



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 12:11 PM EDT

PDB ID : 5S5W  
Title : Tubulin-Z53860899-complex  
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Deposited on : 2020-11-08  
Resolution : 2.35 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

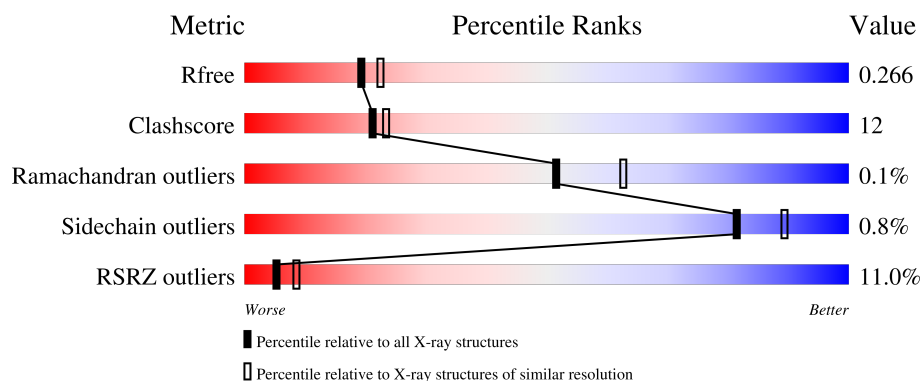
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	C	451	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
2	B	445	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>.</div> </div> </div>
2	D	445	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>.</div> </div> </div>
3	E	143	<div> <div>16%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>21%</div><div>67%</div><div>24%</div><div>8%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18068 atoms, of which 26 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	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	1	1	0
			3359	2109	577	646	27			
2	D	426	Total	C	N	O	S	5	0	0
			3343	2098	570	648	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	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
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	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
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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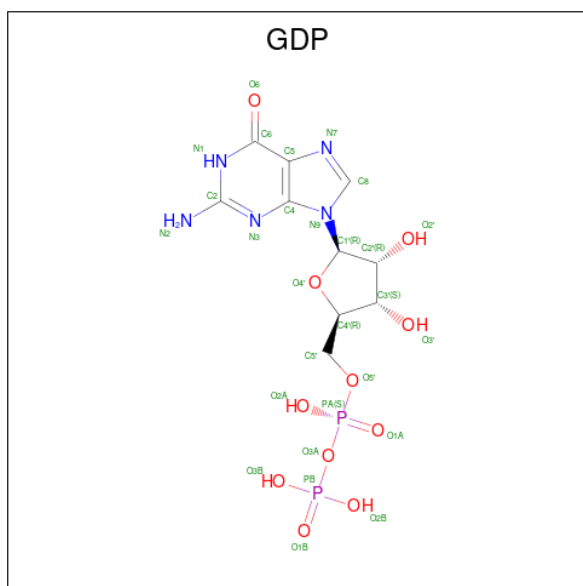
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



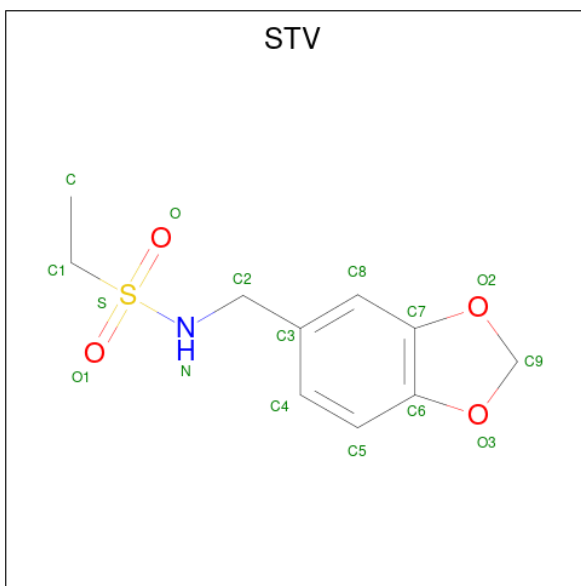
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



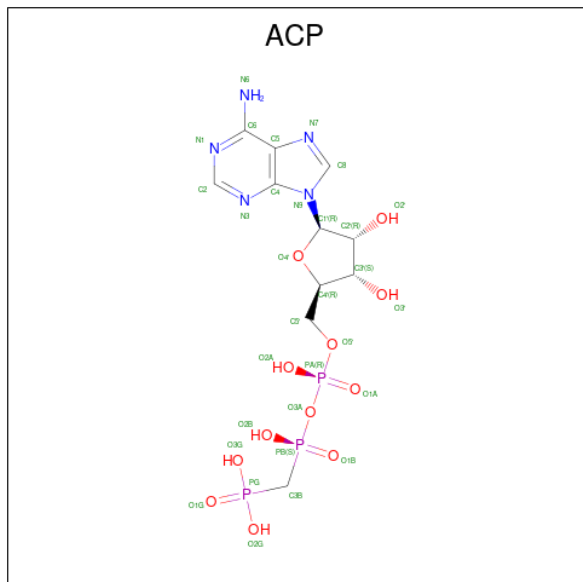
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is {N}-(1,3-benzodioxol-5-ylmethyl)ethanesulfonamide (three-letter code: STV) (formula: C<sub>10</sub>H<sub>13</sub>NO<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			29	10	13	1	4	1		
10	C	1	Total	C	H	N	O	S	0	0
			29	10	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
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

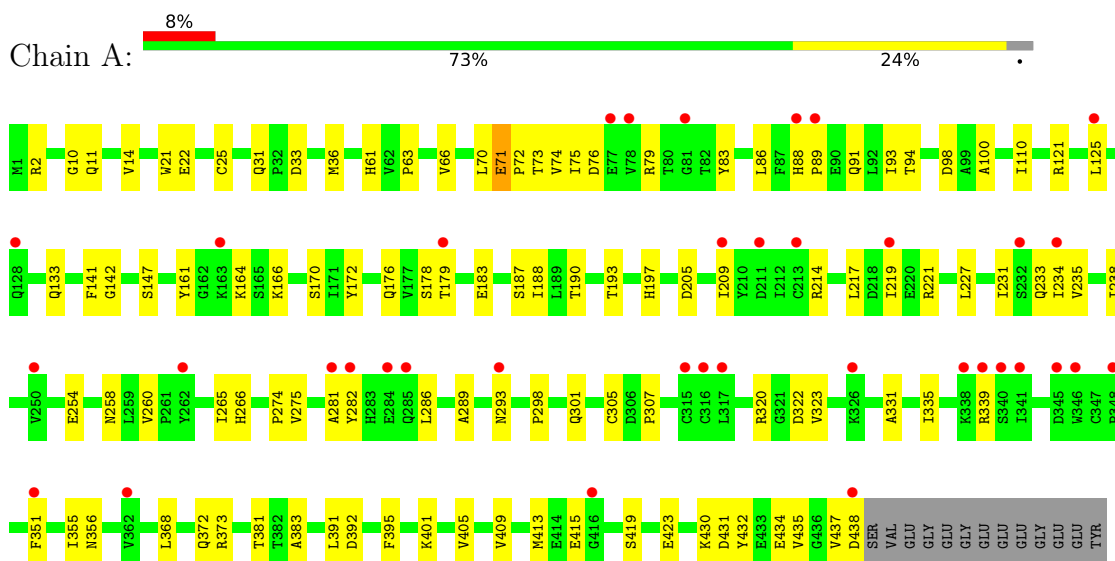
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	62	Total	O	0	0
			62	62		
12	B	84	Total	O	0	0
			84	84		
12	C	180	Total	O	0	0
			180	180		
12	D	32	Total	O	0	0
			32	32		
12	E	9	Total	O	0	0
			9	9		
12	F	11	Total	O	0	0
			11	11		



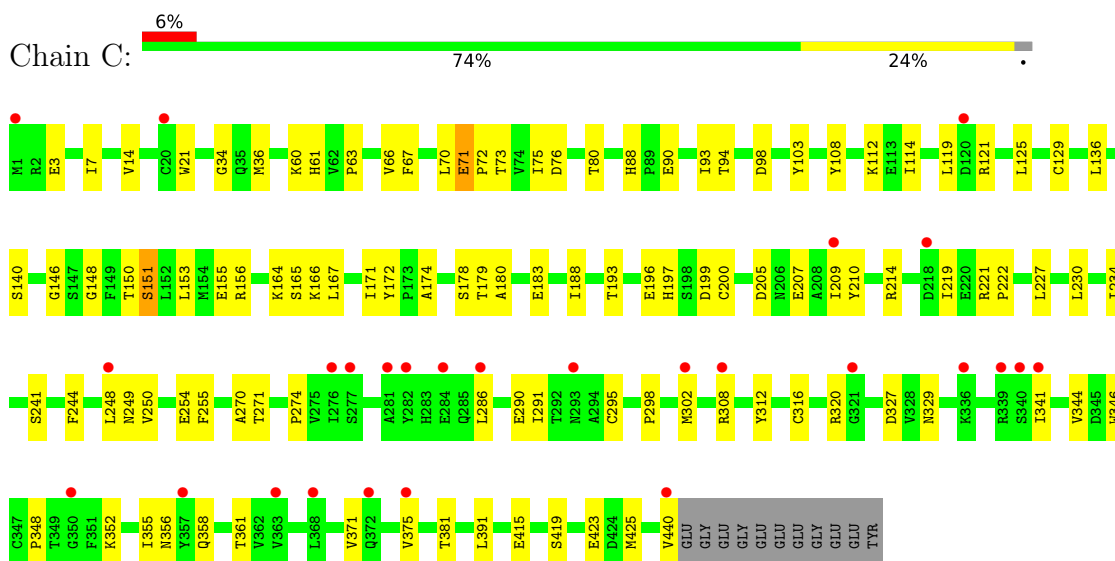
### 3 Residue-property plots

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.

