



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:07 pm BST

PDB ID : 5NG1
Title : TUBULIN-MTC-zampanolide complex
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Deposited on : 2017-03-16
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

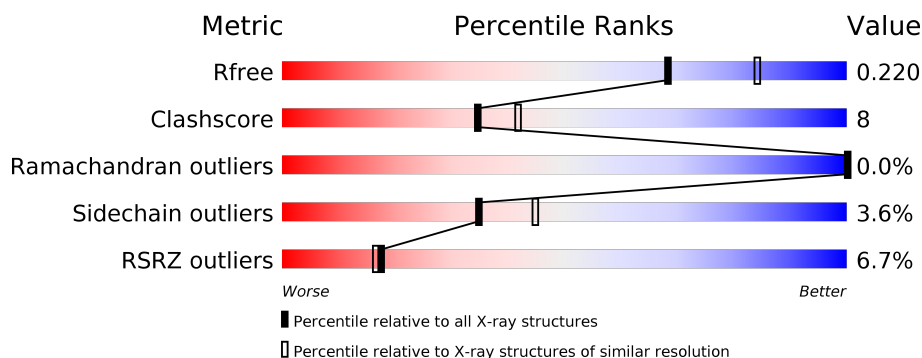
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>• •</div> </div> </div>
2	B	445	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>6%</div> </div> </div>
2	D	445	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
3	E	143	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>14%</div> </div> </div>
4	F	384	<div> <div>21%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18437 atoms, of which 68 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	440	Total	C	N	O	S	0	2	0
			3448	2182	587	656	23			
1	C	440	Total	C	N	O	S	0	4	0
			3462	2191	587	662	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3302	2076	561	638	27			
2	D	431	Total	C	N	O	S	0	2	0
			3402	2135	583	656	28			

- 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

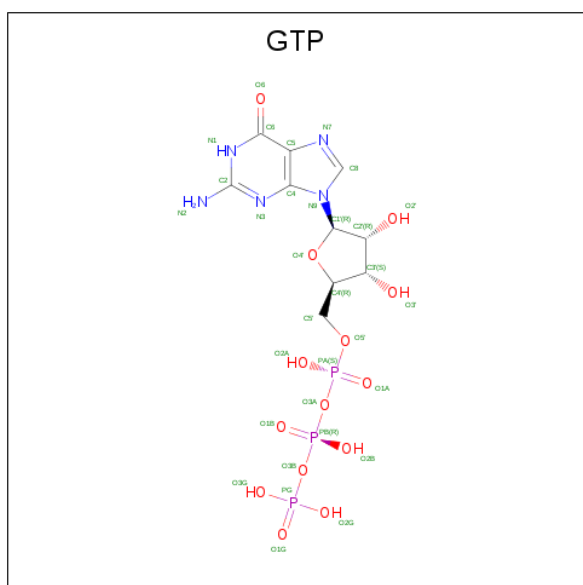
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	353	Total	C	N	O	S	0	0	0
			2879	1844	493	528	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	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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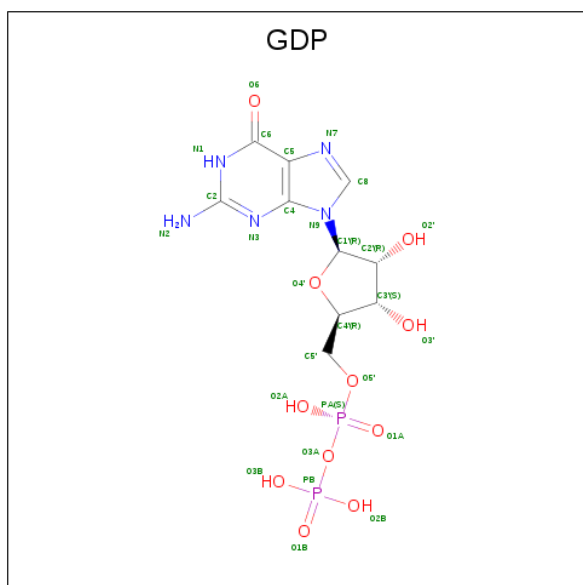
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

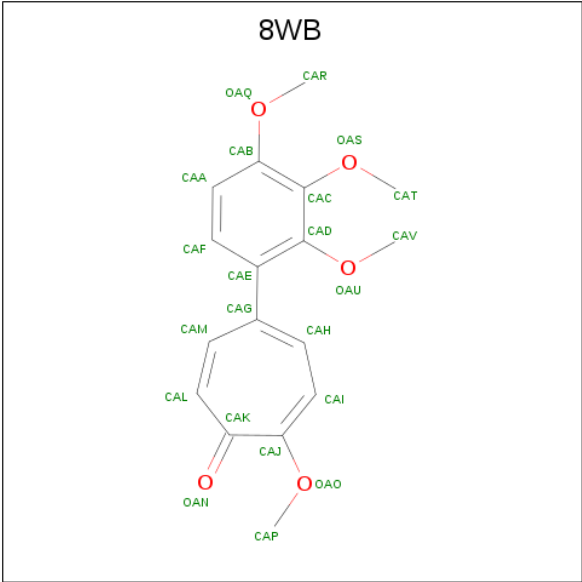
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



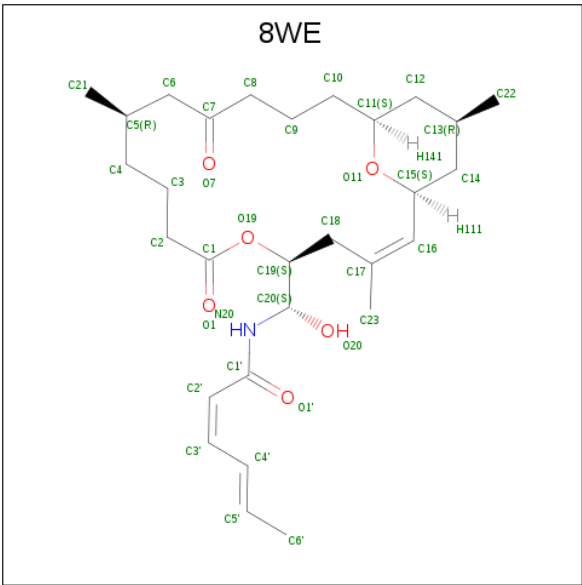
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-methoxy-5-(2,3,4-trimethoxyphenyl)cyclohepta-2,4,6-trien-1-one (three-letter code: 8WB) (formula: C₁₇H₁₈O₅).



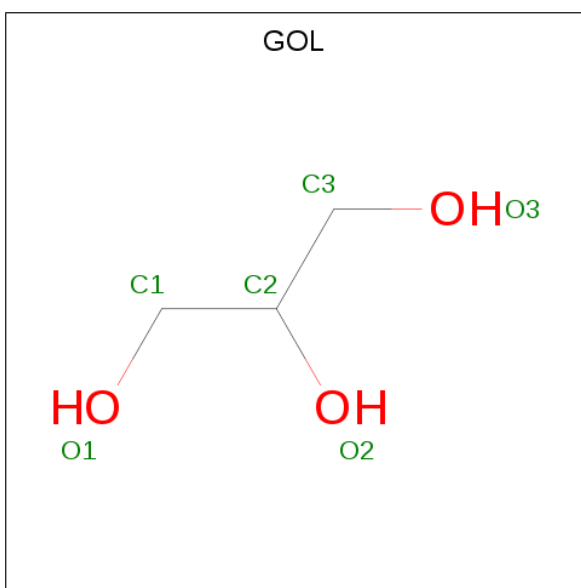
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			22	17	5		
9	D	1	Total	C	O	0	0
			22	17	5		

- Molecule 10 is (2 {Z},4 {E})- {N}-[({S})-oxidanyl-[(1 {S},2 {E},5 {S},11 {R},17 {S},19 {R})]-3,11,19-trimethyl-7,13-bis(oxidanylidene)-6,21-dioxabicyclo[15.3.1]henicos-2-en-5-yl]methyl]hexa-2,4-dienamide (three-letter code: 8WE) (formula: C₂₉H₄₅NO₆).



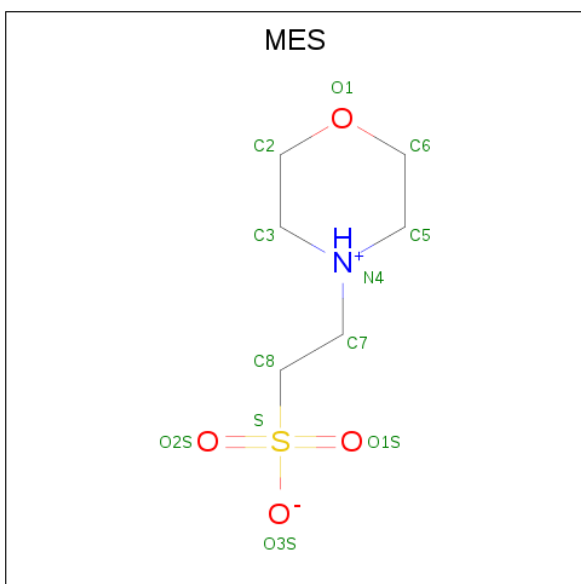
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			70	29	34	1	6		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



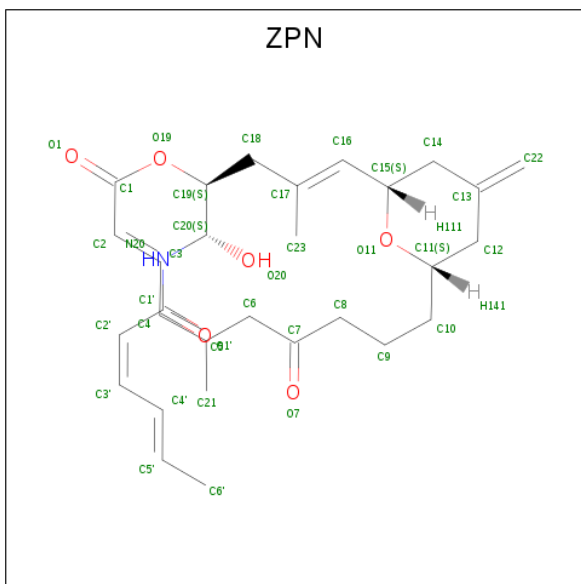
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



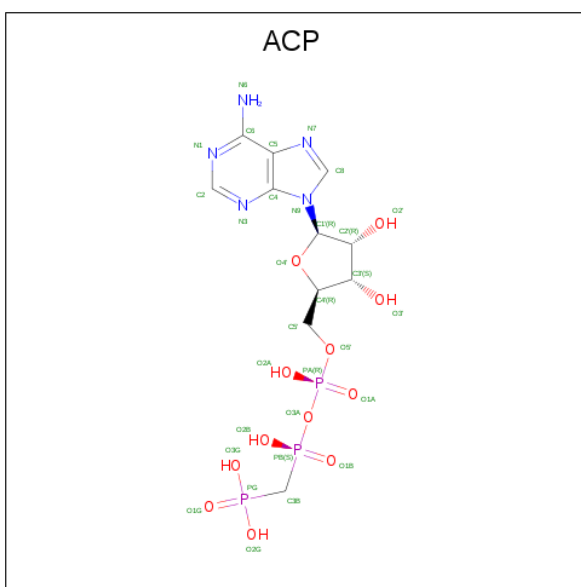
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 13 is (2Z,4E)-N-[(S)-[(1S,2E,5S,8E,10Z,17S)-3,11-dimethyl-19-methylidene-7,13-dioxo-6,21-dioxabicyclo[15.3.1]henicosa-2,8,10-trien-5-yl](hydroxy)methyl]hexa-2,4-dienamide (three-letter code: ZPN) (formula: C₂₉H₃₉NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N	O	
13	D	1	70	29	34	1	6	0

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

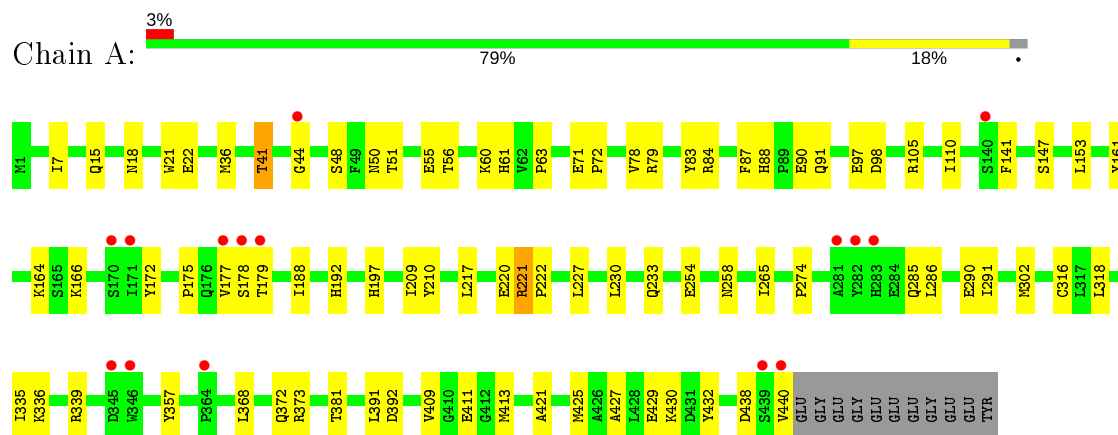
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	101	Total	O	0	0
			101	101		
15	B	92	Total	O	0	0
			92	92		
15	C	195	Total	O	0	0
			195	195		
15	D	104	Total	O	0	0
			104	104		
15	E	22	Total	O	0	0
			22	22		
15	F	56	Total	O	0	0
			56	56		

