EZW	CBF-CBB	-3.87	1.34	1.42
9	B	503	EZW	OAT-CAU	3.86	1.44	1.36
5	C	501	GTP	C5-C6	-3.76	1.39	1.47
9	D	503	EZW	OAT-CAU	3.66	1.44	1.36
11	F	401	ACP	PB-O3A	3.40	1.62	1.58
9	B	503	EZW	CAG-CAE	-3.40	1.34	1.42
11	F	401	ACP	PB-O2B	-3.38	1.48	1.56
9	D	503	EZW	CAR-CAL	-3.29	1.34	1.40
9	D	503	EZW	CAF-CAE	-3.27	1.34	1.42
9	B	503	EZW	CAJ-CAF	-3.26	1.34	1.42
9	D	503	EZW	CAG-CAE	-3.25	1.34	1.42
9	D	503	EZW	CAJ-CAF	-3.16	1.34	1.42
9	B	503	EZW	CAR-CAL	-3.15	1.34	1.40
9	B	503	EZW	CAF-CAE	-3.08	1.35	1.42
9	B	503	EZW	CAD-CAE	-3.07	1.34	1.41
9	D	503	EZW	CAA-CAF	-3.01	1.34	1.41
9	D	503	EZW	CAD-CAE	-2.97	1.34	1.41
9	B	503	EZW	CAA-CAF	-2.92	1.34	1.41
11	F	401	ACP	PG-O2G	2.88	1.61	1.54
11	F	401	ACP	PG-O3G	2.88	1.61	1.54
9	D	503	EZW	OAO-CAI	2.68	1.44	1.40
8	D	501	GDP	C6-N1	-2.65	1.33	1.37
8	B	501	GDP	C6-N1	-2.46	1.34	1.37
11	F	401	ACP	C5-C4	2.32	1.47	1.40
9	D	503	EZW	CAV-CAU	2.16	1.57	1.49
9	B	503	EZW	CAV-CAU	2.11	1.56	1.49
8	B	501	GDP	O4'-C1'	2.03	1.43	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	EZW	OAT-CAU-CAV	7.29	124.55	110.75
9	B	503	EZW	OAT-CAU-CAV	5.56	121.27	110.75
10	B	504	MES	C6-C5-N4	-4.80	102.82	110.10
11	F	401	ACP	N3-C2-N1	-3.90	122.58	128.68
10	B	504	MES	O1S-S-C8	3.77	111.46	106.92
9	D	503	EZW	OAO-CAI-CAH	3.61	127.84	121.20
5	A	501	GTP	C5-C6-N1	3.37	119.90	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	EZW	CAS-CBB-CBA	3.34	120.95	117.15
11	F	401	ACP	PB-O3A-PA	-3.21	122.38	132.56
5	C	501	GTP	C8-N7-C5	3.09	108.88	102.99
9	D	503	EZW	OAT-CAU-OAW	-3.07	117.04	122.36
9	B	503	EZW	CAS-CBB-CBA	3.07	120.64	117.15
9	B	503	EZW	CBD-NBC-CBA	3.06	121.66	116.93
11	F	401	ACP	C4-C5-N7	-3.01	106.26	109.40
9	D	503	EZW	CBD-NBC-CBA	2.93	121.46	116.93
10	B	504	MES	C7-N4-C5	2.91	118.69	111.23
5	A	501	GTP	C8-N7-C5	2.87	108.46	102.99
5	C	501	GTP	C5-C6-N1	2.81	118.91	113.95
5	A	501	GTP	C2-N1-C6	-2.79	119.97	125.10
9	B	503	EZW	OAO-CAI-CAH	2.77	126.29	121.20
5	A	501	GTP	PB-O3B-PG	-2.77	123.31	132.83
5	A	501	GTP	PA-O3A-PB	-2.73	123.46	132.83
11	F	401	ACP	C2'-C3'-C4'	2.64	107.78	102.64
9	B	503	EZW	CBE-CBD-NBC	-2.57	120.00	123.94
9	D	503	EZW	OAO-CAI-CAJ	-2.55	112.97	117.59
5	C	501	GTP	C2-N1-C6	-2.51	120.47	125.10
9	D	503	EZW	CBE-CBD-NBC	-2.46	120.17	123.94
5	A	501	GTP	O6-C6-C5	-2.46	119.57	124.37
5	C	501	GTP	PB-O3B-PG	-2.46	124.39	132.83
8	B	501	GDP	O2B-PB-O3A	2.45	112.86	104.64
8	D	501	GDP	C8-N7-C5	2.42	107.59	102.99
8	B	501	GDP	C8-N7-C5	2.37	107.51	102.99
10	B	504	MES	C5-N4-C3	2.32	114.06	108.83
8	B	501	GDP	PA-O3A-PB	-2.32	124.88	132.83
11	F	401	ACP	C3'-C2'-C1'	2.27	104.40	100.98
9	B	503	EZW	CBB-CBA-NBC	-2.25	120.43	122.83
11	F	401	ACP	O4'-C4'-C3'	-2.25	100.66	105.11
9	B	503	EZW	OAT-CAU-OAW	-2.23	118.49	122.36
8	B	501	GDP	C5-C6-N1	2.23	117.89	113.95
9	D	503	EZW	CAU-OAT-CAM	-2.21	113.83	117.60
10	B	504	MES	O3S-S-C8	2.20	109.32	105.77
8	D	501	GDP	PA-O3A-PB	-2.19	125.30	132.83
9	B	503	EZW	OAO-CAI-CAJ	-2.18	113.65	117.59
9	B	503	EZW	CAU-OAT-CAM	-2.17	113.90	117.60
8	D	501	GDP	C5-C6-N1	2.14	117.73	113.95

There are no chirality outliers.

