



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 02:27 PM EDT

PDB ID : 5S64  
Title : Tubulin-Z28870646-complex  
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Deposited on : 2020-11-08  
Resolution : 2.75 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

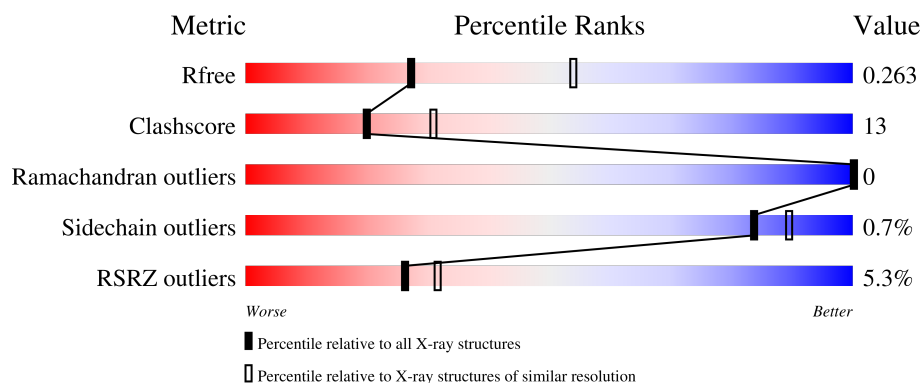
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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>10%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>.</div> </div> </div>
1	C	451	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
2	B	445	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>.</div> </div> </div>
2	D	445	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>
3	E	143	<div> <div>15%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	TVP	C	504	-	-	X	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17802 atoms, of which 30 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	2	0	0
			3348	2103	573	645	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	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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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	2	Total	Ca	0	0
			2	2		
7	B	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>).



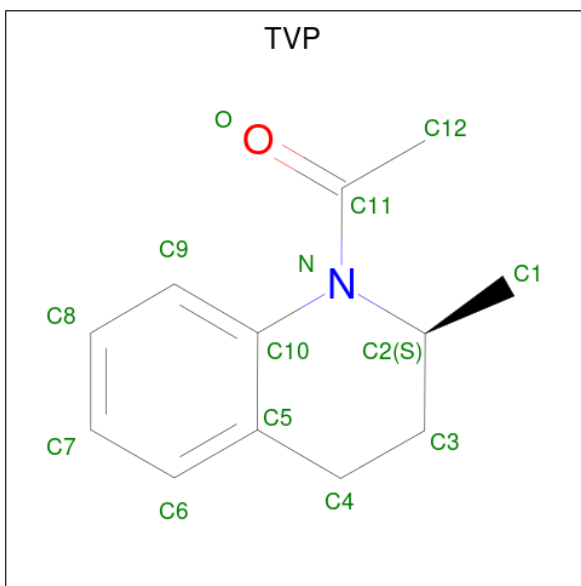
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



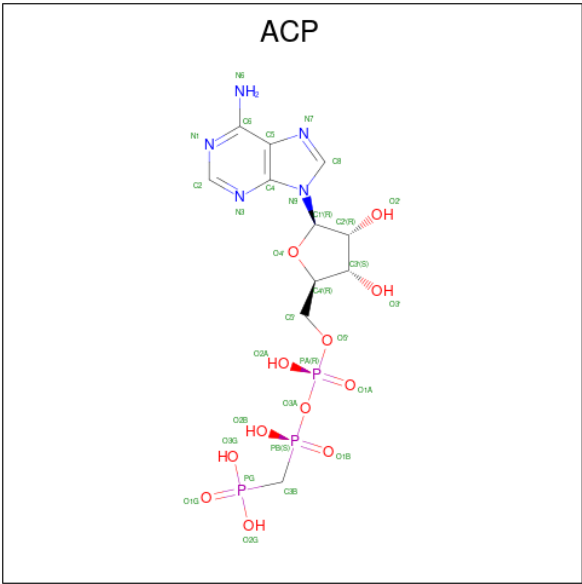
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is (2S)-1-ACETYL-2-METHYL-1,2,3,4-TETRAHYDROQUINOLINE (three-letter code: TVP) (formula: C<sub>12</sub>H<sub>15</sub>NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
10	B	1	29	12	15	1	1	0	0
10	C	1	29	12	15	1	1	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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.

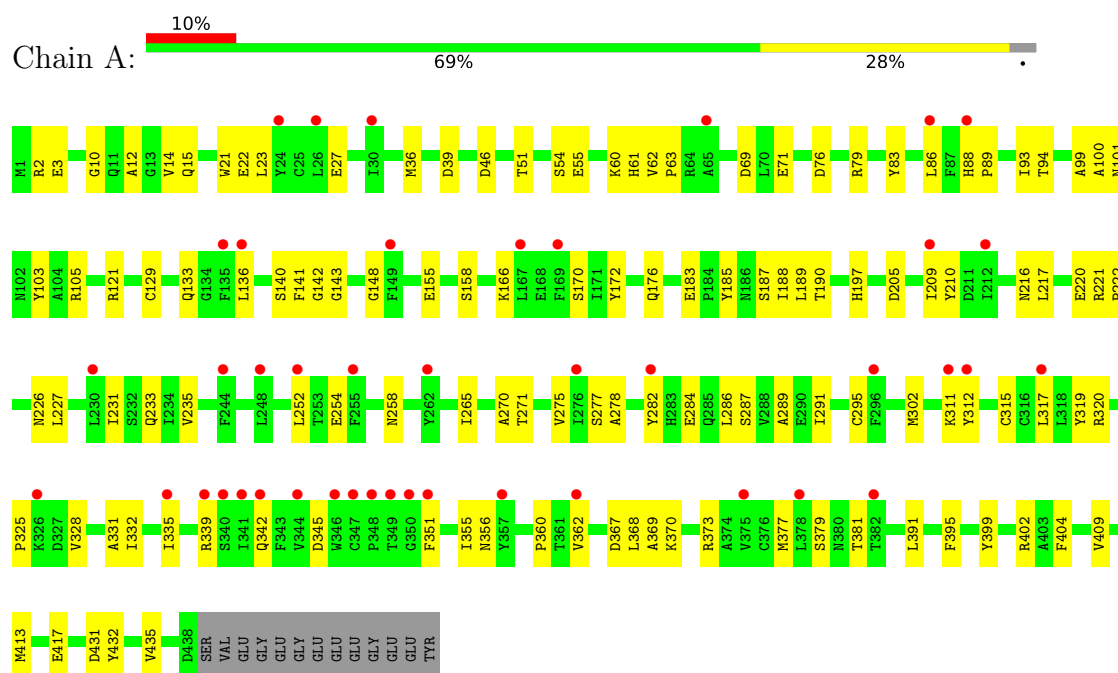
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	13	Total	O	0	0
			13	13		
12	B	24	Total	O	0	0
			24	24		
12	C	55	Total	O	0	0
			55	55		
12	D	3	Total	O	0	0
			3	3		
12	F	3	Total	O	0	0
			3	3		



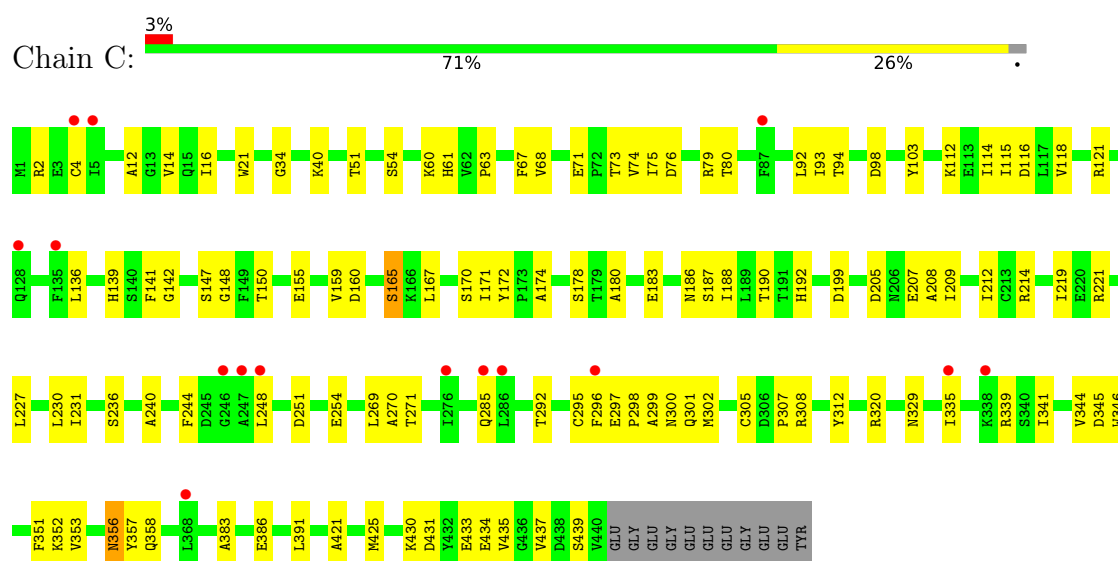
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

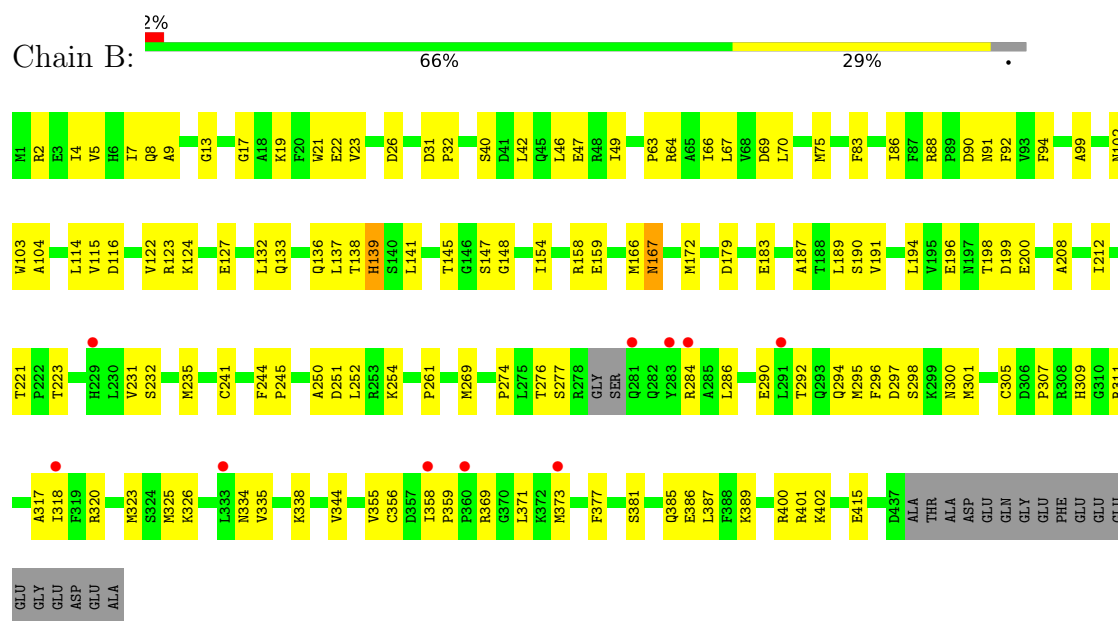
#### • Molecule 1: Tubulin alpha-1B chain