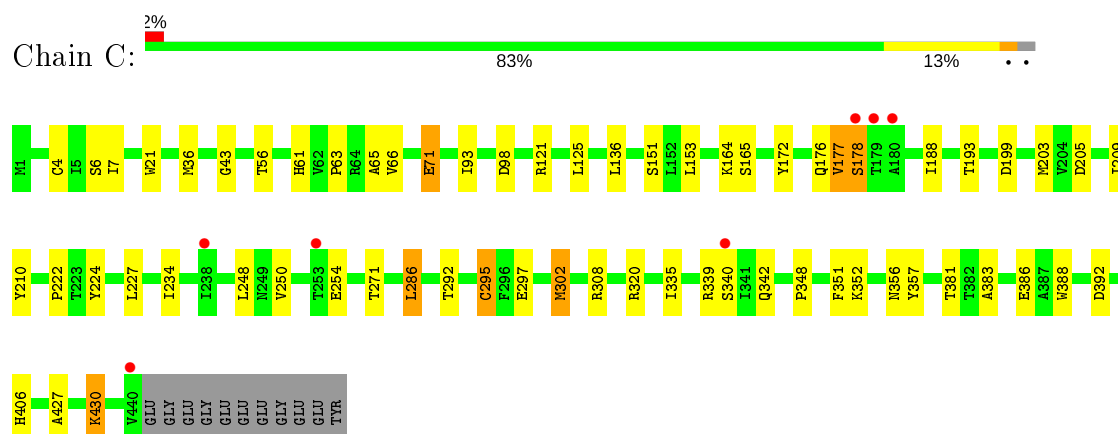
3 Residue-property plots [i](#)

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

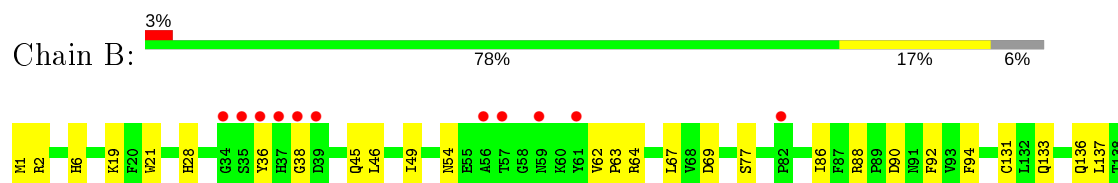
- Molecule 1: Tubulin alpha-1B chain

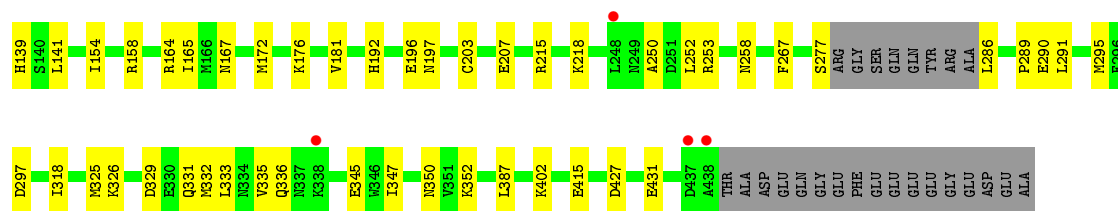


- Molecule 1: Tubulin alpha-1B chain

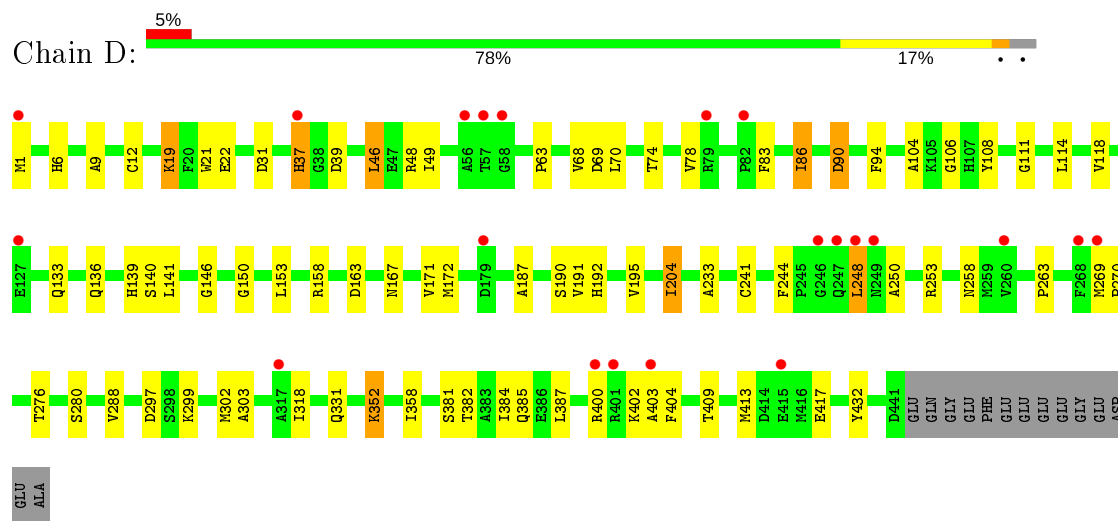


- Molecule 2: Tubulin beta-2B chain

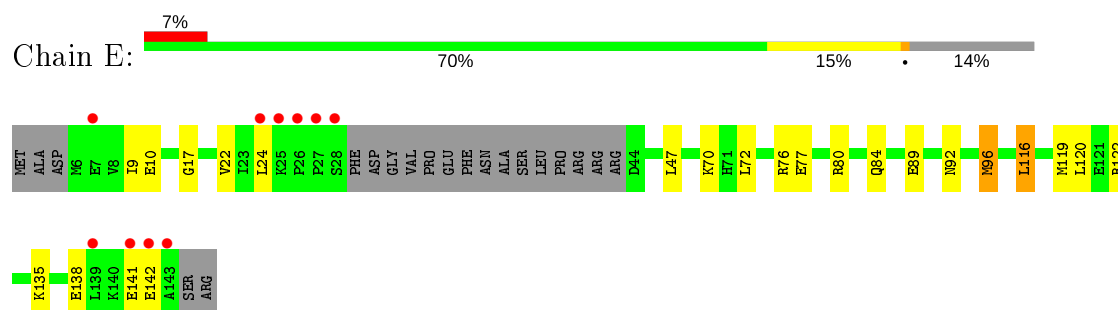




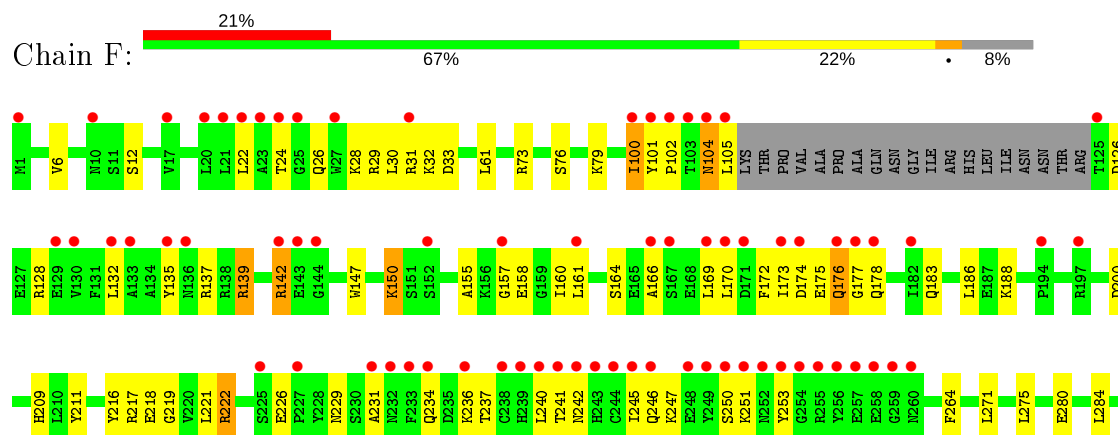
• Molecule 2: Tubulin beta-2B chain

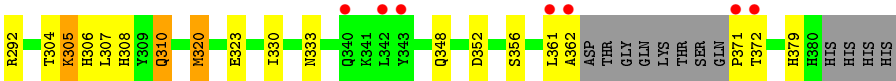


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.24Å 157.42Å 178.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.69 – 2.20 47.69 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.69-2.20) 99.4 (47.69-2.19)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.20Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, R_{free}	0.173 , 0.220 0.173 , 0.220	Depositor DCC
R_{free} test set	7527 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18437	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, CA, GTP, ACP, MES, ZPN, 8WE, 8WB

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	0.43	0/3532	0.58	0/4794
1	C	0.50	1/3552 (0.0%)	0.62	0/4821
2	B	0.43	0/3375	0.58	1/4571 (0.0%)
2	D	0.40	0/3483	0.56	0/4717
3	E	0.43	0/1022	0.52	0/1356
4	F	0.44	0/2945	0.55	0/3979
All	All	0.44	1/17909 (0.0%)	0.58	1/24238 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-6.75	1.70	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	ASN	N-CA-C	5.28	125.26	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3448	0	3367	63	1
1	C	3462	0	3377	39	1
2	B	3302	0	3185	46	0
2	D	3402	0	3288	63	0
3	E	1014	0	1029	13	0
4	F	2879	0	2848	72	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	22	0	0	3	0
9	D	22	0	0	7	0
10	B	36	34	0	0	0
11	B	6	0	8	0	0
12	B	12	0	13	1	0
13	D	36	34	38	2	0
14	F	31	0	14	2	0
15	A	101	0	0	3	0
15	B	92	0	0	1	0
15	C	195	0	0	4	0
15	D	104	0	0	3	0
15	E	22	0	0	1	0
15	F	56	0	0	4	0
All	All	18369	68	17215	291	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 8.