All (43) torsion outliers are listed below:

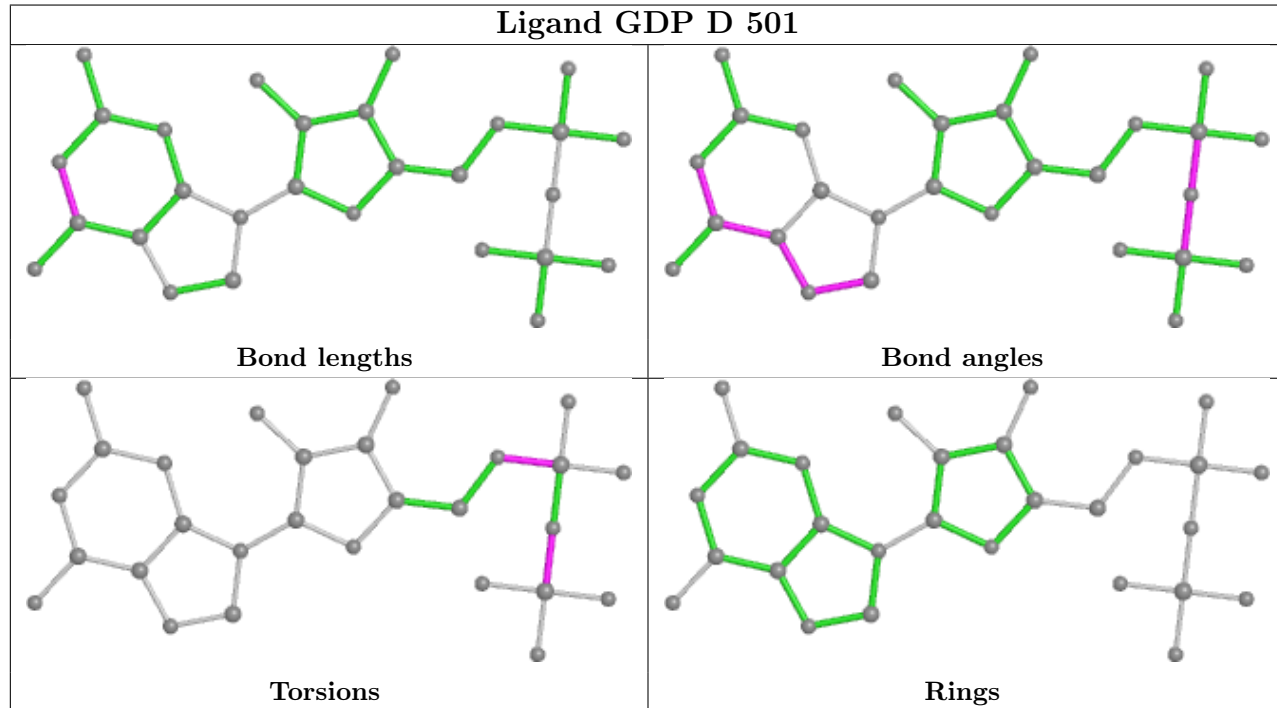
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
9	B	503	EZW	CAV-CAU-OAT-CAM
9	B	503	EZW	OAW-CAU-OAT-CAM
9	D	503	EZW	CAV-CAU-OAT-CAM
9	D	503	EZW	OAW-CAU-OAT-CAM
5	C	501	GTP	PB-O3B-PG-O1G
9	B	503	EZW	OAO-CAN-CAS-CAX
9	D	503	EZW	OAO-CAN-CAS-CAX
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	PG-C3B-PB-O2B
9	B	503	EZW	CAM-CAN-CAS-CAX
9	D	503	EZW	CAM-CAN-CAS-CAX
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	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	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
10	B	504	MES	C8-C7-N4-C3

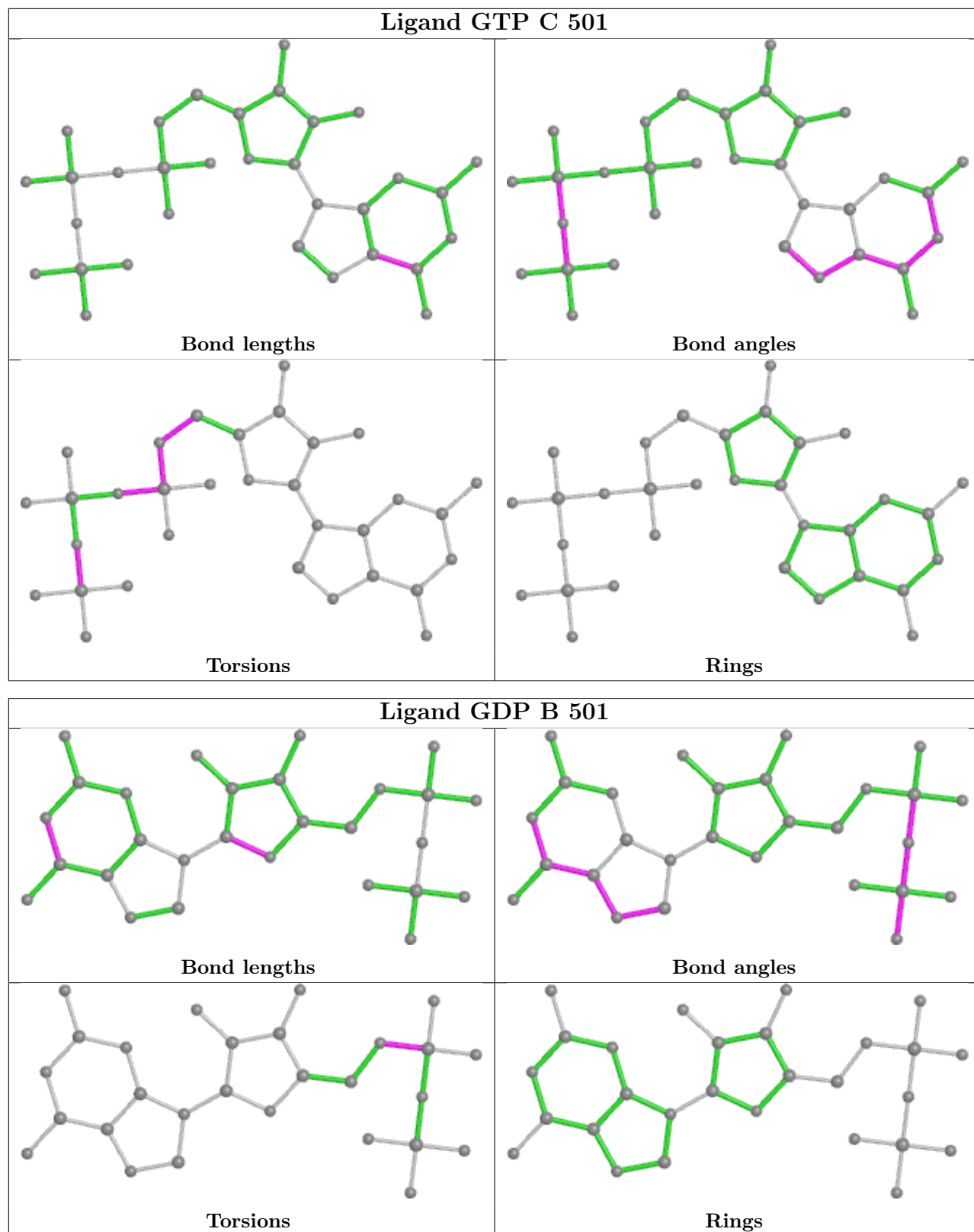
There are no ring outliers.