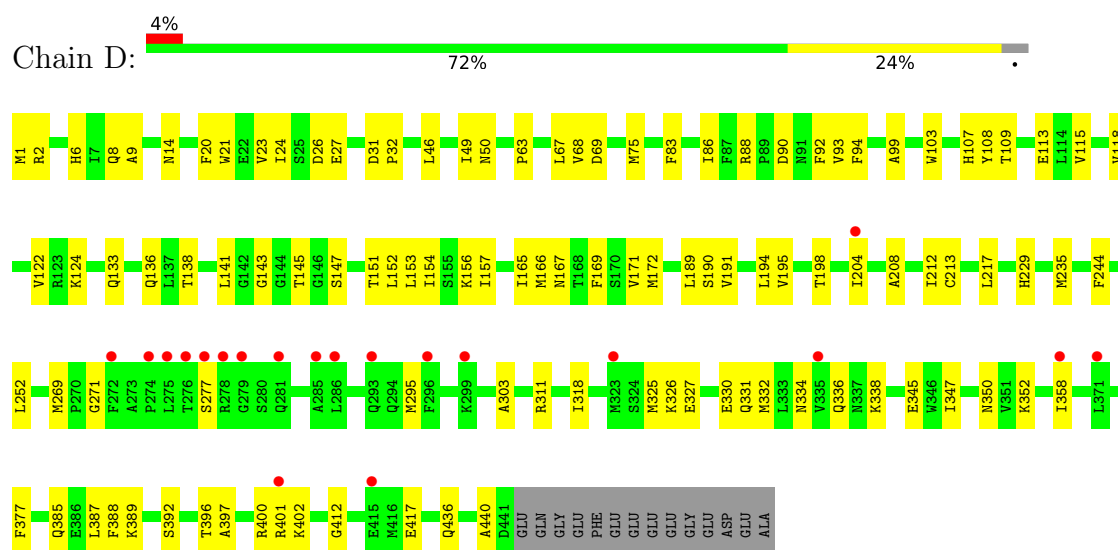
#### • Molecule 1: Tubulin alpha-1B chain



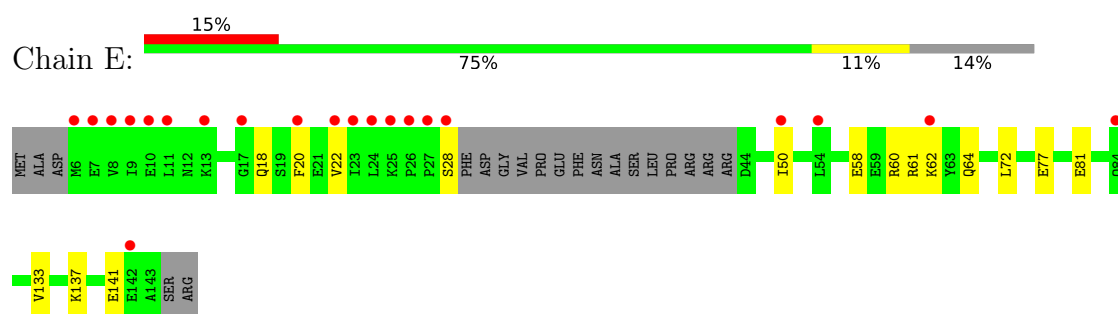
- Molecule 2: Tubulin beta-2B chain



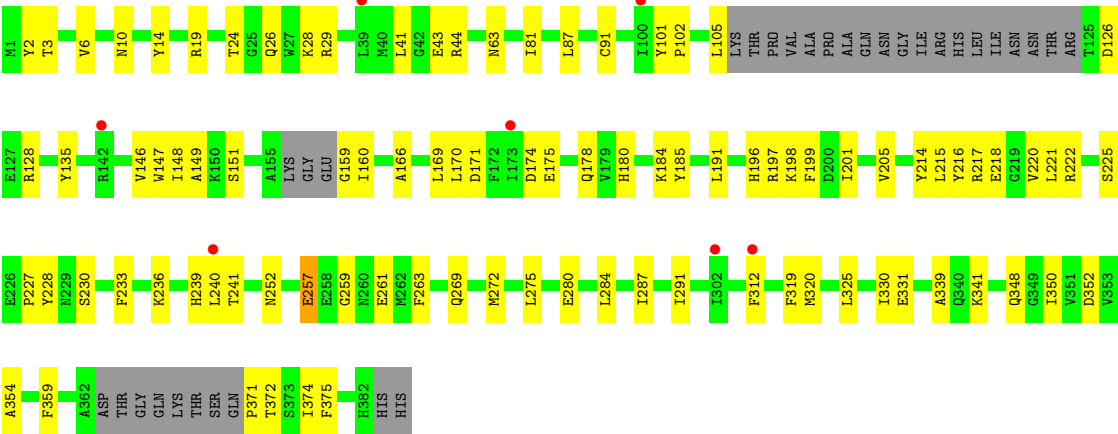
- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin-Tyrosine Ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.62Å 158.42Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.30 – 2.75 118.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (87.30-2.75) 99.4 (118.91-2.75)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.213 , 0.262 0.214 , 0.263	Depositor DCC
$R_{free}$ test set	3905 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.5	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.1	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	17802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: MG, MES, ACP, CA, TVP, GDP, GTP

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	0.26	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.26	0/3422	0.42	0/4633
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17853	0.41	0/24165

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	87	0
1	C	3443	0	3353	94	1
2	B	3348	0	3223	100	0
2	D	3368	0	3236	84	0
3	E	1014	0	1029	15	0
4	F	2877	0	2839	70	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	2	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	1	0
8	D	28	0	12	3	0
9	B	12	0	12	1	0
10	B	14	15	15	4	0
10	C	14	15	15	7	0
11	F	31	0	14	3	0
12	A	13	0	0	1	0
12	B	24	0	0	0	0
12	C	55	0	0	5	0
12	D	3	0	0	0	0
12	F	3	0	0	0	0
All	All	17772	30	17118	439	1

