



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:34 AM UTC

PDB ID : 4O4J / pdb_00004o4j
Title : Tubulin-Peloruside 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 : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

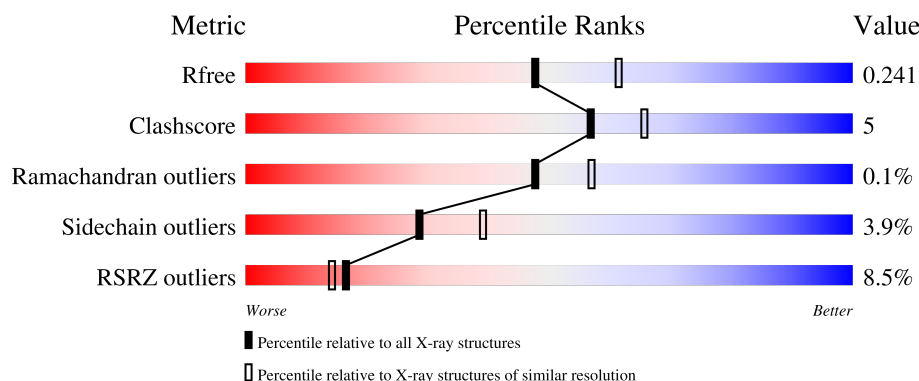
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of 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	2% 88% 8% ..
1	C	451	2% 90% 7% ..
2	B	445	2% 84% 11% ..
2	D	445	4% 81% 15% .
3	E	143	4% 78% 8% . 14%

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Mol	Chain	Length	Quality of chain
4	F	384	35% 48% 18% . 31%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18124 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	439	Total	C	N	O	S	0	12	0
			3485	2213	587	661	24			
1	C	440	Total	C	N	O	S	0	15	0
			3496	2218	585	667	26			

- 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	12	0
			3424	2151	581	664	28			
2	D	431	Total	C	N	O	S	0	6	0
			3413	2145	580	659	29			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	6	0
			1044	645	188	206	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	265	Total	C	N	O	S	0	1	0
			2179	1409	370	386	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 (CCD ID: 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		

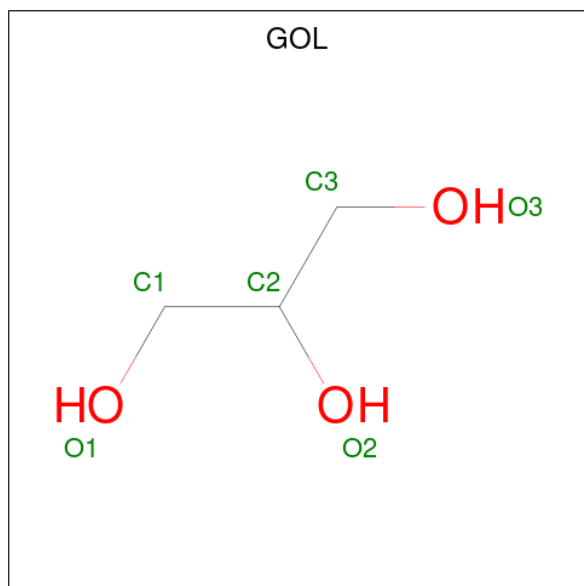
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

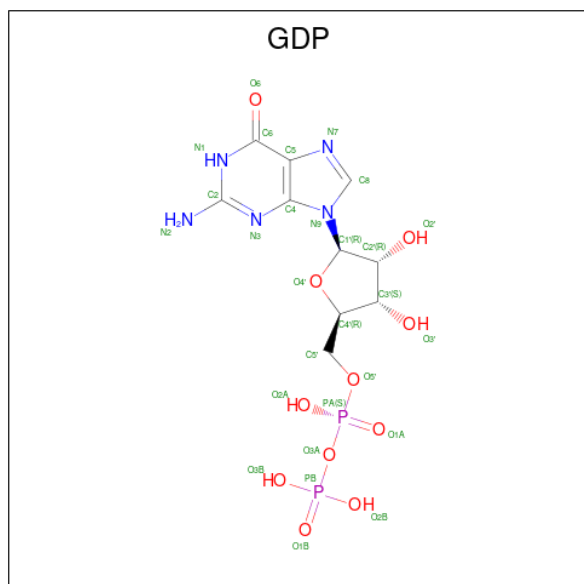
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