5 monomers are involved in 8 short contacts:

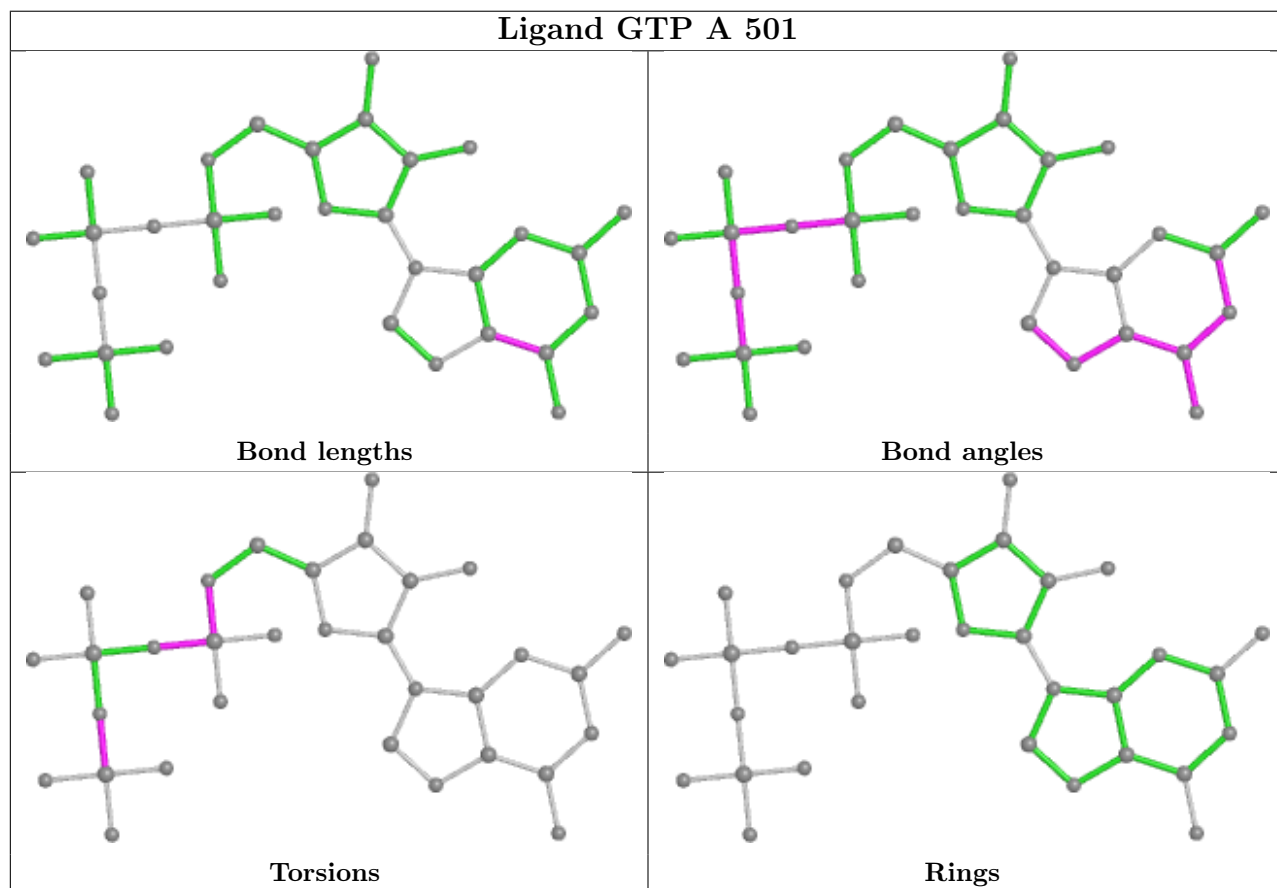
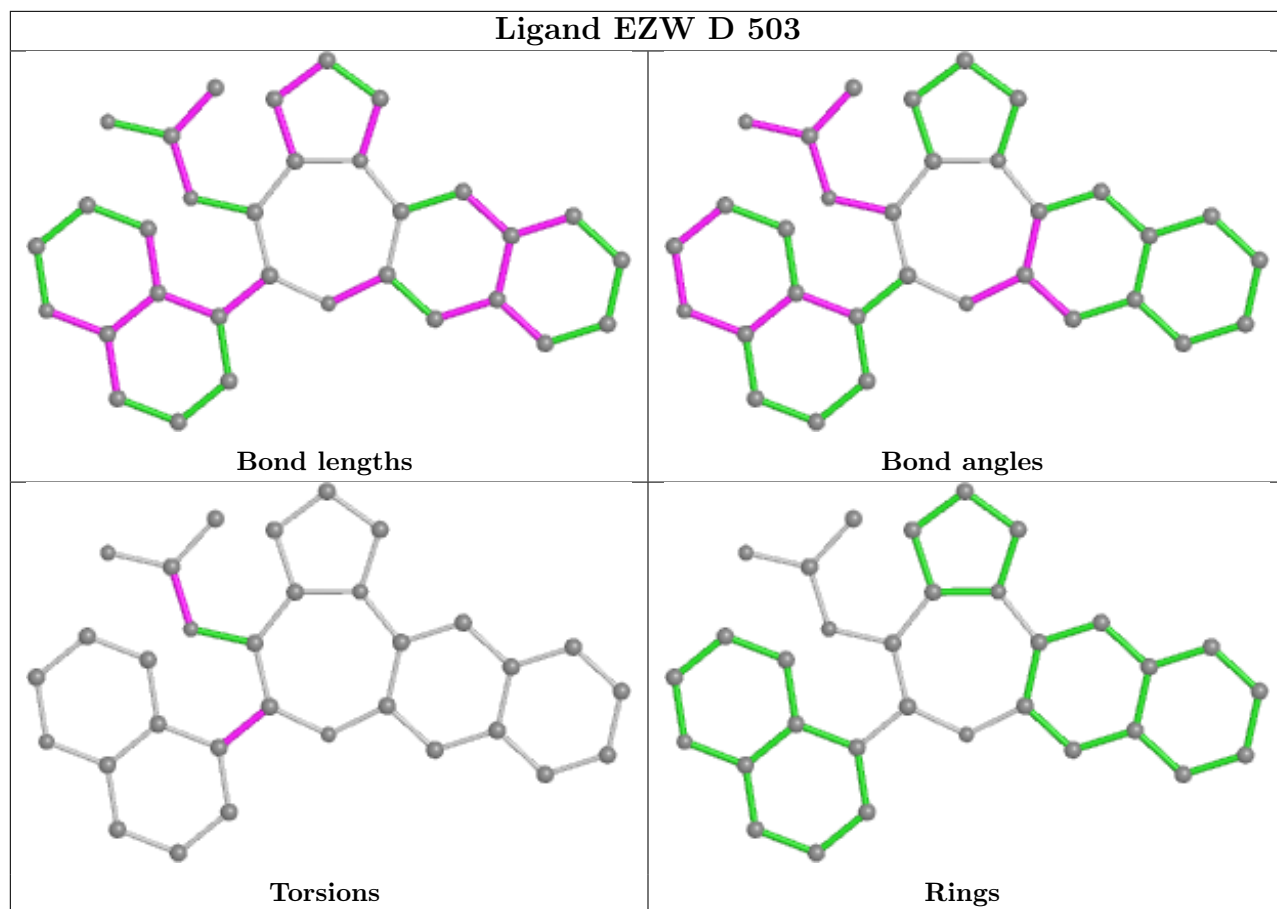
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	3	0
5	C	501	GTP	1	0
8	B	501	GDP	1	0
10	B	504	MES	1	0
11	F	401	ACP	2	0