All (291) 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:248:LEU:HD23	2:D:250:ALA:HB2	1.42	1.02
4:F:160:ILE:HD11	4:F:240:LEU:HD21	1.48	0.93
2:D:250:ALA:HB1	9:D:503:8WB:CAR	2.06	0.86
14:F:701:ACP:O2G	15:F:801:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.15	0.78
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.64	0.78
1:A:41:THR:HB	1:A:44:GLY:O	1.82	0.77
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.48	0.77
2:B:286:LEU:N	2:B:290:GLU:OE1	2.17	0.77
4:F:172:PHE:O	4:F:176:GLN:NE2	2.17	0.77
2:D:19:LYS:NZ	15:D:602:HOH:O	2.17	0.75
2:D:250:ALA:HB1	9:D:503:8WB:OAQ	1.86	0.75
4:F:142:ARG:N	4:F:142:ARG:HD2	2.02	0.74
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.71	0.73
4:F:348:GLN:NE2	4:F:352:ASP:OD2	2.22	0.73
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.69	0.72
4:F:160:ILE:HD11	4:F:240:LEU:CD2	2.18	0.71
4:F:241:THR:OG1	14:F:701:ACP:O3'	2.07	0.71
2:B:69:ASP:O	2:B:94:PHE:HA	1.92	0.70
2:D:352:LYS:HD2	9:D:503:8WB:CAK	2.22	0.69
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.91	0.69
2:D:167:ASN:ND2	15:D:603:HOH:O	2.23	0.69
2:B:1:MET:HG2	2:B:133:GLN:HA	1.75	0.69
3:E:142:GLU:N	3:E:142:GLU:OE1	2.25	0.69
2:D:432:TYR:OH	15:D:601:HOH:O	2.08	0.69
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.76	0.67
4:F:356:SER:HB2	4:F:361:LEU:HD11	1.75	0.67
4:F:73:ARG:HB2	4:F:76:SER:OG	1.95	0.67
1:A:175:PRO:HA	1:A:179:THR:CG2	2.25	0.67
1:C:151:SER:HB3	1:C:193:THR:HG21	1.76	0.66
1:C:340:SER:HA	15:C:601:HOH:O	1.94	0.66
1:A:285:GLN:HG3	1:A:372:GLN:NE2	2.10	0.66
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.78	0.65
4:F:139:ARG:O	4:F:142:ARG:NH2	2.29	0.65
4:F:333:ASN:HB3	15:F:839:HOH:O	1.97	0.65
1:C:308[B]:ARG:NH1	15:C:602:HOH:O	2.31	0.64
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.34	0.63
2:B:402:LYS:HD3	2:B:415:GLU:OE2	1.97	0.63
2:D:1:MET:SD	2:D:253[B]:ARG:NH1	2.71	0.63
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.79	0.63
1:A:88:HIS:O	1:A:91:GLN:HG2	1.99	0.63
3:E:80:ARG:O	3:E:84:GLN:HG3	1.99	0.62
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.81	0.62
1:A:105[B]:ARG:NH2	15:A:603:HOH:O	2.32	0.62
1:A:221:ARG:HG3	2:B:325:MET:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.35	0.61
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.82	0.61
3:E:9:ILE:HD12	3:E:10:GLU:H	1.66	0.60
4:F:102:PRO:HG3	4:F:178:GLN:N	2.15	0.60
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.83	0.60
3:E:84:GLN:NE2	15:E:201:HOH:O	2.33	0.60
4:F:305:LYS:NZ	15:F:802:HOH:O	2.34	0.60
2:B:250:ALA:HB1	9:B:503:8WB:CAR	2.32	0.59
1:A:427:ALA:HA	1:A:430:LYS:HE3	1.84	0.59
2:D:69:ASP:O	2:D:94:PHE:HA	2.03	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.59
2:B:352:LYS:HG3	9:B:503:8WB:CAK	2.32	0.59
4:F:24:THR:O	4:F:26:GLN:NE2	2.32	0.58
2:D:192:HIS:O	2:D:195:VAL:HG12	2.03	0.58
2:D:171:VAL:HA	2:D:204:ILE:O	2.03	0.58
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.84	0.58
2:D:409:THR:HA	2:D:413:MET:O	2.03	0.58
2:D:1:MET:HG2	2:D:133:GLN:HA	1.86	0.58
4:F:128:ARG:HH22	4:F:174:ASP:CG	2.05	0.58
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.38	0.58
1:A:105[B]:ARG:HD3	1:A:411:GLU:OE1	2.04	0.58
4:F:102:PRO:HG3	4:F:178:GLN:H	1.68	0.58
2:B:318:ILE:N	2:B:318:ILE:HD12	2.19	0.57
1:A:220:GLU:HG2	2:B:326:LYS:HD2	1.87	0.57
1:A:48:SER:O	1:A:51:THR:HG23	2.03	0.57
4:F:356:SER:HB2	4:F:361:LEU:CD1	2.34	0.57
1:C:286:LEU:H	1:C:286:LEU:HD12	1.70	0.57
2:D:1:MET:HE3	2:D:133:GLN:HB3	1.87	0.57
4:F:126:ASP:OD2	4:F:128:ARG:HB2	2.04	0.57
4:F:361:LEU:O	4:F:362:ALA:HB2	2.05	0.56
4:F:188:LYS:HB3	4:F:323:GLU:HG2	1.86	0.56
4:F:371:PRO:HA	4:F:372:THR:HB	1.88	0.55
2:B:158:ARG:NH1	2:B:196:GLU:O	2.39	0.55
1:C:43:GLY:HA2	1:C:56:THR:O	2.07	0.55
4:F:158:GLU:HA	4:F:158:GLU:OE1	2.07	0.55
1:C:339:ARG:O	15:C:601:HOH:O	2.18	0.55
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.88	0.54
1:C:165:SER:HA	1:C:199:ASP:OD2	2.06	0.54
1:C:320:ARG:HA	1:C:356:ASN:O	2.07	0.54
2:D:352:LYS:HD2	9:D:503:8WB:OAN	2.06	0.54
1:C:427:ALA:O	1:C:430:LYS:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.54
4:F:356:SER:CB	4:F:361:LEU:HD11	2.36	0.54
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.88	0.54
4:F:242:ASN:HB2	4:F:245:ILE:HG12	1.89	0.54
2:D:258:ASN:HB3	9:D:503:8WB:CAK	2.37	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.53
4:F:246:GLN:O	4:F:250:SER:HB3	2.08	0.53
2:D:382:THR:O	2:D:385:GLN:HG2	2.08	0.53
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.48	0.53
2:D:46:LEU:HA	2:D:49:ILE:HB	1.91	0.53
2:D:163:ASP:O	2:D:253[A]:ARG:NH2	2.42	0.53
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.43	0.53
2:B:164:ARG:O	12:B:506:MES:H31	2.09	0.52
1:A:79:ARG:O	1:A:84:ARG:HB2	2.10	0.52
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.44	0.52
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.45	0.52
2:D:48:ARG:NH1	2:D:241:CYS:O	2.43	0.52
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.52
4:F:100:ILE:O	4:F:100:ILE:HG22	2.10	0.52
1:C:234:ILE:HD13	1:C:302:MET:SD	2.50	0.52
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.44	0.51
2:D:269[A]:MET:CE	2:D:381:SER:HB3	2.39	0.51
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.93	0.51
2:D:258:ASN:HB3	9:D:503:8WB:CAJ	2.40	0.51
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.46	0.51
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.92	0.51
2:B:67:LEU:HD12	2:B:67:LEU:N	2.25	0.51
1:A:175:PRO:HA	1:A:179:THR:HG21	1.92	0.51
4:F:161:LEU:HD22	4:F:172:PHE:HB2	1.92	0.51
4:F:292:ARG:HD2	4:F:379:HIS:O	2.11	0.51
4:F:226:GLU:HG3	4:F:237:THR:HG22	1.93	0.51
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.44	0.51
1:A:141:PHE:O	1:A:147:SER:HB3	2.11	0.50
2:D:141:LEU:HD12	2:D:172:MET:CE	2.40	0.50
3:E:72:LEU:O	3:E:76:ARG:HG2	2.10	0.50
4:F:226:GLU:OE1	4:F:251:LYS:HB2	2.11	0.50
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.11	0.50
4:F:155:ALA:O	4:F:157:GLY:HA2	2.11	0.50
2:B:136:GLN:HA	2:B:167:ASN:O	2.12	0.50
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.94	0.50
1:C:383:ALA:O	1:C:386[A]:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.27	0.50
2:B:427:ASP:O	2:B:431:GLU:HG3	2.12	0.50
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.47	0.49
15:A:656:HOH:O	2:B:352:LYS:HG2	2.12	0.49
4:F:105:LEU:HD12	4:F:177:GLY:O	2.12	0.49
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.46	0.49
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.46	0.49
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.93	0.49
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.49
2:D:141:LEU:HD12	2:D:172:MET:SD	2.53	0.49
4:F:371:PRO:HA	4:F:372:THR:O	2.12	0.49
1:A:175:PRO:HA	1:A:179:THR:HG22	1.95	0.49
2:B:1:MET:SD	2:B:253:ARG:NH1	2.86	0.49
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.47	0.49
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.22	0.49
4:F:209:HIS:HB2	4:F:310:GLN:CG	2.43	0.49
2:D:297:ASP:OD2	2:D:299:LYS:HE2	2.13	0.48
2:D:70:LEU:HD23	2:D:114:LEU:HD22	1.94	0.48
2:D:276:THR:CG2	2:D:280:SER:HB2	2.43	0.48
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.40	0.48
2:D:46:LEU:H	2:D:46:LEU:CD2	2.26	0.48
1:A:336:LYS:HG2	3:E:24:LEU:HD13	1.96	0.48
2:D:403:ALA:HB1	2:D:404:PHE:CD1	2.48	0.48
4:F:101:TYR:N	4:F:126:ASP:OD1	2.41	0.48
4:F:242:ASN:HB2	4:F:245:ILE:CG1	2.43	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.48
4:F:209:HIS:HB2	4:F:310:GLN:HG2	1.95	0.48
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.95	0.48
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.95	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.53	0.48
4:F:372:THR:O	4:F:372:THR:HG22	2.13	0.47
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.46	0.47
4:F:229:ASN:OD1	4:F:231:ALA:HB3	2.15	0.47
1:A:98:ASP:O	1:A:105[B]:ARG:NH2	2.48	0.47
2:B:62:VAL:HG11	2:B:88:ARG:CG	2.44	0.47
1:C:177:VAL:O	1:C:178:SER:C	2.53	0.47
2:D:74:THR:O	2:D:78:VAL:HG23	2.15	0.47
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.49	0.47
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:HIS:HB3	2:B:49:ILE:HD13	1.96	0.47
2:D:269[A]:MET:HG2	2:D:303:ALA:HB3	1.97	0.46
2:B:215:ARG:O	2:B:218:LYS:NZ	2.48	0.46
4:F:371:PRO:CA	4:F:372:THR:HB	2.45	0.46
1:A:105[B]:ARG:CZ	1:A:110:ILE:HD11	2.45	0.46
2:B:289:PRO:HA	2:B:331:GLN:HG2	1.96	0.46
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.15	0.46
2:D:241:CYS:HB3	2:D:250:ALA:CB	2.46	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.50	0.46
1:A:55:GLU:HA	1:A:60:LYS:O	2.15	0.46
1:C:351:PHE:CD1	1:C:351:PHE:N	2.81	0.46
2:D:90:ASP:N	2:D:90:ASP:OD1	2.48	0.46
1:A:15:GLN:NE2	15:A:602:HOH:O	2.29	0.46
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.51	0.46
4:F:28:LYS:HE2	4:F:28:LYS:HB3	1.72	0.46
1:A:105[B]:ARG:HG2	1:A:411:GLU:CD	2.36	0.46
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.51	0.46
2:B:286:LEU:O	2:B:286:LEU:HD12	2.16	0.46
2:B:329:ASP:O	2:B:333:LEU:HG	2.15	0.46
1:C:430:LYS:HD2	15:C:757:HOH:O	2.15	0.46
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.27	0.46
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.51	0.45
4:F:361:LEU:HD12	4:F:361:LEU:H	1.81	0.45
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.47	0.45
1:A:409:VAL:HA	1:A:413:MET:O	2.17	0.45
2:B:295:MET:HE3	2:B:295:MET:HB2	1.76	0.45
1:C:286:LEU:N	1:C:286:LEU:HD12	2.30	0.45
1:C:4:CYS:HB3	1:C:136:LEU:CD2	2.46	0.45
2:D:46:LEU:HD22	2:D:46:LEU:H	1.82	0.45
4:F:31:ARG:HB3	4:F:31:ARG:CZ	2.47	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.45
2:D:104:ALA:HB2	2:D:413:MET:SD	2.57	0.45
1:C:188:ILE:HD11	1:C:392:ASP:OD1	2.17	0.45
2:D:118:VAL:CG1	2:D:153:LEU:HD21	2.47	0.45
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.98	0.45
3:E:119:MET:HA	3:E:122:ARG:NH2	2.31	0.45
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.99	0.45
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.45
2:D:288:VAL:HG12	2:D:331:GLN:HG3	2.00	0.44
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.97	0.44
2:B:88:ARG:NH2	2:B:90:ASP:OD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:LYS:HD2	2:D:402:LYS:N	2.32	0.44
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.99	0.44
2:B:258:ASN:HB3	9:B:503:8WB:CAK	2.47	0.44
1:A:56:THR:OG1	1:A:60:LYS:HB3	2.18	0.44
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.57	0.44
2:B:332:MET:O	2:B:336:GLN:HG3	2.18	0.44
3:E:96:MET:CE	3:E:96:MET:HA	2.48	0.44
4:F:305:LYS:HG2	4:F:306:HIS:N	2.32	0.44
4:F:200:ASP:O	4:F:221:LEU:HA	2.18	0.44
1:A:97:GLU:HG2	2:B:131:CYS:SG	2.58	0.43
4:F:275:LEU:HD23	15:F:807:HOH:O	2.18	0.43
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.53	0.43
1:C:151:SER:HB3	1:C:193:THR:CG2	2.45	0.43
1:C:178:SER:HB2	1:C:224:TYR:OH	2.19	0.43
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.00	0.43
1:C:164:LYS:HB2	1:C:164:LYS:HE2	1.82	0.43
4:F:371:PRO:HA	4:F:372:THR:C	2.38	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.49	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.53	0.43
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.01	0.43
1:C:271:THR:HG21	1:C:295:CYS:O	2.18	0.43
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.43
4:F:320:MET:HE2	4:F:320:MET:HB3	1.79	0.43
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.53	0.43
3:E:116:LEU:O	3:E:120:LEU:HD23	2.19	0.43
3:E:80:ARG:HG2	3:E:80:ARG:HH11	1.84	0.43
1:A:177:VAL:O	1:A:178:SER:C	2.58	0.42
1:A:265:ILE:N	1:A:265:ILE:HD13	2.34	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.02	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.18	0.42
2:D:276:THR:HG22	2:D:280:SER:HB2	2.02	0.42
4:F:104:ASN:OD1	4:F:104:ASN:N	2.41	0.42
2:D:244:PHE:CD1	2:D:358:ILE:HD12	2.54	0.42
4:F:226:GLU:OE1	4:F:251:LYS:HD2	2.19	0.42
4:F:361:LEU:HD12	4:F:361:LEU:N	2.34	0.42
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.54	0.42
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.83	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.02	0.42
2:D:118:VAL:HG11	2:D:153:LEU:HD21	2.01	0.42
3:E:9:ILE:HG13	3:E:10:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:234:GLN:O	4:F:236:LYS:HE2	2.20	0.42
1:A:438:ASP:O	1:A:440:VAL:HG23	2.20	0.42
2:D:146:GLY:O	2:D:150:GLY:HA3	2.20	0.42
2:D:248:LEU:CD2	2:D:250:ALA:HB2	2.31	0.42
2:D:12:CYS:CB	2:D:140:SER:HB3	2.50	0.41
2:D:269[A]:MET:HE2	2:D:381:SER:HB3	2.02	0.41
4:F:100:ILE:HG22	4:F:173:ILE:HG21	2.02	0.41
4:F:147:TRP:HB2	4:F:169:LEU:HD11	2.02	0.41
4:F:6:VAL:HB	4:F:29:ARG:NH2	2.35	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.41
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.01	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.55	0.41
2:B:181:VAL:HG12	1:C:348:PRO:HG2	2.02	0.41
1:C:6:SER:O	1:C:65:ALA:HA	2.21	0.41
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.55	0.41
2:D:187:ALA:O	2:D:191:VAL:HG23	2.20	0.41
1:A:50:ASN:ND2	1:A:55:GLU:OE2	2.34	0.41
1:A:63:PRO:HG2	1:A:87:PHE:CE1	2.56	0.41
2:B:164:ARG:HD2	15:B:673:HOH:O	2.21	0.41
3:E:47:LEU:HD12	3:E:47:LEU:O	2.21	0.41
4:F:161:LEU:HD22	4:F:172:PHE:CB	2.50	0.41
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.55	0.41
1:A:22:GLU:HG3	1:A:83:TYR:HE2	1.84	0.41
4:F:172:PHE:O	4:F:175:GLU:HB2	2.20	0.41
4:F:150:LYS:NZ	4:F:183:GLN:OE1	2.48	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HG3	2.01	0.41
2:B:141:LEU:HD12	2:B:172:MET:SD	2.61	0.41
2:D:31:ASP:HB3	2:D:37:HIS:CD2	2.56	0.41
13:D:504:ZPN:O1'	13:D:504:ZPN:H4'1	2.21	0.41
1:A:392:ASP:OD2	1:A:429:GLU:OE1	2.39	0.41
2:B:28:HIS:HB3	2:B:49:ILE:CD1	2.51	0.40
2:D:233:ALA:HA	13:D:504:ZPN:C22	2.51	0.40
2:D:258:ASN:ND2	9:D:503:8WB:CAL	2.84	0.40
1:A:105[B]:ARG:HG2	1:A:411:GLU:HG3	2.03	0.40
1:C:203:MET:SD	1:C:388:TRP:CH2	3.15	0.40
2:D:86:ILE:HA	2:D:86:ILE:HD13	1.76	0.40
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.89	0.40
4:F:61:LEU:CD1	4:F:310:GLN:HB3	2.51	0.40
4:F:361:LEU:O	4:F:362:ALA:CB	2.70	0.40
2:D:9:ALA:HA	2:D:68:VAL:O	2.21	0.40
4:F:247:LYS:HG3	4:F:253:TYR:CZ	2.56	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:A:290:GLU:OE1	1:C:308[A]:ARG:NH2[3_555]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
1	C	442/451 (98%)	429 (97%)	12 (3%)	1 (0%)	47	55
2	B	416/445 (94%)	404 (97%)	12 (3%)	0	100	100
2	D	431/445 (97%)	423 (98%)	8 (2%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	347/384 (90%)	327 (94%)	20 (6%)	0	100	100
All	All	2195/2319 (95%)	2130 (97%)	64 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	178	SER

