



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:29 PM BST

PDB ID : 4O4I
Title : Tubulin-Laulimalide-Epothilone A complex
Authors : Prota, A.E.; Bargsten, K.; Northcote, P.T.; Marsh, M.; Altmann, K.H.; Miller, J.H.; Diaz, J.F.; Steinmetz, M.O.
Deposited on : 2013-12-18
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

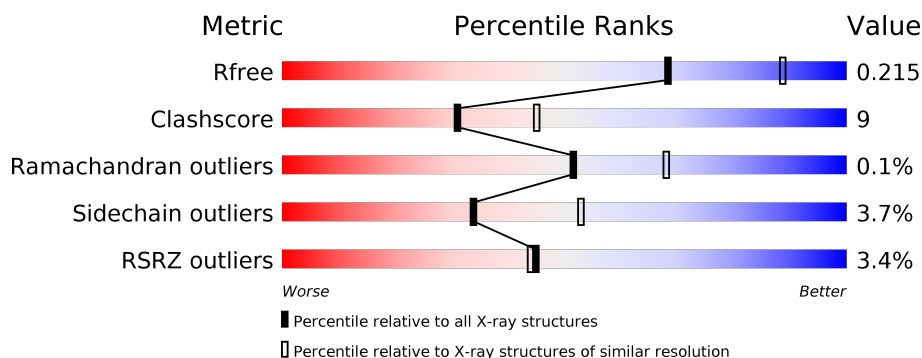
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>76%</div> <div>20%</div> <div>.</div> </div>
1	C	451	<div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	B	445	<div> <div>2%</div> <div>72%</div> <div>22%</div> <div>..</div> </div>
2	D	445	<div> <div>%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
3	E	143	<div> <div>%</div> <div>52%</div> <div>27%</div> <div>5%</div> <div>15%</div> </div>
4	F	384	<div> <div>16%</div> <div>76%</div> <div>14%</div> <div>.</div> <div>9%</div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18304 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	1	0
			3440	2177	584	656	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	1	0
			3372	2117	577	651	27			
2	D	431	Total	C	N	O	S	0	1	0
			3381	2120	579	654	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1013	625	184	199	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	CLONING ARTIFACT	UNP P63043
E	4	ALA	SER	CLONING ARTIFACT	UNP P63043

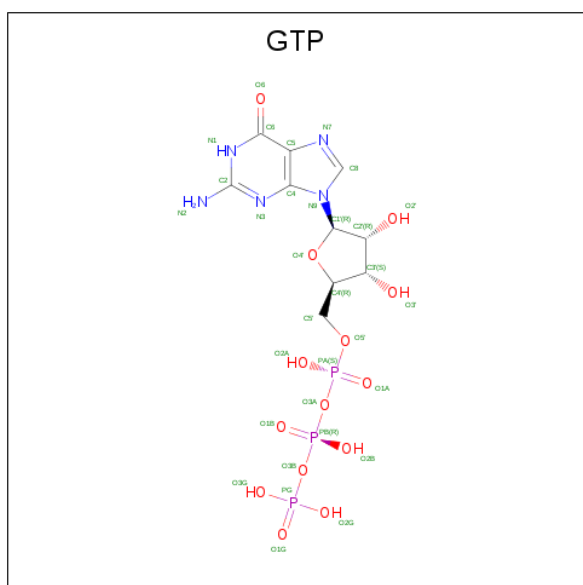
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	0	8	0
			2898	1867	490	527	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	2	Total	Mg	0	0
			2	2		
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		

Continued on next page...

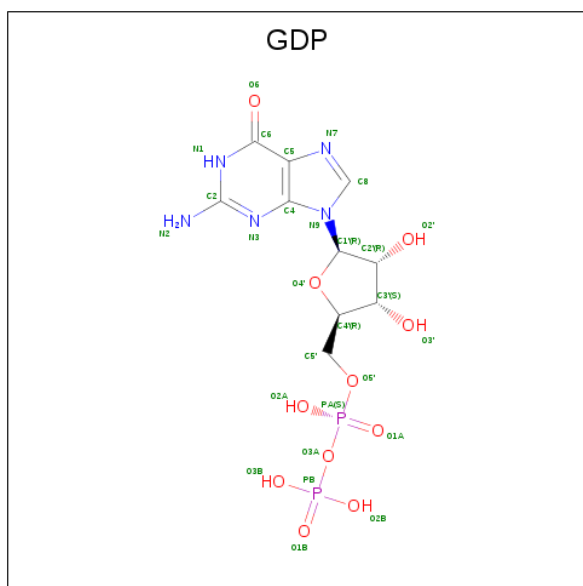
Continued from previous page...

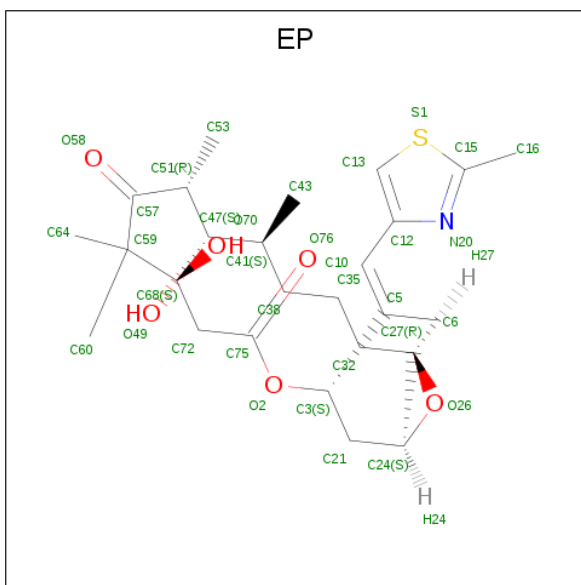
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

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

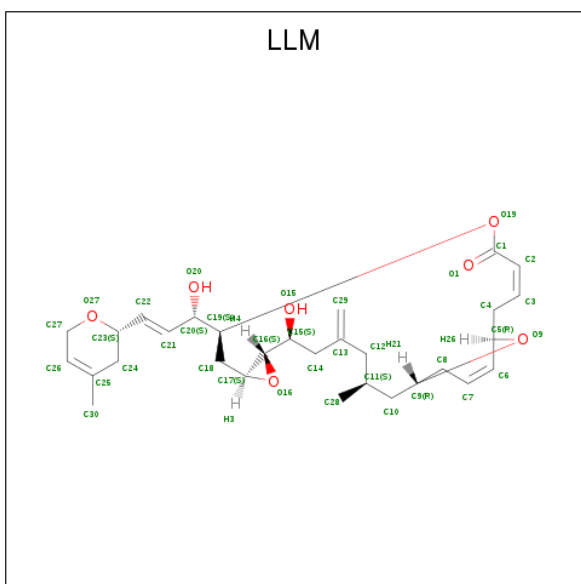
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			34	26	1	6	1		
9	D	1	Total	C	N	O	S	0	0
			34	26	1	6	1		

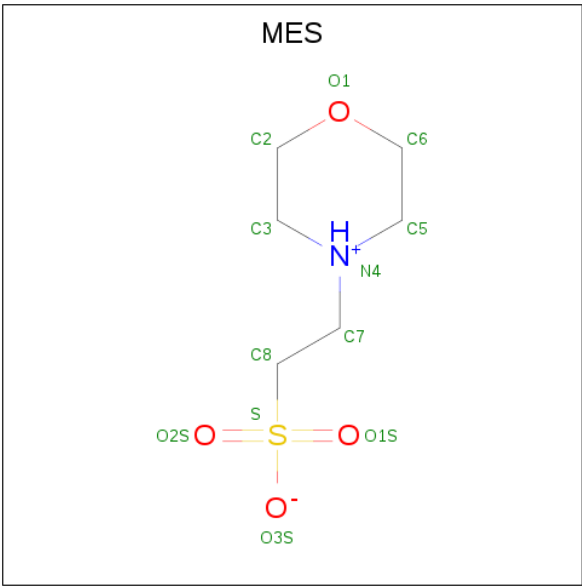
- Molecule 10 is Laulimalide (three-letter code: LLM) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	5	0
			37	30	7		

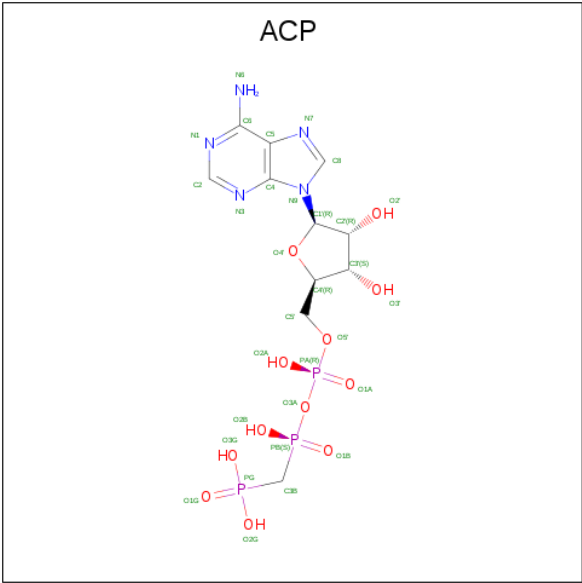
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: C₆H₁₃NO₄S).



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



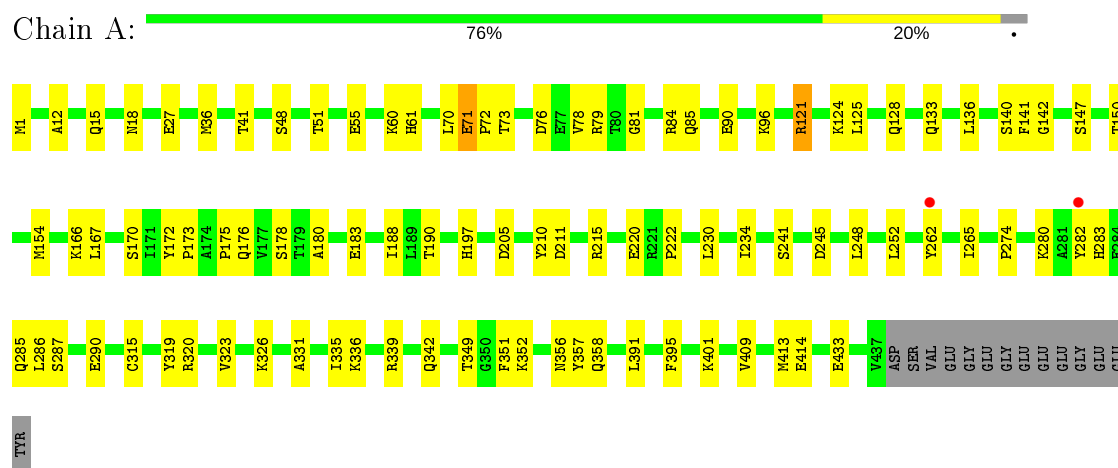
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	112	Total 112	O 112	0	0
13	B	90	Total 90	O 90	0	0
13	C	161	Total 161	O 161	0	0
13	D	63	Total 63	O 63	0	0
13	E	34	Total 34	O 34	0	0
13	F	47	Total 47	O 47	0	0