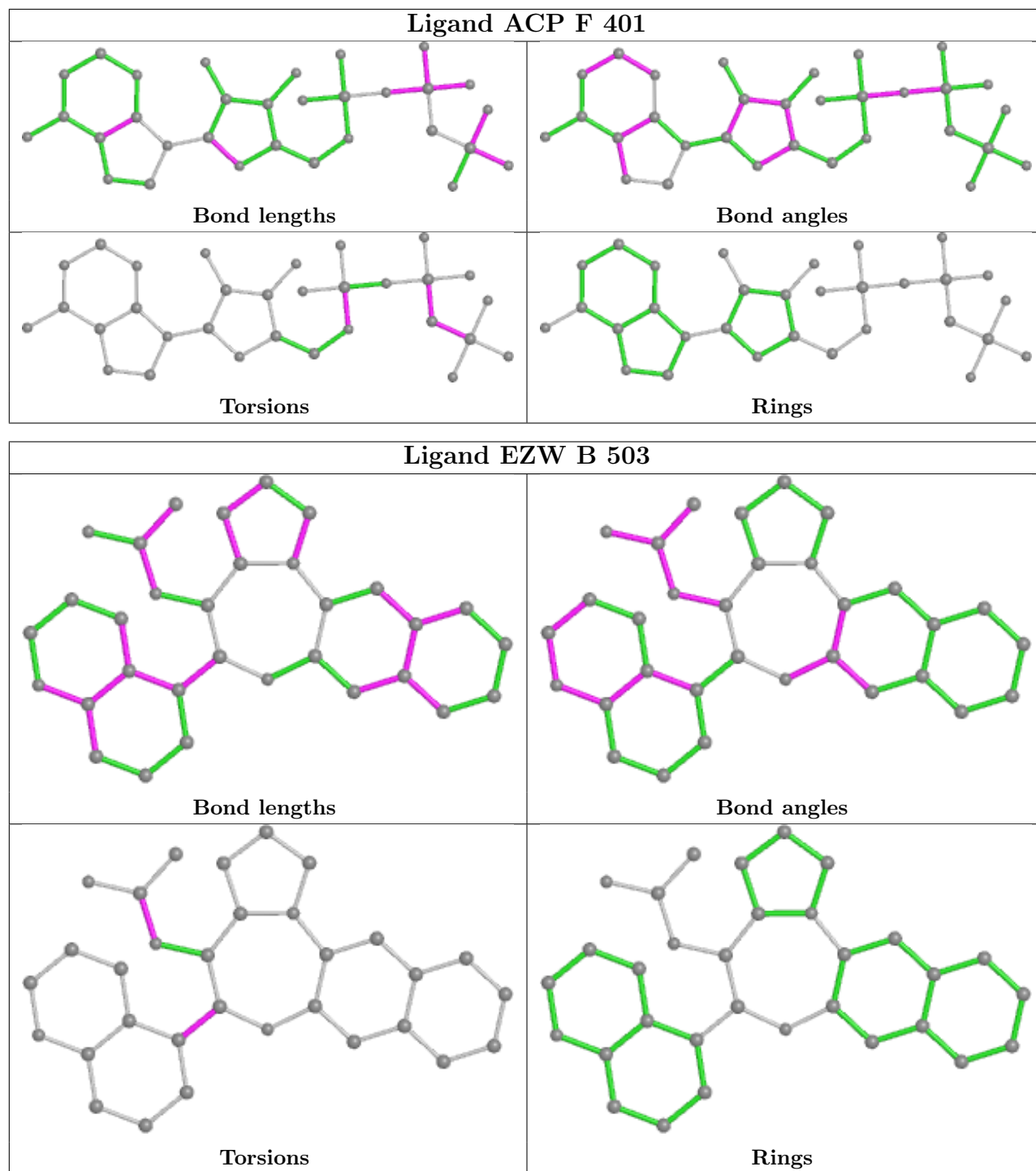
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	435/451 (96%)	-0.08	3 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span>   <span style="border: 1px solid blue; padding: 2px;">86</span>	44, 68, 109, 133	0
1	C	440/451 (97%)	-0.33	1 (0%) <span style="border: 1px solid blue; padding: 2px;">95</span>   <span style="border: 1px solid blue; padding: 2px;">94</span>	36, 52, 88, 116	0
2	B	428/445 (96%)	-0.10	11 (2%) <span style="border: 1px solid gray; padding: 2px;">56</span>   <span style="border: 1px solid gray; padding: 2px;">54</span>	40, 58, 98, 156	0
2	D	422/445 (94%)	0.01	10 (2%) <span style="border: 1px solid gray; padding: 2px;">59</span>   <span style="border: 1px solid gray; padding: 2px;">57</span>	45, 75, 110, 134	0
3	E	120/143 (83%)	0.11	8 (6%) <span style="border: 1px solid red; padding: 2px;">17</span>   <span style="border: 1px solid red; padding: 2px;">16</span>	48, 81, 128, 152	0
4	F	330/384 (85%)	0.85	74 (22%) <span style="border: 1px solid red; padding: 2px;">0</span>   <span style="border: 1px solid red; padding: 2px;">0</span>	53, 96, 156, 184	0
All	All	2175/2319 (93%)	0.03	107 (4%) <span style="border: 1px solid red; padding: 2px;">29</span>   <span style="border: 1px solid red; padding: 2px;">28</span>	36, 69, 122, 184	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	6.4
4	F	254	GLY	6.2
4	F	173	ILE	6.0
4	F	130	VAL	6.0
4	F	250	SER	5.9
4	F	249	TYR	5.8
4	F	240	LEU	5.8
4	F	253	TYR	5.4
4	F	131	PHE	5.2
2	B	437	ASP	5.1
2	B	56	ALA	5.0
4	F	169	LEU	4.7
3	E	25	LYS	4.6
4	F	177	GLY	4.6
4	F	225	SER	4.6
3	E	24	LEU	4.6
2	B	1	MET	4.4
4	F	223	THR	4.4
4	F	241	THR	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	252	ASN	4.3
2	B	438	ALA	4.2
4	F	259	GLY	4.1
2	B	278	ARG	4.0
4	F	166	ALA	4.0
2	B	59	ASN	4.0
1	A	346	TRP	4.0
4	F	256	TYR	3.8
4	F	238	CYS	3.8
4	F	251	LYS	3.8
4	F	182	ILE	3.8
4	F	164	SER	3.7
2	D	219	LEU	3.7
4	F	170	LEU	3.7
4	F	167	SER	3.6
3	E	26	PRO	3.6
4	F	248	GLU	3.6
4	F	100	ILE	3.5
4	F	161	LEU	3.4
4	F	246	GLN	3.4
4	F	149	ALA	3.3
4	F	239	HIS	3.3
4	F	132	LEU	3.3
4	F	226	GLU	3.3
2	D	276	THR	3.1
4	F	194	PRO	3.1
4	F	137	ARG	3.1
1	A	280	LYS	3.1
4	F	228	TYR	3.1
3	E	28	SER	3.0
4	F	192	LEU	2.9
4	F	129	GLU	2.9
1	C	340	SER	2.9
4	F	20	LEU	2.9
4	F	244	CYS	2.8
4	F	245	ILE	2.8
4	F	135	TYR	2.8
4	F	90	SER	2.7
4	F	361	LEU	2.7
2	D	1	MET	2.7
4	F	24	THR	2.7
4	F	133	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	179	VAL	2.7
4	F	229	ASN	2.7
4	F	101	TYR	2.7
4	F	197	ARG	2.7
2	D	57	THR	2.7
2	D	401	ARG	2.6
4	F	247	LYS	2.6
2	D	37	HIS	2.6
4	F	243	HIS	2.6
4	F	134	ALA	2.6
4	F	146	VAL	2.6
4	F	160	ILE	2.6
2	B	280	SER	2.5
4	F	165	GLU	2.5
2	D	222	PRO	2.5
4	F	99	VAL	2.5
4	F	379	HIS	2.5
2	D	286	LEU	2.5
3	E	139	LEU	2.5
4	F	180	HIS	2.5
2	B	37	HIS	2.4
2	B	36	TYR	2.4
4	F	148	ILE	2.4
4	F	147	TRP	2.4
4	F	138	ARG	2.4
4	F	224	SER	2.4
4	F	172	PHE	2.4
2	D	96	GLN	2.3
3	E	6	MET	2.3
2	B	38	GLY	2.3
4	F	21	LEU	2.3
4	F	102	PRO	2.2
4	F	176	GLN	2.2
4	F	17	VAL	2.2
2	B	61	TYR	2.2
4	F	25	GLY	2.2
4	F	28	LYS	2.2
3	E	135	LYS	2.1
4	F	22	LEU	2.1
4	F	162	ILE	2.1
1	A	262	TYR	2.1
2	D	203	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	258	GLU	2.1
4	F	23	ALA	2.0
4	F	13	VAL	2.0
4	F	336	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](#)