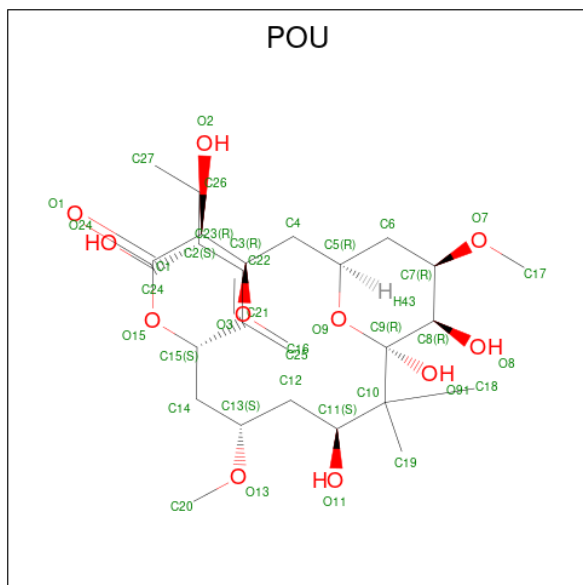
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



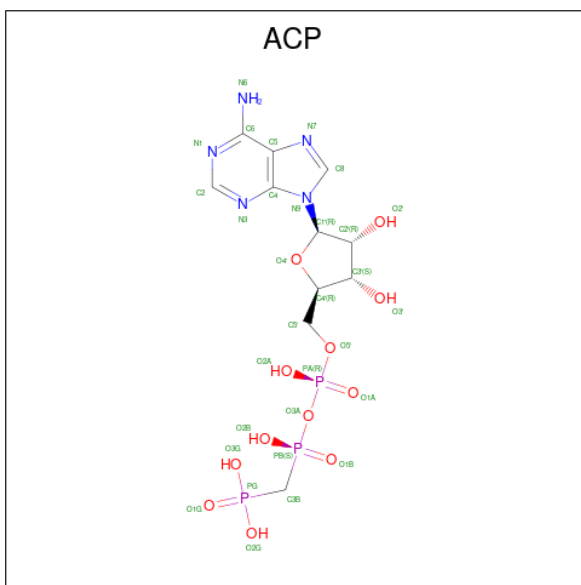
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is Peloruside A (CCD ID: POU) (formula: $C_{27}H_{48}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			38	27	11		
10	D	1	Total	C	O	0	0
			38	27	11		

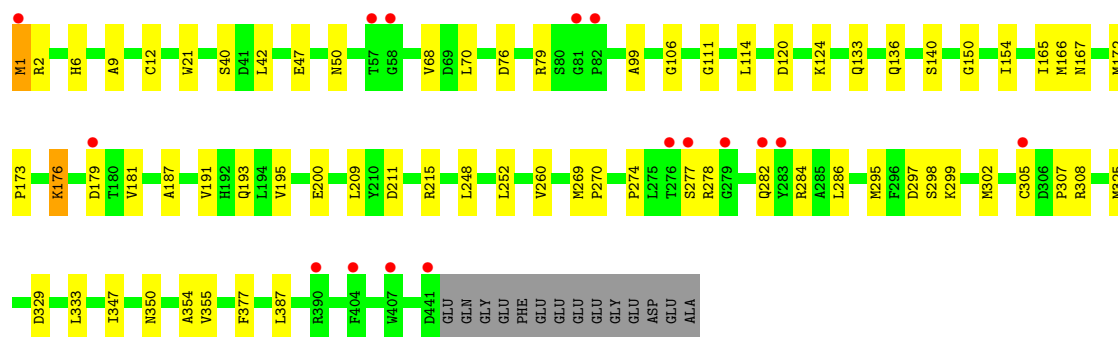
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



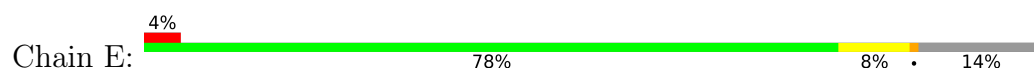
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 12 is water.