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	373/379 (98%)	370 (99%)	3 (1%)	81	90
1	C	375/379 (99%)	366 (98%)	9 (2%)	49	62
2	B	364/383 (95%)	354 (97%)	10 (3%)	44	57
2	D	374/383 (98%)	360 (96%)	14 (4%)	34	43
3	E	110/127 (87%)	100 (91%)	10 (9%)	9	9
4	F	315/342 (92%)	293 (93%)	22 (7%)	15	16
All	All	1911/1993 (96%)	1843 (96%)	68 (4%)	35	45

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	221	ARG
1	A	381	THR
2	B	2	ARG
2	B	19	LYS
2	B	77	SER
2	B	86	ILE
2	B	139	HIS
2	B	192	HIS
2	B	277	SER
2	B	297	ASP
2	B	335	VAL
2	B	345	GLU
1	C	71	GLU
1	C	176	GLN
1	C	177	VAL
1	C	286	LEU
1	C	297	GLU
1	C	302	MET
1	C	342	GLN
1	C	381	THR
1	C	430	LYS
2	D	19	LYS
2	D	37	HIS
2	D	39	ASP
2	D	46	LEU
2	D	86	ILE
2	D	90	ASP
2	D	139	HIS
2	D	158	ARG

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Mol	Chain	Res	Type
2	D	190	SER
2	D	204	ILE
2	D	248	LEU
2	D	352	LYS
2	D	384	ILE
2	D	400	ARG
3	E	22	VAL
3	E	70	LYS
3	E	77	GLU
3	E	89	GLU
3	E	92	ASN
3	E	96	MET
3	E	116	LEU
3	E	135	LYS
3	E	138	GLU
3	E	141	GLU
4	F	12	SER
4	F	22	LEU
4	F	30	LEU
4	F	32	LYS
4	F	33	ASP
4	F	79	LYS
4	F	100	ILE
4	F	104	ASN
4	F	137	ARG
4	F	139	ARG
4	F	142	ARG
4	F	150	LYS
4	F	164	SER
4	F	176	GLN
4	F	186	LEU
4	F	211	TYR
4	F	217	ARG
4	F	222	ARG
4	F	271	LEU
4	F	305	LYS
4	F	310	GLN
4	F	320	MET

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

Mol	Chain	Res	Type
1	A	18	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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$
12	MES	B	506	-	12,12,12	2.39	1 (8%)	14,16,16	1.56	1 (7%)
9	8WB	D	503	-	20,23,23	1.54	1 (5%)	22,31,31	1.12	1 (4%)
11	GOL	B	505	-	5,5,5	0.33	0	5,5,5	0.61	0
10	8WE	B	504	2	36,37,37	1.74	5 (13%)	42,48,48	2.05	13 (30%)
9	8WB	B	503	-	20,23,23	1.62	2 (10%)	22,31,31	1.20	2 (9%)
8	GDP	B	501	6	24,30,30	1.13	3 (12%)	31,47,47	2.01	7 (22%)
5	GTP	C	501	6	26,34,34	1.03	1 (3%)	33,54,54	1.82	8 (24%)
13	ZPN	D	504	2	36,37,37	0.96	2 (5%)	35,48,48	1.16	4 (11%)
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.70	6 (18%)
8	GDP	D	501	6	24,30,30	1.10	1 (4%)	31,47,47	2.04	8 (25%)
14	ACP	F	701	6	27,33,33	2.02	7 (25%)	32,52,52	1.36	5 (15%)

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
12	MES	B	506	-	-	5/6/14/14	0/1/1/1
9	8WB	D	503	-	-	2/6/12/12	0/2/2/2
11	GOL	B	505	-	-	3/4/4/4	-
10	8WE	B	504	2	-	11/41/53/53	0/1/2/2
9	8WB	B	503	-	-	0/6/12/12	0/2/2/2
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
13	ZPN	D	504	2	-	3/41/53/53	0/1/2/2
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
8	GDP	D	501	6	-	5/12/32/32	0/3/3/3
14	ACP	F	701	6	-	5/15/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	506	MES	C8-S	-8.19	1.65	1.77
9	B	503	8WB	CAE-CAG	-6.32	1.38	1.49
10	B	504	8WE	C22-C13	-6.03	1.33	1.52
9	D	503	8WB	CAE-CAG	-6.01	1.38	1.49
14	F	701	ACP	PG-O1G	5.50	1.61	1.50
10	B	504	8WE	C3-C2	-4.82	1.34	1.52
10	B	504	8WE	C20-N20	3.99	1.48	1.43
13	D	504	ZPN	C20-N20	3.92	1.48	1.43
14	F	701	ACP	PG-O3G	-3.71	1.46	1.54
10	B	504	8WE	C4-C5	-3.55	1.33	1.52
5	C	501	GTP	C6-N1	3.51	1.39	1.33
14	F	701	ACP	PB-O2B	-3.42	1.48	1.56
14	F	701	ACP	C2'-C1'	-3.32	1.48	1.53
14	F	701	ACP	PB-O1B	3.32	1.59	1.51
8	D	501	GDP	C6-C5	3.30	1.47	1.41
14	F	701	ACP	PB-O3A	3.11	1.61	1.58
8	B	501	GDP	C6-C5	3.08	1.46	1.41
5	A	501	GTP	C6-N1	2.67	1.37	1.33
14	F	701	ACP	PG-O2G	2.53	1.60	1.54
10	B	504	8WE	O19-C19	-2.52	1.41	1.46
8	B	501	GDP	O4'-C1'	2.51	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C2'-C1'	-2.22	1.50	1.53
9	B	503	8WB	OAU-CAD	-2.18	1.34	1.38
13	D	504	ZPN	O19-C19	-2.07	1.42	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	8WE	C22-C13-C14	5.77	121.01	111.18
5	C	501	GTP	N3-C2-N1	-5.52	119.85	127.22
8	B	501	GDP	C6-C5-C4	-5.49	115.56	120.80
5	A	501	GTP	N3-C2-N1	-4.91	120.67	127.22
10	B	504	8WE	C22-C13-C12	4.71	119.19	111.18
8	D	501	GDP	C6-N1-C2	4.61	123.25	115.93
8	D	501	GDP	C5-C6-N1	-4.44	117.36	123.43
8	D	501	GDP	C6-C5-C4	-4.40	116.60	120.80
8	D	501	GDP	C2-N3-C4	4.17	120.12	115.36
8	B	501	GDP	C6-N1-C2	4.11	122.45	115.93
8	B	501	GDP	N3-C2-N1	-3.99	121.89	127.22
9	B	503	8WB	CAP-OAO-CAJ	3.99	123.55	117.53
10	B	504	8WE	C14-C13-C12	3.95	115.93	110.10
8	B	501	GDP	C2-N3-C4	3.88	119.79	115.36
9	D	503	8WB	CAP-OAO-CAJ	3.86	123.35	117.53
12	B	506	MES	O1S-S-C8	3.85	111.55	106.92
5	A	501	GTP	C5-C6-N1	-3.74	118.31	123.43
8	D	501	GDP	N3-C2-N1	-3.71	122.27	127.22
10	B	504	8WE	C4-C5-C6	3.65	121.49	112.00
14	F	701	ACP	N3-C2-N1	-3.54	123.14	128.68
14	F	701	ACP	C3'-C2'-C1'	3.33	106.00	100.98
5	C	501	GTP	C2-N3-C4	3.32	119.15	115.36
8	B	501	GDP	C5-C6-N1	-3.23	119.02	123.43
5	A	501	GTP	C6-N1-C2	3.22	121.05	115.93
8	B	501	GDP	C1'-N9-C4	-3.16	121.08	126.64
10	B	504	8WE	C12-C11-C10	-3.15	107.28	113.24
5	C	501	GTP	C1'-N9-C4	-3.07	121.25	126.64
10	B	504	8WE	O1'-C1'-N20	-3.06	118.31	122.35
5	C	501	GTP	C6-N1-C2	3.05	120.78	115.93
5	C	501	GTP	C5-C6-N1	-3.05	119.26	123.43
10	B	504	8WE	C5-C6-C7	-3.05	109.07	115.94
8	D	501	GDP	C4-C5-N7	-2.91	106.36	109.40
5	A	501	GTP	C2-N3-C4	2.90	118.66	115.36
5	C	501	GTP	C6-C5-C4	-2.83	118.10	120.80
13	D	504	ZPN	C12-C13-C22	-2.67	120.07	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	8WE	O19-C1-O1	-2.66	117.27	123.70
10	B	504	8WE	C4-C3-C2	2.66	120.59	113.36
8	D	501	GDP	PA-O3A-PB	-2.51	124.22	132.83
14	F	701	ACP	N6-C6-N1	2.50	123.77	118.57
10	B	504	8WE	C21-C5-C6	2.45	116.96	110.00
9	B	503	8WB	CAI-CAH-CAG	2.38	131.97	129.34
14	F	701	ACP	O3G-PG-C3B	2.38	112.16	106.40
10	B	504	8WE	C3-C2-C1	2.36	122.19	113.62
13	D	504	ZPN	C3'-C4'-C5'	-2.35	120.25	124.69
5	C	501	GTP	C5'-C4'-C3'	-2.29	106.60	115.18
10	B	504	8WE	C3-C4-C5	2.28	123.27	115.92
13	D	504	ZPN	O19-C1-O1	-2.26	119.67	123.35
10	B	504	8WE	O1'-C1'-C2'	2.21	128.07	123.03
8	D	501	GDP	O2B-PB-O3A	2.19	111.97	104.64
5	A	501	GTP	C1'-N9-C4	-2.13	122.90	126.64
8	B	501	GDP	O3'-C3'-C4'	-2.11	104.93	111.05
5	A	501	GTP	N2-C2-N1	2.10	120.52	117.25
13	D	504	ZPN	O1'-C1'-N20	-2.09	119.60	122.35
14	F	701	ACP	PA-O3A-PB	-2.04	126.10	132.56
5	C	501	GTP	PB-O3B-PG	-2.01	125.94	132.83

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	504	8WE	C21-C5-C6-C7
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
11	B	505	GOL	O1-C1-C2-C3
14	F	701	ACP	PG-C3B-PB-O1B
14	F	701	ACP	PG-C3B-PB-O2B
14	F	701	ACP	PG-C3B-PB-O3A
12	B	506	MES	C7-C8-S-O3S
11	B	505	GOL	C1-C2-C3-O3
10	B	504	8WE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	B	504	8WE	C3-C4-C5-C6
10	B	504	8WE	C3-C4-C5-C21
11	B	505	GOL	O1-C1-C2-O2
12	B	506	MES	C8-C7-N4-C3
12	B	506	MES	C8-C7-N4-C5
9	D	503	8WB	CAC-CAB-OAQ-CAR
14	F	701	ACP	O4'-C4'-C5'-O5'
10	B	504	8WE	O1-C1-O19-C19
13	D	504	ZPN	C11-C10-C9-C8
12	B	506	MES	C7-C8-S-O1S
12	B	506	MES	C7-C8-S-O2S
10	B	504	8WE	O7-C7-C8-C9
10	B	504	8WE	C5-C6-C7-O7
9	D	503	8WB	CAA-CAB-OAQ-CAR
5	C	501	GTP	C4'-C5'-O5'-PA
8	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
8	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	504	8WE	C11-C10-C9-C8
8	B	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O3G
10	B	504	8WE	C17-C18-C19-C20
13	D	504	ZPN	C17-C18-C19-C20
8	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
13	D	504	ZPN	O7-C7-C8-C9
5	A	501	GTP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O1A
10	B	504	8WE	C4-C5-C6-C7
14	F	701	ACP	C5'-O5'-PA-O1A
10	B	504	8WE	C9-C10-C11-O11

There are no ring outliers.