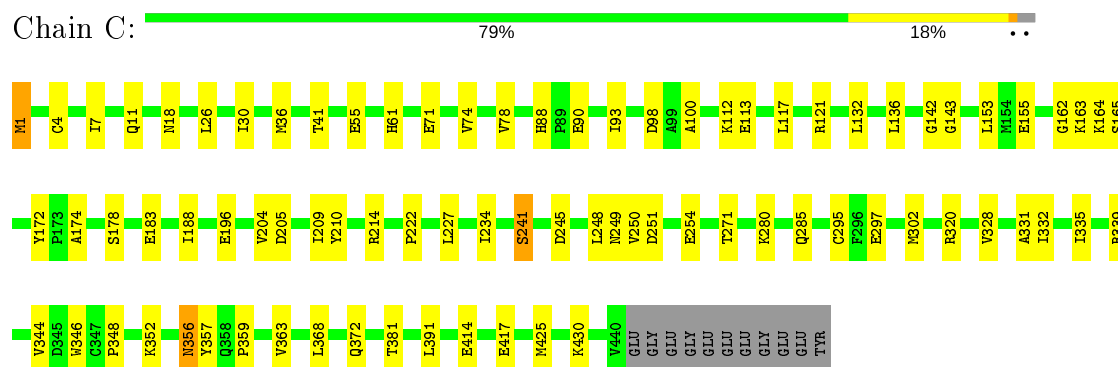
3 Residue-property plots

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

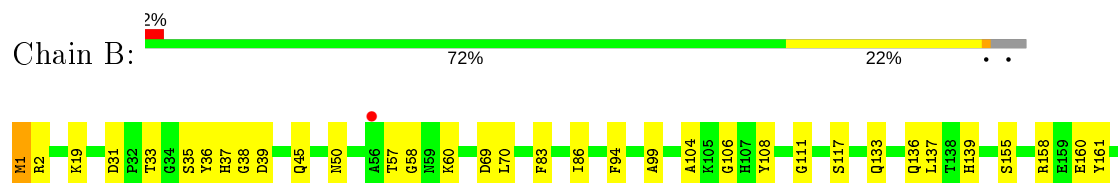
• Molecule 1: Tubulin alpha-1B chain

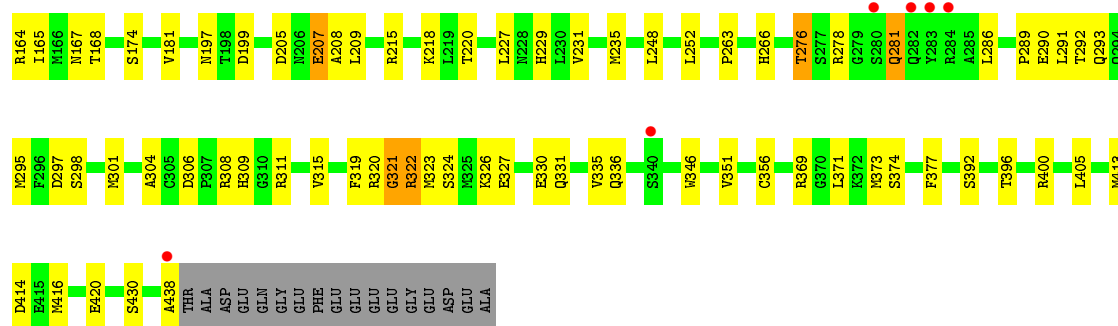


• Molecule 1: Tubulin alpha-1B chain

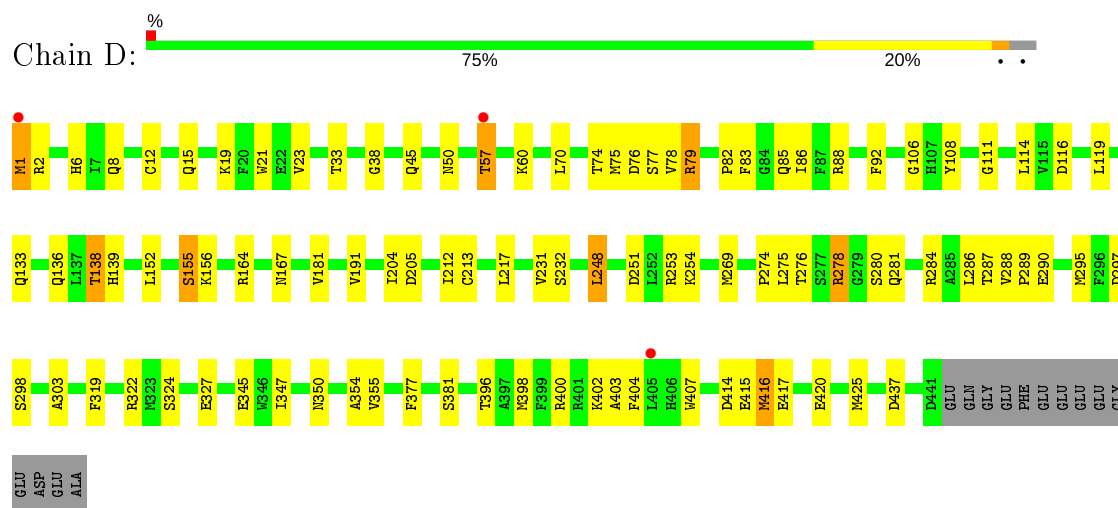


• Molecule 2: Tubulin beta-2B chain

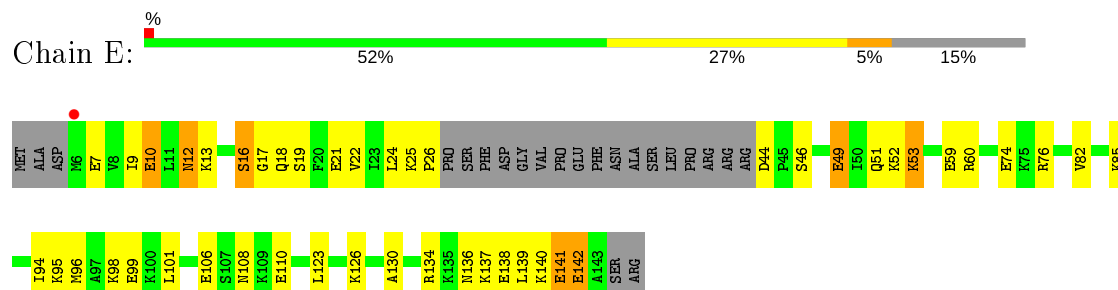




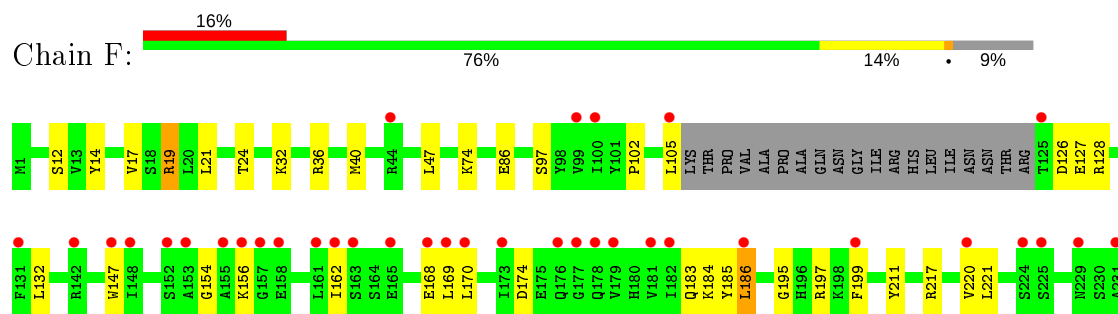
• Molecule 2: Tubulin beta-2B chain

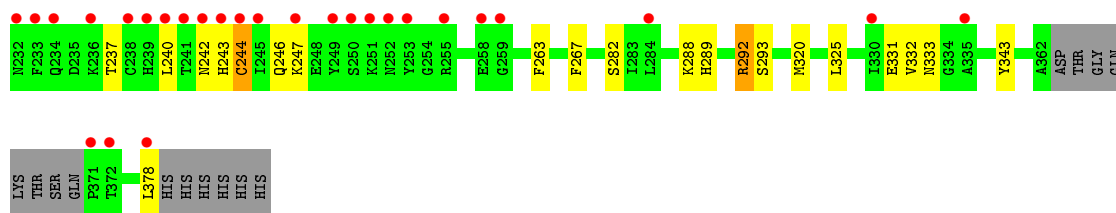


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.20Å 158.03Å 180.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.21 – 2.40 78.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (52.21-2.40) 99.7 (78.78-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.188 , 0.214 0.189 , 0.215	Depositor DCC
R_{free} test set	5886 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18304	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/3494	0.49	0/4743
1	C	0.36	0/3521	0.56	1/4780 (0.0%)
2	B	0.33	0/3450	0.50	0/4672
2	D	0.33	0/3458	0.54	0/4684
3	E	0.32	0/1027	0.46	0/1362
4	F	0.31	0/2985	0.51	0/4032
All	All	0.33	0/17935	0.52	1/24273 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	LEU	CA-CB-CG	-5.00	103.80	115.30