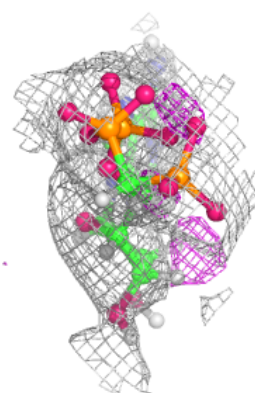
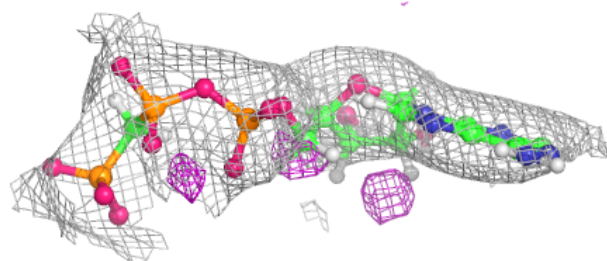
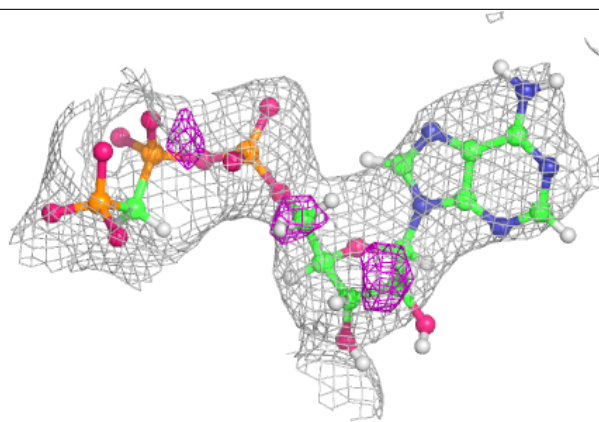
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	F	402	1/1	0.79	0.18	87,87,87,87	0
11	ACP	F	401	31/31	0.84	0.16	87,121,148,174	0
7	CA	A	503	1/1	0.92	0.06	119,119,119,119	0
6	MG	B	502	1/1	0.92	0.29	48,48,48,48	0
8	GDP	D	501	28/28	0.94	0.13	52,66,83,94	0
9	EZW	D	503	32/32	0.95	0.15	57,82,105,121	0
10	MES	B	504	12/12	0.95	0.13	60,83,101,104	0
8	GDP	B	501	28/28	0.95	0.21	37,44,62,85	0
6	MG	A	502	1/1	0.96	0.30	68,68,68,68	0
9	EZW	B	503	32/32	0.97	0.15	46,58,72,81	0
6	MG	D	502	1/1	0.97	0.03	65,65,65,65	0
5	GTP	C	501	32/32	0.98	0.16	32,43,55,63	0
5	GTP	A	501	32/32	0.98	0.21	42,50,57,58	0
6	MG	C	502	1/1	0.99	0.14	49,49,49,49	0
7	CA	C	503	1/1	0.99	0.12	77,77,77,77	0