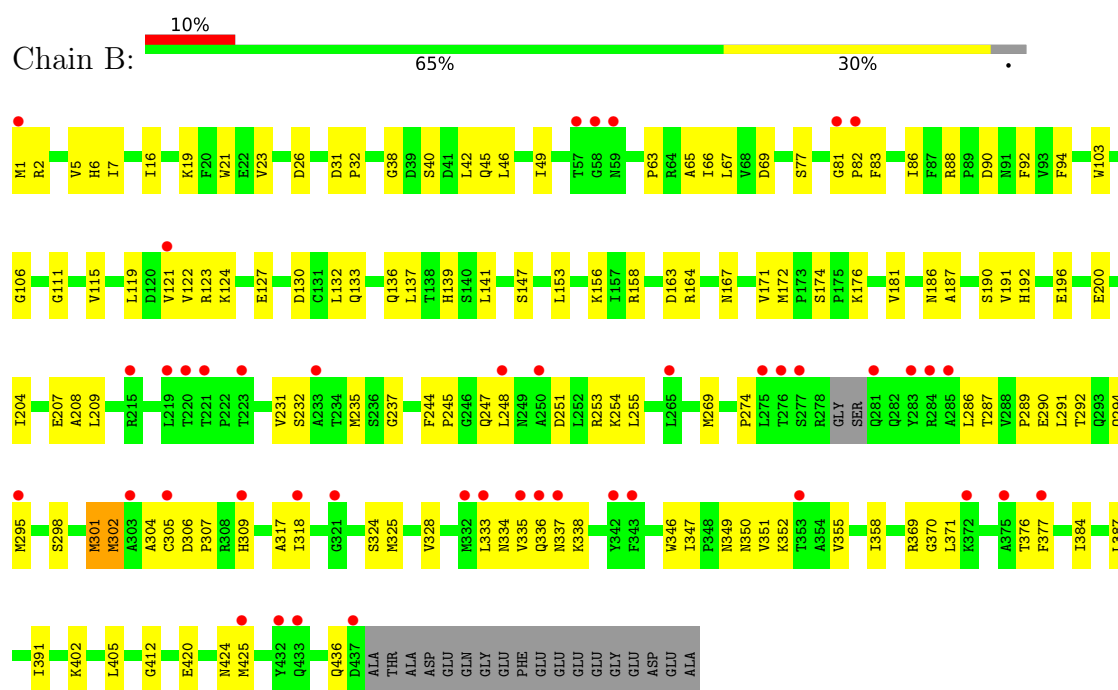
#### • Molecule 1: Tubulin alpha-1B chain



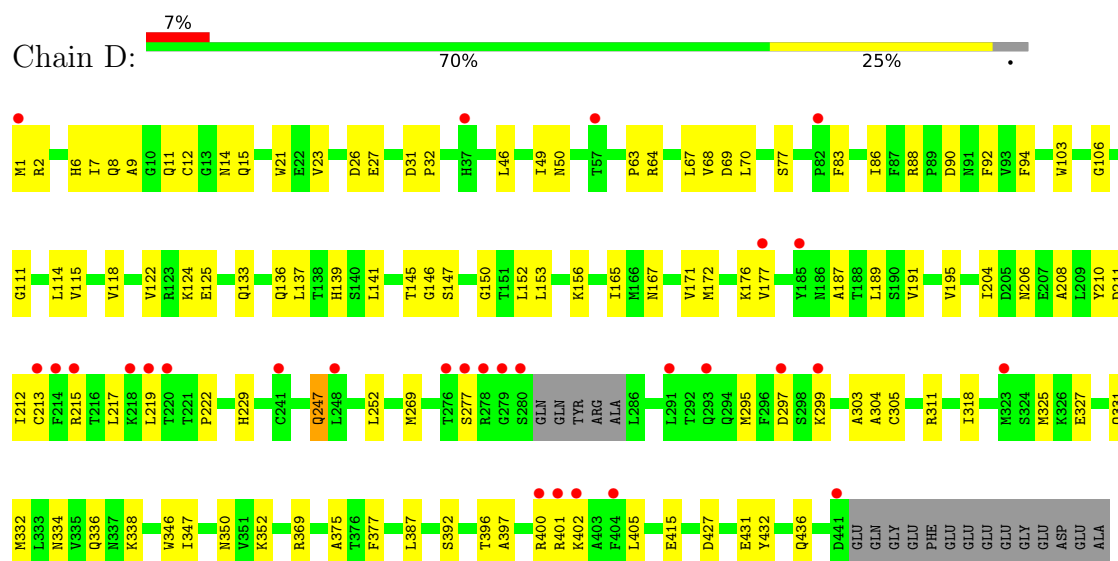
#### • Molecule 1: Tubulin alpha-1B chain



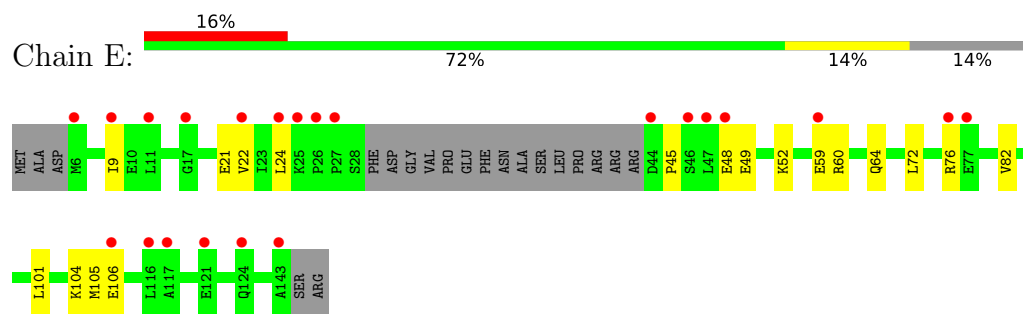
#### • Molecule 2: Tubulin beta-2B chain



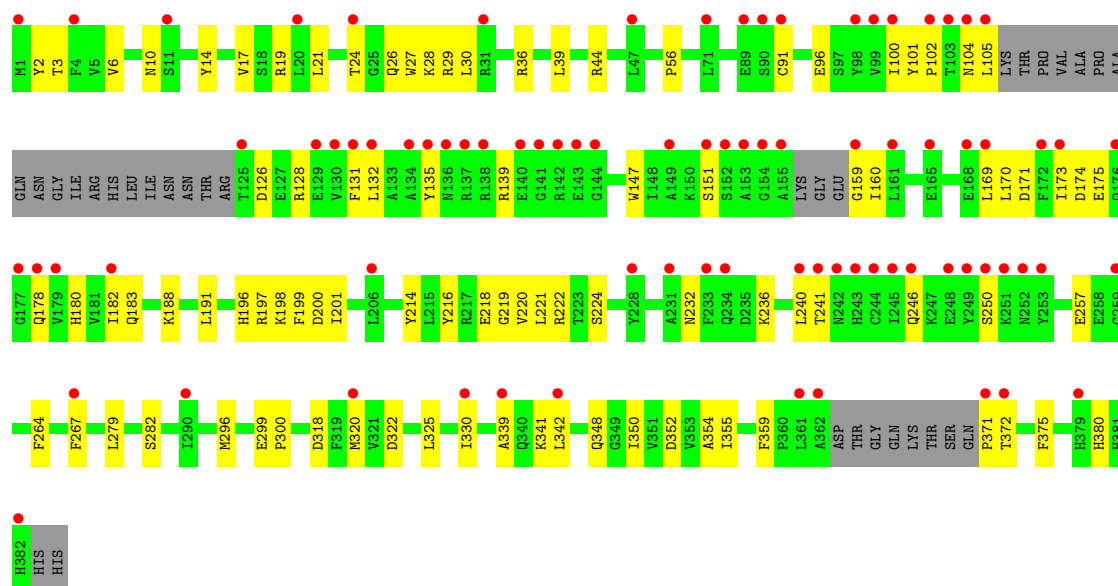
• Molecule 2: Tubulin beta-2B chain



• 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, $\alpha$ , $\beta$ , $\gamma$	104.87Å 158.35Å 178.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.19 – 2.35 118.57 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (63.19-2.35) 99.7 (118.57-2.35)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.224 , 0.265 0.226 , 0.266	Depositor DCC
$R_{free}$ test set	6164 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/3502	0.41	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.25	0/3433	0.41	0/4647
2	D	0.25	0/3416	0.41	0/4626
3	E	0.25	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17838	0.41	0/24141

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	91	0
1	C	3443	0	3352	74	0
2	B	3359	0	3235	105	0
2	D	3343	0	3222	80	0
3	E	1014	0	1029	18	0
4	F	2877	0	2839	70	0
5	A	32	0	12	1	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	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	12	2	0
10	B	16	13	0	0	0
10	C	16	13	0	1	0
11	F	31	0	14	4	0
12	A	62	0	0	5	0
12	B	84	0	0	5	0
12	C	180	0	0	3	0
12	D	32	0	0	4	0
12	E	9	0	0	1	0
12	F	11	0	0	0	0
All	All	18042	26	17085	420	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 12.