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	3416	0	3331	60	0
1	C	3440	0	3354	53	0
2	B	3372	0	3255	76	0
2	D	3381	0	3258	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1013	0	1030	39	0
4	F	2898	0	2914	41	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	2	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	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	34	0	39	6	0
9	D	34	0	39	1	0
10	B	37	0	42	4	0
11	B	12	0	12	3	0
12	F	31	0	14	4	0
13	A	112	0	0	4	0
13	B	90	0	0	6	0
13	C	161	0	0	10	0
13	D	63	0	0	6	0
13	E	34	0	0	6	0
13	F	47	0	0	4	0
All	All	18304	0	17336	319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (319) 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)
4:F:184:LYS:NZ	4:F:185:TYR:O	2.01	0.94
2:B:276:THR:OG1	9:B:503:EP:N20	2.00	0.92
4:F:74:LYS:NZ	4:F:331:GLU:OE2	2.02	0.92
1:C:163:LYS:NZ	13:C:749:HOH:O	2.03	0.91
3:E:10:GLU:O	3:E:12:ASN:ND2	2.03	0.91
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.04	0.89
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.95	0.85
2:D:33:THR:O	2:D:60:LYS:NZ	2.10	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.58	0.84
2:B:36:TYR:O	2:B:37:HIS:ND1	2.11	0.83
2:B:311:ARG:NH1	13:B:602:HOH:O	2.10	0.82
4:F:21:LEU:O	4:F:24:THR:OG1	1.98	0.81
3:E:130:ALA:HB1	3:E:134:ARG:HH12	1.44	0.81
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.13	0.80
2:B:164:ARG:NH1	13:B:689:HOH:O	2.14	0.80
1:C:280:LYS:NZ	13:C:756:HOH:O	2.15	0.79
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.17	0.78
3:E:9:ILE:HG22	3:E:10:GLU:HG2	1.64	0.78
1:A:356:ASN:ND2	13:A:692:HOH:O	2.17	0.77
4:F:331:GLU:OE1	12:F:500:ACP:O2G	2.03	0.77
3:E:46:SER:OG	3:E:49:GLU:OE1	2.03	0.76
2:D:402:LYS:NZ	2:D:415:GLU:OE1	2.13	0.76
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.04	0.75
1:A:280:LYS:HE2	1:A:283:HIS:HB3	1.69	0.73
2:D:181:VAL:O	13:D:657:HOH:O	2.05	0.73
2:B:1:MET:HB3	2:B:50:ASN:OD1	1.88	0.72
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.24	0.72
2:B:215:ARG:NH1	13:B:654:HOH:O	2.09	0.72
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.24	0.71
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.26	0.71
2:D:164:ARG:NH2	13:D:663:HOH:O	2.25	0.70
2:D:85:GLN:N	2:D:85:GLN:OE1	2.22	0.69
3:E:137:LYS:NZ	13:E:214:HOH:O	2.24	0.69
1:C:414:GLU:OE1	13:C:727:HOH:O	2.11	0.68
1:A:349:THR:OG1	13:A:663:HOH:O	2.11	0.68
4:F:168:GLU:OE2	13:F:625:HOH:O	2.11	0.68
2:B:276:THR:O	9:B:503:EP:H722	1.93	0.68
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.35	0.66
1:C:132:LEU:O	1:C:164:LYS:HE3	1.94	0.66
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.29	0.66
2:B:326:LYS:O	2:B:330:GLU:HG3	1.96	0.65
2:D:287:THR:HB	2:D:289:PRO:HD2	1.79	0.65
2:D:437:ASP:OD1	13:D:637:HOH:O	2.13	0.65
2:B:324:SER:HB3	2:B:327:GLU:HB2	1.79	0.64
4:F:86:GLU:O	13:F:621:HOH:O	2.15	0.64
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.07	0.63
3:E:137:LYS:HA	3:E:140:LYS:HD3	1.79	0.63
2:B:33:THR:OG1	2:B:35:SER:OG	2.14	0.63
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:407:TRP:NE1	13:D:618:HOH:O	2.30	0.63
1:A:81:GLY:O	1:A:84:ARG:HD3	1.99	0.62
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.65	0.62
1:A:287:SER:OG	1:A:290:GLU:HG3	2.00	0.62
4:F:292:ARG:HG2	4:F:292:ARG:HH11	1.66	0.61
1:A:133:GLN:OE1	1:A:252:LEU:N	2.26	0.61
2:B:286:LEU:HG	2:B:290:GLU:HB3	1.83	0.60
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.83	0.60
2:D:322:ARG:HG3	2:D:322:ARG:HH21	1.67	0.60
2:B:229:HIS:ND1	9:B:503:EP:H321	2.16	0.60
2:B:276:THR:HG22	2:B:281:GLN:HG3	1.82	0.60
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.36	0.60
2:B:276:THR:CG2	2:B:281:GLN:HG3	2.31	0.60
2:B:289:PRO:O	2:B:293:GLN:HG3	2.02	0.60
2:B:136:GLN:HA	2:B:167:ASN:O	2.01	0.59
2:D:1:MET:SD	2:D:1:MET:N	2.64	0.59
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.84	0.59
1:C:271:THR:HG21	1:C:295:CYS:O	2.03	0.58
2:D:74:THR:O	2:D:78:VAL:HG23	2.04	0.58
1:A:414:GLU:OE1	3:E:60:ARG:NH1	2.36	0.58
1:A:352:LYS:HG3	3:E:21:GLU:HG3	1.85	0.58
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.85	0.58
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.33	0.58
2:B:308:ARG:HD3	10:B:505:LLM:H34	1.86	0.57
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.86	0.57
2:B:320:ARG:O	2:B:374:SER:N	2.34	0.57
1:C:430:LYS:HE2	13:C:673:HOH:O	2.03	0.57
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.86	0.57
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.87	0.57
1:A:166:LYS:HE2	1:A:197:HIS:O	2.05	0.57
1:A:1:MET:HG2	1:A:51:THR:HG22	1.87	0.57
2:D:295:MET:CG	2:D:377:PHE:HB2	2.34	0.56
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.23	0.56
4:F:40:MET:HE1	4:F:47:LEU:HG	1.86	0.56
1:C:234:ILE:HG21	1:C:302:MET:SD	2.45	0.56
2:B:321:GLY:HA2	2:B:356:CYS:O	2.06	0.56
2:B:297:ASP:HA	10:B:505:LLM:O20	2.06	0.56
1:C:204:VAL:HG13	1:C:302:MET:HG2	1.87	0.56
1:C:331:ALA:O	1:C:335:ILE:HD12	2.05	0.56
2:D:274:PRO:HG3	2:D:286:LEU:HD11	1.87	0.56
3:E:44:ASP:HB2	13:E:218:HOH:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:TYR:HB3	13:A:687:HOH:O	2.05	0.55
3:E:95:LYS:O	3:E:99:GLU:HG3	2.05	0.55
2:D:204:ILE:HG21	2:D:231:VAL:HG22	1.87	0.55
1:A:175:PRO:HA	1:A:178:SER:HB3	1.88	0.55
2:B:323:MET:HB3	2:B:373:MET:CE	2.36	0.55
1:C:1:MET:HG2	1:C:1:MET:O	2.06	0.55
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.88	0.55
4:F:186:LEU:HG	12:F:500:ACP:N1	2.22	0.54
2:B:158:ARG:CZ	11:B:507:MES:H21	2.38	0.54
2:D:106:GLY:O	2:D:111:GLY:HA3	2.08	0.54
2:B:315:VAL:HB	2:B:351:VAL:HG22	1.88	0.53
2:B:295:MET:HE1	2:B:319:PHE:CZ	2.43	0.53
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.43	0.53
1:A:60:LYS:NZ	1:A:85:GLN:O	2.24	0.53
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.91	0.53
9:B:503:EP:H62	9:B:503:EP:H13	1.91	0.53
3:E:137:LYS:O	3:E:141:GLU:HG2	2.09	0.53
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.42	0.53
1:C:368:LEU:O	13:C:760:HOH:O	2.19	0.53
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.43	0.53
1:C:204:VAL:HG22	1:C:302:MET:CE	2.39	0.53
2:B:199:ASP:OD2	11:B:507:MES:H52	2.09	0.53
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.44	0.53
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.91	0.52
3:E:52:LYS:HG2	3:E:53:LYS:NZ	2.24	0.52
4:F:333:ASN:HD21	12:F:500:ACP:PG	2.32	0.52
1:C:196:GLU:OE1	13:C:662:HOH:O	2.18	0.52
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.92	0.52
1:A:358:GLN:NE2	13:A:610:HOH:O	2.23	0.52
2:B:36:TYR:C	2:B:37:HIS:HD1	2.08	0.52
3:E:16:SER:OG	13:E:201:HOH:O	2.19	0.52
4:F:36:ARG:NH1	13:F:635:HOH:O	2.37	0.52
2:B:392:SER:O	2:B:396:THR:HG23	2.09	0.51
1:C:11:GLN:HG3	1:C:74:VAL:HG21	1.92	0.51
2:D:116:ASP:HA	2:D:119:LEU:HD12	1.92	0.51
2:D:297:ASP:OD1	2:D:298:SER:N	2.43	0.51
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.76	0.51
2:D:136:GLN:HA	2:D:167:ASN:O	2.10	0.51
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.45	0.51
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.92	0.51
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HD12	1:C:363:VAL:HG12	1.93	0.50
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.12	0.50
4:F:331:GLU:HG2	4:F:332:VAL:N	2.25	0.50
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.93	0.50
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.93	0.50
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.93	0.50
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.93	0.49
4:F:186:LEU:HG	12:F:500:ACP:C2	2.41	0.49
1:A:401:LYS:HE2	2:B:346:TRP:CG	2.46	0.49
1:C:204:VAL:HG22	1:C:302:MET:HE3	1.93	0.49
1:A:336:LYS:HD3	3:E:24:LEU:HD23	1.95	0.49
2:B:336:GLN:OE1	13:B:637:HOH:O	2.20	0.49
2:D:284:ARG:HG2	2:D:290:GLU:OE1	2.13	0.49
1:A:409:VAL:HA	1:A:413:MET:O	2.13	0.49
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.94	0.49
2:D:322:ARG:NH2	2:D:322:ARG:HG3	2.27	0.49
3:E:108:ASN:ND2	13:E:229:HOH:O	2.45	0.49
2:D:278:ARG:HH11	2:D:278:ARG:CG	2.26	0.49
3:E:44:ASP:N	13:E:221:HOH:O	2.46	0.49
2:B:263:PRO:O	2:B:266:HIS:ND1	2.42	0.48
3:E:106:GLU:O	3:E:110:GLU:HG3	2.13	0.48
4:F:288:LYS:NZ	13:F:634:HOH:O	2.44	0.48
1:C:417:GLU:OE1	13:C:717:HOH:O	2.19	0.48
4:F:292:ARG:HG2	4:F:292:ARG:NH1	2.28	0.48
2:D:155:SER:OG	3:E:126:LYS:HE2	2.14	0.48
1:A:150:THR:O	1:A:154:MET:HG2	2.13	0.48
1:A:180:ALA:O	1:A:183:GLU:HG3	2.14	0.48
3:E:140:LYS:HB3	3:E:140:LYS:HZ2	1.79	0.48
4:F:12:SER:HG	4:F:343:TYR:HH	1.62	0.48
2:D:213:CYS:HA	2:D:217:LEU:HD12	1.96	0.47
4:F:243:HIS:HD1	4:F:243:HIS:C	2.18	0.47
2:B:83:PHE:O	2:B:86:ILE:HG22	2.14	0.47
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.97	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.47
2:B:331:GLN:O	2:B:335:VAL:HG23	2.14	0.47
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.15	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.50	0.47
3:E:123:LEU:O	3:E:126:LYS:HB2	2.15	0.47
2:D:398:MET:HE2	2:D:398:MET:HB3	1.77	0.47
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.97	0.47
2:B:39:ASP:OD1	2:B:39:ASP:N	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:25:LYS:HG3	3:E:26:PRO:HD2	1.97	0.47
2:D:152:LEU:O	2:D:156:LYS:HG2	2.15	0.47
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.97	0.47
2:D:276:THR:HG22	2:D:280:SER:HB2	1.97	0.46
2:B:231:VAL:O	2:B:235:MET:HG3	2.16	0.46
4:F:247:LYS:O	4:F:247:LYS:HG2	2.14	0.46
2:D:19:LYS:O	2:D:23:VAL:HG23	2.15	0.46
1:A:90:GLU:O	1:A:121:ARG:HG2	2.16	0.46
1:A:262:TYR:CD1	1:A:265:ILE:HD12	2.51	0.46
1:A:331:ALA:O	1:A:335:ILE:HG12	2.15	0.46
2:B:293:GLN:O	10:B:505:LLM:H30	2.15	0.46
1:A:280:LYS:CE	1:A:283:HIS:HB3	2.44	0.46
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.46
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.51	0.46
4:F:292:ARG:HD3	4:F:378[B]:LEU:HB3	1.97	0.46
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.98	0.45
2:B:2:ARG:HB3	2:B:133:GLN:HG3	1.98	0.45
1:C:30:ILE:HG12	1:C:36:MET:HB2	1.98	0.45
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.45
3:E:136:ASN:O	3:E:140:LYS:HD3	2.15	0.45
3:E:138:GLU:HA	3:E:138:GLU:OE1	2.17	0.45
2:B:158:ARG:NH1	2:B:197:ASN:OD1	2.43	0.45
2:D:286:LEU:HD13	9:D:503:EP:H163	1.98	0.45
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.97	0.45
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE2	2.52	0.45
2:B:286:LEU:HG	2:B:290:GLU:CB	2.45	0.45
4:F:186:LEU:HD11	4:F:320:MET:CE	2.46	0.45
2:B:174:SER:OG	2:B:207:GLU:HB2	2.17	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.45
2:B:286:LEU:HD12	2:B:286:LEU:HA	1.74	0.44
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.99	0.44
2:D:57:THR:HA	13:D:650:HOH:O	2.17	0.44
2:D:74:THR:O	2:D:77:SER:OG	2.21	0.44
3:E:142:GLU:HG3	3:E:142:GLU:H	1.67	0.44
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.85	0.44
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.32	0.44
1:C:359:PRO:HB3	13:C:658:HOH:O	2.17	0.44
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.98	0.44
2:D:416:MET:O	2:D:420:GLU:HG3	2.17	0.44
1:A:230:LEU:O	1:A:234:ILE:HD13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:ILE:HG21	2:D:275:LEU:HD13	1.99	0.44
3:E:53:LYS:HA	3:E:53:LYS:HD3	1.82	0.44
3:E:85:LYS:NZ	13:E:207:HOH:O	2.27	0.44
1:A:315:CYS:HG	1:A:351:PHE:HE2	1.65	0.44
2:B:218:LYS:HA	2:B:218:LYS:HD3	1.73	0.44
2:B:438:ALA:O	13:B:602:HOH:O	2.21	0.44
2:D:83:PHE:O	2:D:86:ILE:HG22	2.17	0.44
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.17	0.44
4:F:97:SER:OG	4:F:183:GLN:NE2	2.48	0.44
2:B:323:MET:HB3	2:B:373:MET:HE1	1.99	0.44
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.21	0.44
2:B:322:ARG:HB2	13:B:627:HOH:O	2.17	0.44
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.53	0.44
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.83	0.44
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.18	0.43
1:A:319:TYR:HB3	1:A:323:VAL:HG21	2.00	0.43
4:F:156:LYS:HB3	4:F:244:CYS:SG	2.58	0.43
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.33	0.43
3:E:134:ARG:HG3	3:E:134:ARG:HH11	1.83	0.43
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.18	0.43
2:D:79:ARG:HB2	2:D:79:ARG:HH11	1.82	0.43
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.43
3:E:13:LYS:HG2	3:E:18:GLN:CG	2.48	0.43
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.54	0.43
2:B:174:SER:CB	2:B:207:GLU:HB2	2.49	0.43
2:D:396:THR:O	2:D:400:ARG:HG2	2.18	0.43
3:E:51:GLN:OE1	3:E:51:GLN:HA	2.18	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.43
1:A:245:ASP:HB3	3:E:16:SER:OG	2.19	0.43
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.43
2:B:301:MET:CE	2:B:301:MET:HA	2.49	0.42
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.54	0.42
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.48	0.42
4:F:186:LEU:HD11	4:F:320:MET:HE3	2.00	0.42
2:B:57:THR:HG22	2:B:58:GLY:N	2.34	0.42
1:C:372:GLN:O	13:C:658:HOH:O	2.21	0.42
1:C:155:GLU:HB3	3:E:101:LEU:HD22	2.00	0.42
2:B:320:ARG:HA	2:B:321:GLY:HA2	1.68	0.42
3:E:9:ILE:HG22	3:E:10:GLU:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:CB	1:A:140:SER:HB3	2.49	0.42
2:D:8:GLN:HB3	2:D:138:THR:CG2	2.50	0.42
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.02	0.42
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.82	0.42
2:D:276:THR:HB	2:D:281:GLN:HG2	2.01	0.42
2:D:403:ALA:HB1	2:D:404:PHE:CE2	2.55	0.42
2:D:75:MET:N	13:D:606:HOH:O	2.25	0.42
4:F:156:LYS:HD2	4:F:156:LYS:HA	1.88	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.55	0.42
2:B:160:GLU:HB3	2:B:161:TYR:CE1	2.54	0.42
2:D:269:MET:HE3	2:D:381:SER:HB3	2.01	0.42
4:F:14:TYR:HA	4:F:17:VAL:HB	2.01	0.42
2:B:371:LEU:HD21	9:B:503:EP:C13	2.50	0.42
2:D:19:LYS:HA	2:D:19:LYS:HD3	1.61	0.42
2:D:295:MET:HE1	2:D:319:PHE:CZ	2.55	0.42
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.19	0.42
4:F:237:THR:O	4:F:246:GLN:NE2	2.50	0.42
2:D:70:LEU:HD23	2:D:114:LEU:HD22	2.01	0.41
4:F:126:ASP:OD1	4:F:127:GLU:N	2.53	0.41
1:A:188:ILE:HD13	1:A:395:PHE:HB2	2.03	0.41
4:F:292:ARG:HD3	4:F:378[A]:LEU:HB3	2.01	0.41
1:A:211:ASP:O	1:A:215:ARG:HB2	2.21	0.41
1:C:174:ALA:O	1:C:178:SER:HB3	2.20	0.41
1:A:336:LYS:HD3	3:E:24:LEU:CD2	2.51	0.41
2:B:276:THR:N	9:B:503:EP:O76	2.33	0.41
2:D:8:GLN:HB3	2:D:138:THR:HG23	2.01	0.41
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.55	0.41
4:F:289:HIS:O	4:F:293:SER:OG	2.33	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.41
2:B:295:MET:CG	2:B:377:PHE:HB2	2.51	0.41
2:B:298:SER:N	10:B:505:LLM:O20	2.41	0.41
1:A:136:LEU:CD2	1:A:167:LEU:HB2	2.50	0.41
2:D:82:PRO:O	2:D:83:PHE:HB2	2.20	0.41
1:A:241:SER:HB2	1:A:248:LEU:O	2.21	0.41
2:B:158:ARG:HG3	11:B:507:MES:H62	2.03	0.41
2:D:205:ASP:HB3	2:D:303:ALA:HA	2.03	0.41
1:A:125:LEU:O	1:A:128:GLN:HB2	2.21	0.41
1:A:283:HIS:CD2	1:A:285:GLN:HE21	2.38	0.41
2:B:2:ARG:HB3	2:B:133:GLN:HG2	2.02	0.41
2:D:251:ASP:OD1	2:D:253:ARG:N	2.52	0.41
2:D:76:ASP:HA	2:D:79:ARG:HH12	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.56	0.41
1:A:220:GLU:OE1	2:B:326:LYS:HD2	2.21	0.41
2:B:396:THR:O	2:B:400:ARG:HG3	2.21	0.41
3:E:7:GLU:O	3:E:22:VAL:HA	2.21	0.41
1:C:143:GLY:HA3	5:C:501:GTP:O3A	2.21	0.41
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.41
4:F:221:LEU:HD11	4:F:267:PHE:CD2	2.55	0.41
4:F:162:ILE:HD11	4:F:240:LEU:HD21	2.03	0.41
1:C:241:SER:HB3	1:C:250:VAL:O	2.20	0.40
1:C:339:ARG:NE	13:C:686:HOH:O	2.31	0.40
2:D:414:ASP:N	2:D:414:ASP:OD1	2.55	0.40
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.85	0.40
2:B:292:THR:HA	2:B:295:MET:CE	2.51	0.40
1:C:328:VAL:O	1:C:332:ILE:HG13	2.22	0.40
4:F:19:ARG:CG	4:F:19:ARG:HH11	2.34	0.40
2:D:319:PHE:HB2	2:D:355:VAL:HG22	2.03	0.40
3:E:134:ARG:HG3	3:E:134:ARG:NH1	2.36	0.40
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.53	0.40
1:A:71:GLU:HG2	1:A:72:PRO:N	2.37	0.40
2:D:79:ARG:HB2	2:D:79:ARG:NH1	2.37	0.40
1:A:265:ILE:O	1:A:265:ILE:HG22	2.21	0.40
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.86	0.40
2:D:324:SER:HB3	2:D:327:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	426 (98%)	9 (2%)	0	100	100
1	C	439/451 (97%)	431 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	427/445 (96%)	412 (96%)	14 (3%)	1 (0%)	47	62
2	D	430/445 (97%)	421 (98%)	9 (2%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	352/384 (92%)	341 (97%)	10 (3%)	1 (0%)	41	55
All	All	2202/2319 (95%)	2150 (98%)	50 (2%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	321	GLY
4	F	154	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	358 (97%)	10 (3%)	44	65
1	C	372/379 (98%)	363 (98%)	9 (2%)	49	68
2	B	371/383 (97%)	353 (95%)	18 (5%)	25	40
2	D	371/383 (97%)	358 (96%)	13 (4%)	36	55
3	E	110/127 (87%)	97 (88%)	13 (12%)	5	7
4	F	321/342 (94%)	313 (98%)	8 (2%)	47	67
All	All	1913/1993 (96%)	1842 (96%)	71 (4%)	34	53