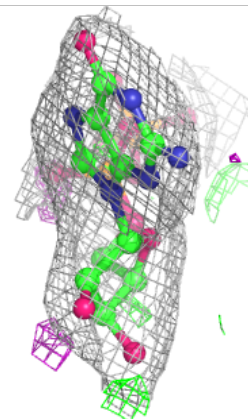
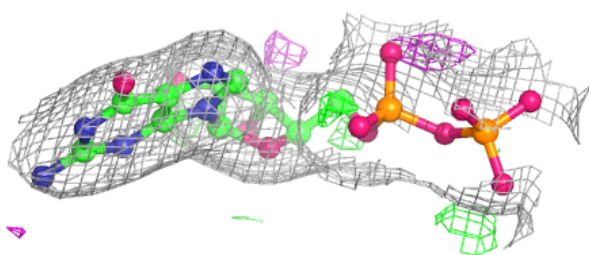
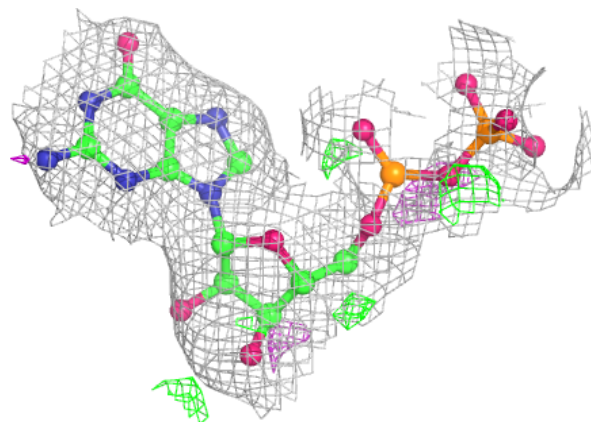
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