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 13.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.34	0.89
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.41	0.84
2:D:141:LEU:HA	2:D:147:SER:HB3	1.60	0.83
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.63	0.81
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.63	0.80
2:D:136:GLN:HA	2:D:167:ASN:O	1.81	0.79
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.15	0.79
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.63	0.78
2:B:325:MET:HG3	2:B:355:VAL:HG21	1.64	0.78
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.66	0.78
1:C:209:ILE:HD11	1:C:302:MET:CE	2.15	0.77
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.50	0.76
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.68	0.74
2:B:223:THR:HA	10:B:505:TVP:H12C	1.69	0.73
2:D:217:LEU:HA	2:D:277:SER:HB3	1.70	0.73
2:D:83:PHE:O	2:D:86:ILE:HG22	1.89	0.72
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.71	0.72
1:A:71:GLU:OE2	2:B:2:ARG:NH2	2.22	0.72
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.26	0.71
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.06	0.71
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.72	0.71
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.71	0.71
1:A:328:VAL:O	1:A:332:ILE:HG13	1.91	0.70
2:D:397:ALA:O	2:D:401:ARG:NH1	2.24	0.70
1:C:165:SER:HA	1:C:199:ASP:OD2	1.92	0.70
2:B:136:GLN:HA	2:B:167:ASN:O	1.91	0.69
1:C:142:GLY:HA3	1:C:183:GLU:OE1	1.93	0.69
2:D:75:MET:SD	2:D:94:PHE:HB3	2.33	0.69
1:C:76:ASP:O	1:C:80:THR:HG22	1.94	0.68
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.29	0.68
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.76	0.67
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.60	0.67
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.76	0.67
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.03	0.67
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.24	0.66
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.10	0.66
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.75	0.66
1:A:351:PHE:O	3:E:22:VAL:HG12	1.96	0.66
1:C:271:THR:HG21	1:C:295:CYS:O	1.95	0.66
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.32	0.65
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.77	0.65
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.78	0.65
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.79	0.64
5:C:501:GTP:O1B	12:C:601:HOH:O	2.15	0.64
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.79	0.64
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.29	0.64
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.33	0.64
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.80	0.63
1:C:329:ASN:HD21	10:C:504:TVP:H121	1.64	0.63
2:B:83:PHE:O	2:B:86:ILE:HG22	1.99	0.63
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.34	0.63
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.64	0.62
2:D:69:ASP:O	2:D:94:PHE:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:VAL:HB	10:C:504:TVP:H42C	1.80	0.62
2:B:199:ASP:OD1	9:B:504:MES:H62	2.00	0.62
2:B:145:THR:HB	8:B:501:GDP:O2B	2.00	0.61
2:B:4:ILE:O	2:B:64:ARG:HD2	2.00	0.61
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.35	0.61
1:C:112:LYS:HE2	12:C:649:HOH:O	2.00	0.61
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.81	0.61
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.36	0.61
2:B:5:VAL:HG23	2:B:132:LEU:HD11	1.82	0.61
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.61
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.82	0.60
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.82	0.60
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.34	0.60
1:C:296:PHE:CE2	1:C:341:ILE:HD11	2.36	0.60
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.01	0.60
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.84	0.60
1:A:217:LEU:HA	1:A:277:SER:HB2	1.84	0.60
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.33	0.60
1:A:345:ASP:O	3:E:28:SER:HB2	2.03	0.59
1:C:298:PRO:HG2	1:C:308:ARG:HH21	1.67	0.59
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.84	0.59
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.18	0.59
2:D:20:PHE:O	2:D:24:ILE:HG12	2.02	0.59
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.15	0.59
2:D:145:THR:HB	8:D:501:GDP:O2B	2.02	0.59
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.32	0.59
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.38	0.58
1:A:431:ASP:O	1:A:435:VAL:HG23	2.03	0.58
2:D:147:SER:O	2:D:151:THR:HG23	2.03	0.58
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.38	0.58
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.44	0.58
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.85	0.58
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.85	0.58
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.17	0.58
2:B:147:SER:HG	2:B:190:SER:HG	1.48	0.57
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.39	0.57
2:B:334:ASN:O	2:B:338:LYS:HG3	2.04	0.57
2:D:327:GLU:O	2:D:331:GLN:HG2	2.04	0.57
3:E:60:ARG:O	3:E:64:GLN:HG3	2.04	0.57
1:A:287:SER:O	1:A:291:ILE:HG23	2.04	0.57
4:F:371:PRO:HA	4:F:372:THR:C	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:MET:CE	2:D:377:PHE:HB2	2.33	0.57
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.40	0.57
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.87	0.57
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.17	0.56
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
4:F:371:PRO:CA	4:F:372:THR:HB	2.35	0.56
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.87	0.56
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.41	0.56
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.39	0.56
2:B:179:ASP:N	2:B:183:GLU:OE2	2.38	0.56
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.87	0.56
2:D:109:THR:O	2:D:113:GLU:HG2	2.05	0.56
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.88	0.56
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.40	0.56
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.42	0.55
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.88	0.55
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.87	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.88	0.55
2:B:231:VAL:O	2:B:235:MET:HG3	2.07	0.55
2:D:152:LEU:O	2:D:156:LYS:HG2	2.06	0.55
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.89	0.55
1:A:166:LYS:HE2	1:A:197:HIS:O	2.06	0.55
4:F:63:ASN:HA	4:F:312:PHE:O	2.07	0.55
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.88	0.55
1:C:186:ASN:O	1:C:190:THR:HG22	2.06	0.55
1:C:251:ASP:HB2	12:C:619:HOH:O	2.06	0.55
1:A:311:LYS:HA	1:A:342:GLN:O	2.06	0.55
2:B:47:GLU:HG2	2:B:245:PRO:HB3	1.89	0.55
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.89	0.55
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.40	0.55
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.72	0.54
2:D:23:VAL:O	2:D:27:GLU:HG3	2.06	0.54
1:A:220:GLU:HB3	2:B:326:LYS:HD2	1.88	0.54
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.90	0.54
2:B:7:ILE:O	2:B:137:LEU:HA	2.06	0.54
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.22	0.54
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.38	0.54
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.07	0.54
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.42	0.54
3:E:137:LYS:HE2	3:E:141:GLU:OE2	2.07	0.54
2:B:141:LEU:HD12	2:B:172:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ASN:OD1	2:B:200:GLU:HB2	2.08	0.54
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.90	0.54
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.89	0.54
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.08	0.53
1:C:431:ASP:O	1:C:435:VAL:HG22	2.08	0.53
1:A:271:THR:HG21	1:A:295:CYS:HA	1.90	0.53
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.23	0.53
4:F:371:PRO:HA	4:F:372:THR:O	2.08	0.53
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.91	0.53
2:D:2:ARG:CB	2:D:133:GLN:HE21	2.20	0.53
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.91	0.53
1:A:3:GLU:OE1	1:A:129:CYS:HB3	2.09	0.53
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.08	0.53
3:E:77:GLU:O	3:E:81:GLU:HG3	2.09	0.53
2:D:412:GLY:C	3:E:133:VAL:HG13	2.29	0.53
2:D:67:LEU:N	2:D:67:LEU:HD12	2.23	0.53
1:C:248:LEU:HD13	10:C:504:TVP:H8	1.91	0.53
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.90	0.52
4:F:101:TYR:N	4:F:126:ASP:OD1	2.25	0.52
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.74	0.52
1:C:114:ILE:O	1:C:118:VAL:HG23	2.08	0.52
4:F:128:ARG:NH1	4:F:170:LEU:HD22	2.24	0.52
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.92	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.44	0.52
3:E:58:GLU:HA	3:E:61:ARG:NH2	2.24	0.52
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.18	0.52
2:B:141:LEU:HA	2:B:147:SER:HB2	1.91	0.52
1:A:10:GLY:O	1:A:14:VAL:HG23	2.09	0.52
2:B:194:LEU:HD22	2:B:198:THR:HG21	1.92	0.52
4:F:196:HIS:O	4:F:227:PRO:HA	2.10	0.51
2:D:271:GLY:HA3	2:D:377:PHE:HB3	1.92	0.51
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.10	0.51
2:D:46:LEU:HA	2:D:49:ILE:HB	1.92	0.51
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.93	0.51
1:A:187:SER:CB	1:A:391:LEU:HD21	2.40	0.51
1:A:69:ASP:O	1:A:94:THR:HA	2.10	0.51
1:A:312:TYR:CE1	1:A:379:SER:HB2	2.46	0.51
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.93	0.51
2:B:208:ALA:O	2:B:212:ILE:HG13	2.11	0.51
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.41	0.51
4:F:24:THR:O	4:F:26:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:O	1:A:51:THR:HG22	2.11	0.51
2:B:297:ASP:OD1	2:B:298:SER:N	2.43	0.51
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.46	0.51
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.91	0.51
1:A:54:SER:O	1:A:61:HIS:HA	2.10	0.50
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.46	0.50
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.46	0.50
2:D:318:ILE:N	2:D:318:ILE:HD12	2.26	0.50
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.46	0.50
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.93	0.50
2:D:124:LYS:C	2:D:124:LYS:HD3	2.31	0.50
4:F:184:LYS:NZ	4:F:185:TYR:O	2.42	0.50
2:D:109:THR:HG21	3:E:137:LYS:NZ	2.26	0.50
4:F:159:GLY:C	4:F:160:ILE:HD12	2.31	0.50
4:F:263:PHE:CE1	4:F:341:LYS:HE2	2.46	0.50
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.93	0.50
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.46	0.50
1:A:136:LEU:HD21	1:A:252:LEU:HD21	1.92	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.11	0.50
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.27	0.50
2:D:99:ALA:HB2	2:D:145:THR:OG1	2.12	0.50
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.50
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.93	0.50
2:B:124:LYS:HD3	2:B:124:LYS:C	2.32	0.50
10:B:505:TVP:H121	10:B:505:TVP:C9	2.42	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
2:D:326:LYS:O	2:D:330:GLU:HG3	2.11	0.50
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.47	0.49
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.47	0.49
4:F:259:GLY:O	4:F:261:GLU:HG3	2.13	0.49
1:C:178:SER:OG	2:D:352:LYS:NZ	2.43	0.49
2:D:392:SER:O	2:D:396:THR:HG22	2.11	0.49
4:F:371:PRO:HA	4:F:372:THR:HB	1.93	0.49
1:A:227:LEU:O	1:A:231:ILE:HG13	2.12	0.49
2:B:301:MET:HE1	2:B:377:PHE:CZ	2.47	0.49
2:B:317:ALA:C	2:B:318:ILE:HD12	2.33	0.49
1:C:40:LYS:HG2	12:C:622:HOH:O	2.11	0.49
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.94	0.49
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.93	0.49
2:B:241:CYS:HB3	2:B:250:ALA:HB2	1.94	0.49
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ASP:HB3	1:C:302:MET:O	2.12	0.49
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.45	0.49
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.94	0.49
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.30	0.49
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.43	0.49
2:B:40:SER:OG	2:B:42:LEU:HD13	2.13	0.49
1:C:270:ALA:O	1:C:302:MET:HG2	2.13	0.49
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.48	0.49
4:F:198:LYS:HG2	4:F:199:PHE:H	1.77	0.49
1:A:319:TYR:HB2	1:A:355:ILE:HG12	1.94	0.48
2:B:187:ALA:O	2:B:191:VAL:HG23	2.13	0.48
2:B:323:MET:HB3	2:B:373:MET:HE2	1.94	0.48
1:A:62:VAL:HG13	1:A:86:LEU:O	2.13	0.48
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.48
1:A:46:ASP:OD1	1:A:46:ASP:N	2.44	0.48
1:A:404:PHE:CE2	2:B:261:PRO:HB3	2.48	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.13	0.48
2:B:323:MET:HB3	2:B:373:MET:CE	2.43	0.48
1:A:325:PRO:HD3	3:E:18:GLN:NE2	2.29	0.48
2:B:223:THR:CA	10:B:505:TVP:H12C	2.39	0.48
1:C:75:ILE:HB	1:C:94:THR:CG2	2.42	0.48
1:C:208:ALA:O	1:C:212:ILE:HG13	2.13	0.48
2:D:9:ALA:HA	2:D:68:VAL:O	2.12	0.48
2:D:244:PHE:CD1	2:D:358:ILE:HD12	2.48	0.48
1:C:430:LYS:O	1:C:434:GLU:HG3	2.14	0.48
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.96	0.48
2:B:67:LEU:N	2:B:67:LEU:HD12	2.29	0.48
1:C:136:LEU:CD2	1:C:167:LEU:HB2	2.44	0.48
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.49	0.48
1:A:413:MET:HG3	1:A:417:GLU:OE1	2.13	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.49	0.47
1:A:55:GLU:HA	1:A:60:LYS:O	2.14	0.47
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.14	0.47
2:B:221:THR:CG2	10:C:504:TVP:H122	2.44	0.47
1:C:271:THR:HG23	1:C:300:ASN:O	2.13	0.47
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.43	0.47
4:F:160:ILE:HD12	4:F:160:ILE:N	2.29	0.47
4:F:217:ARG:CZ	4:F:374:ILE:HA	2.44	0.47
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.49	0.47
1:C:180:ALA:HB3	1:C:183:GLU:CG	2.44	0.47
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:222:ARG:O	4:F:241:THR:HB	2.15	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.47
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.29	0.47
2:B:318:ILE:HD12	2:B:318:ILE:N	2.30	0.47
1:C:269:LEU:HD11	1:C:301:GLN:HB3	1.95	0.47
1:C:341:ILE:HD12	1:C:351:PHE:HZ	1.79	0.47
1:C:433:GLU:O	1:C:437:VAL:HG23	2.15	0.47
2:D:208:ALA:O	2:D:212:ILE:HG13	2.14	0.47
1:A:12:ALA:CB	1:A:140:SER:HB3	2.45	0.47
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.97	0.47
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.96	0.47
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.50	0.47
1:C:174:ALA:HB2	1:C:207:GLU:N	2.30	0.47
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.50	0.47
2:B:19:LYS:NZ	2:B:22:GLU:OE1	2.40	0.47
2:B:138:THR:O	2:B:139:HIS:HB3	2.15	0.47
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.50	0.47
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.96	0.47
1:C:12:ALA:HB2	5:C:501:GTP:C8	2.49	0.47
3:E:58:GLU:O	3:E:62:LYS:HG3	2.15	0.47
1:C:192:HIS:CG	1:C:421:ALA:HA	2.50	0.46
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.79	0.46
2:B:221:THR:HG23	10:C:504:TVP:H122	1.96	0.46
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.50	0.46
2:D:332:MET:O	2:D:336:GLN:HG3	2.15	0.46
2:B:294:GLN:HB3	2:B:300:ASN:ND2	2.30	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.15	0.46
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.44	0.46
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.16	0.46
1:A:141:PHE:HB3	1:A:187:SER:OG	2.15	0.46
1:A:317:LEU:CD2	1:A:377:MET:HG3	2.45	0.46
2:B:276:THR:HG22	2:B:277:SER:O	2.16	0.46
2:D:145:THR:N	8:D:501:GDP:O2B	2.48	0.46
4:F:350:ILE:O	4:F:354:ALA:HB3	2.16	0.46
4:F:3:THR:HA	4:F:28:LYS:O	2.16	0.46
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.44	0.46
1:C:345:ASP:OD2	1:C:439:SER:N	2.39	0.46
4:F:371:PRO:N	4:F:372:THR:HB	2.30	0.46
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.51	0.46
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.81	0.46
2:B:158:ARG:NH1	2:B:196:GLU:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.51	0.46
1:C:2:ARG:O	1:C:51:THR:HG22	2.17	0.45
1:A:289:ALA:HA	1:A:331:ALA:HB2	1.98	0.45
2:B:241:CYS:HB3	2:B:250:ALA:CB	2.46	0.45
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.16	0.45
4:F:146:VAL:HG21	4:F:233:PHE:CZ	2.51	0.45
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.51	0.45
1:A:155:GLU:HB3	3:E:50:ILE:CD1	2.46	0.45
2:B:320:ARG:HA	2:B:356:CYS:O	2.15	0.45
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.51	0.45
1:A:362:VAL:HG22	12:A:604:HOH:O	2.16	0.45
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.46	0.45
1:C:115:ILE:HG23	1:C:116:ASP:N	2.32	0.45
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.17	0.45
1:C:214:ARG:HG2	1:C:219:ILE:O	2.17	0.45
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.15	0.45
4:F:171:ASP:O	4:F:175:GLU:HG3	2.17	0.45
2:B:295:MET:CG	2:B:377:PHE:HB2	2.47	0.45
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.49	0.44
1:C:305:CYS:O	1:C:307:PRO:HD3	2.17	0.44
4:F:19:ARG:HD2	4:F:19:ARG:O	2.17	0.44
2:B:138:THR:CG2	2:B:235:MET:HE3	2.47	0.44
1:A:315:CYS:HG	1:A:351:PHE:HD2	1.64	0.44
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.47	0.44
1:A:320:ARG:HA	1:A:356:ASN:O	2.17	0.44
1:A:101:ASN:OD1	2:B:254:LYS:HE2	2.18	0.44
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.81	0.44
1:C:271:THR:CG2	1:C:295:CYS:HA	2.47	0.44
2:D:385:GLN:O	2:D:389:LYS:HG3	2.17	0.44
4:F:205:VAL:HG22	4:F:215:LEU:HD13	1.99	0.44
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.52	0.44
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.44
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.99	0.44
1:C:74:VAL:HB	12:C:602:HOH:O	2.17	0.44
10:C:504:TVP:H121	10:C:504:TVP:H2	1.88	0.44
2:B:19:LYS:HB2	2:B:232:SER:OG	2.18	0.44
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.82	0.44
1:C:2:ARG:HA	1:C:2:ARG:HD3	1.76	0.44
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.47	0.44
1:C:236:SER:O	1:C:240:ALA:HB2	2.18	0.44
1:C:248:LEU:HB3	10:C:504:TVP:H8	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:269:GLN:HA	4:F:272:MET:HE2	1.98	0.44
2:B:9:ALA:O	2:B:13:GLY:HA3	2.17	0.44
1:C:75:ILE:HB	1:C:94:THR:HG21	2.00	0.44
1:C:155:GLU:O	1:C:159:VAL:HG23	2.18	0.44
1:C:174:ALA:HB2	1:C:207:GLU:H	1.83	0.43
1:C:383:ALA:O	1:C:386:GLU:HG3	2.18	0.43
2:B:46:LEU:HA	2:B:49:ILE:HB	1.99	0.43
2:D:68:VAL:HA	2:D:93:VAL:O	2.18	0.43
2:D:387:LEU:HD23	2:D:387:LEU:C	2.38	0.43
1:A:289:ALA:HA	1:A:331:ALA:CB	2.49	0.43
4:F:225:SER:HB2	4:F:252:ASN:O	2.18	0.43
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.00	0.43
1:A:99:ALA:HA	1:A:105:ARG:HD3	1.99	0.43
4:F:220:VAL:HG11	4:F:339:ALA:HB2	2.00	0.43
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.49	0.43
1:A:399:TYR:O	1:A:402:ARG:NH1	2.49	0.43
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.54	0.43
1:A:142:GLY:HA3	1:A:183:GLU:HG2	2.00	0.43
2:D:147:SER:HB2	2:D:190:SER:OG	2.18	0.43
2:B:359:PRO:HB2	2:B:371:LEU:O	2.19	0.43
2:B:385:GLN:HG3	2:B:386:GLU:N	2.34	0.43
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.49	0.43
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.49	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.19	0.42
4:F:128:ARG:HH12	4:F:170:LEU:HB3	1.84	0.42
4:F:178:GLN:HE21	4:F:180:HIS:HE1	1.66	0.42
4:F:320:MET:HG3	4:F:330:ILE:HD11	2.01	0.42
4:F:372:THR:O	4:F:372:THR:HG22	2.18	0.42
1:C:192:HIS:CD2	1:C:421:ALA:HA	2.54	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.00	0.42
2:B:8:GLN:OE1	2:B:17:GLY:HA3	2.19	0.42
1:C:54:SER:O	1:C:61:HIS:HA	2.20	0.42
2:D:345:GLU:H	2:D:345:GLU:HG2	1.69	0.42
1:A:286:LEU:O	1:A:373:ARG:NH1	2.49	0.42
2:B:305:CYS:O	2:B:307:PRO:HD3	2.19	0.42
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.01	0.42
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.88	0.42
2:B:325:MET:HE2	2:B:355:VAL:HG11	2.01	0.42
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.55	0.42
1:C:297:GLU:HG3	1:C:299:ALA:HB3	2.02	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:275:LEU:N	4:F:275:LEU:HD22	2.34	0.42
1:A:158:SER:OG	1:A:166:LYS:HE3	2.20	0.42
1:A:284:GLU:CD	1:A:284:GLU:H	2.24	0.42
1:C:79:ARG:NH2	1:C:92:LEU:O	2.48	0.42
2:D:46:LEU:O	2:D:49:ILE:HG22	2.19	0.42
4:F:320:MET:CG	4:F:330:ILE:HD11	2.50	0.42
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.55	0.42
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.55	0.41
2:B:102:ASN:OD1	2:B:104:ALA:N	2.53	0.41
1:C:147:SER:OG	1:C:148:GLY:N	2.53	0.41
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.55	0.41
4:F:228:TYR:HE2	4:F:230:SER:HB3	1.85	0.41
1:A:103:TYR:CD1	1:A:189:LEU:HD13	2.55	0.41
2:B:311:ARG:NH2	2:B:344:VAL:HA	2.36	0.41
2:D:8:GLN:HB3	2:D:138:THR:OG1	2.20	0.41
4:F:6:VAL:HB	4:F:29:ARG:NH2	2.36	0.41
1:A:185:TYR:O	1:A:189:LEU:HG	2.20	0.41
2:B:269:MET:HE3	2:B:301:MET:SD	2.61	0.41
2:D:118:VAL:O	2:D:122:VAL:HG23	2.21	0.41
1:C:34:GLY:HA3	1:C:60:LYS:HG3	2.03	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.55	0.41
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.56	0.41
4:F:149:ALA:O	4:F:160:ILE:HG23	2.20	0.41
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.02	0.41
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.03	0.41
1:A:188:ILE:HD12	1:A:395:PHE:CG	2.56	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.56	0.41
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.20	0.41
2:B:42:LEU:H	2:B:42:LEU:HD12	1.86	0.41
2:B:269:MET:HE1	2:B:307:PRO:HG3	2.02	0.41
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.21	0.41
2:D:21:TRP:CH2	2:D:63:PRO:HB3	2.56	0.41
1:A:270:ALA:HB3	1:A:302:MET:HG3	2.03	0.41
1:C:68:VAL:HG11	1:C:118:VAL:HG21	2.02	0.41
2:D:107:HIS:O	2:D:152:LEU:HD22	2.20	0.41
4:F:199:PHE:CA	4:F:241:THR:HG21	2.51	0.41
1:C:227:LEU:O	1:C:231:ILE:HG13	2.21	0.41
2:D:387:LEU:HD23	2:D:388:PHE:N	2.36	0.41
2:D:401:ARG:O	2:D:402:LYS:HB2	2.20	0.41
4:F:240:LEU:HD12	4:F:240:LEU:N	2.35	0.41
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.45	0.40
10:B:505:TVP:H12C	10:B:505:TVP:O	2.21	0.40
2:D:311:ARG:NH1	2:D:436:GLN:O	2.53	0.40
1:A:23:LEU:O	1:A:27:GLU:HG3	2.20	0.40
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.04	0.40
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.86	0.40
2:B:114:LEU:HG	2:B:114:LEU:O	2.21	0.40
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.40
2:D:153:LEU:O	2:D:157:ILE:HG13	2.21	0.40
1:A:155:GLU:HB3	3:E:50:ILE:HD13	2.02	0.40
2:B:115:VAL:HG13	2:B:116:ASP:N	2.37	0.40
1:A:187:SER:O	1:A:190:THR:HG22	2.21	0.40
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.04	0.40
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.57	0.40
1:A:360:PRO:O	1:A:370:LYS:NZ	2.47	0.40
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ASP:O	1:C:285:GLN:NE2[4_555]	2.18	0.02