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	71	GLU
1	A	96	LYS
1	A	121	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	LYS
1	A	176	GLN
1	A	326	LYS
1	A	342	GLN
1	A	433	GLU
2	B	1	MET
2	B	19	LYS
2	B	60	LYS
2	B	117	SER
2	B	139	HIS
2	B	207	GLU
2	B	220	THR
2	B	248	LEU
2	B	276	THR
2	B	278	ARG
2	B	281	GLN
2	B	322	ARG
2	B	369	ARG
2	B	405	LEU
2	B	414	ASP
2	B	416	MET
2	B	420	GLU
2	B	430	SER
1	C	1	MET
1	C	41	THR
1	C	165	SER
1	C	241	SER
1	C	245	ASP
1	C	251	ASP
1	C	297	GLU
1	C	356	ASN
1	C	381	THR
2	D	1	MET
2	D	15	GLN
2	D	50	ASN
2	D	57	THR
2	D	79	ARG
2	D	88	ARG
2	D	138	THR
2	D	139	HIS
2	D	155	SER
2	D	248	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	278	ARG
2	D	345	GLU
2	D	416	MET
3	E	10	GLU
3	E	12	ASN
3	E	16	SER
3	E	19	SER
3	E	49	GLU
3	E	53	LYS
3	E	59	GLU
3	E	74	GLU
3	E	96	MET
3	E	98	LYS
3	E	139	LEU
3	E	141	GLU
3	E	142	GLU
4	F	19	ARG
4	F	32	LYS
4	F	186	LEU
4	F	211	TYR
4	F	217	ARG
4	F	242	ASN
4	F	244	CYS
4	F	292	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	339	ASN
3	E	12	ASN
3	E	108	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ACP	F	500	6	27,33,33	1.37	5 (18%)	32,52,52	1.52	6 (18%)
9	EP	D	503	-	32,36,36	1.40	4 (12%)	39,53,53	2.08	12 (30%)
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	2.02	9 (29%)
9	EP	B	503	-	32,36,36	1.23	3 (9%)	39,53,53	2.51	13 (33%)
5	GTP	A	501	6	26,34,34	1.03	1 (3%)	33,54,54	1.85	8 (24%)
5	GTP	C	501	6	26,34,34	1.02	1 (3%)	33,54,54	1.70	6 (18%)
8	GDP	B	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.92	8 (25%)
10	LLM	B	505	-	38,40,40	2.49	16 (42%)	44,55,55	1.98	10 (22%)
11	MES	B	507	-	12,12,12	2.20	1 (8%)	14,16,16	2.13	4 (28%)

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	ACP	F	500	6	-	6/15/38/38	0/3/3/3
9	EP	D	503	-	-	5/49/55/55	0/2/3/3
8	GDP	D	501	6	-	5/12/32/32	0/3/3/3
9	EP	B	503	-	-	12/49/55/55	0/2/3/3
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
5	GTP	C	501	6	-	3/18/38/38	0/3/3/3
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LLM	B	505	-	-	19/39/64/64	0/3/4/4
11	MES	B	507	-	-	4/6/14/14	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	MES	C8-S	-7.36	1.67	1.77
10	B	505	LLM	C22-C21	6.80	1.52	1.32
10	B	505	LLM	C5-C6	-5.30	1.40	1.50
10	B	505	LLM	C30-C25	-4.83	1.38	1.50
9	D	503	EP	C27-C24	4.59	1.54	1.46
8	D	501	GDP	C6-C5	3.95	1.48	1.41
8	B	501	GDP	C6-C5	3.94	1.48	1.41
9	B	503	EP	C27-C24	3.92	1.53	1.46
10	B	505	LLM	C8-C7	-3.91	1.41	1.49
9	D	503	EP	O2-C75	3.89	1.45	1.34
9	B	503	EP	O2-C75	3.86	1.45	1.34
10	B	505	LLM	C2-C1	-3.82	1.39	1.48
10	B	505	LLM	C27-C26	-3.76	1.40	1.48
10	B	505	LLM	C14-C13	-3.61	1.38	1.50
10	B	505	LLM	C4-C3	-3.59	1.39	1.50
10	B	505	LLM	C24-C25	-3.39	1.41	1.50
10	B	505	LLM	C12-C13	-3.25	1.39	1.50
5	A	501	GTP	C6-N1	3.18	1.38	1.33
5	C	501	GTP	C6-N1	3.17	1.38	1.33
12	F	500	ACP	PG-O2G	3.05	1.61	1.54
10	B	505	LLM	C6-C7	2.99	1.40	1.32
12	F	500	ACP	PB-O3A	2.91	1.61	1.58
9	D	503	EP	O2-C3	-2.85	1.40	1.45
10	B	505	LLM	C2-C3	2.81	1.39	1.32
10	B	505	LLM	C29-C13	2.77	1.39	1.32
9	D	503	EP	C13-S1	2.71	1.74	1.70
12	F	500	ACP	C5-C4	2.58	1.47	1.40
10	B	505	LLM	C16-C17	2.52	1.50	1.46
12	F	500	ACP	PG-O3G	2.43	1.60	1.54
8	B	501	GDP	C5-C4	2.26	1.46	1.40
8	D	501	GDP	C5-C4	2.20	1.46	1.40
12	F	500	ACP	PB-O2B	2.13	1.61	1.56
10	B	505	LLM	O19-C19	-2.04	1.42	1.46
10	B	505	LLM	C26-C25	2.04	1.40	1.33
9	B	503	EP	C59-C57	-2.03	1.51	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	LLM	C20-C21-C22	-7.18	113.66	124.93
9	B	503	EP	C32-C27-C24	-6.89	113.93	123.31
11	B	507	MES	C5-N4-C3	6.20	122.78	108.83
9	D	503	EP	C27-O26-C24	6.07	65.07	60.69
9	B	503	EP	C27-O26-C24	5.78	64.85	60.69
5	A	501	GTP	N3-C2-N1	-5.72	119.60	127.22
9	B	503	EP	C21-C24-C27	-5.43	114.50	124.78
5	C	501	GTP	N3-C2-N1	-5.42	119.99	127.22
9	B	503	EP	O26-C27-C32	-4.85	109.20	116.57
8	B	501	GDP	C6-C5-C4	-4.74	116.27	120.80
10	B	505	LLM	C23-C22-C21	-4.72	114.27	124.93
8	D	501	GDP	C2-N3-C4	4.60	120.61	115.36
8	B	501	GDP	C2-N3-C4	4.56	120.57	115.36
8	D	501	GDP	C6-N1-C2	4.35	122.83	115.93
8	D	501	GDP	C6-C5-C4	-4.34	116.65	120.80
8	B	501	GDP	C6-N1-C2	4.30	122.76	115.93
5	A	501	GTP	C2-N3-C4	4.27	120.23	115.36
8	D	501	GDP	C5-C6-N1	-4.19	117.70	123.43
9	D	503	EP	O26-C27-C32	-4.11	110.32	116.57
5	C	501	GTP	C2-N3-C4	4.04	119.97	115.36
12	F	500	ACP	PA-O3A-PB	-4.00	119.89	132.56
10	B	505	LLM	C19-C20-C21	-3.85	105.94	111.33
10	B	505	LLM	C18-C17-C16	-3.84	115.85	124.18
8	B	501	GDP	C5-C6-N1	-3.80	118.23	123.43
9	B	503	EP	O26-C24-C21	-3.74	108.43	116.33
9	D	503	EP	O26-C24-C27	-3.71	57.28	59.65
9	D	503	EP	C16-C15-S1	-3.63	115.24	120.12
8	D	501	GDP	N3-C2-N1	-3.61	122.41	127.22
8	B	501	GDP	N3-C2-N1	-3.55	122.49	127.22
9	B	503	EP	C16-C15-S1	-3.43	115.50	120.12
9	B	503	EP	O26-C27-C24	-3.38	57.49	59.65
9	D	503	EP	O26-C24-C21	-3.37	109.21	116.33
9	B	503	EP	C16-C15-N20	3.27	132.40	123.80
9	D	503	EP	C32-C27-C24	-3.27	118.86	123.31
8	D	501	GDP	PA-O3A-PB	-3.24	121.72	132.83
10	B	505	LLM	C16-O16-C17	3.23	62.66	60.59
12	F	500	ACP	N3-C2-N1	-3.19	123.70	128.68
5	C	501	GTP	C5-C6-N1	-3.18	119.08	123.43
9	D	503	EP	C16-C15-N20	3.14	132.06	123.80
9	B	503	EP	C21-C3-C5	-3.13	109.14	113.50
9	D	503	EP	O26-C27-C24	-3.13	57.65	59.65
9	B	503	EP	O26-C24-C27	-3.13	57.65	59.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	EP	C53-C51-C47	-3.07	107.25	112.37
12	F	500	ACP	C3'-C2'-C1'	3.01	105.50	100.98
5	A	501	GTP	C5-C6-N1	-2.96	119.39	123.43
9	B	503	EP	O2-C75-C72	2.93	116.84	111.46
5	C	501	GTP	C6-N1-C2	2.83	120.42	115.93
5	A	501	GTP	C6-N1-C2	2.81	120.40	115.93
9	B	503	EP	C53-C51-C47	-2.75	107.77	112.37
5	A	501	GTP	O2G-PG-O3B	2.75	113.87	104.64
5	A	501	GTP	N2-C2-N1	2.69	121.44	117.25
9	D	503	EP	C21-C24-C27	-2.65	119.76	124.78
12	F	500	ACP	O2G-PG-C3B	2.57	112.64	106.40
10	B	505	LLM	C9-C8-C7	2.54	114.77	109.52
8	B	501	GDP	C4-C5-N7	-2.52	106.77	109.40
8	D	501	GDP	C4-C5-N7	-2.49	106.80	109.40
5	A	501	GTP	PA-O3A-PB	-2.46	124.37	132.83
10	B	505	LLM	O27-C23-C22	2.33	112.20	107.46
12	F	500	ACP	C2-N1-C6	2.29	122.68	118.75
5	C	501	GTP	N2-C2-N1	2.28	120.80	117.25
10	B	505	LLM	C4-C5-C6	-2.25	109.05	113.00
9	D	503	EP	C21-C3-C5	-2.23	110.40	113.50
8	D	501	GDP	C1'-N9-C4	-2.22	122.74	126.64
8	B	501	GDP	C1'-N9-C4	-2.21	122.75	126.64
5	A	501	GTP	C6-C5-C4	-2.21	118.69	120.80
11	B	507	MES	C2-C3-N4	2.20	113.45	110.10
11	B	507	MES	O3S-S-C8	2.15	109.25	105.77
11	B	507	MES	O2S-S-C8	2.15	109.50	106.92
10	B	505	LLM	C19-C18-C17	-2.12	108.94	113.81
9	B	503	EP	C64-C59-C68	2.10	113.24	109.43
8	D	501	GDP	C2'-C3'-C4'	2.08	106.69	102.64
9	D	503	EP	O2-C75-C72	2.06	115.25	111.46
12	F	500	ACP	C4-C5-N7	-2.03	107.28	109.40
8	B	501	GDP	O2B-PB-O3A	2.03	111.44	104.64
5	C	501	GTP	C6-C5-C4	-2.03	118.86	120.80
10	B	505	LLM	C15-C14-C13	-2.02	110.19	115.53