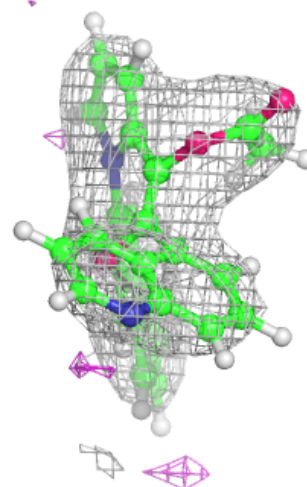
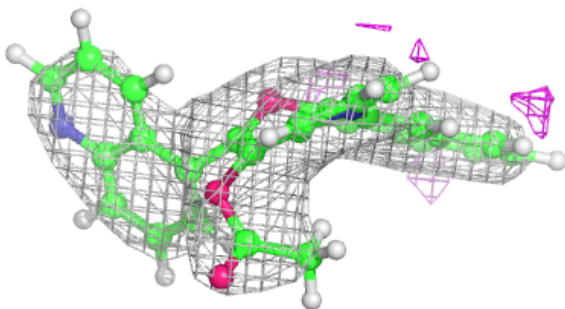
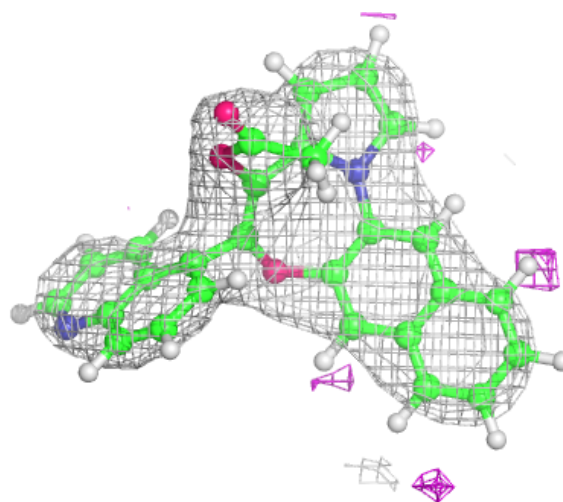
**Electron density around GDP D 501:**