## 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%)	415 (95%)	21 (5%)	0	100	100
1	C	439/451 (97%)	424 (97%)	15 (3%)	0	100	100
2	B	421/445 (95%)	400 (95%)	21 (5%)	0	100	100
2	D	429/445 (96%)	419 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	320 (93%)	24 (7%)	0	100	100
All	All	2188/2319 (94%)	2095 (96%)	93 (4%)	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	369/379 (97%)	365 (99%)	4 (1%)	73	84
1	C	372/379 (98%)	370 (100%)	2 (0%)	88	92
2	B	367/383 (96%)	364 (99%)	3 (1%)	81	88
2	D	368/383 (96%)	366 (100%)	2 (0%)	88	92
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	312 (99%)	3 (1%)	76	85
All	All	1901/1993 (95%)	1887 (99%)	14 (1%)	84	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	221	ARG
1	A	282	TYR
1	A	381	THR
2	B	139	HIS
2	B	167	ASN
2	B	381	SER
1	C	165	SER
1	C	356	ASN
2	D	26	ASP
2	D	229	HIS
4	F	43	GLU

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Mol	Chain	Res	Type
4	F	91	CYS
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	133	GLN
2	B	15	GLN
2	B	294	GLN
1	C	11	GLN
1	C	300	ASN
1	C	329	ASN
1	C	356	ASN
2	D	8	GLN
2	D	133	GLN
2	D	247	GLN
2	D	294	GLN
3	E	108	ASN
4	F	180	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN
4	F	380	HIS

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	B	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.94	7 (22%)
10	TVP	B	505	-	15,15,15	1.17	2 (13%)	21,21,21	1.47	4 (19%)
10	TVP	C	504	-	15,15,15	1.30	2 (13%)	21,21,21	1.99	3 (14%)
11	ACP	F	401	6	27,33,33	1.41	5 (18%)	32,52,52	1.50	4 (12%)
8	GDP	D	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.94	8 (25%)
5	GTP	C	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.76	6 (18%)
9	MES	B	504	-	12,12,12	2.26	1 (8%)	14,16,16	2.04	5 (35%)
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.73	7 (21%)

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	B	501	6	-	3/12/32/32	0/3/3/3
10	TVP	B	505	-	-	0/4/17/17	0/2/2/2
10	TVP	C	504	-	-	2/4/17/17	0/2/2/2
11	ACP	F	401	6	-	11/15/38/38	0/3/3/3
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.53	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C6-C5	4.16	1.48	1.41
8	D	501	GDP	C6-C5	3.99	1.48	1.41
10	C	504	TVP	C11-N	3.49	1.43	1.37
10	B	505	TVP	C11-N	3.37	1.43	1.37
5	C	501	GTP	C6-N1	3.07	1.38	1.33
5	A	501	GTP	C6-N1	3.07	1.38	1.33
11	F	401	ACP	PB-O3A	2.98	1.61	1.58
11	F	401	ACP	PG-O2G	2.97	1.61	1.54
11	F	401	ACP	PG-O3G	2.91	1.61	1.54
10	C	504	TVP	C2-N	2.62	1.50	1.48
11	F	401	ACP	C5-C4	2.54	1.47	1.40
8	D	501	GDP	C5-C4	2.38	1.47	1.40
8	B	501	GDP	C5-C4	2.36	1.47	1.40
11	F	401	ACP	PB-O2B	2.27	1.61	1.56
10	B	505	TVP	C10-N	2.03	1.45	1.42