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	500	ACP	C5'-O5'-PA-O2A
9	D	503	EP	C5-C10-C12-N20
8	D	501	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
10	B	505	LLM	O15-C15-C16-C17
10	B	505	LLM	C14-C15-C16-C17
10	B	505	LLM	O15-C15-C16-O16
10	B	505	LLM	C14-C15-C16-O16
10	B	505	LLM	C11-C12-C13-C14
10	B	505	LLM	C11-C12-C13-C29
10	B	505	LLM	C9-C10-C11-C12
10	B	505	LLM	C9-C10-C11-C28
10	B	505	LLM	C11-C10-C9-O9
10	B	505	LLM	C18-C19-C20-O20
10	B	505	LLM	C18-C19-C20-C21
10	B	505	LLM	O19-C19-C20-O20
10	B	505	LLM	O19-C19-C20-C21
10	B	505	LLM	O20-C20-C21-C22
9	B	503	EP	C5-C10-C12-N20
9	B	503	EP	C24-C21-C3-C5
9	B	503	EP	C24-C21-C3-O2
9	B	503	EP	C64-C59-C68-O70
9	B	503	EP	C60-C59-C68-O70
11	B	507	MES	C7-C8-S-O2S
12	F	500	ACP	O4'-C4'-C5'-O5'
12	F	500	ACP	C3'-C4'-C5'-O5'
11	B	507	MES	C7-C8-S-O3S
10	B	505	LLM	C11-C10-C9-C8
9	D	503	EP	C21-C3-C5-C10
9	D	503	EP	C21-C3-C5-C6
10	B	505	LLM	C19-C20-C21-C22
11	B	507	MES	C8-C7-N4-C5
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	503	EP	C64-C59-C68-C72
9	B	503	EP	C60-C59-C68-C72
9	B	503	EP	C57-C59-C68-C72
8	D	501	GDP	C5'-O5'-PA-O2A
11	B	507	MES	C7-C8-S-O1S
10	B	505	LLM	C12-C13-C14-C15
8	D	501	GDP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3A-PA-O2A
9	B	503	EP	C21-C3-C5-C10
9	B	503	EP	C21-C3-C5-C6
10	B	505	LLM	C29-C13-C14-C15
9	D	503	EP	O2-C3-C5-C10
8	B	501	GDP	PB-O3A-PA-O2A
12	F	500	ACP	PB-C3B-PG-O1G
9	D	503	EP	O2-C3-C5-C6
12	F	500	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C3'-C4'-C5'-O5'
8	B	501	GDP	PB-O3A-PA-O1A
9	B	503	EP	C68-C72-C75-O2
12	F	500	ACP	C5'-O5'-PA-O1A
9	B	503	EP	C57-C59-C68-O70
10	B	505	LLM	C17-C18-C19-O19

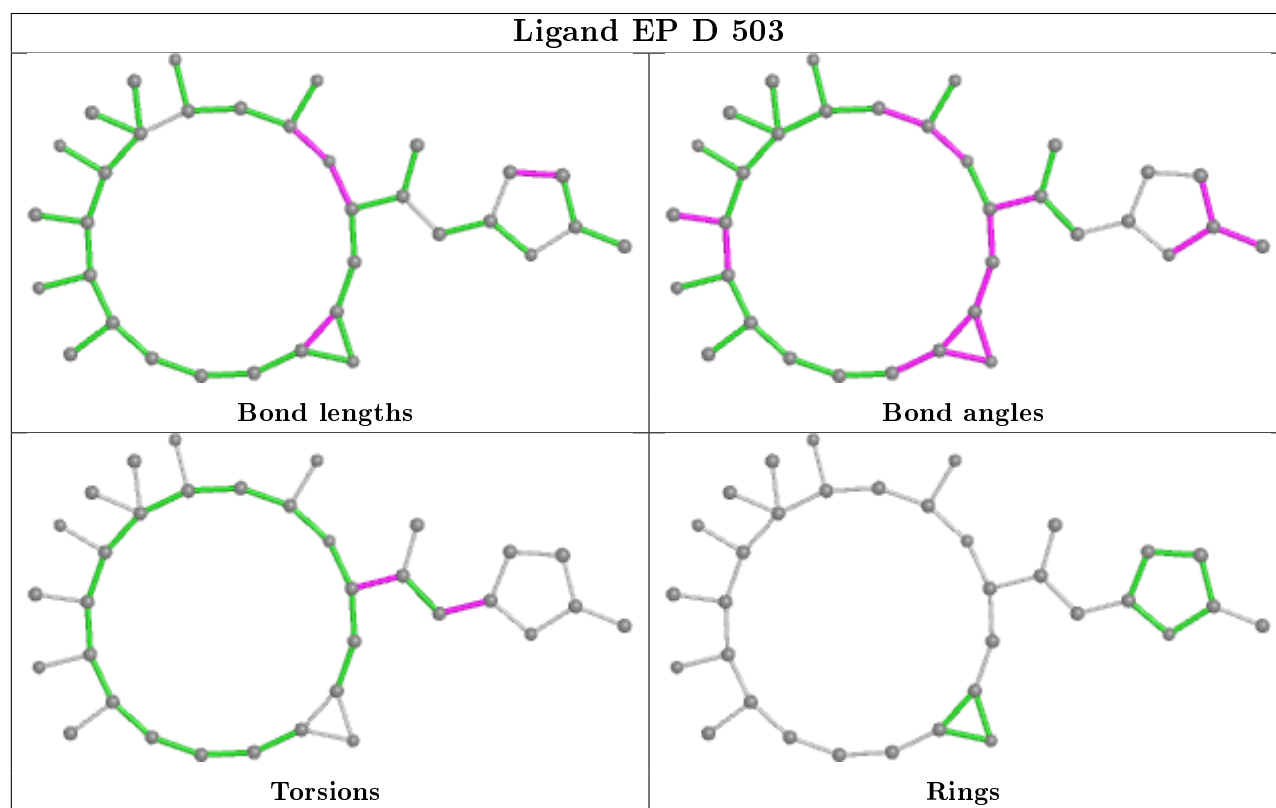
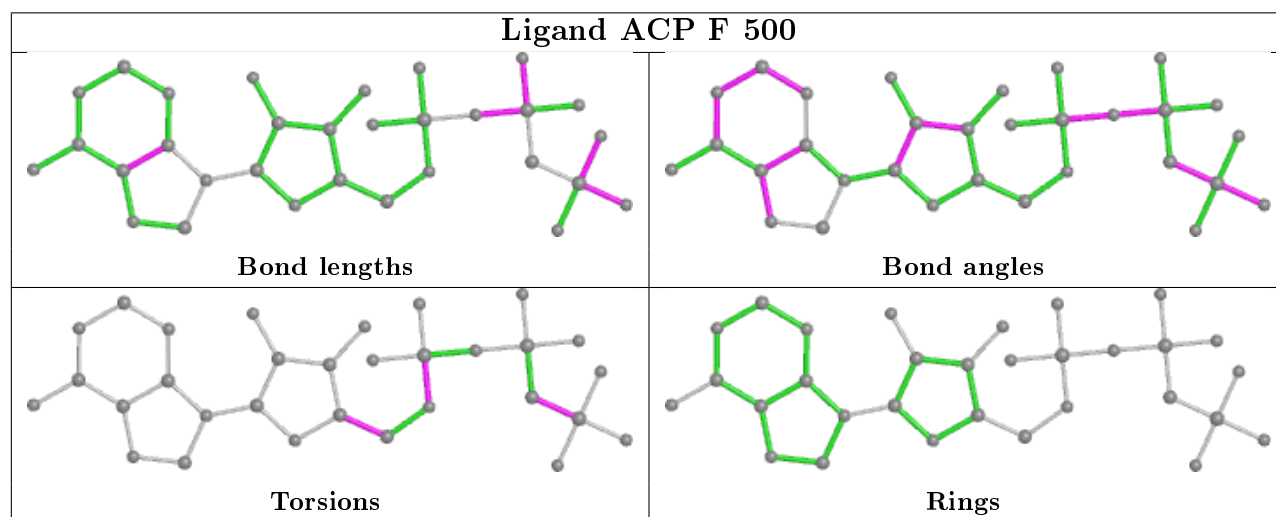
There are no ring outliers.