All (420) 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:221:ARG:HG3	2:D:325:MET:HG2	1.36	1.02
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.59	0.84
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.95	0.84
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.60	0.83
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.19	0.80
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.64	0.80
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.64	0.79
2:B:83:PHE:O	2:B:86:ILE:HG22	1.83	0.77
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.19	0.74
2:B:88:ARG:NH1	2:B:90:ASP:OD2	2.20	0.73
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.68	0.73
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:LEU:HA	2:D:277:SER:HB3	1.70	0.73
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.71	0.72
1:C:209:ILE:HD11	1:C:302:MET:CE	2.19	0.72
2:B:2:ARG:O	2:B:133:GLN:NE2	2.15	0.72
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.20	0.72
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.25	0.72
2:B:69:ASP:O	2:B:94:PHE:HA	1.90	0.71
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.69	0.71
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.20	0.71
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.56	0.71
1:C:165:SER:HA	1:C:199:ASP:OD2	1.91	0.71
2:D:136:GLN:HA	2:D:167:ASN:O	1.90	0.71
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.26	0.70
2:B:115:VAL:HG23	2:B:153:LEU:HD23	1.72	0.70
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.73	0.70
2:B:167:ASN:OD1	2:B:200:GLU:HB2	1.91	0.69
2:B:163:ASP:OD1	12:B:601:HOH:O	2.11	0.69
2:B:136:GLN:HA	2:B:167:ASN:O	1.93	0.68
1:C:76:ASP:O	1:C:80:THR:HG22	1.93	0.68
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.75	0.68
1:A:179:THR:HA	2:B:352:LYS:HD2	1.75	0.67
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.77	0.67
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.58	0.67
2:D:432:TYR:OH	12:D:601:HOH:O	2.12	0.67
1:C:180:ALA:O	1:C:183:GLU:HG3	1.95	0.67
2:B:324:SER:O	2:B:328:VAL:HG23	1.95	0.66
2:D:145:THR:HB	8:D:501:GDP:O2B	1.94	0.66
2:D:208:ALA:O	2:D:212:ILE:HG13	1.95	0.66
1:C:329:ASN:OD1	10:C:504:STV:N	2.29	0.66
2:B:147:SER:HG	2:B:190:SER:HG	1.43	0.66
1:C:327:ASP:OD1	12:C:601:HOH:O	2.12	0.66
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.95	0.65
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.78	0.65
4:F:320:MET:CG	4:F:330:ILE:HD11	2.27	0.65
2:B:82:PRO:O	12:B:602:HOH:O	2.14	0.65
2:D:83:PHE:O	2:D:86:ILE:HG22	1.96	0.64
1:C:271:THR:HG21	1:C:295:CYS:O	1.98	0.64
2:D:106:GLY:O	2:D:111:GLY:HA3	1.98	0.63
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.28	0.63
1:C:286:LEU:HA	1:C:290:GLU:OE1	1.99	0.63
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HB2	2:B:133:GLN:HG2	1.81	0.63
2:D:171:VAL:HA	2:D:204:ILE:O	1.99	0.62
4:F:371:PRO:HA	4:F:372:THR:O	1.99	0.62
4:F:246:GLN:O	4:F:250:SER:HB3	1.98	0.62
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.81	0.62
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.35	0.62
2:B:420:GLU:OE1	12:B:603:HOH:O	2.16	0.62
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.35	0.62
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.34	0.62
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.81	0.62
2:D:392:SER:O	2:D:396:THR:HG22	1.99	0.62
2:D:1:MET:CE	2:D:50:ASN:HB2	2.30	0.61
2:B:231:VAL:O	2:B:235:MET:HG3	2.00	0.61
4:F:371:PRO:HA	4:F:372:THR:HB	1.81	0.61
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.83	0.61
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.81	0.61
1:C:320:ARG:HA	1:C:356:ASN:O	2.00	0.60
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.32	0.60
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.83	0.60
1:A:214:ARG:HG2	1:A:219:ILE:O	2.01	0.60
2:B:66:ILE:HD13	2:B:121:VAL:HG12	1.83	0.59
4:F:371:PRO:CA	4:F:372:THR:HB	2.33	0.59
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.85	0.59
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.68	0.59
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.85	0.59
4:F:159:GLY:C	4:F:160:ILE:HD12	2.23	0.59
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.38	0.59
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.83	0.59
2:B:192:HIS:HB2	12:B:647:HOH:O	2.03	0.58
2:B:209:LEU:HD21	2:B:302:MET:HG2	1.85	0.58
1:C:155:GLU:HB3	3:E:101:LEU:HD22	1.84	0.58
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.36	0.58
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.39	0.58
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.86	0.58
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.85	0.58
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.85	0.58
3:E:85:LYS:NZ	12:E:201:HOH:O	2.36	0.58
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.39	0.58
2:B:209:LEU:CD2	2:B:302:MET:HG2	2.34	0.57
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.86	0.57
2:B:123:ARG:O	2:B:127:GLU:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.05	0.57
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.39	0.57
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.20	0.57
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.86	0.57
2:D:152:LEU:O	2:D:156:LYS:HG2	2.04	0.57
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.22	0.57
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.40	0.57
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.70	0.56
2:B:42:LEU:H	2:B:42:LEU:HD12	1.69	0.56
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.40	0.56
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.88	0.56
2:B:187:ALA:O	2:B:191:VAL:HG23	2.05	0.56
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.34	0.56
1:A:431:ASP:O	1:A:435:VAL:HG23	2.06	0.56
2:B:424:ASN:HB3	12:B:669:HOH:O	2.06	0.56
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.88	0.56
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.36	0.56
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.41	0.56
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.41	0.56
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.88	0.56
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.71	0.55
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.06	0.55
2:B:174:SER:CB	2:B:207:GLU:HB2	2.36	0.55
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.38	0.55
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.87	0.55
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.87	0.55
1:A:187:SER:CB	1:A:391:LEU:HD21	2.37	0.55
2:D:141:LEU:HA	2:D:147:SER:HB3	1.89	0.55
1:C:151:SER:OG	1:C:193:THR:HG21	2.07	0.55
1:C:108:TYR:O	1:C:112:LYS:HG2	2.06	0.55
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.42	0.55
1:C:108:TYR:OH	3:E:104:LYS:HD2	2.07	0.55
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.40	0.55
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.89	0.55
2:D:11:GLN:O	2:D:15:GLN:HG2	2.07	0.54
3:E:101:LEU:O	3:E:105:MET:HG2	2.07	0.54
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.89	0.54
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.37	0.54
2:B:115:VAL:HG23	2:B:153:LEU:CD2	2.38	0.54
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.23	0.54
2:D:146:GLY:O	2:D:150:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:CB	2:B:253[B]:ARG:HG2	2.37	0.54
1:A:178:SER:OG	1:A:183:GLU:OE1	2.19	0.54
2:D:187:ALA:O	2:D:191:VAL:HG23	2.08	0.54
2:B:46:LEU:HA	2:B:49:ILE:HB	1.89	0.54
2:D:431:GLU:OE1	12:D:602:HOH:O	2.18	0.54
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.23	0.54
4:F:17:VAL:O	4:F:21:LEU:HG	2.07	0.54
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.31	0.53
2:B:333:LEU:HD23	2:B:336:GLN:NE2	2.24	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.53
2:B:124:LYS:HD3	2:B:124:LYS:C	2.29	0.53
1:A:179:THR:HA	2:B:352:LYS:CD	2.39	0.53
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.24	0.53
2:B:317:ALA:C	2:B:318:ILE:HD12	2.28	0.53
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.38	0.53
4:F:101:TYR:N	4:F:126:ASP:OD1	2.32	0.53
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.90	0.53
2:D:295:MET:CE	2:D:375:ALA:HB1	2.39	0.53
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.41	0.53
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.44	0.53
1:A:179:THR:HG21	2:B:248:LEU:CB	2.39	0.53
2:B:66:ILE:CD1	2:B:121:VAL:HG12	2.37	0.53
1:A:430:LYS:O	1:A:434:GLU:HG3	2.09	0.52
1:A:419:SER:O	1:A:423:GLU:HG3	2.10	0.52
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.90	0.52
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.91	0.52
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.45	0.52
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.91	0.52
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.52
1:A:275:VAL:HG13	1:A:368:LEU:HD22	1.91	0.52
2:D:318:ILE:N	2:D:318:ILE:HD12	2.24	0.52
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.92	0.52
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.10	0.52
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.45	0.52
1:C:234:ILE:HD12	1:C:234:ILE:H	1.75	0.52
2:D:247:GLN:NE2	12:D:603:HOH:O	2.34	0.52
4:F:371:PRO:HA	4:F:372:THR:C	2.29	0.52
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.23	0.51
2:D:297:ASP:OD2	2:D:299:LYS:HB2	2.11	0.51
2:D:311:ARG:NH1	2:D:436:GLN:O	2.43	0.51
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.91	0.51
3:E:9:ILE:HG13	3:E:21:GLU:HB3	1.92	0.51
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.93	0.51
1:A:234:ILE:O	1:A:238:ILE:HG13	2.11	0.51
3:E:85:LYS:O	3:E:89:GLU:HG3	2.10	0.50
2:B:2:ARG:HG3	2:B:133:GLN:NE2	2.26	0.50
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.47	0.50
1:C:270:ALA:O	1:C:302:MET:HG2	2.12	0.50
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.46	0.50
1:A:193:THR:HG23	12:A:649:HOH:O	2.11	0.50
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.47	0.50
2:D:70:LEU:HD23	2:D:114:LEU:HD22	1.94	0.50
1:A:71:GLU:HG2	1:A:72:PRO:N	2.26	0.50
1:A:305:CYS:O	1:A:307:PRO:HD3	2.12	0.50
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.12	0.50
1:C:179:THR:HG21	12:D:603:HOH:O	2.12	0.50
3:E:72:LEU:O	3:E:76:ARG:HG2	2.11	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.46	0.49
2:D:332:MET:O	2:D:336:GLN:HG3	2.12	0.49
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.27	0.49
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.94	0.49
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.12	0.49
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.47	0.49
2:B:298:SER:HA	2:B:301:MET:HG3	1.93	0.49
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.49
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.48	0.49
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.42	0.49
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.47	0.49
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.94	0.49
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.47	0.49
2:B:40:SER:OG	2:B:42:LEU:HD13	2.13	0.49
2:D:64:ARG:HG3	2:D:125:GLU:OE1	2.13	0.49
1:A:381:THR:HG22	1:A:383:ALA:H	1.78	0.49
2:B:174:SER:OG	2:B:207:GLU:HB2	2.13	0.49
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.43	0.49
1:A:289:ALA:HA	1:A:331:ALA:CB	2.43	0.49