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	504	TVP	C10-N-C11	-5.62	119.13	125.19
5	A	501	GTP	N3-C2-N1	-5.36	120.07	127.22
5	C	501	GTP	N3-C2-N1	-5.32	120.13	127.22
8	B	501	GDP	C2-N3-C4	4.88	120.93	115.36
8	D	501	GDP	C2-N3-C4	4.77	120.80	115.36
10	C	504	TVP	C1-C2-N	4.57	115.15	111.19
8	B	501	GDP	C6-N1-C2	4.20	122.60	115.93
5	A	501	GTP	C2-N3-C4	4.15	120.10	115.36
5	C	501	GTP	C2-N3-C4	4.06	119.99	115.36
8	D	501	GDP	C6-N1-C2	4.04	122.35	115.93
8	B	501	GDP	C5-C6-N1	-4.03	117.92	123.43
8	D	501	GDP	C5-C6-N1	-4.02	117.94	123.43
10	B	505	TVP	C10-N-C11	-4.00	120.88	125.19
11	F	401	ACP	PA-O3A-PB	-4.00	119.87	132.56
8	B	501	GDP	C6-C5-C4	-3.80	117.17	120.80
9	B	504	MES	C5-N4-C3	3.75	117.27	108.83
8	D	501	GDP	C6-C5-C4	-3.63	117.33	120.80
11	F	401	ACP	C3'-C2'-C1'	3.61	106.41	100.98
8	B	501	GDP	N3-C2-N1	-3.52	122.52	127.22
9	B	504	MES	C6-C5-N4	-3.38	104.98	110.10
8	D	501	GDP	N3-C2-N1	-3.31	122.81	127.22
8	D	501	GDP	PA-O3A-PB	-3.29	121.52	132.83
8	B	501	GDP	PA-O3A-PB	-3.27	121.62	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	504	TVP	C2-N-C11	3.16	128.08	119.36
11	F	401	ACP	N3-C2-N1	-3.15	123.75	128.68
5	C	501	GTP	PA-O3A-PB	-3.11	122.16	132.83
5	C	501	GTP	C5-C6-N1	-3.01	119.32	123.43
5	A	501	GTP	C5-C6-N1	-2.94	119.41	123.43
9	B	504	MES	O1S-S-C8	2.93	110.45	106.92
5	C	501	GTP	PB-O3B-PG	-2.90	122.89	132.83
5	A	501	GTP	PB-O3B-PG	-2.86	123.02	132.83
8	B	501	GDP	C4-C5-N7	-2.84	106.43	109.40
10	B	505	TVP	C1-C2-N	2.83	113.64	111.19
8	D	501	GDP	C4-C5-N7	-2.69	106.60	109.40
8	D	501	GDP	C3'-C2'-C1'	2.65	104.97	100.98
5	A	501	GTP	C6-N1-C2	2.64	120.12	115.93
11	F	401	ACP	C4-C5-N7	-2.61	106.68	109.40
5	C	501	GTP	C6-N1-C2	2.59	120.04	115.93
5	A	501	GTP	PA-O3A-PB	-2.45	124.42	132.83
9	B	504	MES	C7-N4-C5	2.42	117.41	111.23
10	B	505	TVP	C3-C2-N	-2.36	105.18	109.83
5	A	501	GTP	N2-C2-N1	2.08	120.49	117.25
9	B	504	MES	O3S-S-C8	2.05	109.09	105.77
10	B	505	TVP	O-C11-N	2.04	123.02	120.73

There are no chirality outliers.

All (36) 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
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
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

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Mol	Chain	Res	Type	Atoms
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	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
8	B	501	GDP	PA-O3A-PB-O2B
5	C	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	PG-C3B-PB-O2B
10	C	504	TVP	O-C11-N-C2
10	C	504	TVP	C12-C11-N-C2
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O1A
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C4'-C5'-O5'-PA

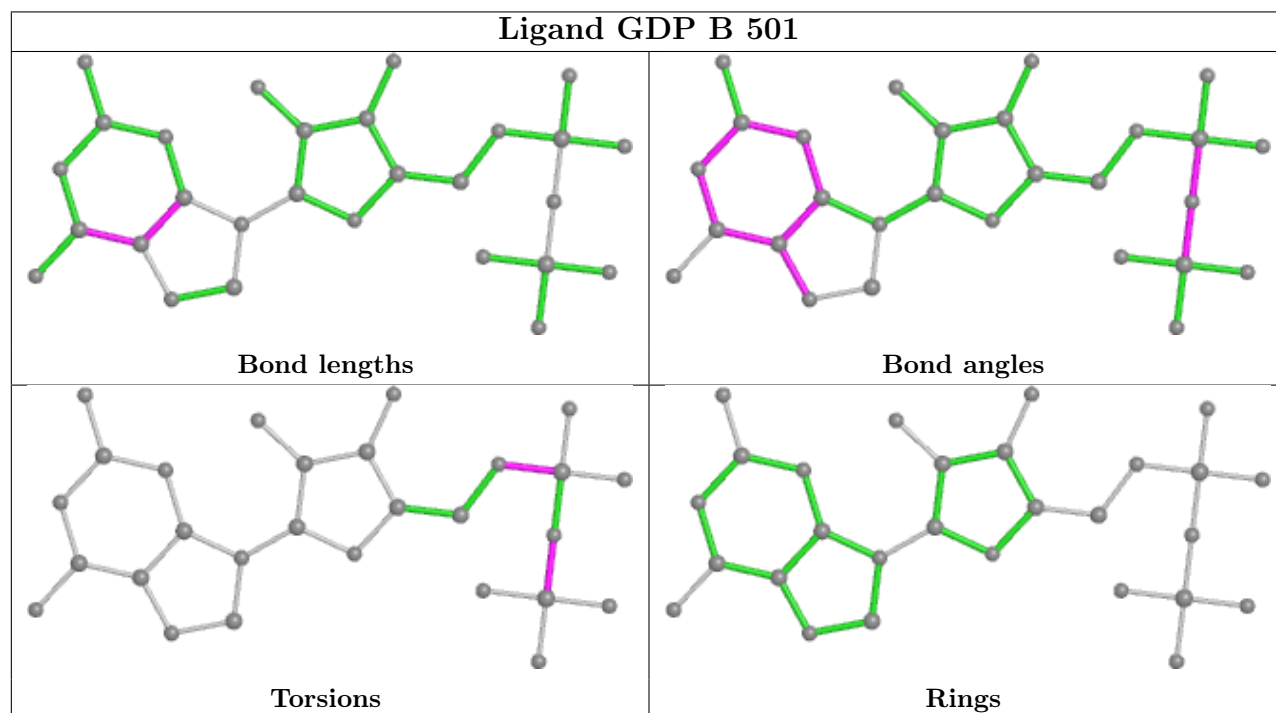
There are no ring outliers.

8 monomers are involved in 23 short contacts:

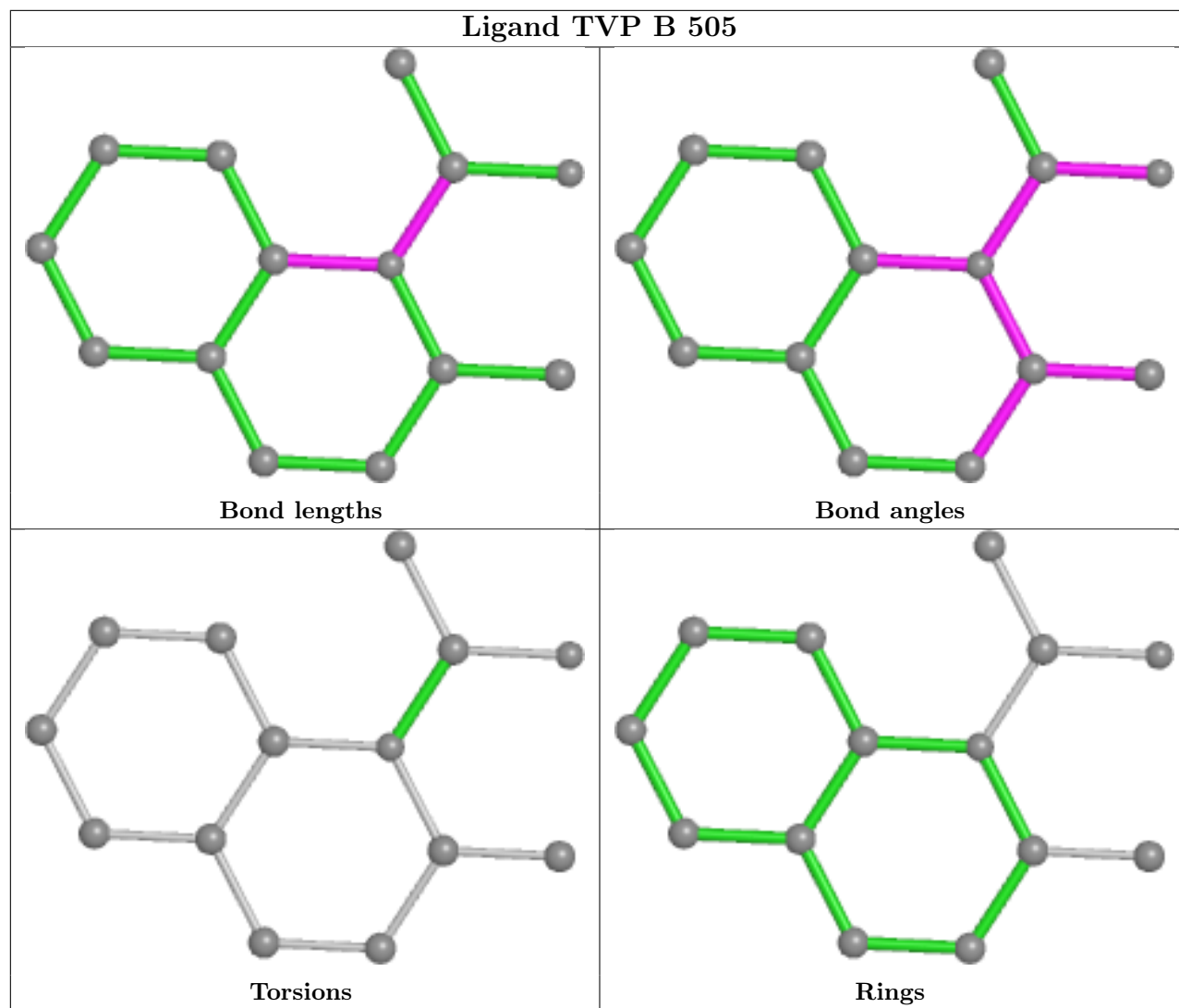
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	1	0
10	B	505	TVP	4	0
10	C	504	TVP	7	0
11	F	401	ACP	3	0
8	D	501	GDP	3	0
5	C	501	GTP	2	0
9	B	504	MES	1	0
5	A	501	GTP	2	0

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

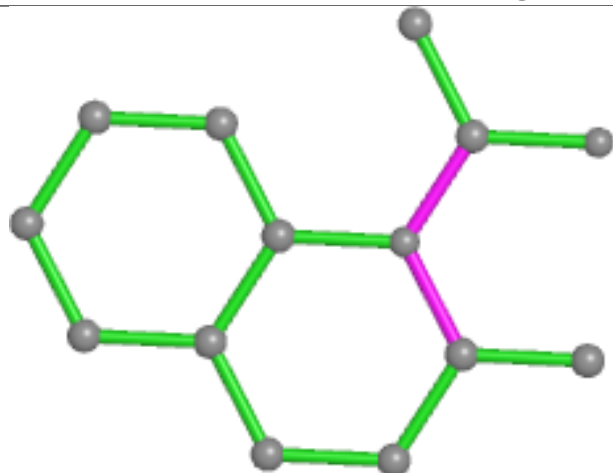
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