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

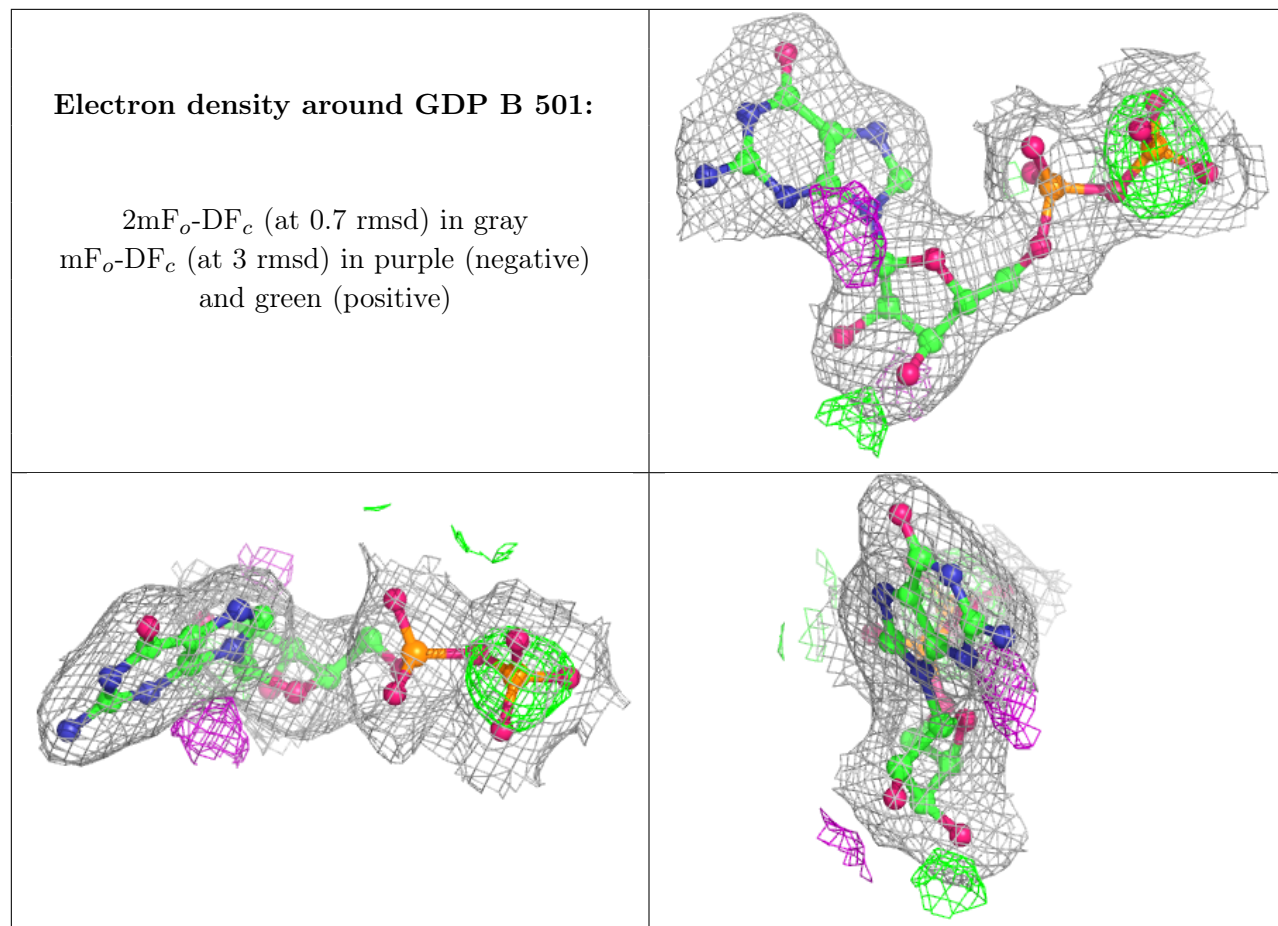


**Electron density around EZW D 503:**

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

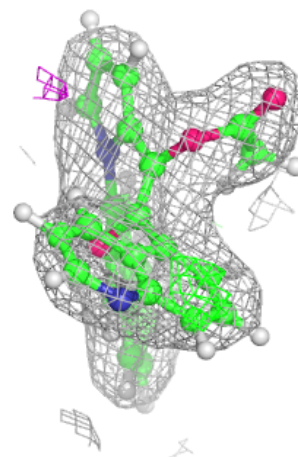
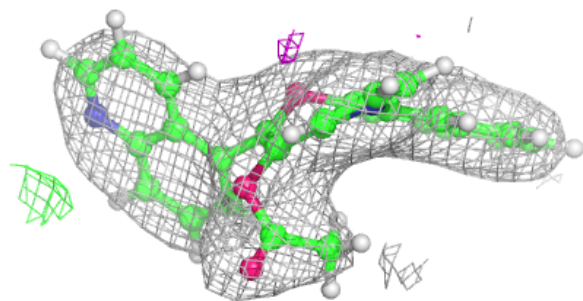
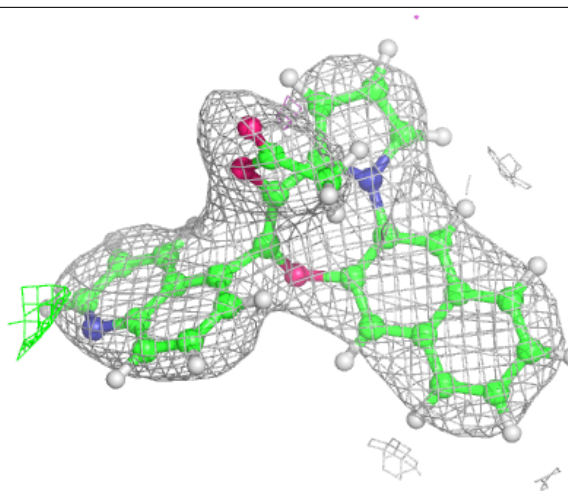


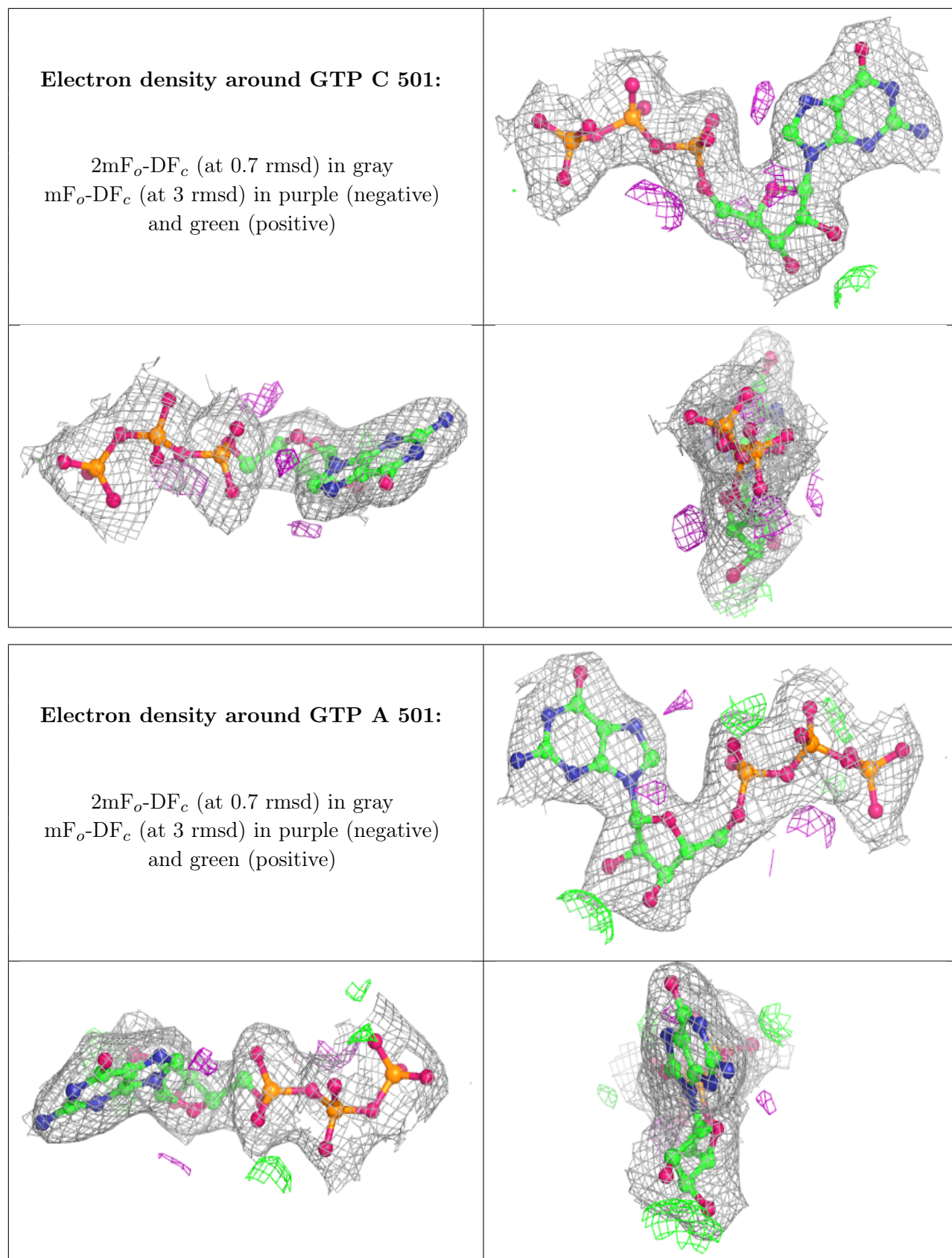




**Electron density around EZW B 503:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.