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.48	0.49
1:A:100:ALA:HB1	2:B:253[B]:ARG:HG2	1.95	0.48
2:D:1:MET:HG3	2:D:50:ASN:CB	2.43	0.48
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.78	0.48
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:MET:HG2	2:B:384:ILE:HD13	1.95	0.48
2:B:391:ILE:HG22	2:B:425:MET:HE1	1.95	0.48
2:D:427:ASP:O	2:D:431:GLU:HG3	2.14	0.48
4:F:341:LYS:HG2	4:F:341:LYS:O	2.14	0.48
4:F:135:TYR:OH	4:F:139:ARG:NH2	2.47	0.48
1:A:356:ASN:HB2	12:A:608:HOH:O	2.13	0.48
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.49	0.48
3:E:106:GLU:HA	3:E:106:GLU:OE1	2.14	0.48
4:F:350:ILE:O	4:F:354:ALA:HB3	2.14	0.48
2:B:77:SER:O	2:B:81:GLY:N	2.47	0.48
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.79	0.48
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.49	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
2:B:42:LEU:HB2	2:B:358:ILE:HD11	1.95	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.47
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.95	0.47
2:D:397:ALA:O	2:D:401:ARG:NH1	2.46	0.47
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.32	0.47
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.47
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.96	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.47
2:D:69:ASP:O	2:D:94:PHE:HA	2.14	0.47
2:B:309:HIS:O	2:B:436:GLN:NE2	2.48	0.47
2:B:318:ILE:HD12	2:B:318:ILE:N	2.30	0.47
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.41	0.47
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.39	0.47
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.97	0.47
2:D:46:LEU:HA	2:D:49:ILE:HB	1.96	0.47
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.97	0.47
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.45	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.47
1:C:440:VAL:HG12	1:C:440:VAL:O	2.15	0.47
2:B:7:ILE:O	2:B:137:LEU:HA	2.14	0.47
2:B:86:ILE:HG12	2:B:86:ILE:O	2.15	0.47
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.50	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.97	0.46
1:C:140:SER:HA	1:C:171:ILE:HB	1.97	0.46
4:F:198:LYS:HG2	4:F:199:PHE:H	1.80	0.46
2:B:1:MET:HB2	2:B:130:ASP:OD2	2.14	0.46
2:B:106:GLY:O	2:B:111:GLY:HA3	2.15	0.46
2:B:295:MET:CG	2:B:377:PHE:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:GLY:O	2:B:371:LEU:HD23	2.15	0.46
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.98	0.46
1:C:234:ILE:HG12	1:C:302:MET:CE	2.46	0.46
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.98	0.46
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.16	0.46
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.44	0.46
2:B:334:ASN:O	2:B:338:LYS:HG3	2.16	0.46
4:F:2:TYR:O	4:F:27:TRP:HA	2.16	0.46
4:F:218:GLU:HB3	4:F:342:LEU:HD13	1.97	0.46
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.97	0.46
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.30	0.46
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.15	0.46
1:C:419:SER:O	1:C:423:GLU:HG3	2.16	0.46
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.98	0.46
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.97	0.46
4:F:178:GLN:N	4:F:178:GLN:OE1	2.49	0.46
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.42	0.46
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.16	0.46
2:D:211:ASP:O	2:D:215:ARG:HB2	2.15	0.46
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.45	0.46
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.46	0.46
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.51	0.45
2:B:19:LYS:O	2:B:23:VAL:HG23	2.17	0.45
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.98	0.45
2:B:305:CYS:O	2:B:307:PRO:HD3	2.16	0.45
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.51	0.45
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.47	0.45
2:B:412:GLY:C	3:E:82:VAL:HG13	2.36	0.45
2:D:23:VAL:O	2:D:27:GLU:HG3	2.16	0.45
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.97	0.45
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.45
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.16	0.45
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.99	0.45
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.99	0.45
1:A:231:ILE:O	1:A:235:VAL:HG23	2.17	0.45
1:C:214:ARG:HG2	1:C:219:ILE:O	2.17	0.45
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.16	0.45
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.99	0.45
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.17	0.45
4:F:171:ASP:O	4:F:175:GLU:HG3	2.16	0.45
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.99	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
2:D:9:ALA:HA	2:D:68:VAL:O	2.18	0.44
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.99	0.44
2:D:327:GLU:O	2:D:331:GLN:HG2	2.15	0.44
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.99	0.44
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.46	0.44
2:B:349:ASN:O	2:B:352:LYS:HE2	2.17	0.44
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.00	0.44
2:D:303:ALA:O	2:D:305:CYS:N	2.46	0.44
4:F:197:ARG:HB2	4:F:224:SER:O	2.17	0.44
1:C:196:GLU:HG2	12:C:644:HOH:O	2.17	0.44
1:C:234:ILE:HD12	1:C:234:ILE:N	2.32	0.44
1:C:291:ILE:HD12	1:C:375:VAL:HG12	2.00	0.44
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.48	0.44
1:A:320:ARG:HD2	12:A:634:HOH:O	2.18	0.44
2:D:387:LEU:HD23	2:D:387:LEU:C	2.38	0.44
4:F:191:LEU:HD13	4:F:196:HIS:CD2	2.52	0.44
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.44
4:F:24:THR:O	4:F:26:GLN:HG3	2.18	0.44
1:A:166:LYS:HE2	1:A:197:HIS:O	2.18	0.44
2:B:176:LYS:HD2	2:B:176:LYS:N	2.33	0.44
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.18	0.44
4:F:296:MET:SD	4:F:380:HIS:HB2	2.58	0.44
1:A:10:GLY:O	1:A:14:VAL:HG23	2.18	0.43
2:B:23:VAL:HG21	2:B:232:SER:HB3	2.00	0.43
2:D:1:MET:CG	2:D:50:ASN:HB2	2.48	0.43
2:B:164:ARG:O	9:B:504:MES:H31	2.18	0.43
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.48	0.43
4:F:188:LYS:O	4:F:322:ASP:HB2	2.17	0.43
1:A:176:GLN:HG3	4:F:56:PRO:HB3	2.00	0.43
2:B:336:GLN:OE1	2:B:351:VAL:HB	2.18	0.43
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.43
4:F:3:THR:HB	4:F:30:LEU:HD11	2.00	0.43
4:F:222:ARG:O	4:F:241:THR:HB	2.18	0.43
1:A:141:PHE:HB3	1:A:187:SER:OG	2.18	0.43
2:B:158:ARG:NH1	2:B:196:GLU:O	2.52	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.00	0.43
4:F:6:VAL:HB	4:F:29:ARG:NH2	2.33	0.43
1:A:176:GLN:HB2	12:A:648:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD12	1:A:234:ILE:N	2.34	0.43
1:A:430:LYS:HE2	1:A:434:GLU:OE2	2.19	0.43
2:B:287:THR:OG1	2:B:289:PRO:HD2	2.19	0.43
2:B:325:MET:HE2	2:B:355:VAL:HG11	2.00	0.43
1:C:3:GLU:OE1	1:C:129:CYS:HB3	2.18	0.43
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.48	0.43
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.18	0.43
4:F:39:LEU:CD2	4:F:355:ILE:HD13	2.49	0.43
4:F:240:LEU:HD12	4:F:240:LEU:N	2.33	0.43
1:A:75:ILE:HB	1:A:94:THR:CG2	2.48	0.43
2:B:42:LEU:HD12	2:B:42:LEU:N	2.33	0.43
1:A:227:LEU:O	1:A:231:ILE:HG13	2.19	0.43
2:D:124:LYS:C	2:D:124:LYS:HD3	2.38	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.43
1:C:178:SER:OG	2:D:352:LYS:NZ	2.52	0.43
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.49	0.43
3:E:22:VAL:HG13	3:E:22:VAL:O	2.19	0.42
4:F:151:SER:HB3	4:F:180:HIS:CG	2.54	0.42
1:A:298:PRO:HA	1:A:301:GLN:CD	2.39	0.42
2:B:251:ASP:HB3	2:B:254:LYS:HB2	2.00	0.42
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.49	0.42
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.55	0.42
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.19	0.42
1:A:66:VAL:HG23	1:A:125:LEU:HD12	2.01	0.42
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.19	0.42
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.19	0.42
4:F:19:ARG:HD2	4:F:19:ARG:O	2.20	0.42
1:A:437:VAL:HG12	1:A:438:ASP:N	2.34	0.42
1:C:70:LEU:HB2	1:C:98:ASP:HA	2.01	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.20	0.42
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.04	0.42
1:A:409:VAL:HA	1:A:413:MET:O	2.20	0.42
2:B:5:VAL:HG23	2:B:132:LEU:HD11	2.00	0.42
2:B:387:LEU:C	2:B:387:LEU:HD23	2.40	0.42
2:D:141:LEU:HD12	2:D:172:MET:SD	2.60	0.42
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.42
3:E:9:ILE:HD11	3:E:21:GLU:OE1	2.19	0.42
3:E:60:ARG:O	3:E:64:GLN:HG3	2.20	0.42
1:A:142:GLY:HA3	1:A:183:GLU:HG2	2.01	0.42
1:C:221:ARG:CG	2:D:325:MET:HG2	2.27	0.42
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:HB3	1:A:373:ARG:HH21	1.85	0.41
2:B:290:GLU:O	2:B:294:GLN:HG3	2.19	0.41
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.92	0.41
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.02	0.41
1:C:241:SER:HA	1:C:249:ASN:OD1	2.20	0.41
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.55	0.41
1:C:71:GLU:OE1	1:C:73:THR:HG23	2.20	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CD2	2.56	0.41
2:B:6:HIS:O	2:B:65:ALA:HA	2.21	0.41
2:D:2:ARG:O	2:D:133:GLN:NE2	2.43	0.41
4:F:14:TYR:HA	4:F:17:VAL:HB	2.03	0.41
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.51	0.41
4:F:199:PHE:HA	4:F:241:THR:HG21	2.03	0.41
1:A:289:ALA:HA	1:A:331:ALA:HB2	2.03	0.41
2:B:141:LEU:HD12	2:B:172:MET:SD	2.61	0.41
2:B:333:LEU:HD23	2:B:336:GLN:HE22	1.85	0.41
2:D:219:LEU:O	2:D:222:PRO:HD3	2.19	0.41
2:D:176:LYS:HD3	2:D:210:TYR:CD1	2.56	0.41
4:F:3:THR:HA	4:F:28:LYS:O	2.21	0.41
2:B:171:VAL:HA	2:B:204:ILE:O	2.21	0.41
1:A:74:VAL:HB	12:A:618:HOH:O	2.21	0.41
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.36	0.41
2:D:191:VAL:O	2:D:195:VAL:HG23	2.22	0.40
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.03	0.40
1:C:146:GLY:O	1:C:150:THR:HB	2.21	0.40
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.40
1:C:415:GLU:HG3	12:C:735:HOH:O	2.21	0.40
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.56	0.40
4:F:267:PHE:CD2	4:F:279:LEU:HD13	2.57	0.40
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.22	0.40
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.03	0.40
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.04	0.40
2:D:69:ASP:OD1	2:D:70:LEU:N	2.54	0.40
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.31	0.40
1:A:281:ALA:O	1:A:282:TYR:HB2	2.21	0.40
1:A:405:VAL:HG11	1:A:415:GLU:HG3	2.04	0.40
1:C:167:LEU:HA	1:C:200:CYS:O	2.21	0.40
2:D:118:VAL:O	2:D:122:VAL:HG23	2.22	0.40
4:F:96:GLU:O	4:F:183:GLN:HA	2.21	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	420 (96%)	16 (4%)	0	100	100
1	C	439/451 (97%)	429 (98%)	9 (2%)	1 (0%)	47	56
2	B	422/445 (95%)	410 (97%)	12 (3%)	0	100	100
2	D	422/445 (95%)	410 (97%)	11 (3%)	1 (0%)	47	56
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	344/384 (90%)	329 (96%)	14 (4%)	1 (0%)	41	47
All	All	2182/2319 (94%)	2117 (97%)	62 (3%)	3 (0%)	51	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	232	ASN
2	D	304	ALA
1	C	72	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	367 (100%)	2 (0%)	88	94
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	B	368/383 (96%)	364 (99%)	4 (1%)	73	84
2	D	368/383 (96%)	364 (99%)	4 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	314 (100%)	1 (0%)	92	96
All	All	1902/1993 (95%)	1887 (99%)	15 (1%)	81	89