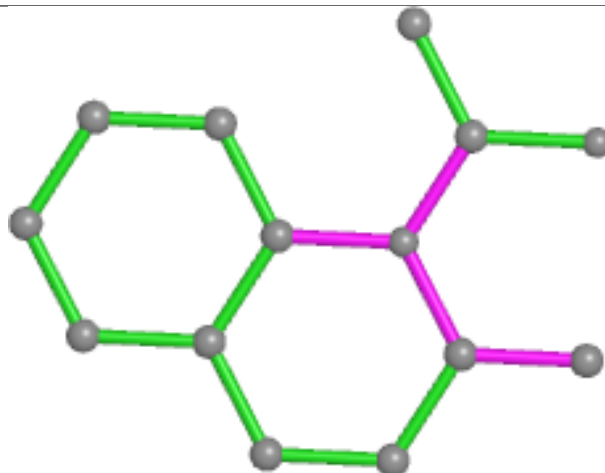




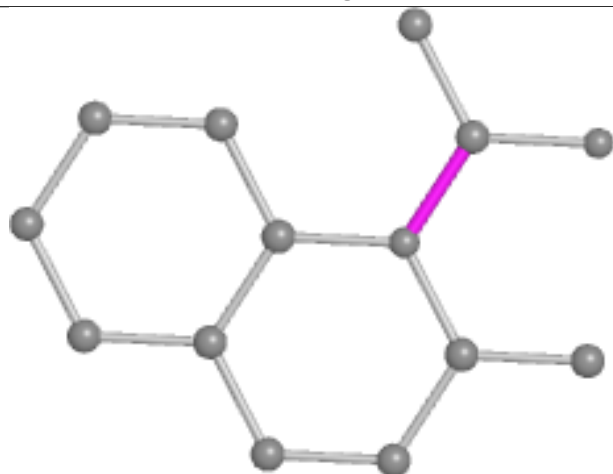
## Ligand TVP C 504



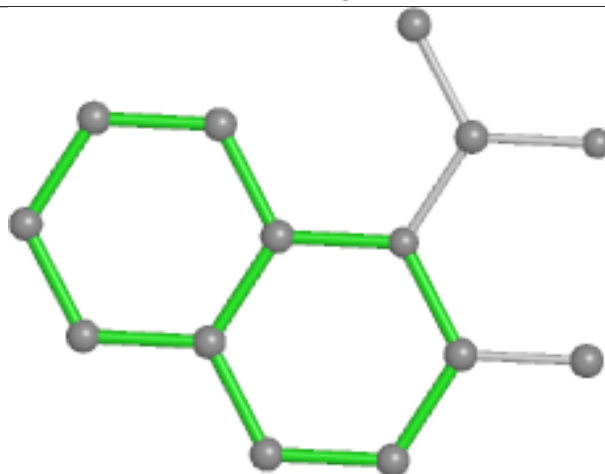
Bond lengths



Bond angles

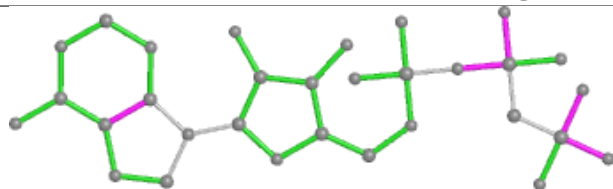


Torsions

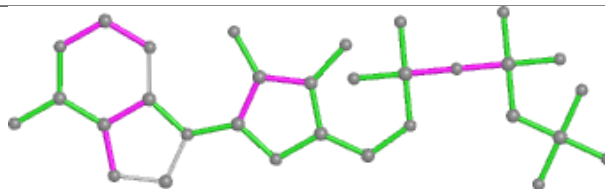


Rings

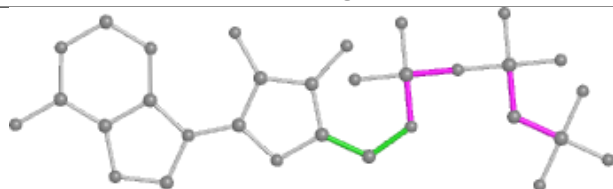
## Ligand ACP F 401



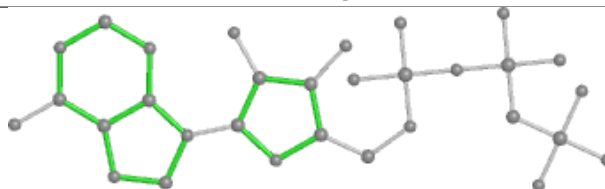
Bond lengths



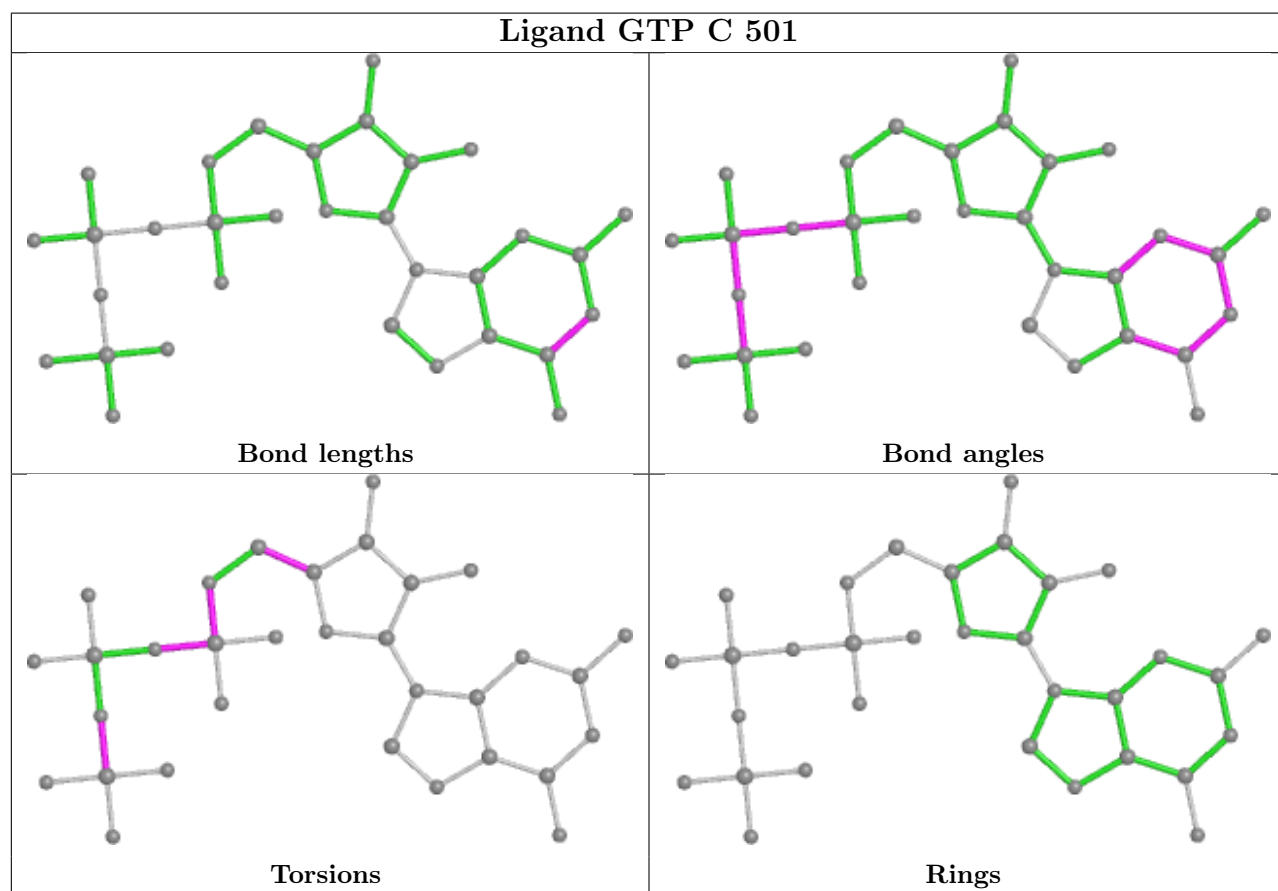
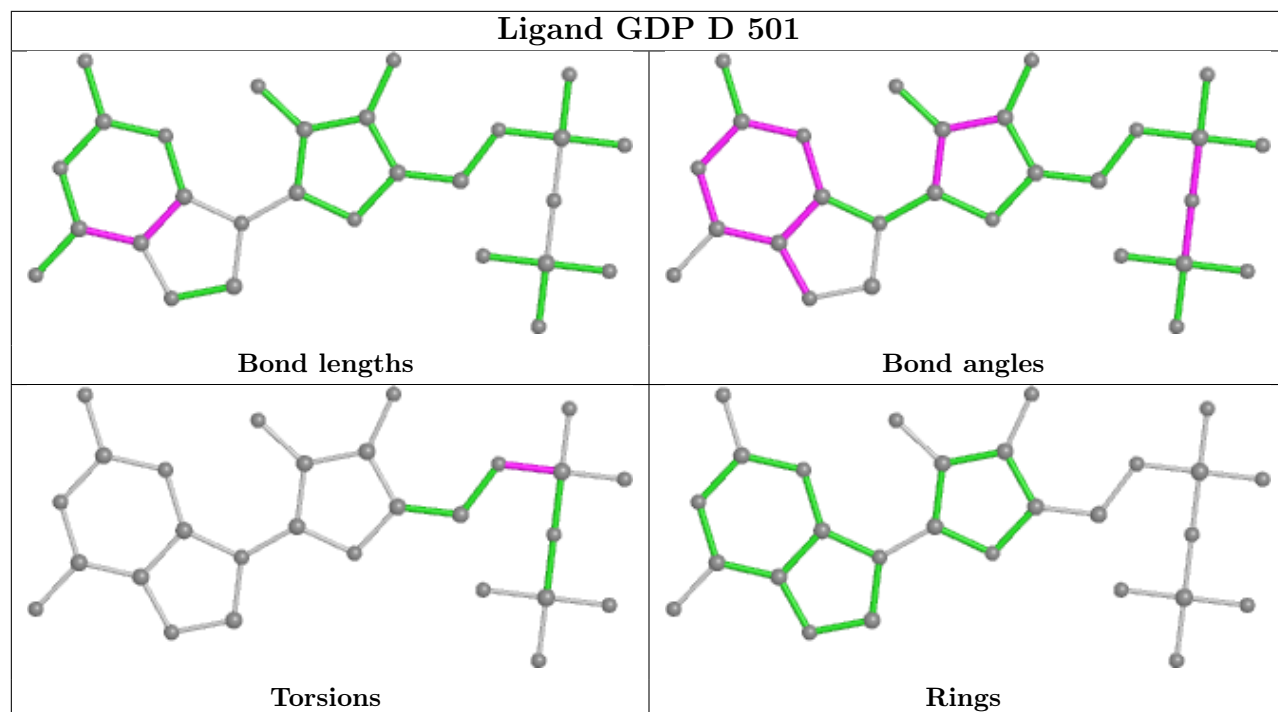
Bond angles