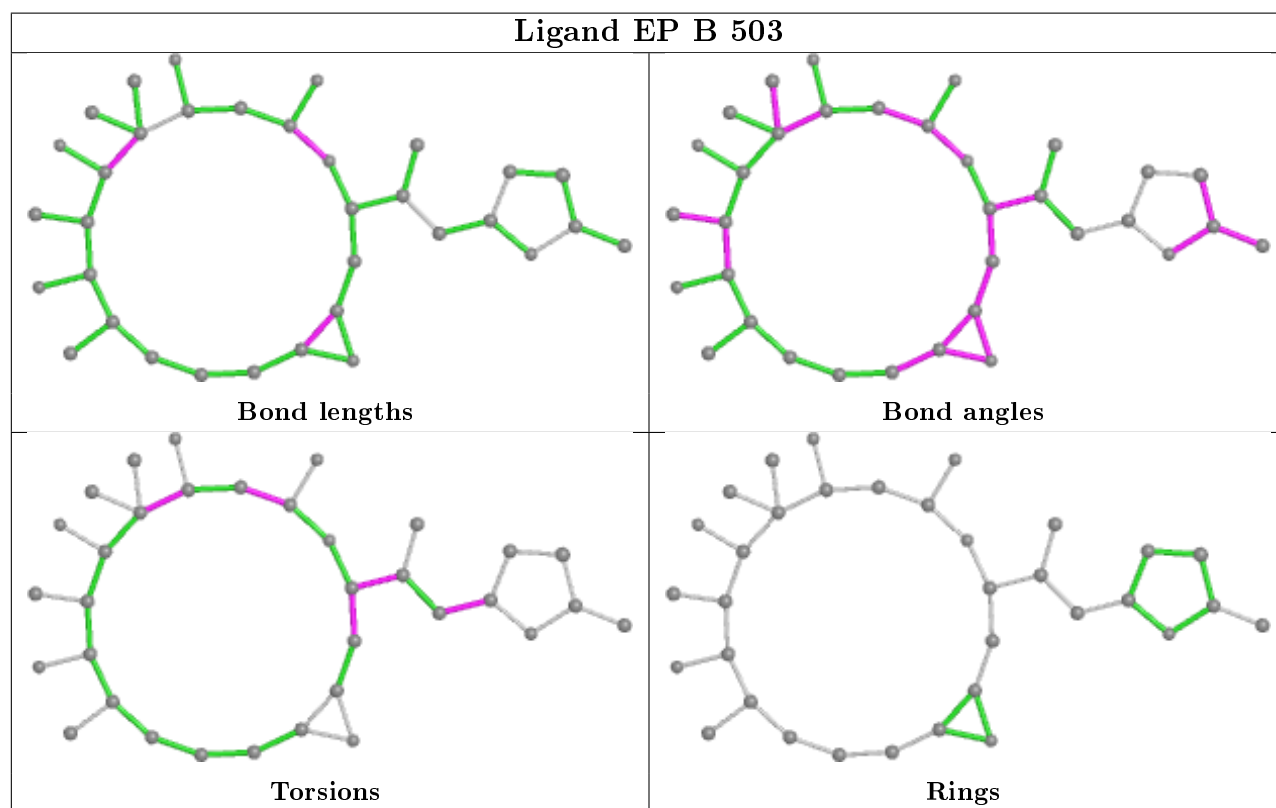
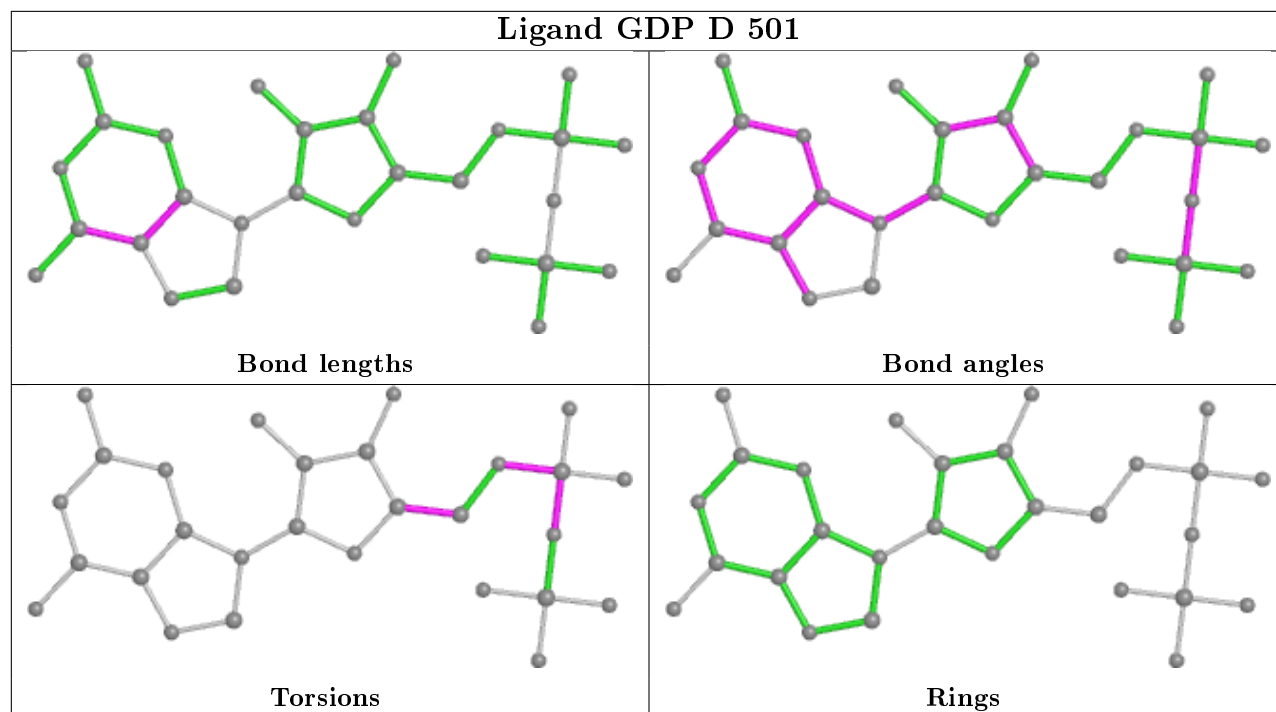
8 monomers are involved in 21 short contacts:

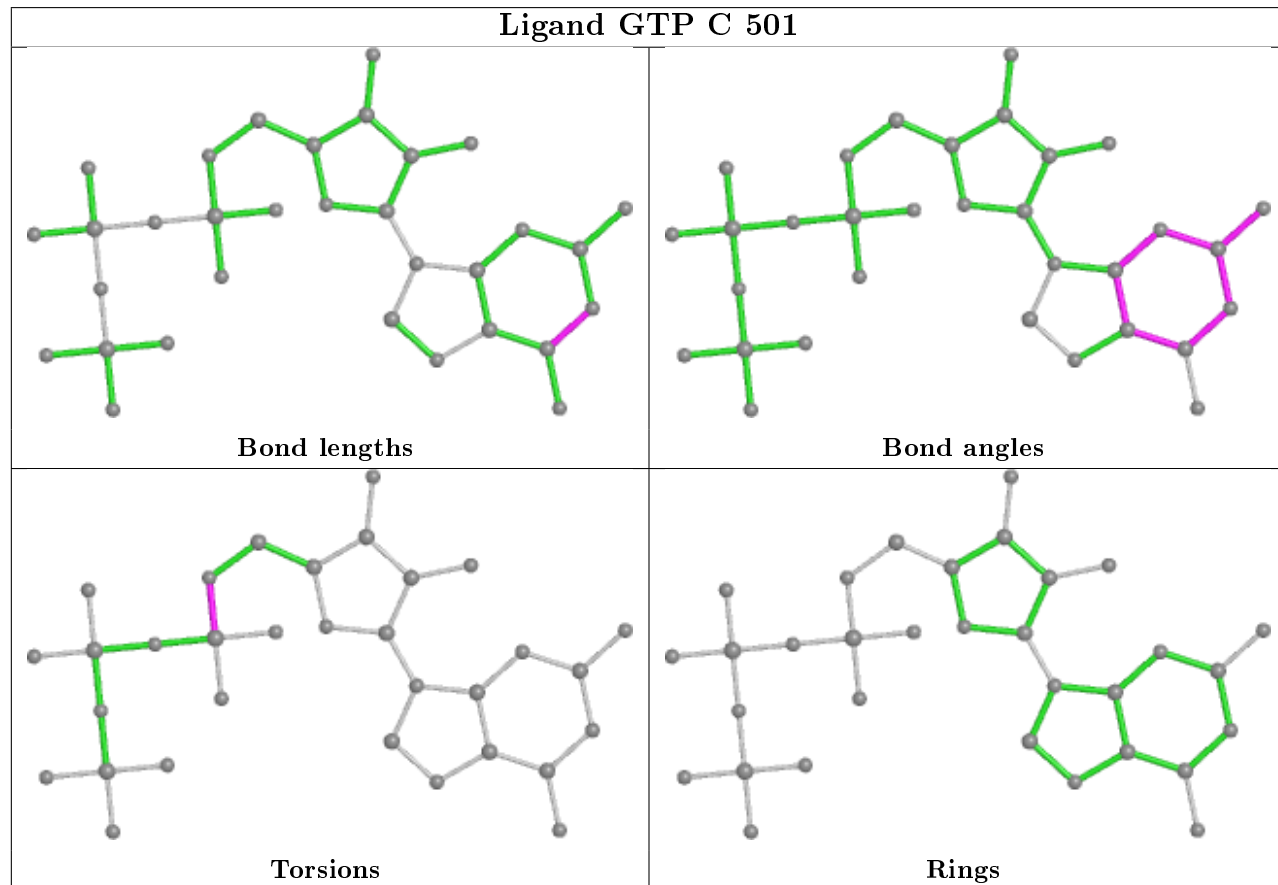
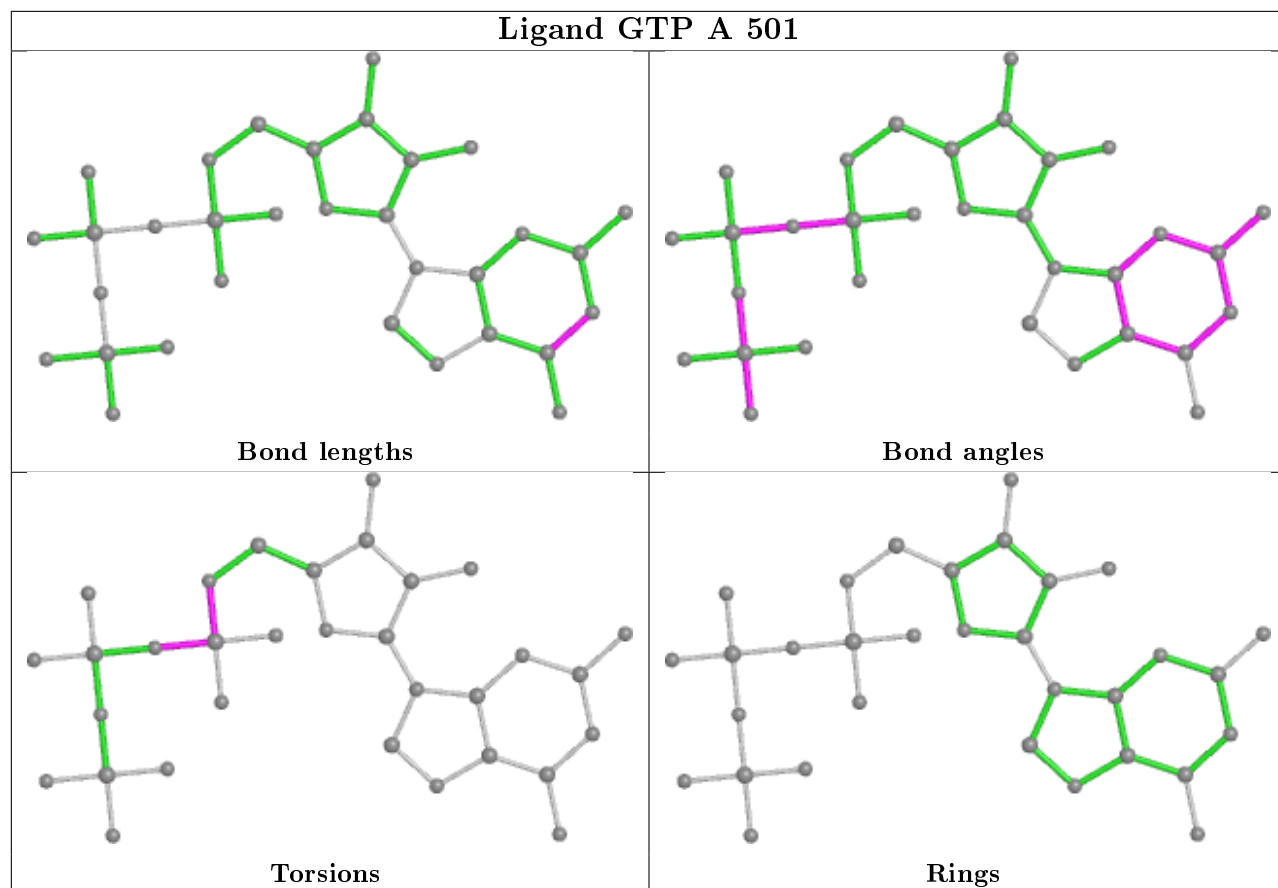
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	500	ACP	4	0
9	D	503	EP	1	0
8	D	501	GDP	1	0
9	B	503	EP	6	0
5	A	501	GTP	1	0
5	C	501	GTP	1	0
10	B	505	LLM	4	0
11	B	507	MES	3	0