6 monomers are involved in 16 short contacts:

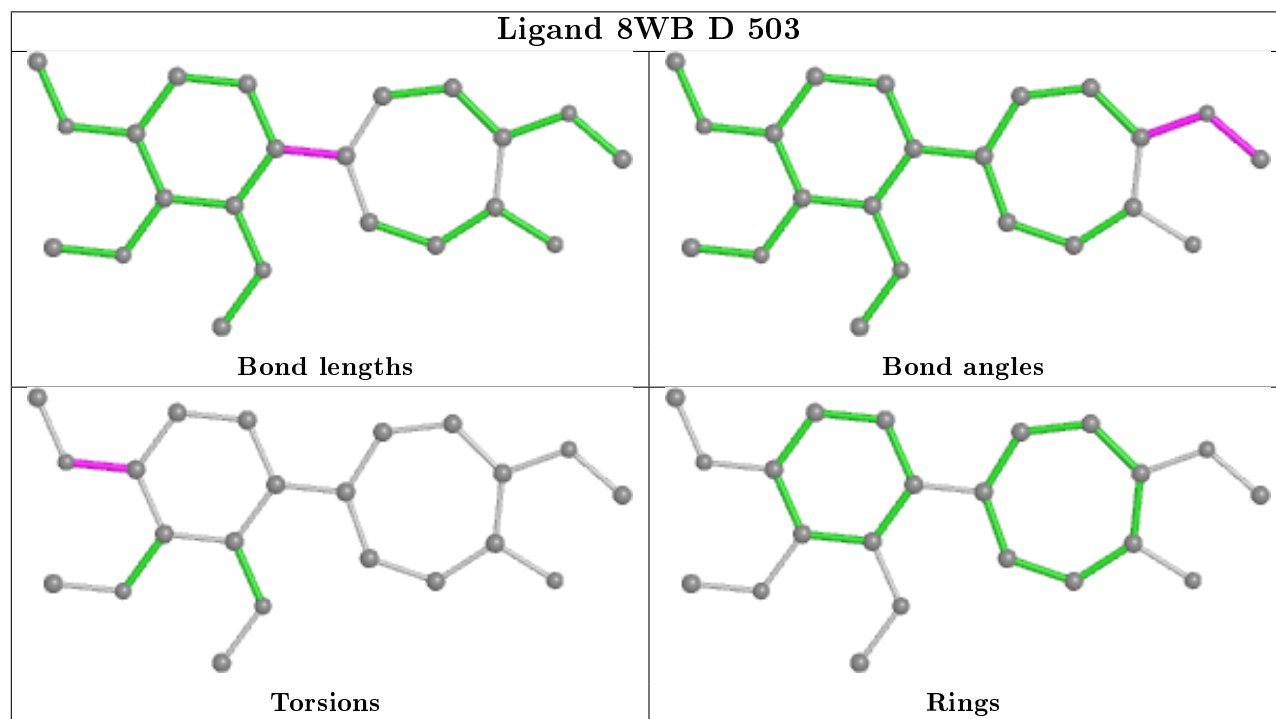
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	506	MES	1	0
9	D	503	8WB	7	0
9	B	503	8WB	3	0