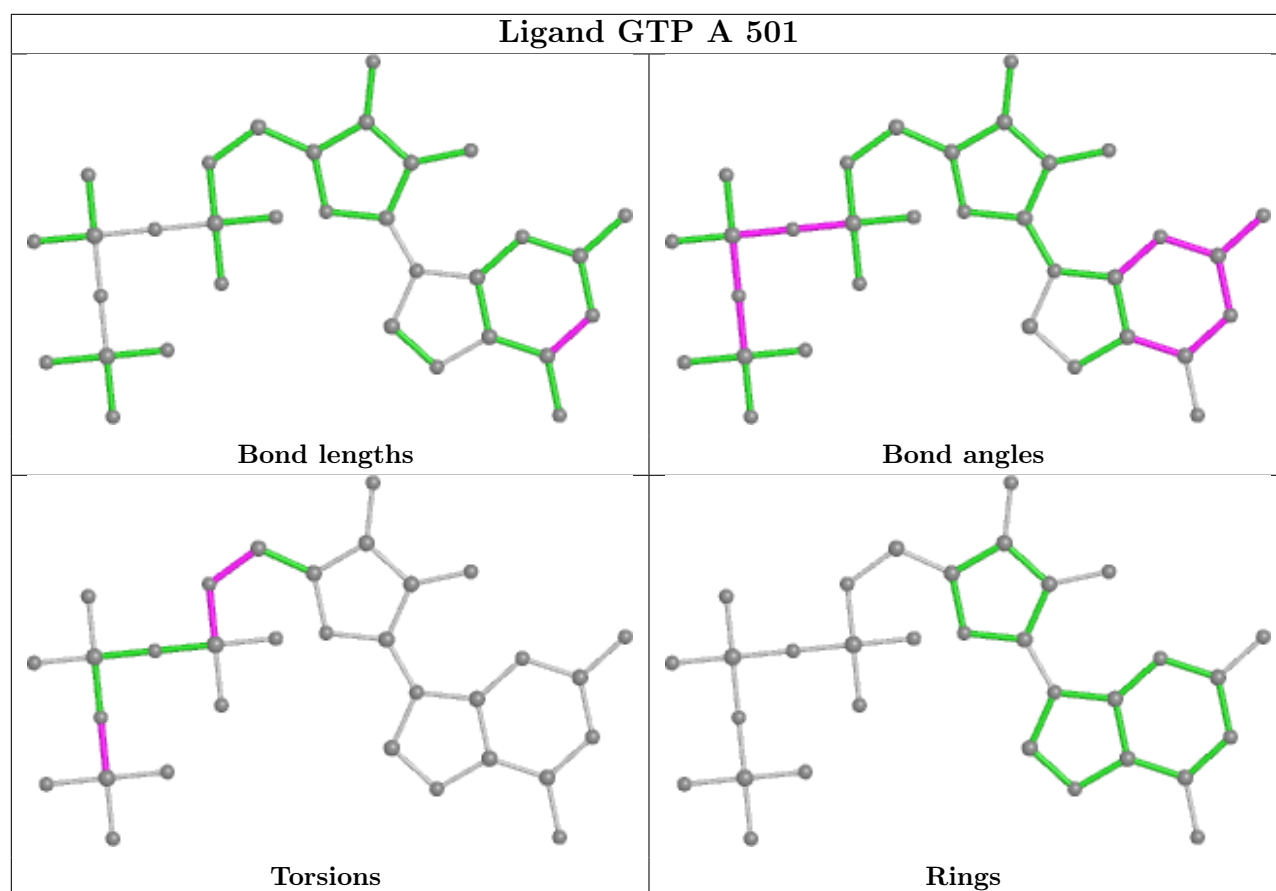


Torsions



Rings





## 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%)	0.69	43 (9%) 7 8	67, 91, 146, 228	0
1	C	440/451 (97%)	0.42	15 (3%) 45 53	58, 76, 115, 161	0
2	B	425/445 (95%)	0.41	10 (2%) 59 68	61, 84, 131, 176	2 (0%)
2	D	431/445 (96%)	0.36	20 (4%) 32 39	72, 101, 143, 191	4 (0%)
3	E	123/143 (86%)	0.90	21 (17%) 1 1	83, 112, 171, 224	0
4	F	352/384 (91%)	0.20	7 (1%) 65 73	86, 131, 201, 261	0
All	All	2209/2319 (95%)	0.45	116 (5%) 26 31	58, 95, 162, 261	6 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	14.2
1	A	349	THR	12.2
1	A	341	ILE	10.4
3	E	24	LEU	8.0
1	A	346	TRP	7.6
1	C	248	LEU	6.7
3	E	26	PRO	6.3
1	A	351	PHE	6.0
1	A	339	ARG	5.6
3	E	6	MET	5.4
2	D	286	LEU	4.9
3	E	22	VAL	4.9
4	F	240	LEU	4.7
3	E	25	LYS	4.6
1	A	344	VAL	4.5
2	B	281	GLN	4.2
1	A	350	GLY	4.0
1	A	86	LEU	3.9
2	D	279	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	284	ARG	3.9
1	A	296	PHE	3.8
2	D	278	ARG	3.7
3	E	28	SER	3.6
1	A	335	ILE	3.6
3	E	54	LEU	3.5
3	E	11	LEU	3.4
1	A	357	TYR	3.3
2	D	285	ALA	3.3
3	E	8	VAL	3.2
4	F	100	ILE	3.2
1	A	317	LEU	3.2
1	A	347	CYS	3.1
3	E	7	GLU	3.1
1	C	135	PHE	3.1
2	D	276	THR	3.0
2	D	277	SER	3.0
1	C	128	GLN	3.0
1	A	167	LEU	3.0
1	A	378	LEU	2.9
1	A	282	TYR	2.9
4	F	142	ARG	2.9
1	C	335	ILE	2.9
4	F	173	ILE	2.8
1	C	286	LEU	2.8
1	A	65	ALA	2.8
1	C	4[A]	CYS	2.8
1	C	296	PHE	2.8
2	D	358	ILE	2.8
1	C	368	LEU	2.7
1	A	252	LEU	2.7
1	A	88	HIS	2.7
1	A	348	PRO	2.7
1	A	212	ILE	2.6
1	A	326	LYS	2.6
2	D	275	LEU	2.6
2	B	318	ILE	2.6
1	A	382	THR	2.6
2	D	323	MET	2.6
2	D	299	LYS	2.5
1	A	24	TYR	2.5
2	D	401	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	10	GLU	2.4
1	A	312	TYR	2.4
1	A	362	VAL	2.4
3	E	142	GLU	2.4
3	E	9	ILE	2.3
1	C	285	GLN	2.3
1	A	30	ILE	2.3
2	D	281	GLN	2.3
1	C	5	ILE	2.3
2	D	274	PRO	2.3
1	A	255	PHE	2.3
1	C	247	ALA	2.3
1	A	26	LEU	2.2
1	A	248	LEU	2.2
1	A	135	PHE	2.2
1	A	276	ILE	2.2
3	E	20	PHE	2.2
1	A	340	SER	2.2
3	E	23	ILE	2.2
2	B	229	HIS	2.2
2	D	371	LEU	2.2
4	F	39	LEU	2.2
1	A	149	PHE	2.2
1	A	230	LEU	2.2
2	D	293	GLN	2.2
1	A	244	PHE	2.2
2	D	204	ILE	2.2
2	B	358	ILE	2.1
1	C	338	LYS	2.1
3	E	62	LYS	2.1
2	D	415	GLU	2.1
2	B	283	TYR	2.1
2	D	335	VAL	2.1
2	B	373	MET	2.1
2	D	296	PHE	2.1
1	A	262	TYR	2.1
1	A	311	LYS	2.1
2	B	333	LEU	2.1
1	A	136	LEU	2.1
3	E	50	ILE	2.1
1	A	169	PHE	2.1
3	E	17	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	272	PHE	2.1
3	E	13	LYS	2.0
2	B	360	PRO	2.0
1	C	246	GLY	2.0
1	C	87	PHE	2.0
4	F	312	PHE	2.0
1	A	375	VAL	2.0
4	F	302	ILE	2.0
3	E	84	GLN	2.0
1	A	209	ILE	2.0
1	C	276	ILE	2.0
1	A	342	GLN	2.0
2	B	291	LEU	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	D	502	1/1	0.80	0.14	89,89,89,89	0
7	CA	A	504	1/1	0.84	0.19	104,104,104,104	0
11	ACP	F	401	31/31	0.88	0.14	127,133,142,154	0
7	CA	B	503	1/1	0.90	0.11	117,117,117,117	0
7	CA	A	503	1/1	0.90	0.09	122,122,122,122	0
6	MG	B	502	1/1	0.94	0.10	70,70,70,70	0
9	MES	B	504	12/12	0.94	0.19	102,108,121,128	0
6	MG	F	402	1/1	0.94	0.13	125,125,125,125	0
10	TVP	C	504	14/14	0.95	0.33	61,74,89,99	29
8	GDP	D	501	28/28	0.95	0.18	84,93,101,105	0

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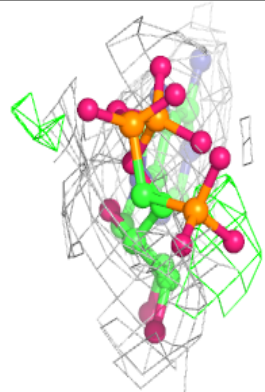
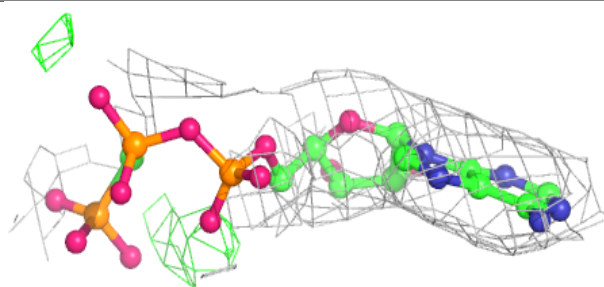
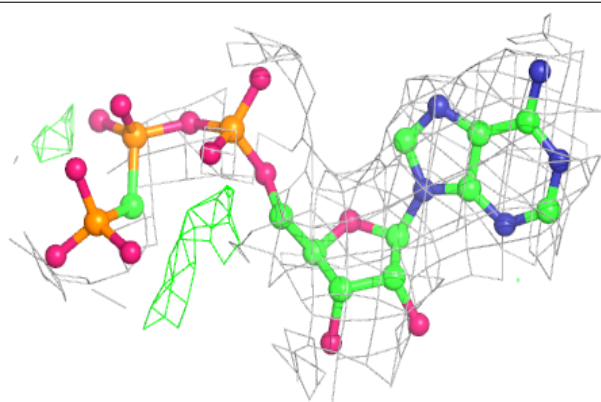
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	TVP	B	505	14/14	0.97	0.26	58,70,88,88	0
5	GTP	A	501	32/32	0.97	0.17	63,70,75,79	0
6	MG	A	502	1/1	0.97	0.20	76,76,76,76	0
8	GDP	B	501	28/28	0.98	0.17	59,65,71,72	0
5	GTP	C	501	32/32	0.98	0.19	56,67,73,80	0
7	CA	C	503	1/1	0.98	0.12	103,103,103,103	0
6	MG	C	502	1/1	0.99	0.16	67,67,67,67	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.