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
2	B	139	HIS
2	B	247	GLN
2	B	301	MET
2	B	302	MET
1	C	71	GLU
1	C	151	SER
1	C	361	THR
1	C	381	THR
2	D	77	SER
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN
4	F	91	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	336	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 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	1.15	2 (8%)	31,47,47	1.92	7 (22%)
9	MES	B	504	-	12,12,12	2.25	1 (8%)	14,16,16	1.99	6 (42%)
8	GDP	B	501	6	24,30,30	1.11	2 (8%)	31,47,47	1.87	7 (22%)
11	ACP	F	401	6	27,33,33	1.40	5 (18%)	32,52,52	1.46	4 (12%)
5	GTP	A	501	6	26,34,34	1.02	1 (3%)	33,54,54	1.74	7 (21%)
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.63	6 (18%)
10	STV	B	505	-	17,17,17	1.30	3 (17%)	21,24,24	1.47	1 (4%)
10	STV	C	504	-	17,17,17	1.28	3 (17%)	21,24,24	1.47	3 (14%)

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	-	2/12/32/32	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	ACP	F	401	6	-	10/15/38/38	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
10	STV	B	505	-	-	6/9/15/15	0/2/2/2
10	STV	C	504	-	-	3/9/15/15	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.55	1.66	1.77
8	D	501	GDP	C6-C5	3.97	1.48	1.41
8	B	501	GDP	C6-C5	3.80	1.47	1.41
5	A	501	GTP	C6-N1	3.23	1.38	1.33
10	C	504	STV	S-N	3.17	1.69	1.61
5	C	501	GTP	C6-N1	3.11	1.38	1.33
10	B	505	STV	S-N	3.04	1.69	1.61
11	F	401	ACP	PG-O3G	2.93	1.61	1.54
11	F	401	ACP	PG-O2G	2.91	1.61	1.54
11	F	401	ACP	PB-O3A	2.79	1.61	1.58
11	F	401	ACP	C5-C4	2.48	1.47	1.40
8	D	501	GDP	C5-C4	2.38	1.47	1.40
10	B	505	STV	O-S	2.36	1.46	1.43
8	B	501	GDP	C5-C4	2.27	1.46	1.40
11	F	401	ACP	PB-O2B	2.25	1.61	1.56
10	B	505	STV	O1-S	2.25	1.46	1.43
10	C	504	STV	O1-S	2.24	1.46	1.43
10	C	504	STV	O-S	2.17	1.46	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.41	120.00	127.22
5	C	501	GTP	N3-C2-N1	-4.96	120.61	127.22
8	D	501	GDP	C2-N3-C4	4.71	120.74	115.36
8	B	501	GDP	C2-N3-C4	4.48	120.47	115.36
8	B	501	GDP	C6-N1-C2	4.28	122.73	115.93
8	B	501	GDP	C6-C5-C4	-4.27	116.72	120.80
11	F	401	ACP	PA-O3A-PB	-4.12	119.50	132.56
8	D	501	GDP	C6-N1-C2	4.11	122.46	115.93
8	D	501	GDP	C6-C5-C4	-3.99	116.98	120.80
8	B	501	GDP	C5-C6-N1	-3.99	117.97	123.43
8	D	501	GDP	C5-C6-N1	-3.97	118.00	123.43
5	A	501	GTP	C2-N3-C4	3.94	119.85	115.36
9	B	504	MES	C5-N4-C3	3.78	117.34	108.83
5	C	501	GTP	C2-N3-C4	3.73	119.62	115.36
8	B	501	GDP	N3-C2-N1	-3.47	122.59	127.22
8	D	501	GDP	N3-C2-N1	-3.37	122.73	127.22
11	F	401	ACP	C3'-C2'-C1'	3.24	105.86	100.98
9	B	504	MES	C6-C5-N4	-3.21	105.23	110.10
11	F	401	ACP	N3-C2-N1	-3.11	123.81	128.68
8	D	501	GDP	PA-O3A-PB	-3.05	122.35	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	-3.05	119.26	123.43
5	C	501	GTP	C5-C6-N1	-2.99	119.34	123.43
5	C	501	GTP	PA-O3A-PB	-2.89	122.90	132.83
5	A	501	GTP	PA-O3A-PB	-2.89	122.92	132.83
5	C	501	GTP	PB-O3B-PG	-2.75	123.40	132.83
5	A	501	GTP	C6-N1-C2	2.75	120.29	115.93
10	C	504	STV	C-C1-S	-2.71	109.12	112.93
9	B	504	MES	O1S-S-C8	2.64	110.10	106.92
8	B	501	GDP	PA-O3A-PB	-2.63	123.79	132.83
8	D	501	GDP	C4-C5-N7	-2.58	106.71	109.40
11	F	401	ACP	C4-C5-N7	-2.50	106.80	109.40
5	C	501	GTP	C6-N1-C2	2.48	119.88	115.93
5	A	501	GTP	PB-O3B-PG	-2.44	124.44	132.83
8	B	501	GDP	C4-C5-N7	-2.36	106.94	109.40
10	B	505	STV	O1-S-O	-2.35	115.94	119.35
10	C	504	STV	O1-S-O	-2.32	115.99	119.35
5	A	501	GTP	N2-C2-N1	2.25	120.75	117.25
9	B	504	MES	C7-N4-C5	2.20	116.85	111.23
9	B	504	MES	O3S-S-C8	2.17	109.28	105.77
9	B	504	MES	O2S-S-C8	2.07	109.41	106.92
10	C	504	STV	C9-O3-C6	-2.06	102.67	105.34

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
10	B	505	STV	C2-N-S-C1
10	B	505	STV	C2-N-S-O1
10	B	505	STV	C-C1-S-N
10	B	505	STV	C-C1-S-O
10	B	505	STV	C-C1-S-O1
10	C	504	STV	C2-N-S-C1
10	C	504	STV	C2-N-S-O1

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Mol	Chain	Res	Type	Atoms
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-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
10	B	505	STV	C3-C2-N-S
10	C	504	STV	C3-C2-N-S
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G

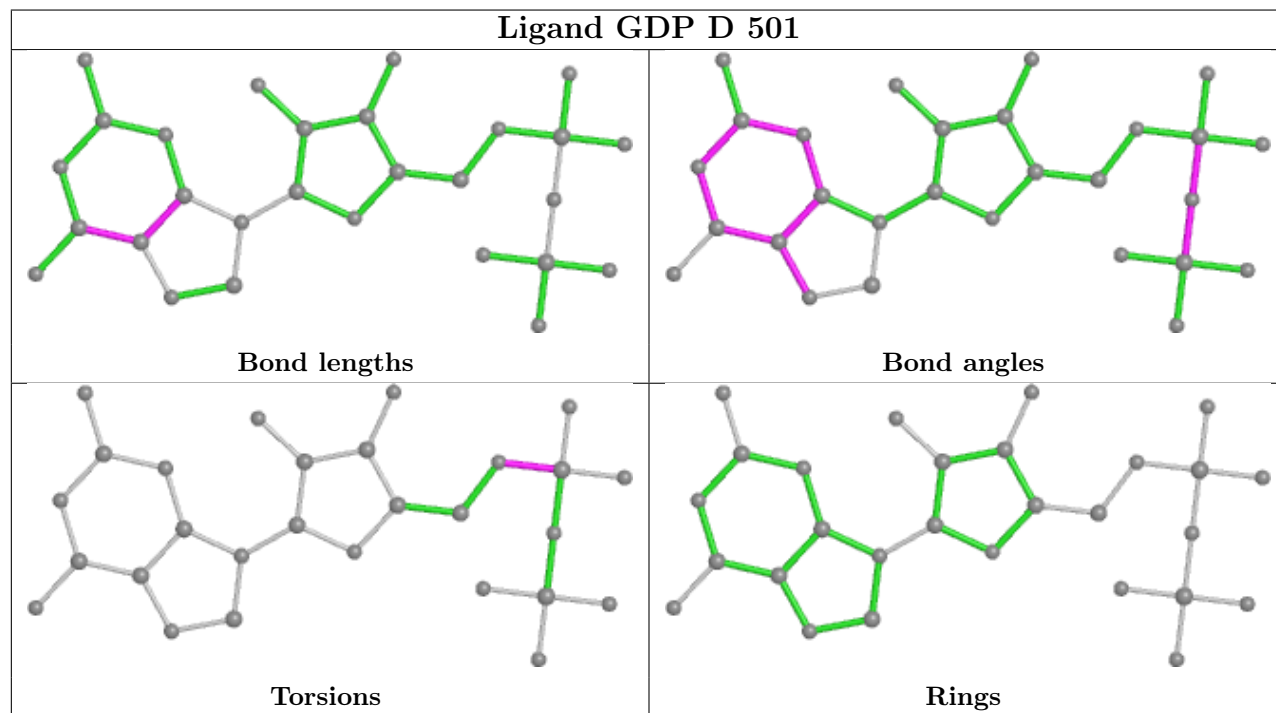
There are no ring outliers.

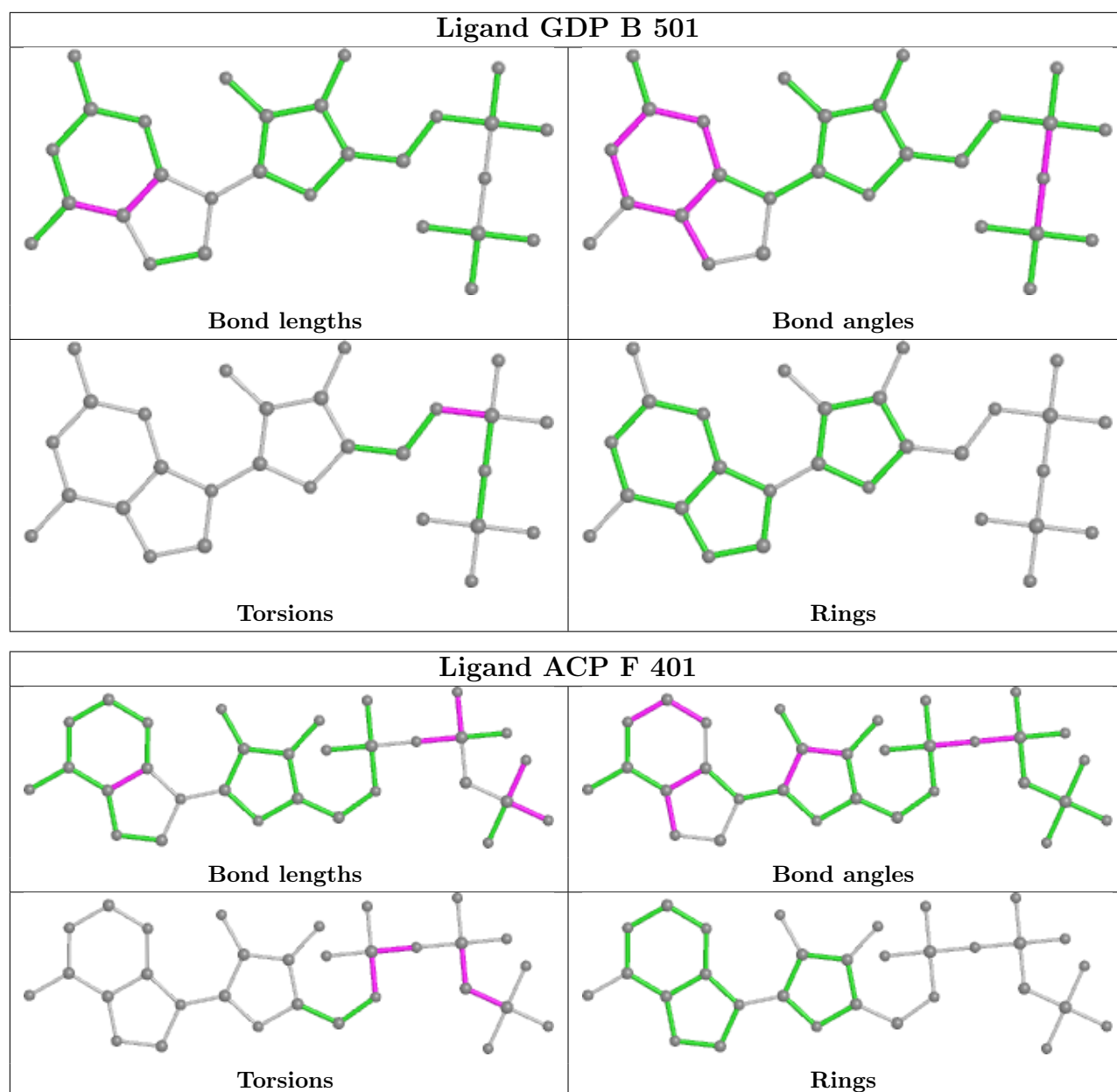
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
9	B	504	MES	2	0
11	F	401	ACP	4	0
5	A	501	GTP	1	0
5	C	501	GTP	1	0
10	C	504	STV	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