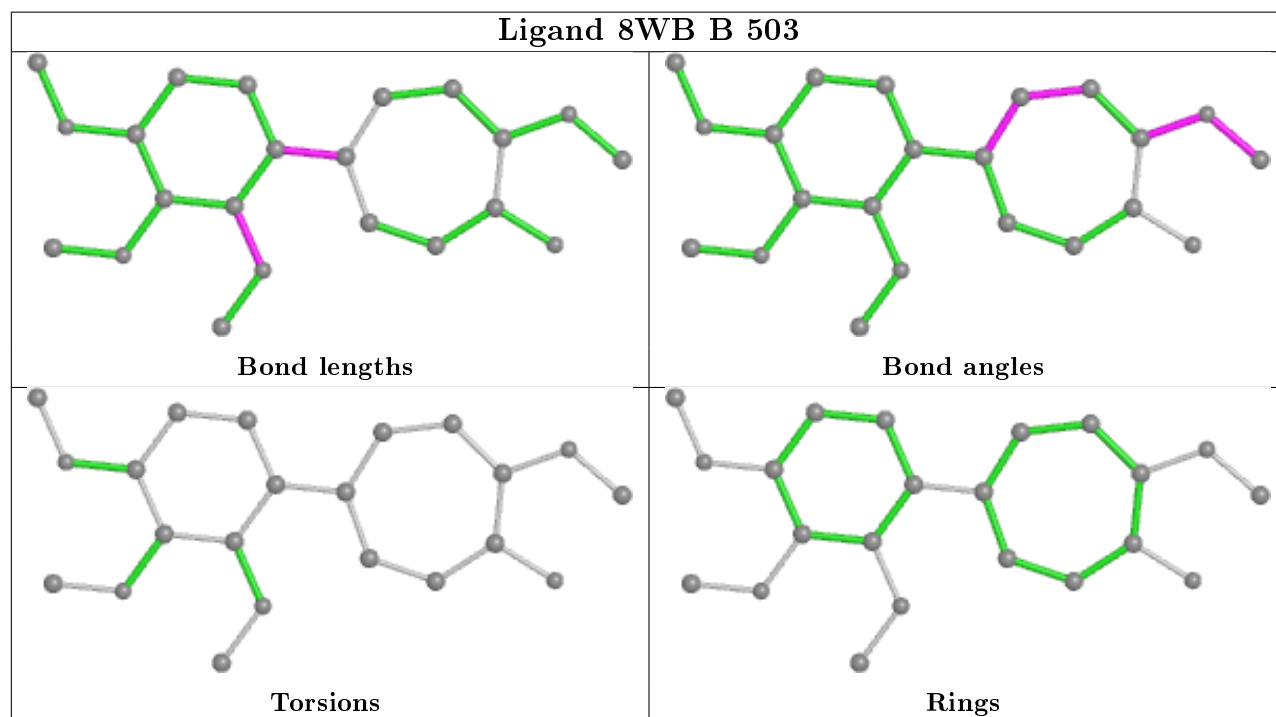
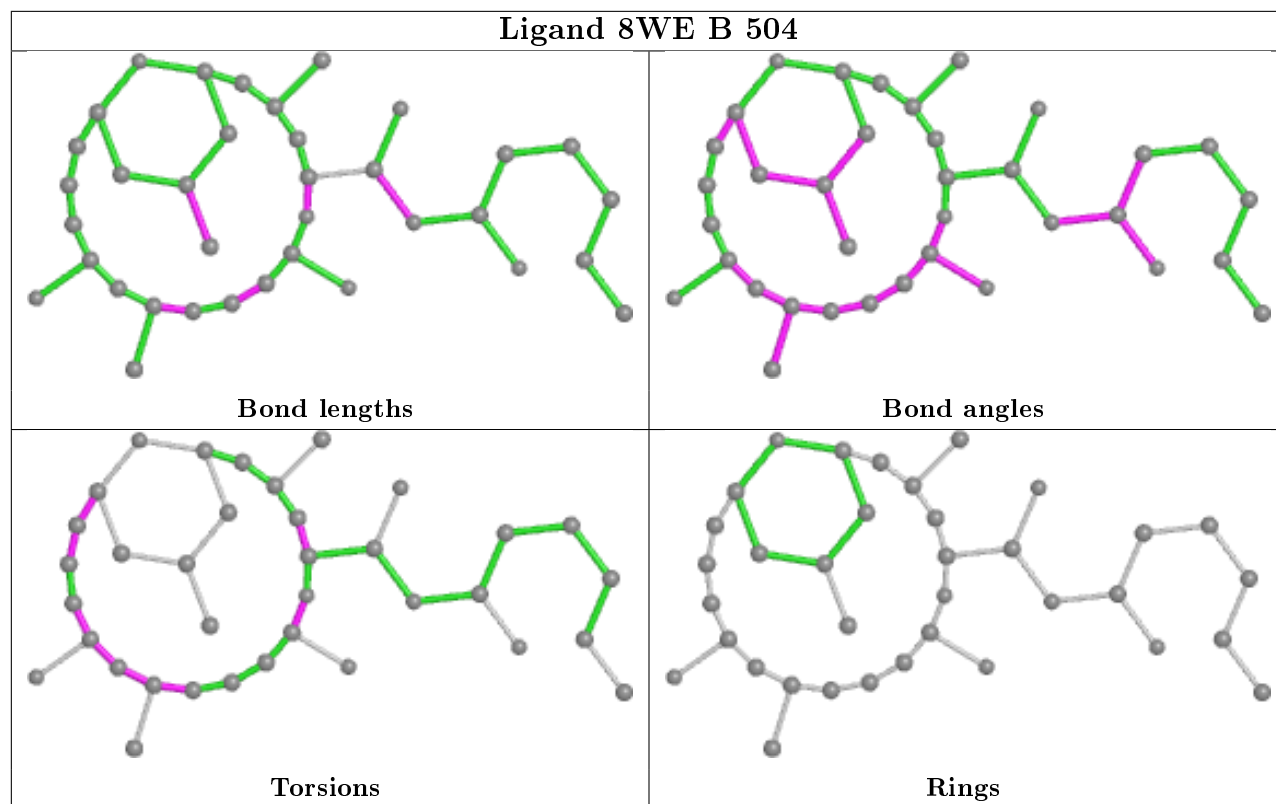
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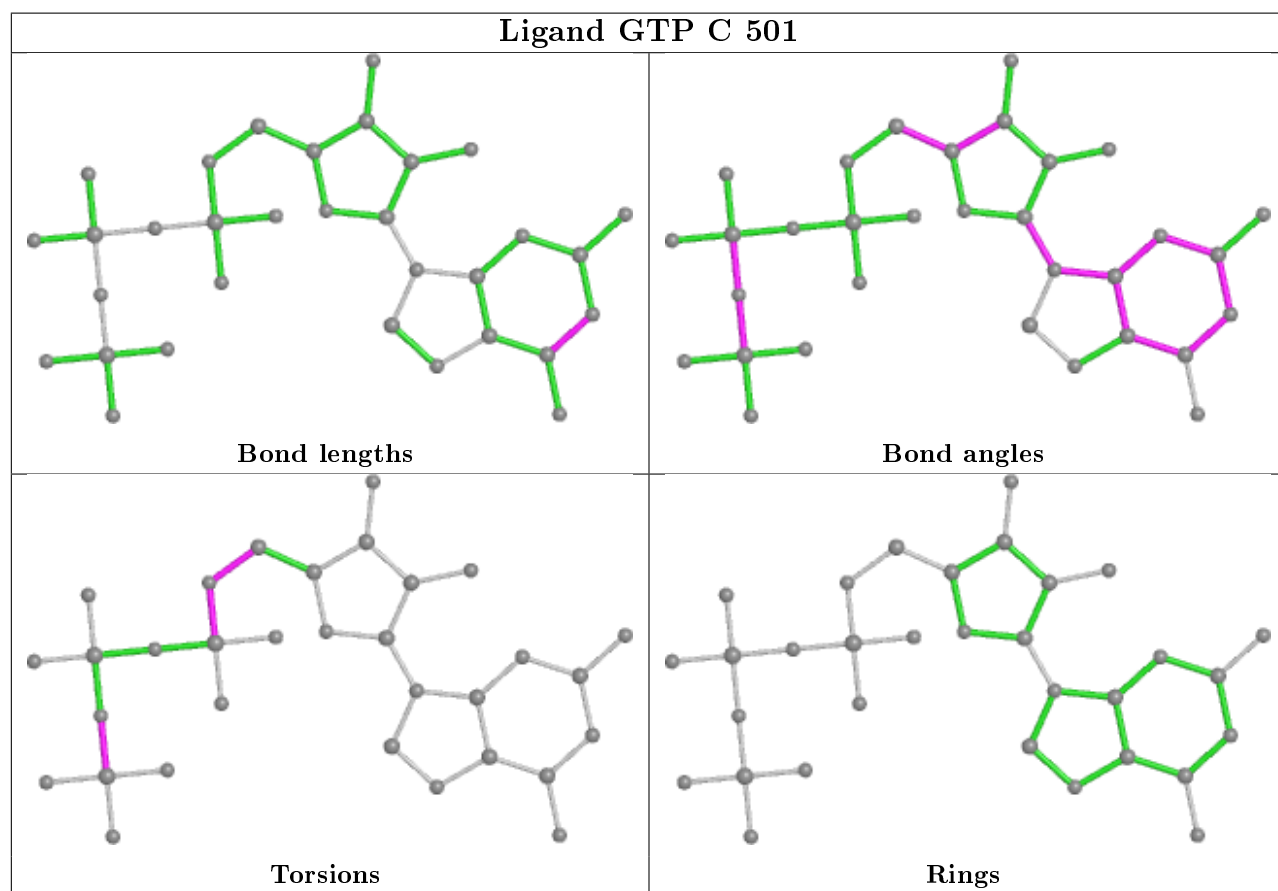
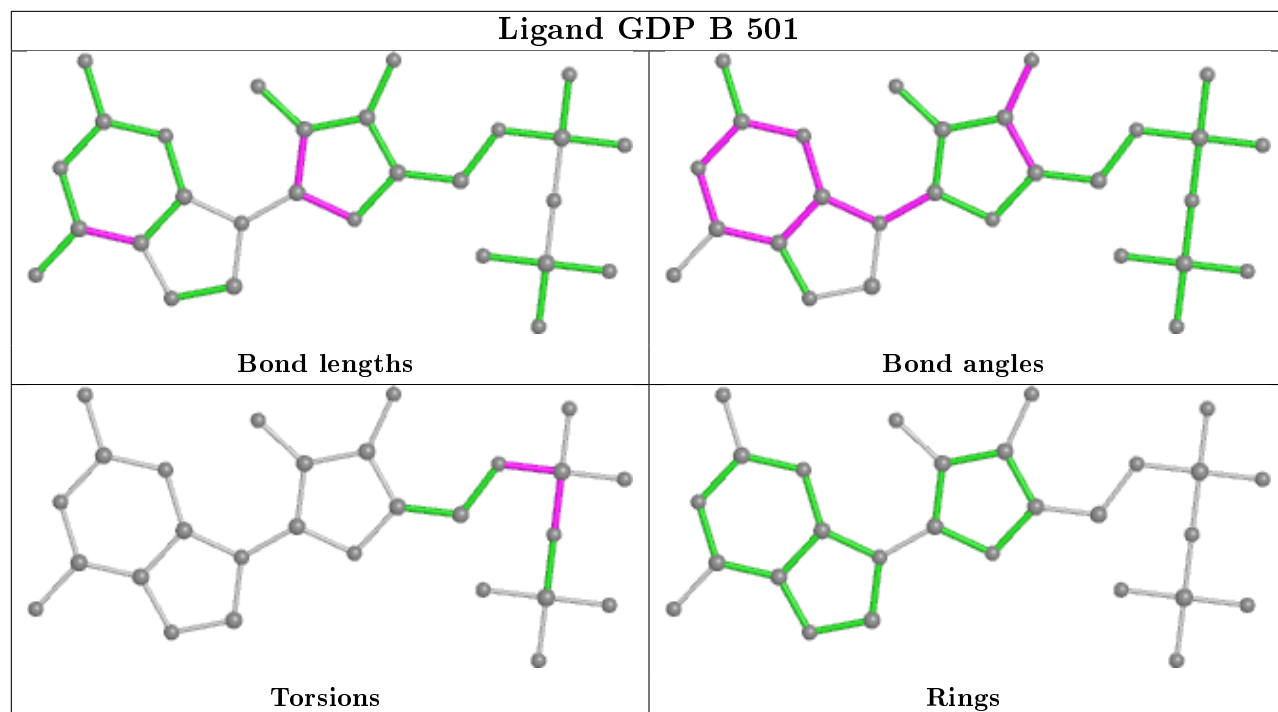
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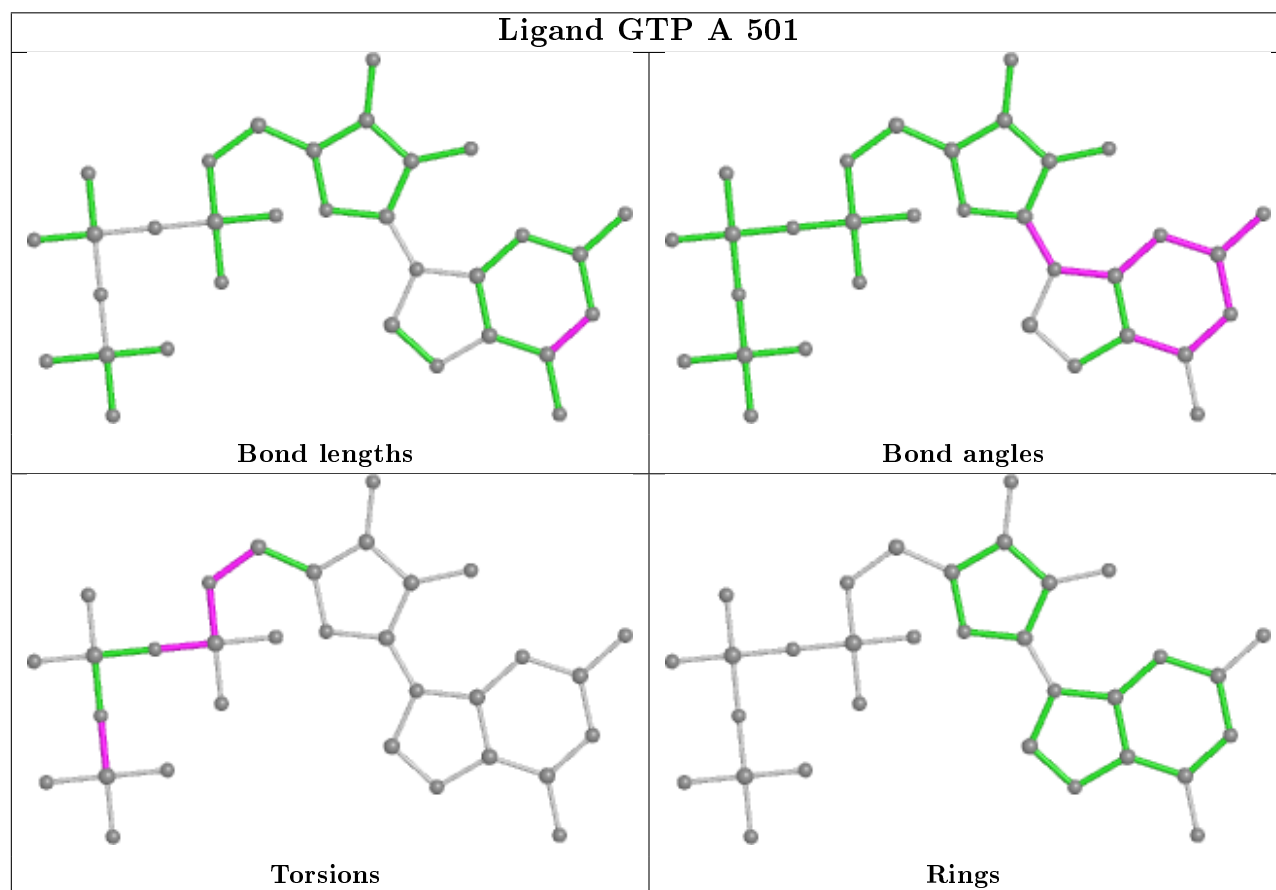
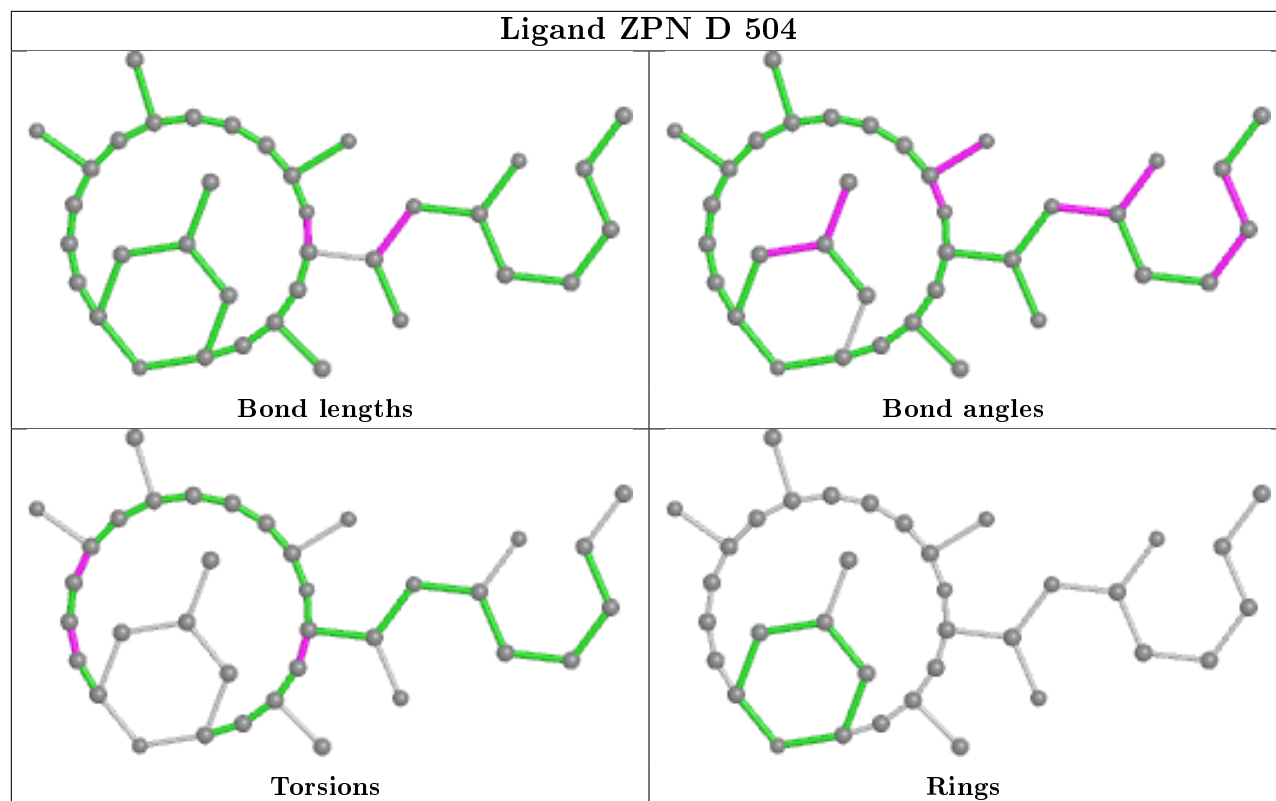
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	504	ZPN	2	0
8	D	501	GDP	1	0
14	F	701	ACP	2	0