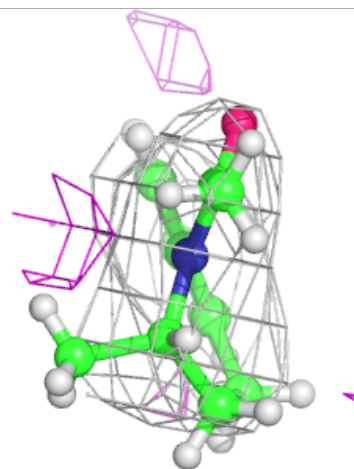
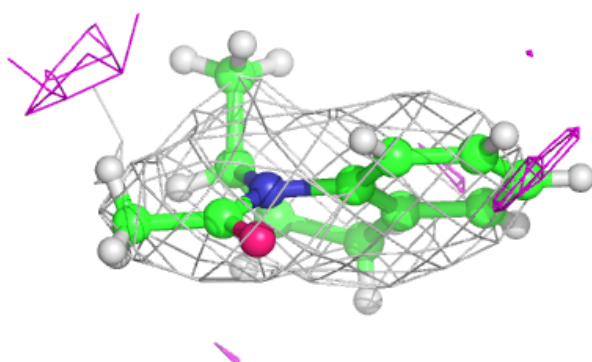
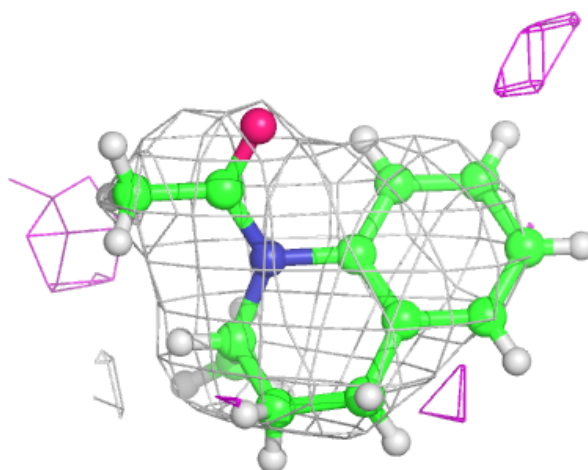
**Electron density around ACP F 401:**

2mF<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)



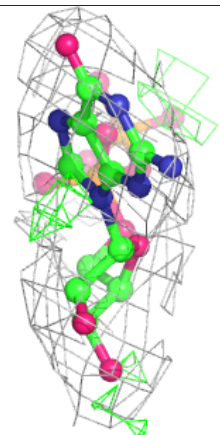
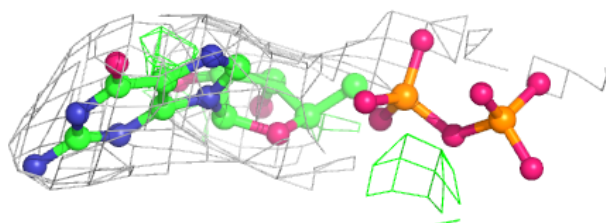
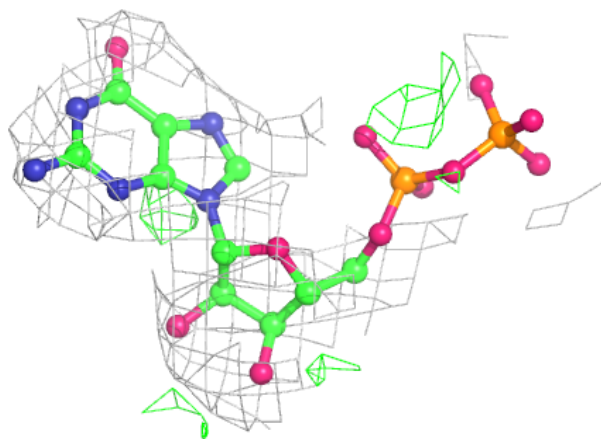
**Electron density around TVP C 504:**

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

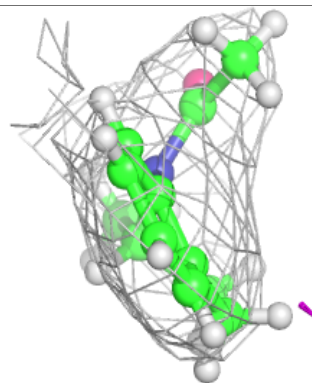
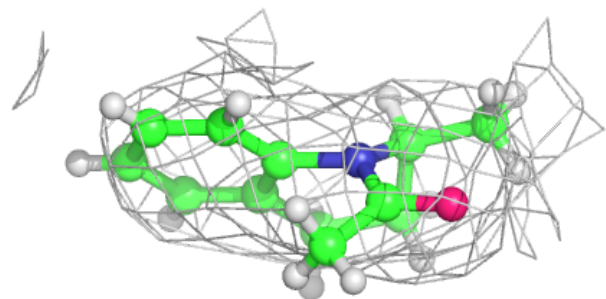
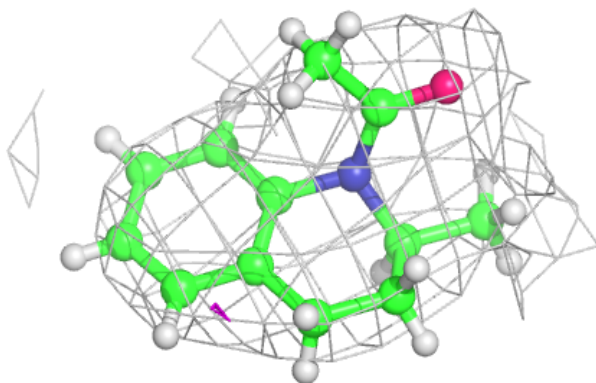


**Electron density around GDP D 501:**

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

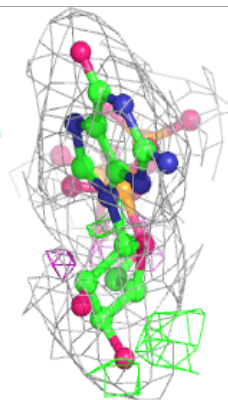
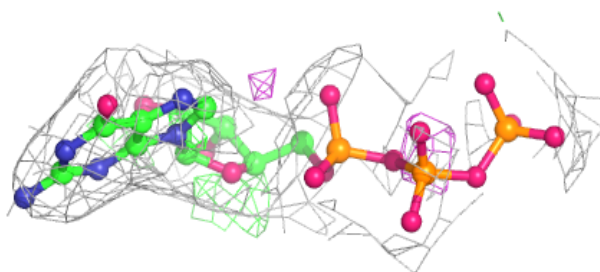
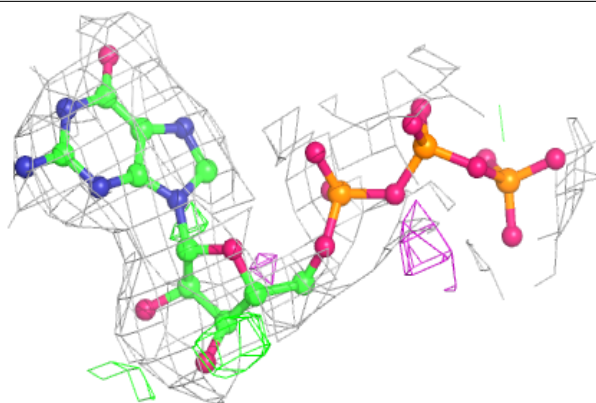
**Electron density around TVP B 505:**

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



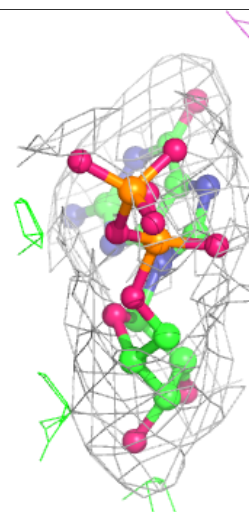
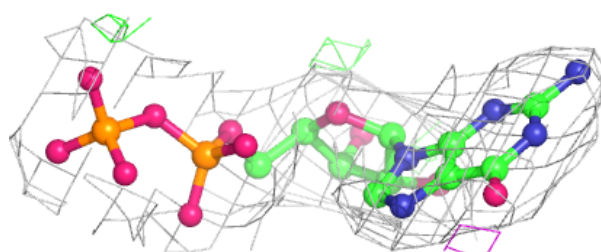
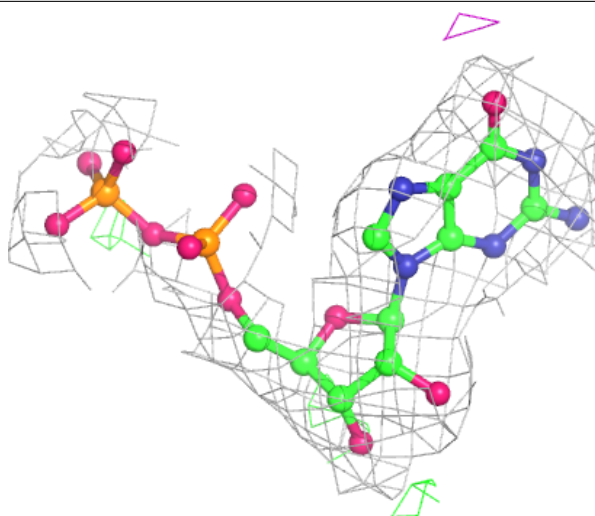
**Electron density around GTP A 501:**

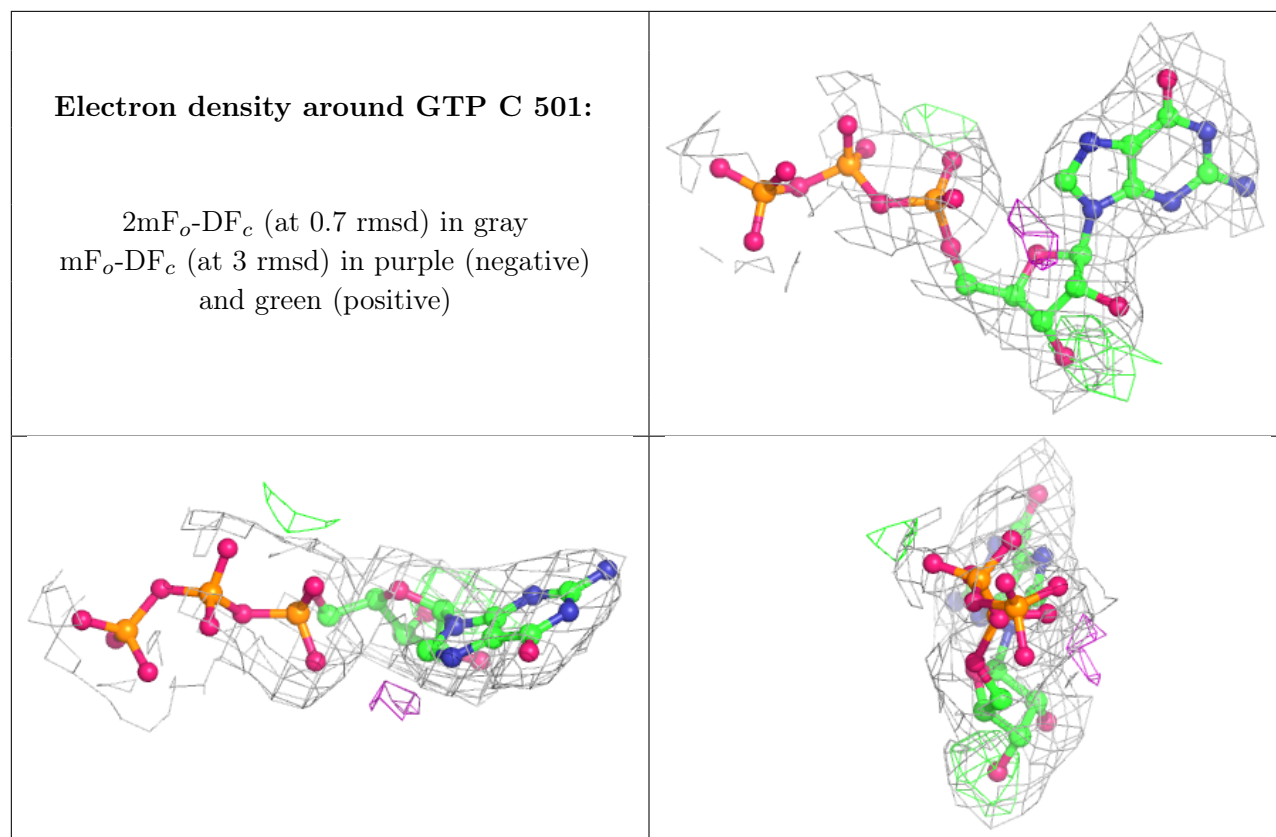
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.