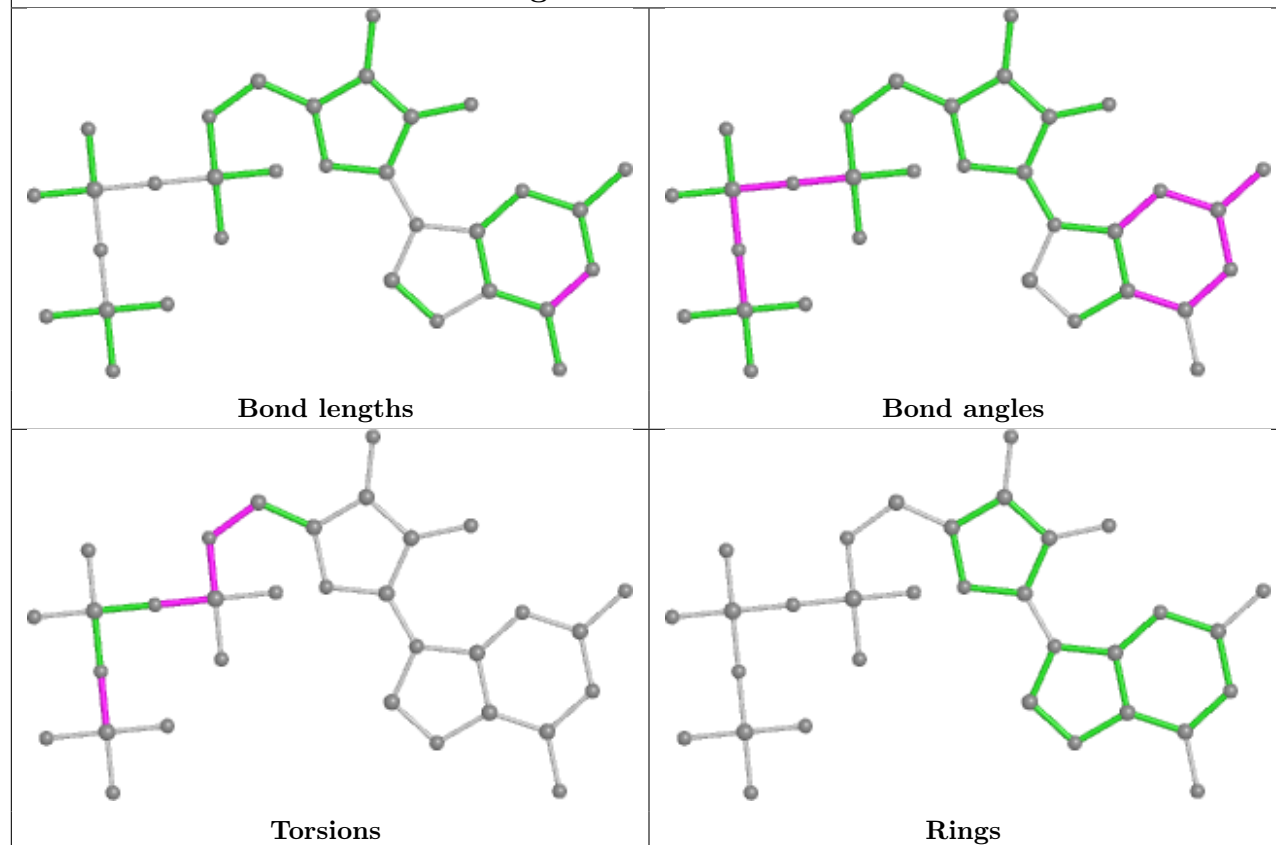
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