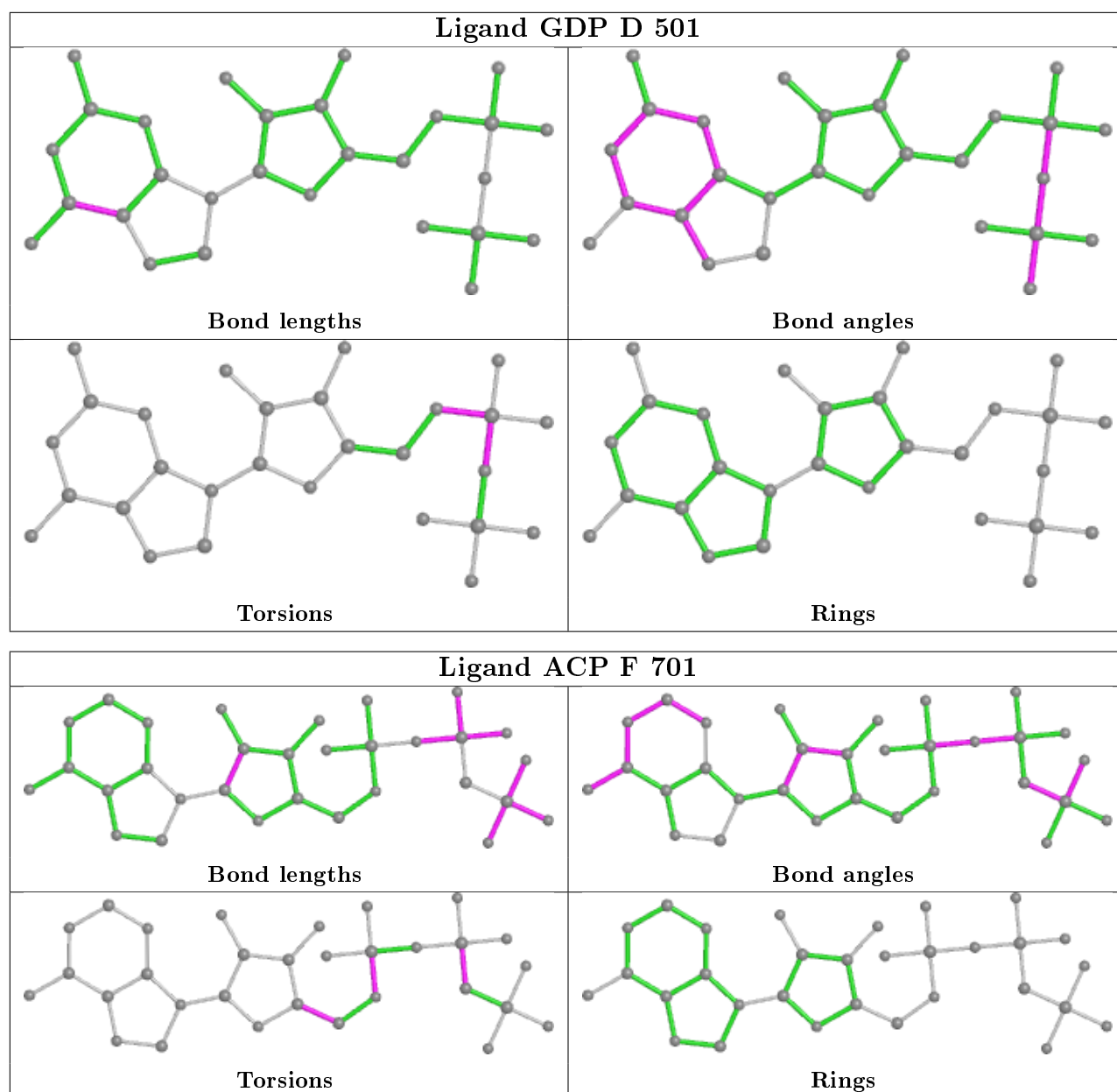
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/451 (97%)	0.04	15 (3%) 45 43	35, 51, 85, 144	0
1	C	440/451 (97%)	-0.19	7 (1%) 72 70	29, 42, 70, 118	0
2	B	420/445 (94%)	-0.07	15 (3%) 42 41	28, 52, 95, 133	2 (0%)
2	D	431/445 (96%)	0.08	21 (4%) 29 28	36, 57, 92, 127	6 (1%)
3	E	123/143 (86%)	0.10	10 (8%) 12 10	38, 66, 104, 138	0
4	F	353/384 (91%)	0.74	79 (22%) 0 0	43, 73, 139, 163	0
All	All	2207/2319 (95%)	0.09	147 (6%) 17 16	28, 54, 103, 163	8 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	8.4
4	F	105	LEU	8.3
1	A	440	VAL	7.3
4	F	249	TYR	6.6
4	F	244	CYS	6.6
4	F	103	THR	6.2
4	F	231	ALA	6.0
4	F	173	ILE	5.9
4	F	104	ASN	5.5
1	A	439	SER	5.5
4	F	253	TYR	5.4
2	D	57	THR	5.3
4	F	243	HIS	5.1
4	F	258	GLU	4.8
4	F	130	VAL	4.7
4	F	248	GLU	4.7
2	D	247	GLN	4.7
4	F	252	ASN	4.6
2	B	57	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	4.6
4	F	129	GLU	4.6
3	E	26	PRO	4.6
3	E	27	PRO	4.5
4	F	142	ARG	4.3
2	B	59	ASN	4.3
4	F	177	GLY	4.3
1	C	340	SER	4.3
4	F	236	LYS	4.2
4	F	251	LYS	4.1
4	F	361	LEU	4.0
4	F	143	GLU	4.0
2	D	179	ASP	4.0
4	F	132	LEU	3.8
4	F	240	LEU	3.8
4	F	25	GLY	3.7
1	C	178	SER	3.7
4	F	133	ALA	3.7
2	D	58	GLY	3.6
4	F	362	ALA	3.6
2	D	248	LEU	3.6
4	F	250	SER	3.5
4	F	254	GLY	3.5
4	F	170	LEU	3.5
4	F	166	ALA	3.5
4	F	372	THR	3.5
4	F	225	SER	3.5
4	F	21	LEU	3.5
4	F	255	ARG	3.5
3	E	7	GLU	3.5
4	F	256	TYR	3.4
4	F	157	GLY	3.4
3	E	24	LEU	3.4
4	F	31	ARG	3.3
4	F	167	SER	3.3
3	E	139	LEU	3.3
2	D	82	PRO	3.3
4	F	371	PRO	3.3
4	F	233	PHE	3.3
1	C	180	ALA	3.3
2	D	400	ARG	3.3
1	C	179	THR	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	234	GLN	3.2
4	F	20	LEU	3.1
4	F	194	PRO	3.1
4	F	176	GLN	3.1
4	F	27	TRP	3.1
4	F	136	ASN	3.1
4	F	144	GLY	3.0
3	E	28	SER	3.0
4	F	340	GLN	3.0
4	F	101	TYR	2.9
2	D	246	GLY	2.9
4	F	102	PRO	2.9
2	B	248	LEU	2.9
4	F	17	VAL	2.9
4	F	238	CYS	2.9
2	D	317	ALA	2.9
4	F	182	ILE	2.8
4	F	24	THR	2.8
2	B	438	ALA	2.8
2	B	61	TYR	2.8
3	E	142	GLU	2.8
4	F	169	LEU	2.7
4	F	227	PRO	2.7
1	C	440	VAL	2.7
3	E	25	LYS	2.7
4	F	152	SER	2.7
4	F	241	THR	2.7
1	A	281	ALA	2.7
1	A	346	TRP	2.6
4	F	23	ALA	2.6
4	F	100	ILE	2.6
2	D	268	PHE	2.6
2	B	37	HIS	2.6
2	B	36	TYR	2.5
4	F	135	TYR	2.5
2	D	249	ASN	2.5
4	F	259	GLY	2.5
4	F	197	ARG	2.5
1	A	179	THR	2.5
1	A	170	SER	2.4
2	D	403	ALA	2.4
4	F	174	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	22	LEU	2.4
2	D	260	VAL	2.4
2	D	1	MET	2.4
4	F	178	GLN	2.4
3	E	141	GLU	2.4
2	B	39	ASP	2.3
1	A	171	ILE	2.3
1	C	238	ILE	2.3
4	F	171	ASP	2.3
1	A	345	ASP	2.3
2	B	437	ASP	2.3
4	F	161	LEU	2.3
2	B	38	GLY	2.3
2	B	82	PRO	2.3
2	D	56	ALA	2.3
2	D	269[A]	MET	2.3
4	F	260	ASN	2.2
1	A	364	PRO	2.2
2	D	401	ARG	2.2
4	F	239	HIS	2.2
2	D	415	GLU	2.2
4	F	125	THR	2.2
4	F	343	TYR	2.2
4	F	246	GLN	2.2
2	B	34	GLY	2.2
4	F	245	ILE	2.2
1	A	140	SER	2.1
2	B	35	SER	2.1
1	A	44	GLY	2.1
4	F	242	ASN	2.1
4	F	1	MET	2.1
2	D	37	HIS	2.1
4	F	232	ASN	2.1
4	F	342	LEU	2.1
1	A	283	HIS	2.1
2	B	56	ALA	2.1
4	F	257	GLU	2.1
1	A	177	VAL	2.1
2	D	79	ARG	2.0
2	D	127	GLU	2.0
1	A	178	SER	2.0
2	B	338	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	10	ASN	2.0
1	C	253	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

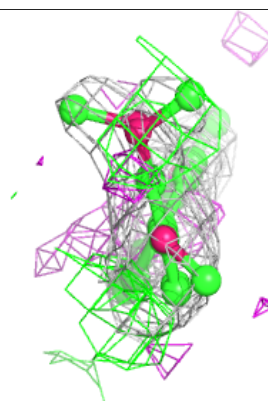
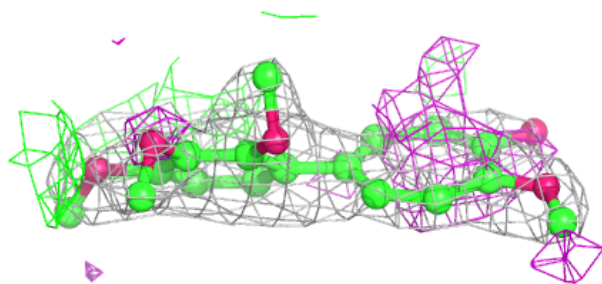
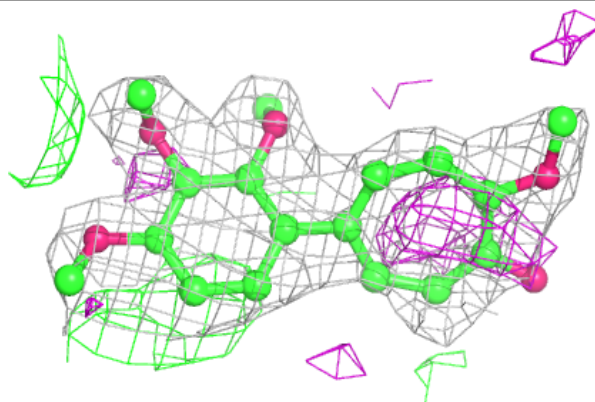
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	8WB	D	503	22/22	0.77	0.30	46,55,64,66	22
7	CA	A	503	1/1	0.82	0.37	191,191,191,191	0
12	MES	B	506	12/12	0.92	0.14	44,60,72,73	0
14	ACP	F	701	31/31	0.92	0.11	59,70,107,113	0
10	8WE	B	504	36/36	0.93	0.17	45,64,78,85	0
11	GOL	B	505	6/6	0.93	0.26	51,70,77,77	0
6	MG	D	502	1/1	0.93	0.05	55,55,55,55	0
9	8WB	B	503	22/22	0.94	0.14	42,58,65,70	0
6	MG	B	502	1/1	0.95	0.26	35,35,35,35	0
13	ZPN	D	504	36/36	0.95	0.12	39,58,80,91	0
6	MG	F	702	1/1	0.95	0.12	61,61,61,61	0
6	MG	A	502	1/1	0.96	0.17	36,36,36,36	0
6	MG	C	502	1/1	0.98	0.15	34,34,34,34	0
7	CA	C	503	1/1	0.98	0.08	63,63,63,63	0
5	GTP	A	501	32/32	0.98	0.18	31,39,45,49	0
8	GDP	D	501	28/28	0.98	0.09	40,51,60,64	0
5	GTP	C	501	32/32	0.99	0.15	29,34,37,44	0
8	GDP	B	501	28/28	0.99	0.16	31,36,40,40	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.

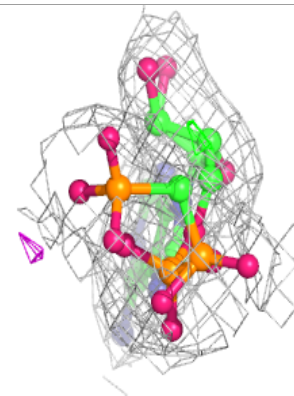
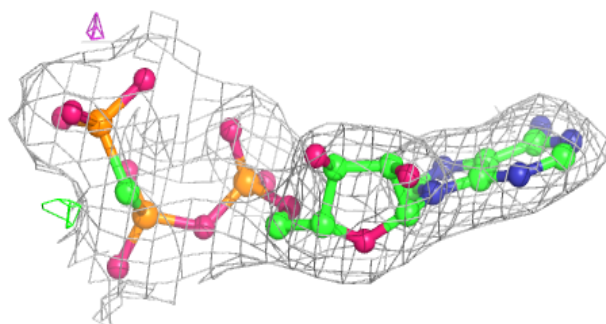
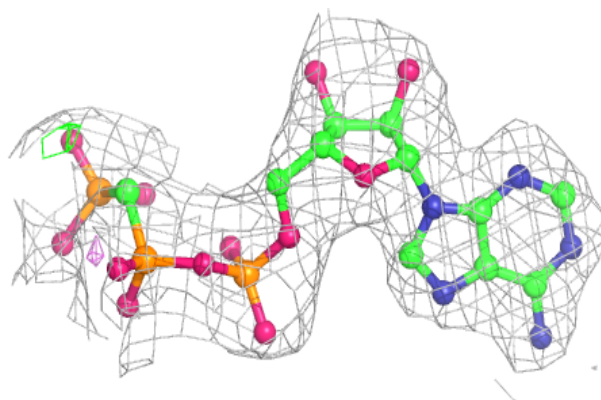
Electron density around 8WB D 503:

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



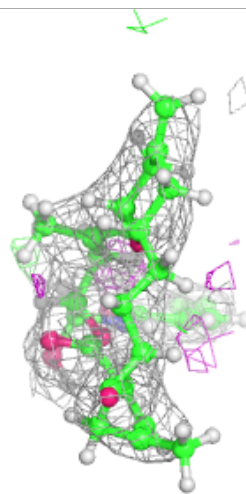
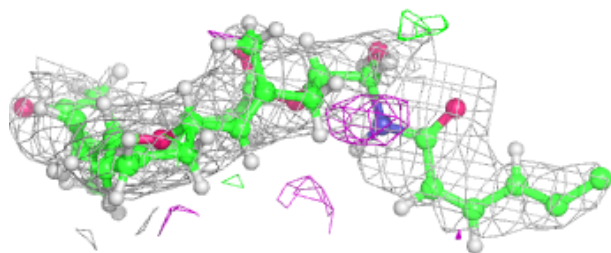
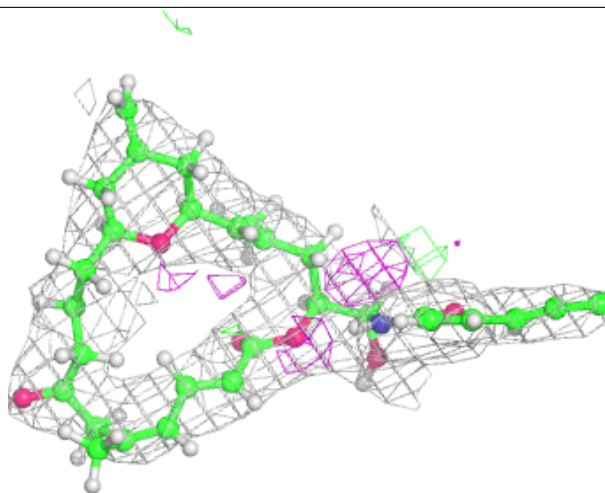
Electron density around ACP F 701:

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



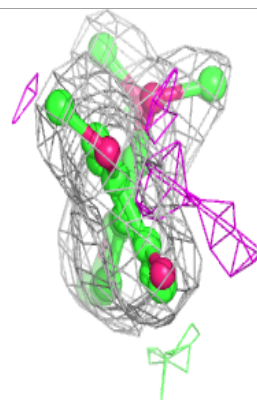
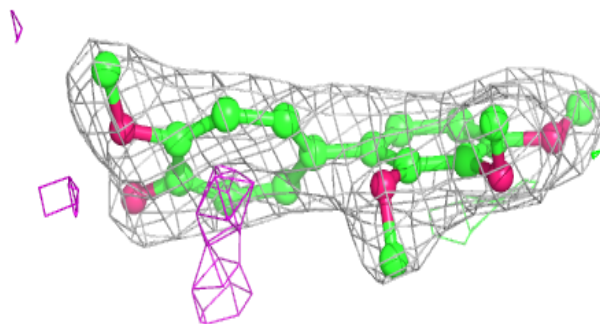
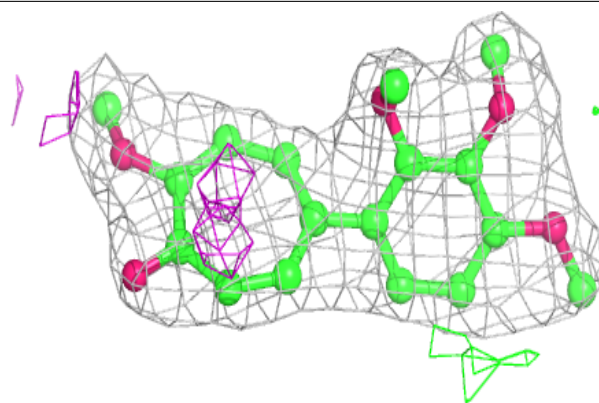
Electron density around 8WE B 504:

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

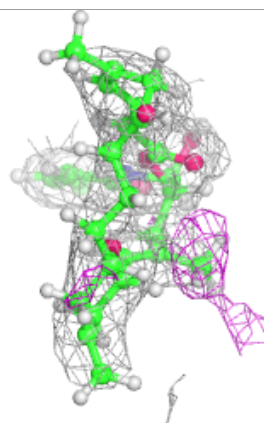
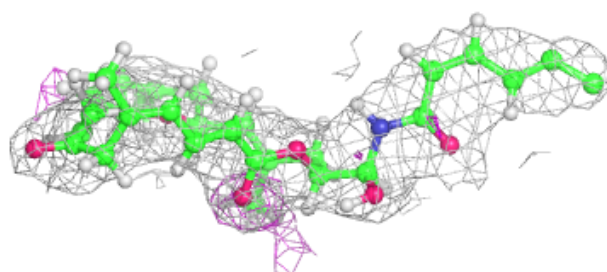
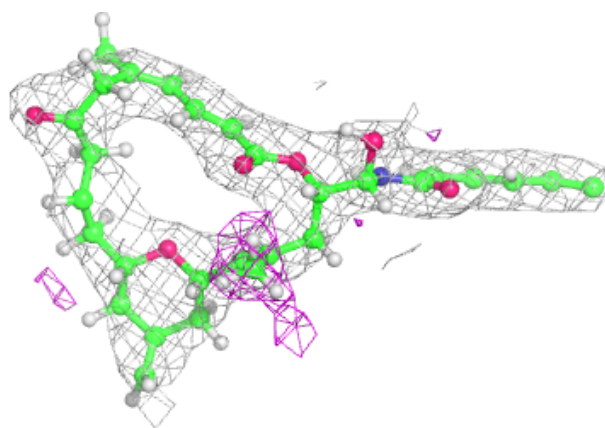


Electron density around 8WB B 503:

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

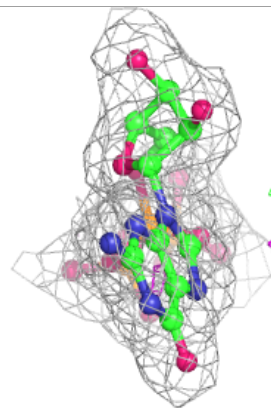
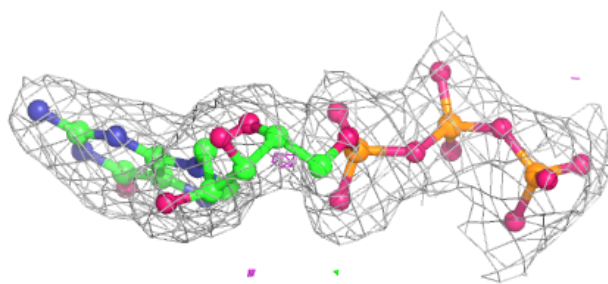
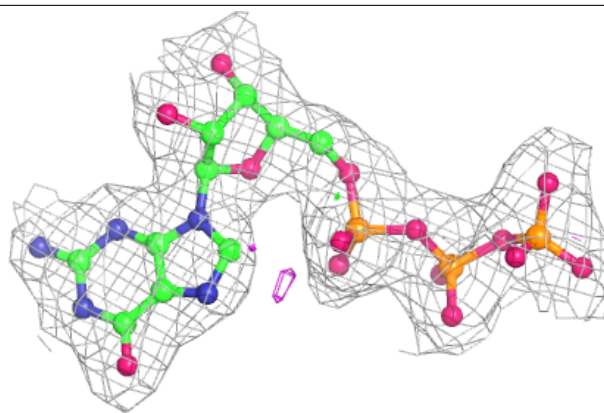
**Electron density around ZPN D 504:**

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



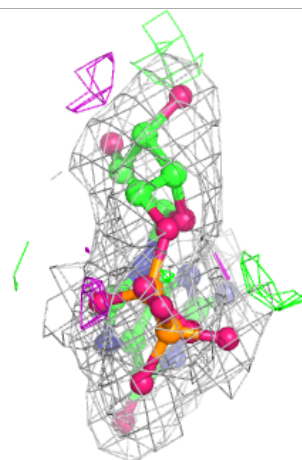
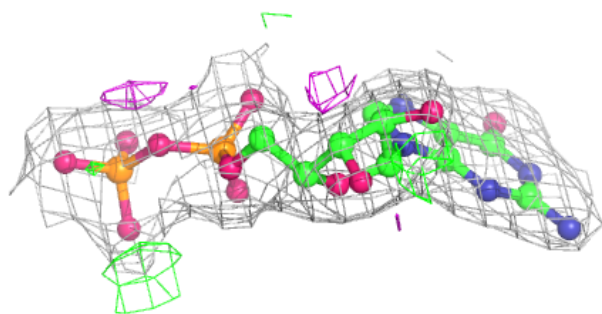
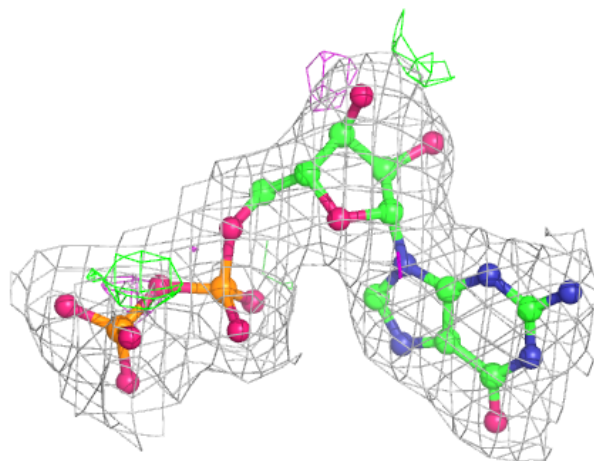
Electron density around GTP A 501:

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



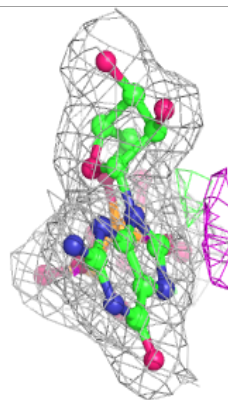
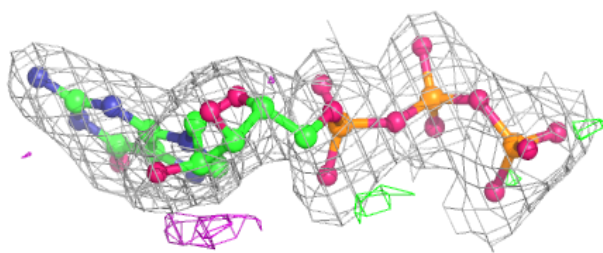
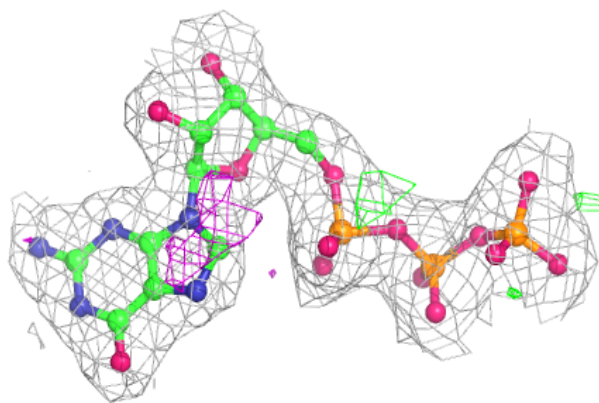
Electron density around GDP D 501:

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

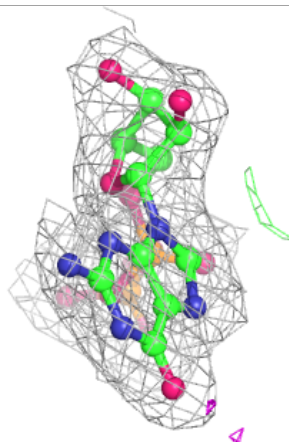
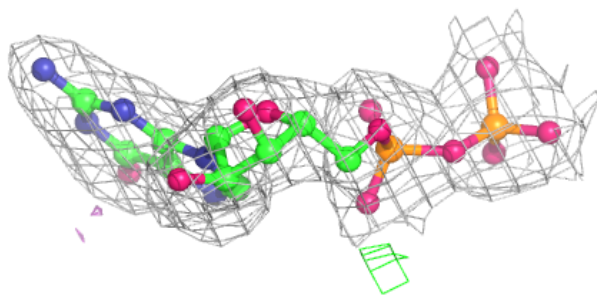
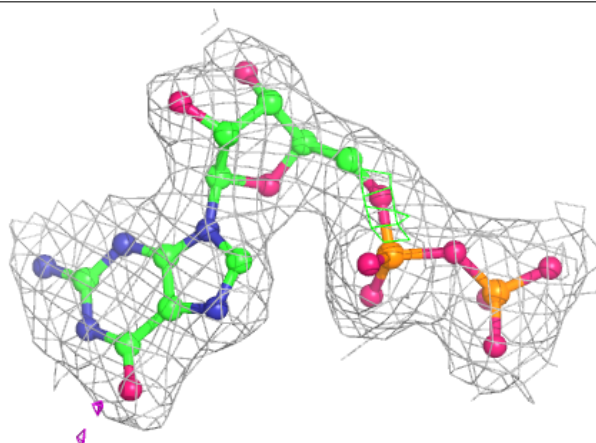


Electron density around GTP C 501:

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

**Electron density around 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.