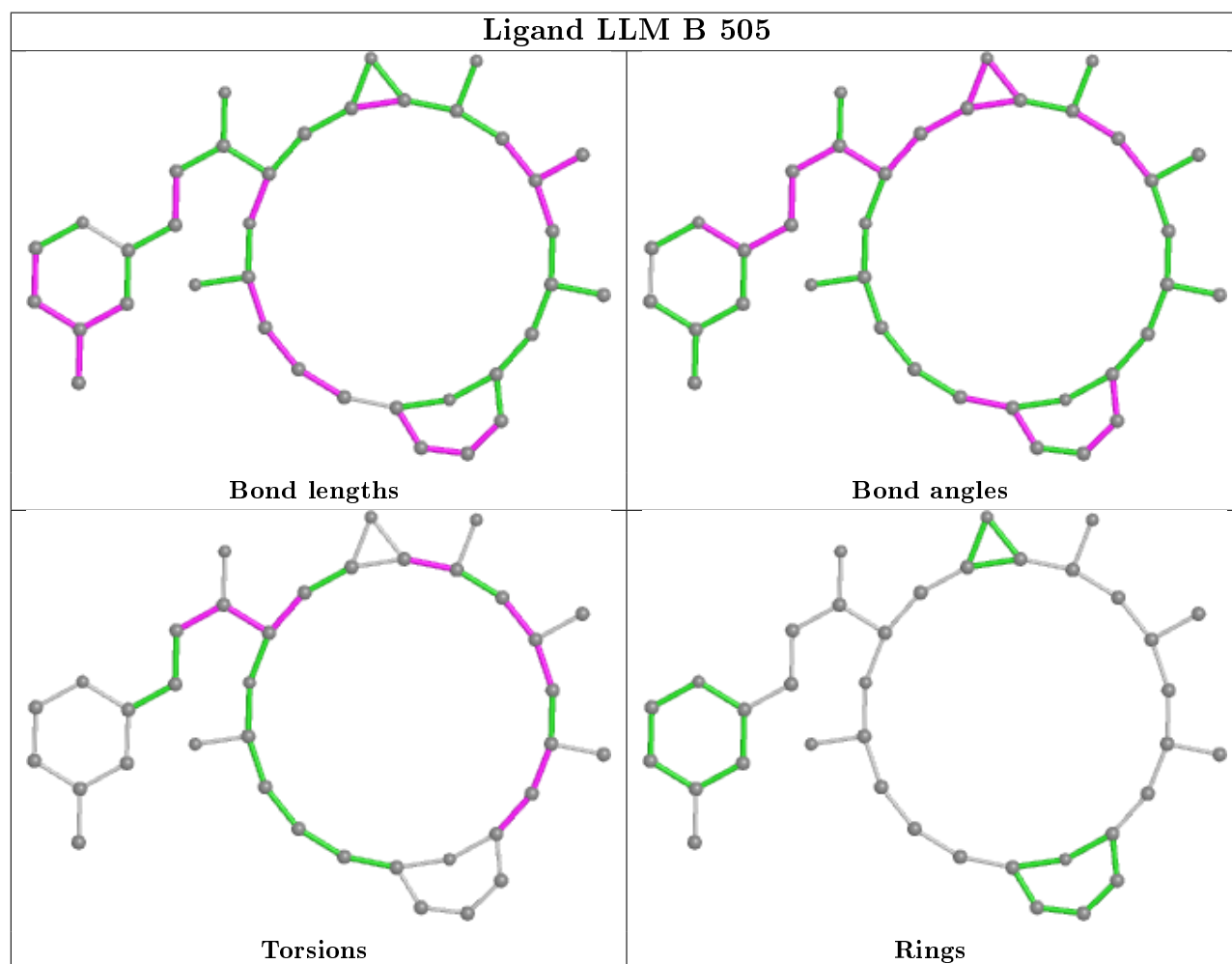
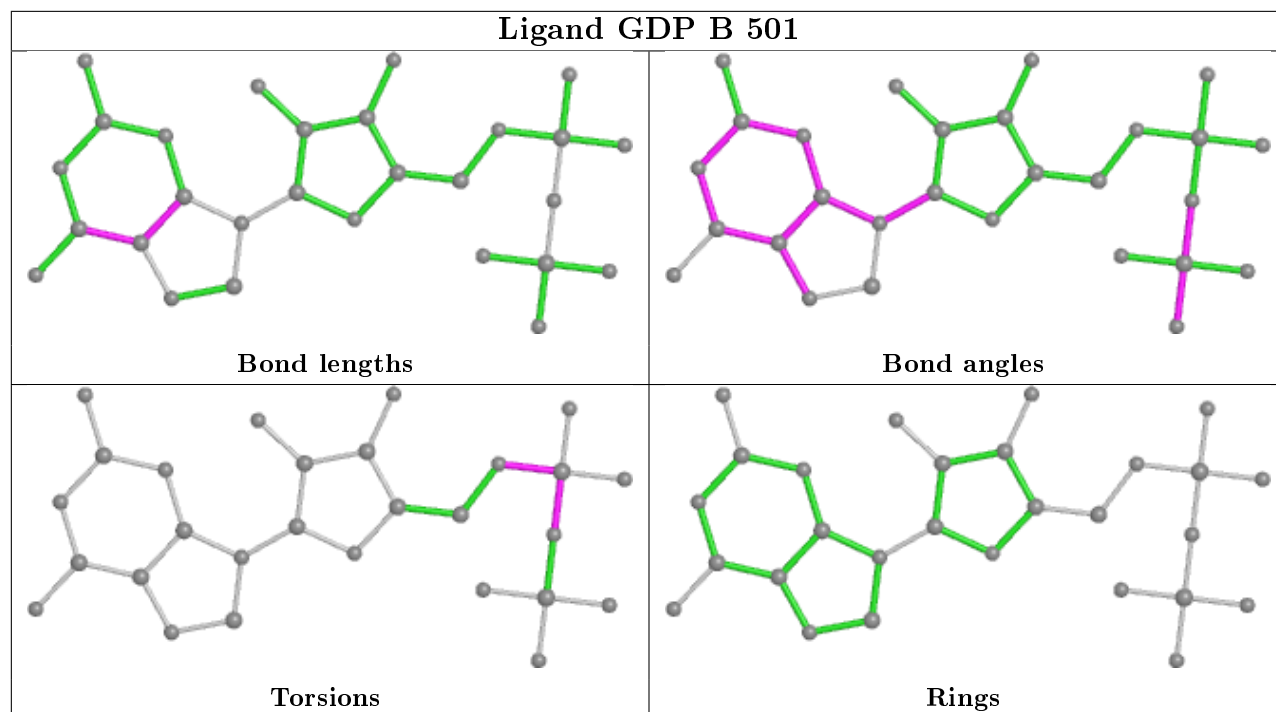
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	-0.18	2 (0%) 91 89	24, 40, 68, 119	0
1	C	440/451 (97%)	-0.21	0 100 100	19, 32, 59, 84	0
2	B	428/445 (96%)	-0.03	7 (1%) 72 70	23, 43, 81, 115	2 (0%)
2	D	431/445 (96%)	-0.17	3 (0%) 87 86	25, 47, 79, 107	6 (1%)
3	E	121/143 (84%)	-0.01	1 (0%) 86 84	30, 53, 100, 118	0
4	F	351/384 (91%)	0.87	63 (17%) 1 1	36, 65, 136, 154	0
All	All	2208/2319 (95%)	0.02	76 (3%) 45 44	19, 44, 99, 154	8 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	240	LEU	7.3
4	F	173	ILE	6.7
4	F	234	GLN	6.4
4	F	249	TYR	5.3
4	F	152	SER	4.7
4	F	236	LYS	4.6
4	F	233	PHE	4.6
4	F	232	ASN	4.5
4	F	157	GLY	4.4
4	F	244	CYS	4.3
4	F	156	LYS	4.3
4	F	162	ILE	4.0
4	F	177	GLY	4.0
4	F	186	LEU	3.9
4	F	131	PHE	3.8
4	F	161	LEU	3.8
4	F	179	VAL	3.7
4	F	243	HIS	3.7
4	F	258	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	238	CYS	3.6
4	F	242	ASN	3.6
4	F	259	GLY	3.5
4	F	225	SER	3.5
4	F	170	LEU	3.4
4	F	253	TYR	3.4
4	F	168	GLU	3.3
4	F	220[A]	VAL	3.3
4	F	245	ILE	3.2
4	F	169	LEU	3.2
4	F	231	ALA	3.1
2	B	438	ALA	3.1
4	F	372	THR	3.1
2	B	56	ALA	3.1
4	F	224	SER	3.1
2	B	280	SER	3.0
2	B	284	ARG	3.0
4	F	239	HIS	3.0
4	F	163	SER	3.0
2	B	283	TYR	3.0
4	F	176	GLN	2.9
2	B	282	GLN	2.9
4	F	255[A]	ARG	2.8
4	F	241	THR	2.8
4	F	182	ILE	2.8
4	F	158	GLU	2.7
4	F	125	THR	2.6
4	F	229	ASN	2.6
4	F	371	PRO	2.6
2	B	340	SER	2.6
4	F	199	PHE	2.5
4	F	142	ARG	2.5
4	F	284[A]	LEU	2.4
1	A	262	TYR	2.4
4	F	178	GLN	2.4
4	F	99	VAL	2.4
4	F	247	LYS	2.4
4	F	330	ILE	2.3
2	D	1	MET	2.3
3	E	6	MET	2.3
4	F	378[A]	LEU	2.3
4	F	100	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	44	ARG	2.3
4	F	147	TRP	2.3
4	F	155	ALA	2.3
4	F	105	LEU	2.2
4	F	335	ALA	2.2
4	F	165	GLU	2.2
4	F	252	ASN	2.2
4	F	181	VAL	2.2
1	A	282	TYR	2.1
4	F	153	ALA	2.1
4	F	251	LYS	2.1
2	D	405	LEU	2.1
4	F	250	SER	2.0
2	D	57	THR	2.0
4	F	148	ILE	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, 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.

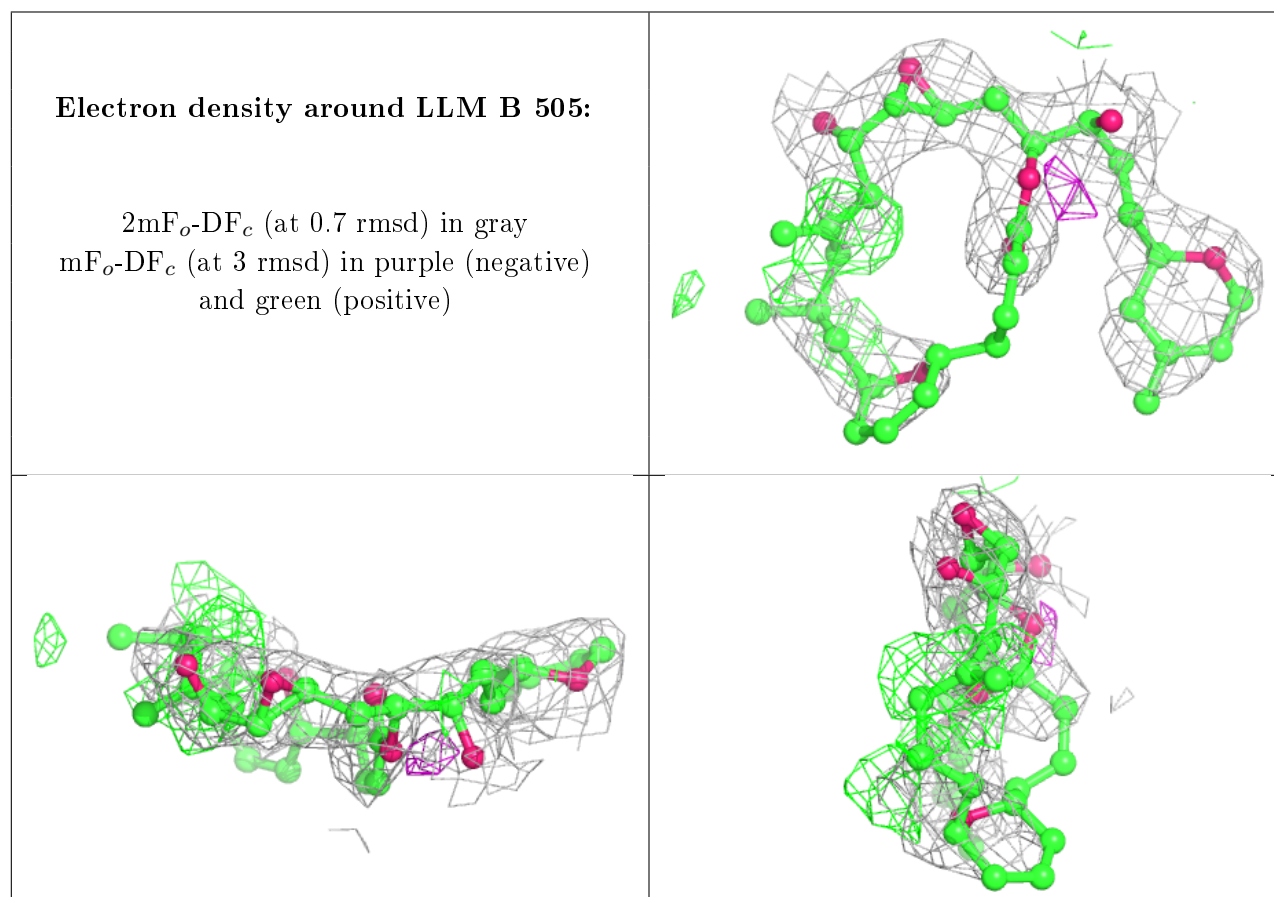
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	LLM	B	505	37/37	0.78	0.26	72,99,120,123	5
6	MG	F	501	1/1	0.79	0.14	77,77,77,77	0
6	MG	B	502	1/1	0.80	0.24	54,54,54,54	0
9	EP	B	503	34/34	0.85	0.27	54,67,75,82	0
6	MG	C	502	1/1	0.85	0.32	29,29,29,29	0
6	MG	D	502	1/1	0.86	0.12	62,62,62,62	0
12	ACP	F	500	31/31	0.90	0.20	69,83,158,200	0
7	CA	C	503	1/1	0.91	0.19	68,68,68,68	0

Continued on next page...

Continued from previous page...