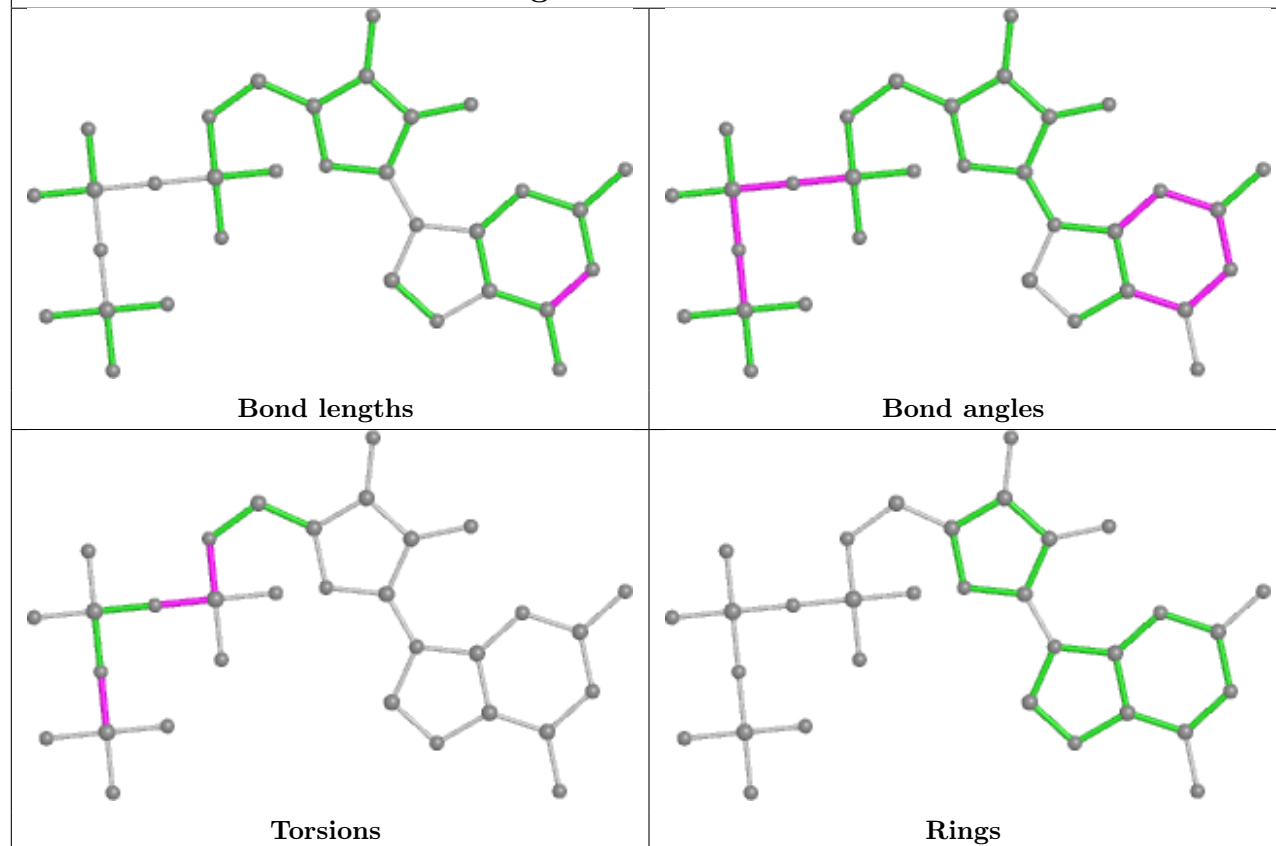


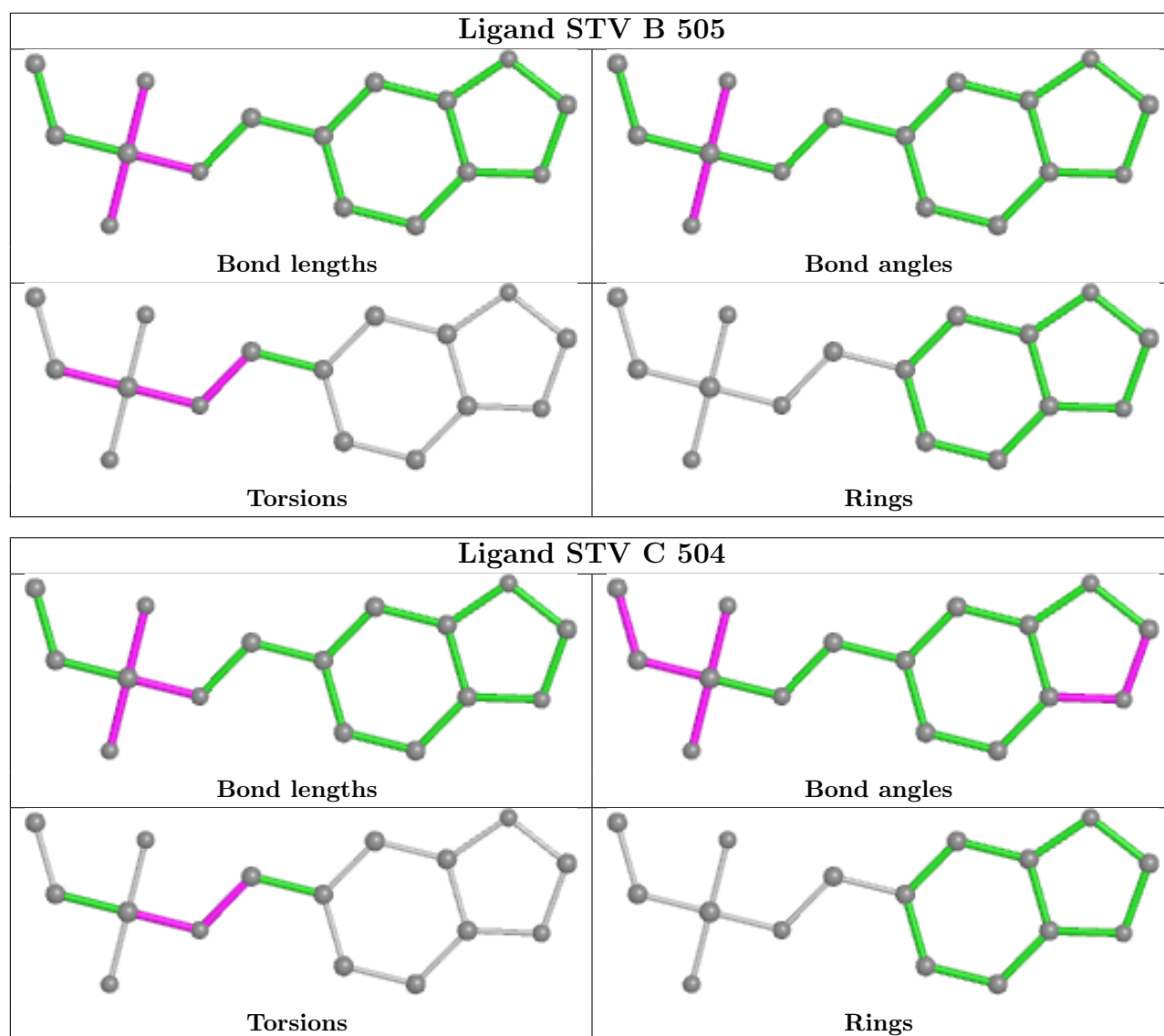


## Ligand GTP A 501



## Ligand GTP C 501





## 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	438/451 (97%)	0.95	37 (8%)	11 16	49, 68, 102, 193	0
1	C	440/451 (97%)	0.88	27 (6%)	21 31	44, 56, 82, 121	0
2	B	425/445 (95%)	1.02	44 (10%)	6 10	45, 66, 110, 195	1 (0%)
2	D	426/445 (95%)	0.87	29 (6%)	17 25	51, 72, 106, 144	4 (0%)
3	E	123/143 (86%)	1.21	23 (18%)	1 2	55, 76, 118, 148	0
4	F	352/384 (91%)	1.50	82 (23%)	0 1	64, 93, 152, 201	0
All	All	2204/2319 (95%)	1.04	242 (10%)	5 8	44, 70, 122, 201	5 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	276	THR	8.8
4	F	173	ILE	8.7
2	B	276	THR	8.2
4	F	104	ASN	7.6
4	F	177	GLY	6.7
3	E	26	PRO	6.1
4	F	154	GLY	6.0
4	F	103	THR	5.9
4	F	153	ALA	5.6
4	F	136	ASN	5.6
2	B	281	GLN	5.6
4	F	152	SER	5.5
3	E	27	PRO	5.1
3	E	6	MET	5.1
4	F	137	ARG	5.0
4	F	253	TYR	5.0
4	F	20	LEU	4.9
2	B	284	ARG	4.9
4	F	169	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
4	F	31	ARG	4.8
4	F	140	GLU	4.8
4	F	251	LYS	4.8
1	A	346	TRP	4.8
4	F	143	GLU	4.8
4	F	89	GLU	4.6
4	F	135	TYR	4.6
2	B	337	ASN	4.4
4	F	142	ARG	4.3
1	A	285	GLN	4.2
1	A	179	THR	4.2
1	A	88	HIS	4.2
4	F	234	GLN	4.2
4	F	250	SER	4.2
2	B	1	MET	4.1
4	F	132	LEU	4.1
4	F	100	ILE	4.1
1	C	357	TYR	4.1
4	F	90	SER	4.1
4	F	259	GLY	4.0
2	B	283	TYR	4.0
4	F	243	HIS	4.0
4	F	330	ILE	3.9
4	F	248	GLU	3.9
1	C	286	LEU	3.9
1	A	282	TYR	3.9
4	F	233	PHE	3.9
4	F	159	GLY	3.8
1	C	284	GLU	3.8
4	F	99	VAL	3.8
1	A	351	PHE	3.7
3	E	44	ASP	3.7
2	D	57	THR	3.7
4	F	176	GLN	3.6
2	D	293	GLN	3.6
1	C	336	LYS	3.6
4	F	134	ALA	3.6
4	F	382	HIS	3.6
4	F	161	LEU	3.6
4	F	178	GLN	3.5
2	B	336	GLN	3.5
1	A	438	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	267	PHE	3.4
4	F	371	PRO	3.4
2	B	59	ASN	3.4
1	C	440	VAL	3.3
4	F	244	CYS	3.3
2	B	303	ALA	3.3
2	D	219	LEU	3.3
2	D	402	LYS	3.3
3	E	24	LEU	3.3
1	A	262	TYR	3.3
2	D	82	PRO	3.3
2	D	401	ARG	3.3
2	D	213	CYS	3.3
2	D	215	ARG	3.3
1	A	341	ILE	3.2
4	F	24	THR	3.2
4	F	339	ALA	3.2
4	F	138	ARG	3.2
1	A	281	ALA	3.2
1	A	340	SER	3.2
2	D	218	LYS	3.2
1	A	345	ASP	3.2
2	B	58	GLY	3.2
1	C	340	SER	3.2
2	D	277	SER	3.1
4	F	130	VAL	3.1
1	C	276	ILE	3.1
1	C	282	TYR	3.1
3	E	116	LEU	3.1
3	E	121	GLU	3.1
4	F	141	GLY	3.1
2	B	275	LEU	3.1
4	F	231	ALA	3.1
4	F	240	LEU	3.1
4	F	91	CYS	3.1
1	A	78	VAL	3.0
1	A	326	LYS	3.0
2	D	280	SER	3.0
3	E	11	LEU	3.0
3	E	48	GLU	3.0
4	F	372	THR	2.9
2	B	333	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	278	ARG	2.9
1	A	316	CYS	2.9
2	D	1	MET	2.9
1	C	218	ASP	2.9
1	A	125	LEU	2.8
4	F	129	GLU	2.8
4	F	151	SER	2.8
4	F	362	ALA	2.8
4	F	249	TYR	2.8
1	A	163	LYS	2.8
4	F	320	MET	2.8
3	E	106	GLU	2.8
4	F	379	HIS	2.8
1	C	350	GLY	2.7
3	E	59	GLU	2.7
1	C	363	VAL	2.7
4	F	131	PHE	2.7
4	F	11	SER	2.7
1	A	250	VAL	2.7
1	A	128	GLN	2.7
2	B	335	VAL	2.7
2	D	400	ARG	2.7
1	A	284	GLU	2.7
1	C	248	LEU	2.7
1	C	20	CYS	2.6
2	D	297	ASP	2.6
4	F	241	THR	2.6
4	F	4	PHE	2.6
1	C	281	ALA	2.6
1	A	348	PRO	2.6
2	B	57	THR	2.6
4	F	105	LEU	2.6
4	F	206	LEU	2.6
4	F	342	LEU	2.6
1	A	338	LYS	2.6
3	E	76	ARG	2.5
1	A	209	ILE	2.5
1	A	234	ILE	2.5
2	D	177	VAL	2.5
3	E	22	VAL	2.5
1	C	341	ILE	2.5
2	B	318	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	433	GLN	2.5
2	B	372	LYS	2.5
3	E	25	LYS	2.5
3	E	96	MET	2.5
2	D	220	THR	2.5
1	C	368	LEU	2.5
2	B	265	LEU	2.5
2	D	441	ASP	2.5
1	C	308	ARG	2.4
2	D	279	GLY	2.4
2	D	37	HIS	2.4
4	F	144	GLY	2.4
4	F	1	MET	2.4
2	D	404	PHE	2.4
4	F	179	VAL	2.4
4	F	168	GLU	2.4
2	B	82	PRO	2.4
3	E	46	SER	2.4
2	B	437	ASP	2.3
2	B	81	GLY	2.3
2	D	291	LEU	2.3
4	F	149	ALA	2.3
2	B	321	GLY	2.3
3	E	17	GLY	2.3
4	F	245	ILE	2.3
4	F	361	LEU	2.3
4	F	252	ASN	2.3
3	E	77	GLU	2.3
4	F	165	GLU	2.3
2	B	342	TYR	2.3
4	F	98	TYR	2.3
2	B	332	MET	2.3
2	D	323	MET	2.3
3	E	124	GLN	2.3
4	F	290	ILE	2.3
1	C	302	MET	2.3
1	C	293	ASN	2.2
4	F	242	ASN	2.2
2	B	121	VAL	2.2
3	E	9	ILE	2.2
4	F	155	ALA	2.2
4	F	125	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	248	LEU	2.2
1	C	375	VAL	2.2
2	B	248	LEU	2.2
2	D	185	TYR	2.2
2	B	250	ALA	2.2
1	A	219	ILE	2.2
1	C	339	ARG	2.2
4	F	228	TYR	2.2
1	A	77	GLU	2.2
1	A	317	LEU	2.2
3	E	47	LEU	2.2
2	B	295	MET	2.2
2	B	432	TYR	2.2
2	D	241	CYS	2.2
2	B	277	SER	2.2
1	A	81	GLY	2.2
2	B	215	ARG	2.1
2	B	221	THR	2.1
2	B	223	THR	2.1
3	E	117	ALA	2.1
1	C	209	ILE	2.1
1	A	339	ARG	2.1
2	B	220	THR	2.1
1	C	277	SER	2.1
2	B	219	LEU	2.1
4	F	71	LEU	2.1
2	B	233	ALA	2.1
2	B	285	ALA	2.1
1	C	120	ASP	2.1
4	F	172	PHE	2.1
1	A	293	ASN	2.1
4	F	182	ILE	2.1
2	B	305	CYS	2.1
2	B	353	THR	2.1
1	A	89	PRO	2.1
4	F	102	PRO	2.1
2	B	309	HIS	2.1
1	A	416	GLY	2.1
1	A	211	ASP	2.1
1	A	213	CYS	2.1
1	A	362	VAL	2.1
2	B	343	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	299	LYS	2.0
1	C	321	GLY	2.0
1	C	372	GLN	2.0
2	D	214	PHE	2.0
2	B	425	MET	2.0
1	A	232	SER	2.0
2	B	375	ALA	2.0
3	E	143	ALA	2.0
4	F	246	GLN	2.0
2	B	377	PHE	2.0
1	A	315	CYS	2.0
4	F	47	LEU	2.0
1	C	1	MET	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( $\text{\AA}^2$ )	Q<0.9
10	STV	C	504	16/16	0.75	0.28	59,70,84,91	29
11	ACP	F	401	31/31	0.78	0.21	89,102,116,120	0
10	STV	B	505	16/16	0.83	0.24	49,80,103,104	29
7	CA	A	504	1/1	0.85	0.14	93,93,93,93	0
9	MES	B	504	12/12	0.86	0.24	93,98,111,115	0
6	MG	C	502	1/1	0.90	0.14	43,43,43,43	0
6	MG	D	502	1/1	0.91	0.10	77,77,77,77	0
8	GDP	D	501	28/28	0.91	0.17	64,71,78,82	0
6	MG	A	502	1/1	0.92	0.12	48,48,48,48	0
6	MG	F	402	1/1	0.92	0.11	101,101,101,101	0

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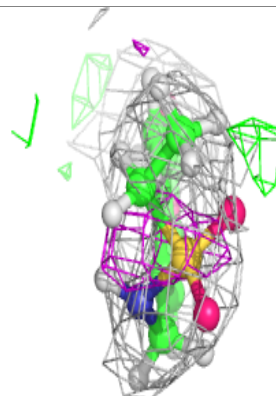
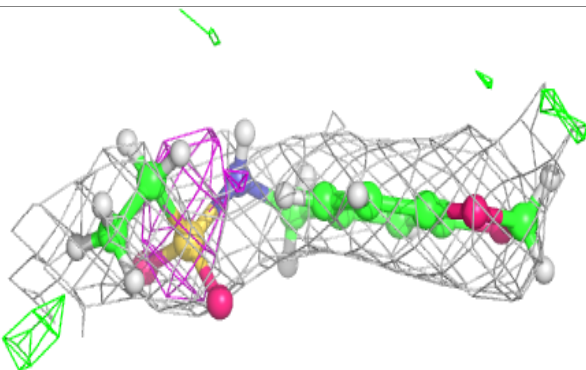
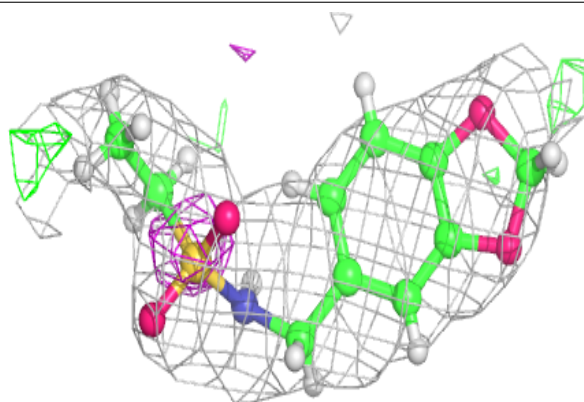
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CA	B	503	1/1	0.93	0.08	104,104,104,104	0
5	GTP	A	501	32/32	0.94	0.17	45,51,57,63	0
8	GDP	B	501	28/28	0.96	0.17	40,49,55,58	0
5	GTP	C	501	32/32	0.96	0.18	42,48,54,55	0
7	CA	A	503	1/1	0.96	0.08	93,93,93,93	0
6	MG	B	502	1/1	0.98	0.14	46,46,46,46	0
7	CA	C	503	1/1	0.98	0.08	71,71,71,71	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.

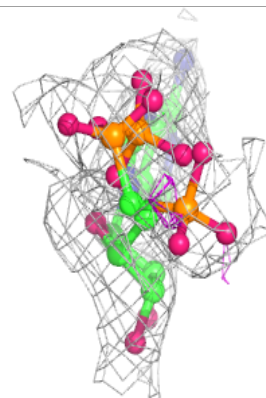
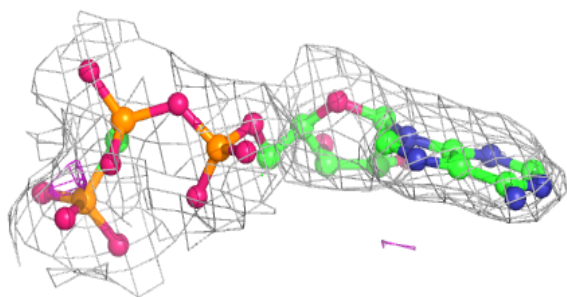
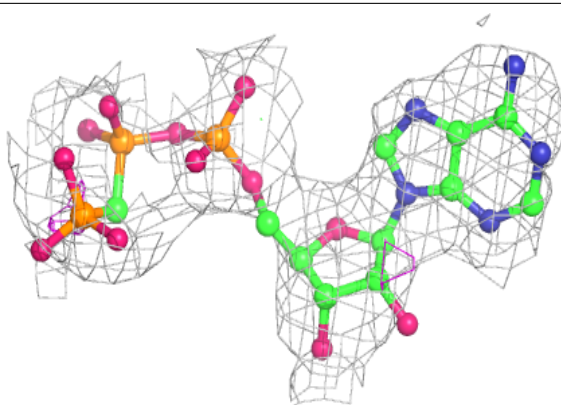
**Electron density around STV C 504:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

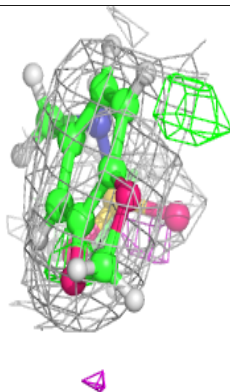
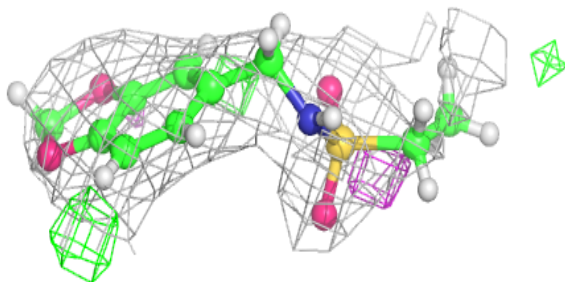
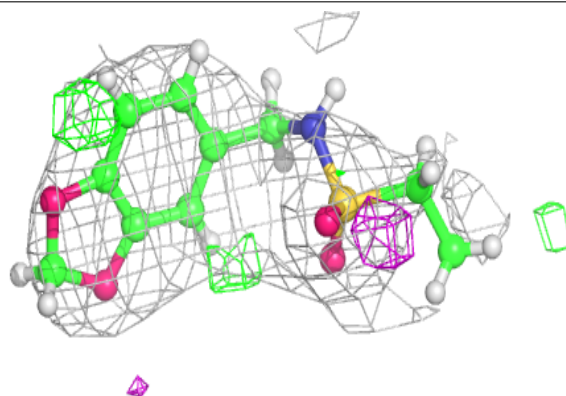


**Electron density around ACP F 401:**

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

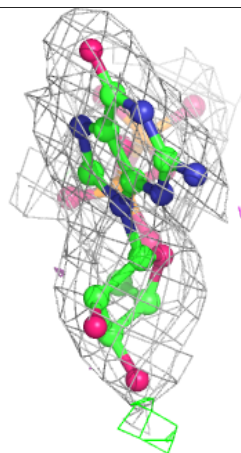
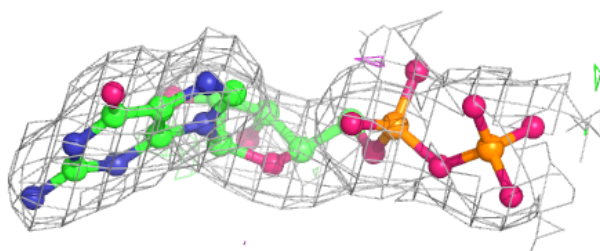
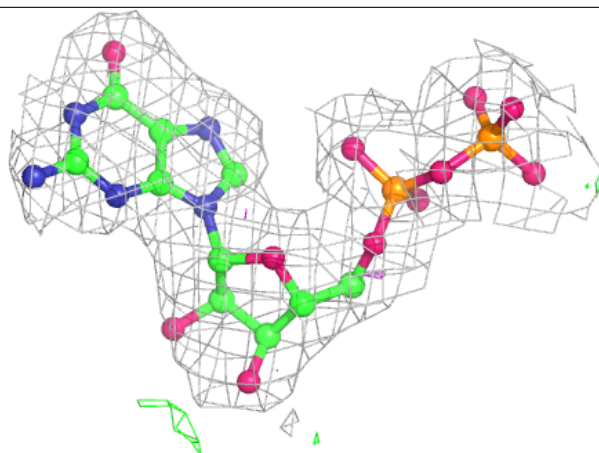
**Electron density around STV B 505:**

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

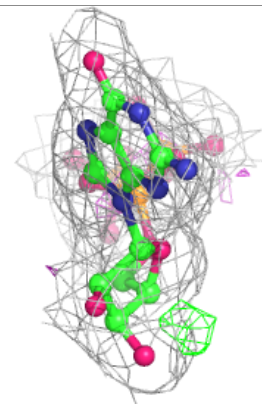
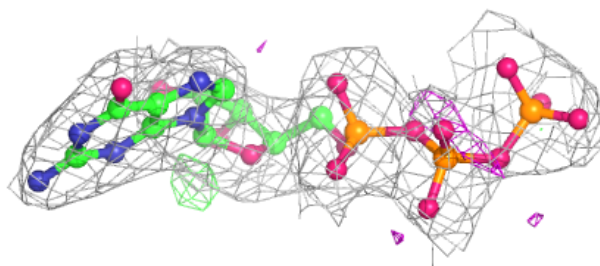
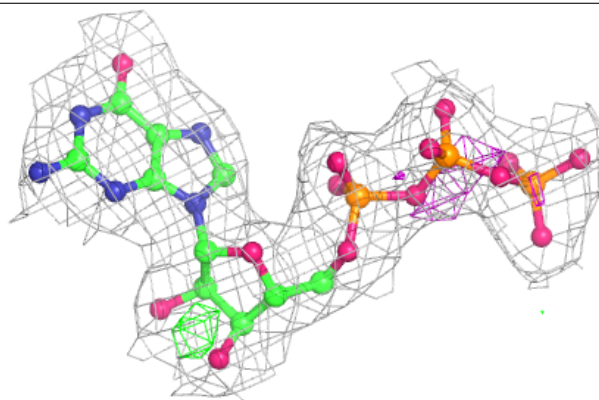


**Electron density around GDP D 501:**

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

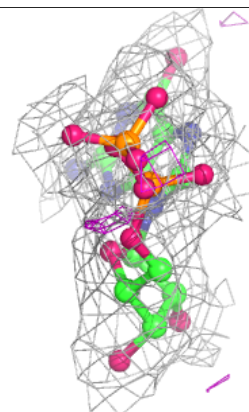
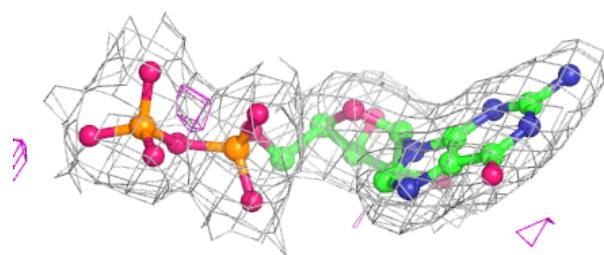
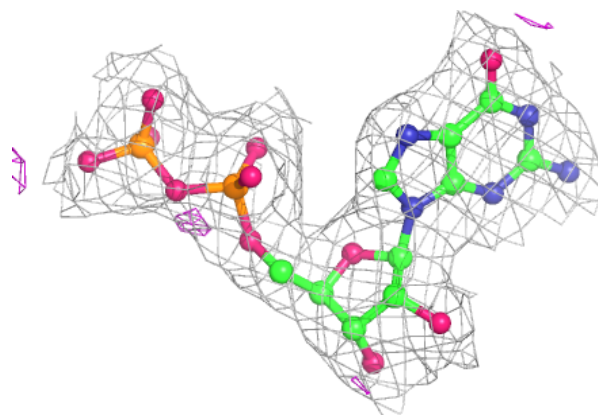
**Electron density around GTP A 501:**

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

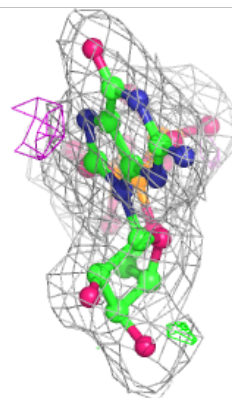
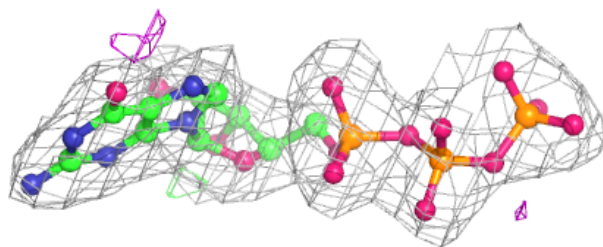
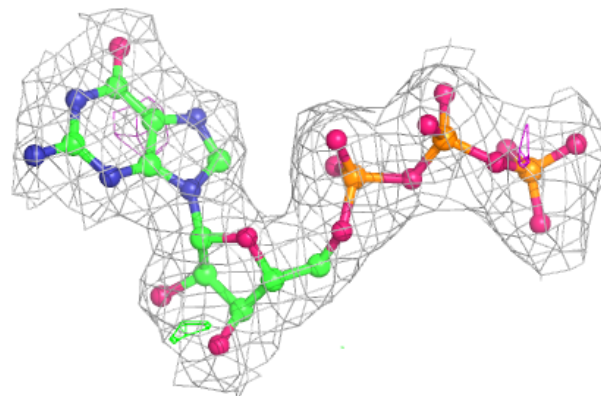


**Electron density around GDP B 501:**

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

**Electron density around GTP C 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.