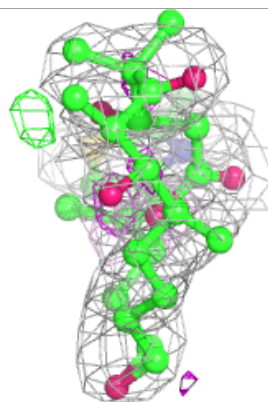
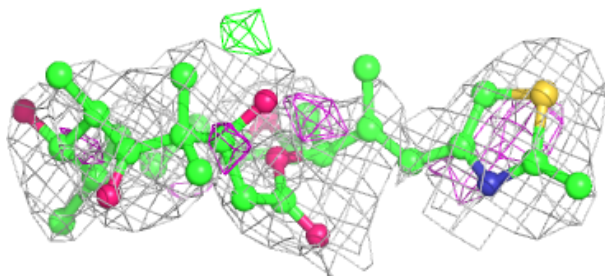
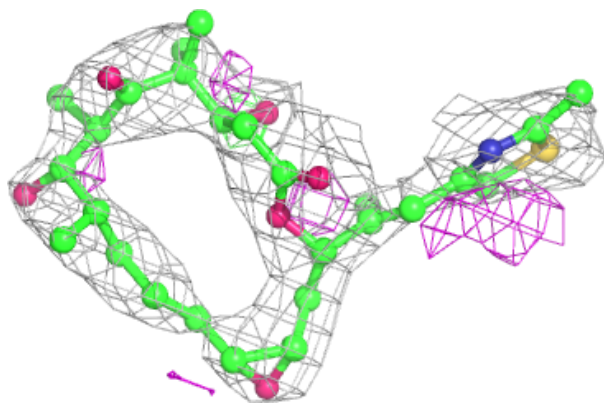
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	MES	B	507	12/12	0.93	0.13	48,55,71,74	0
7	CA	B	506	1/1	0.94	0.20	80,80,80,80	0
7	CA	A	503	1/1	0.95	0.18	64,64,64,64	0
9	EP	D	503	34/34	0.96	0.16	35,46,60,63	0
6	MG	A	502	1/1	0.97	0.35	30,30,30,30	0
8	GDP	D	501	28/28	0.98	0.12	29,34,46,51	0
5	GTP	A	501	32/32	0.98	0.17	19,26,34,42	0
5	GTP	C	501	32/32	0.98	0.16	16,22,27,42	0
8	GDP	B	501	28/28	0.98	0.17	18,27,32,35	0
6	MG	B	504	1/1	0.99	0.29	28,28,28,28	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.

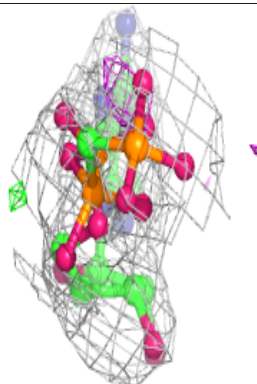
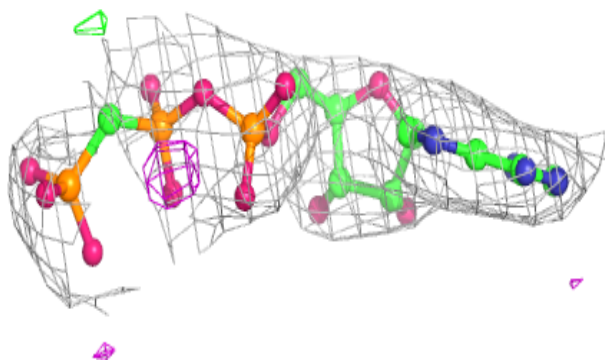
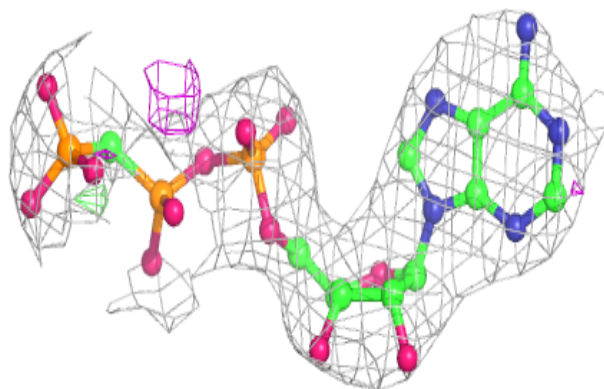


Electron density around EP B 503:

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

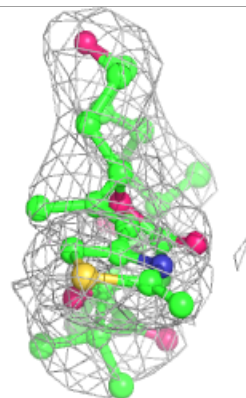
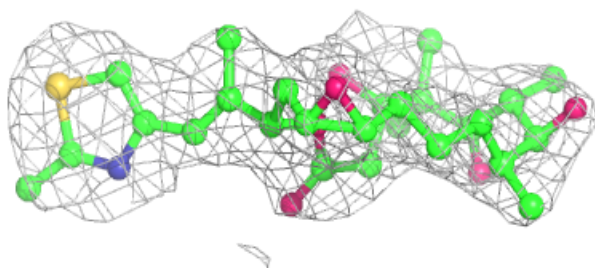
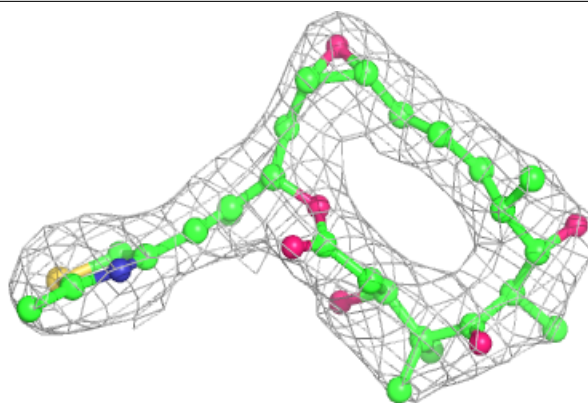
**Electron density around ACP F 500:**

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



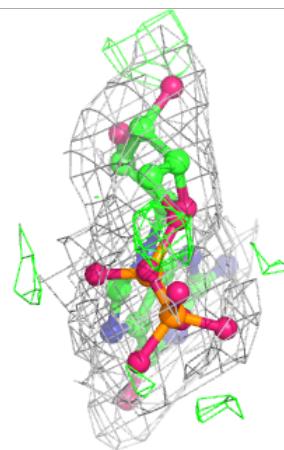
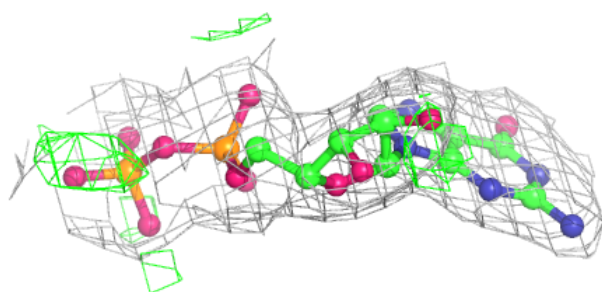
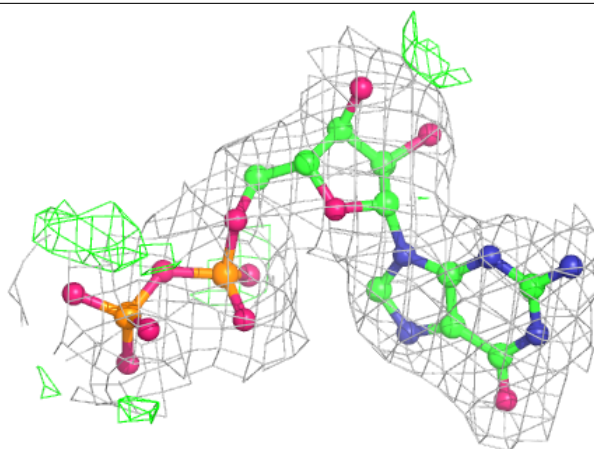
Electron density around EP D 503:

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



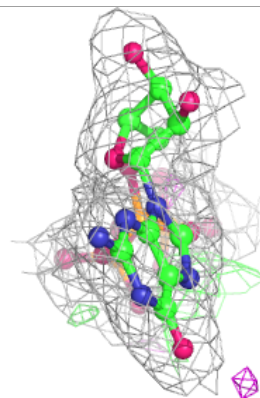
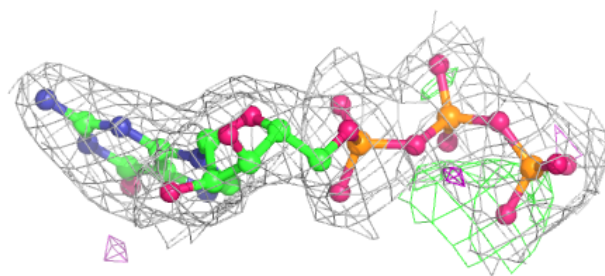
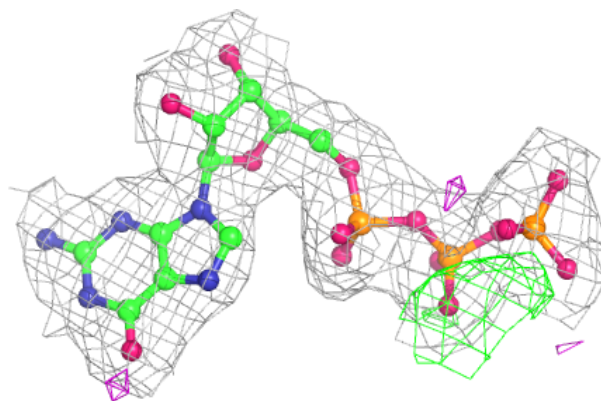
Electron density around GDP D 501:

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

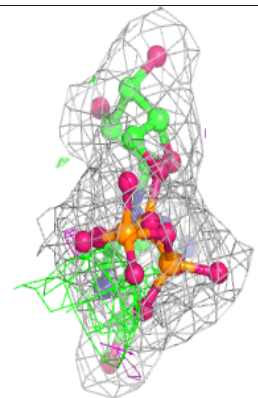
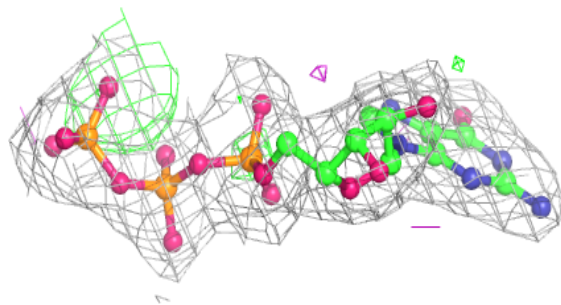
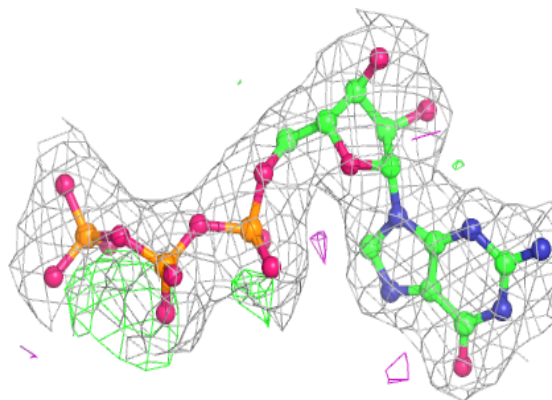


Electron density around GTP A 501:

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

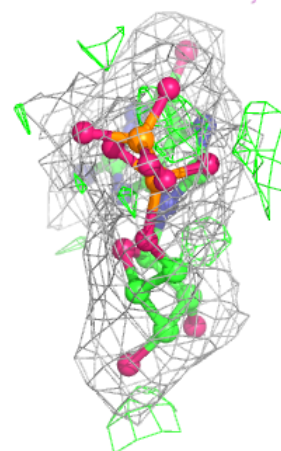
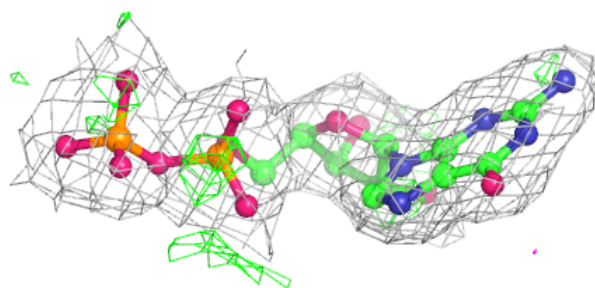
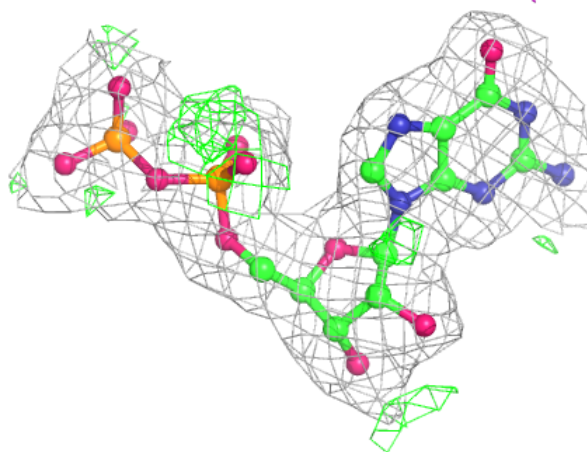
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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.