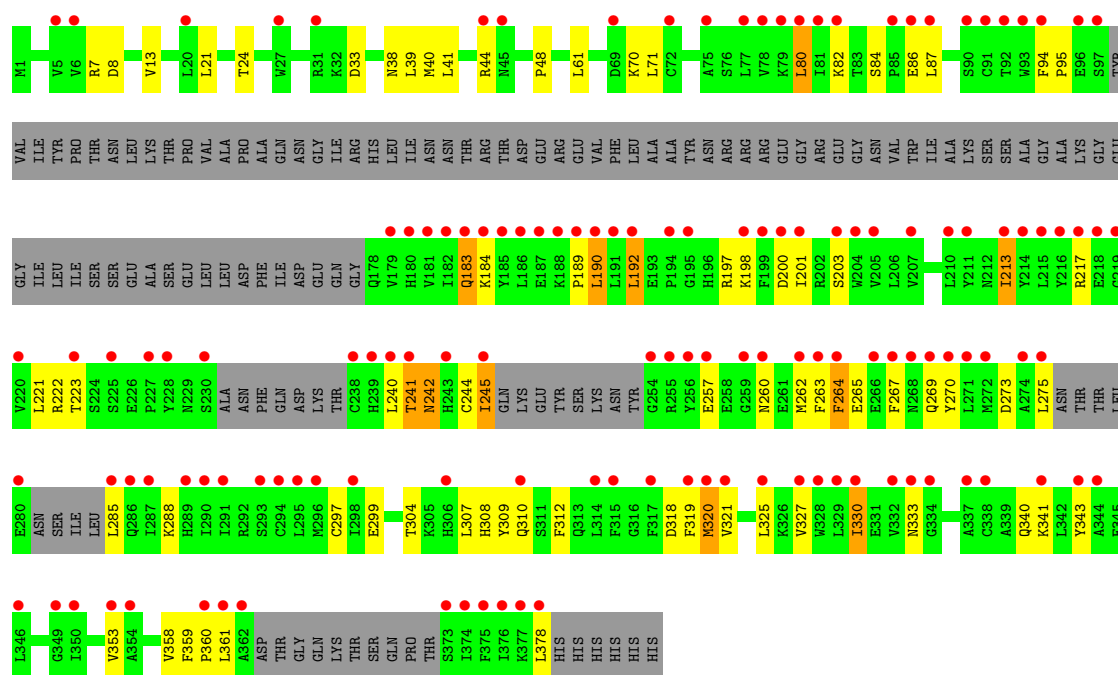
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	191	Total O 191 191	0	0
12	B	210	Total O 210 210	0	0
12	C	264	Total O 264 264	0	0
12	D	116	Total O 116 116	0	0
12	E	43	Total O 43 43	0	0
12	F	21	Total O 21 21	0	0



- 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	104.37Å 157.84Å 180.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.30 – 2.20 72.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.30-2.20) 99.7 (72.30-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.201 , 0.239 0.204 , 0.241	Depositor DCC
R_{free} test set	7568 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	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	0.95	EDS
Total number of atoms	18124	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: CA, GTP, MG, POU, GDP, ACP, GOL

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	0.38	0/3599	0.76	3/4887 (0.1%)
1	C	0.43	0/3619	0.77	1/4917 (0.0%)
2	B	0.40	0/3532	0.75	3/4783 (0.1%)
2	D	0.35	0/3506	0.73	2/4751 (0.0%)
3	E	0.35	0/1071	0.69	0/1423
4	F	0.30	0/2230	0.76	0/3006
All	All	0.38	0/17557	0.75	9/23767 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	ASN	N-CA-C	6.15	120.82	112.88
2	B	260	VAL	N-CA-C	5.37	113.46	108.15
1	A	359	PRO	O-C-N	5.24	123.61	121.15
2	B	56	ALA	CA-C-O	5.22	120.97	117.94
2	D	260	VAL	CA-C-N	5.13	124.83	119.64
2	D	260	VAL	C-N-CA	5.13	124.83	119.64
1	A	262	TYR	CA-C-N	5.12	125.15	119.32
1	A	262	TYR	C-N-CA	5.12	125.15	119.32
1	C	357	TYR	N-CA-C	5.02	117.65	111.82

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	3485	0	3436	19	0
1	C	3496	0	3440	22	0
2	B	3424	0	3319	31	0
2	D	3413	0	3310	39	0
3	E	1044	0	1068	6	0
4	F	2179	0	2178	40	0
5	A	32	0	12	1	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
7	A	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	38	0	48	4	0
10	D	38	0	48	2	0
11	F	31	0	14	1	0
12	A	191	0	0	1	0
12	B	210	0	0	5	0
12	C	264	0	0	4	0
12	D	116	0	0	2	0
12	E	43	0	0	1	0
12	F	21	0	0	0	0
All	All	18124	0	16917	156	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 5.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:ILE:HG22	3:E:10:GLU:HG3	1.70	0.74
1:C:381:THR:HG22	1:C:383:ALA:H	1.51	0.73
2:B:298:SER:HB3	2:B:307:PRO:HD2	1.71	0.71
2:B:22:GLU:OE2	12:B:802:HOH:O	2.09	0.70
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.23	0.70
2:D:176:LYS:NZ	2:D:211:ASP:OD1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.73	0.68
4:F:61[B]:LEU:HG	4:F:310:GLN:HB2	1.76	0.68
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.75	0.68
2:D:2:ARG:HH21	2:D:50:ASN:HB2	1.63	0.64
4:F:318:ASP:HB3	4:F:330:ILE:HD12	1.79	0.64
4:F:321:VAL:HG12	4:F:327:VAL:HG22	1.80	0.62
1:A:356:ASN:ND2	12:A:664:HOH:O	2.31	0.62
1:C:297:GLU:OE2	12:C:755:HOH:O	2.16	0.61
3:E:53:LYS:NZ	12:E:217:HOH:O	2.34	0.60
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.82	0.60
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.59
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.20	0.59
1:A:47:ASP:N	1:A:47:ASP:OD1	2.35	0.58
2:B:217:LEU:O	12:B:795:HOH:O	2.17	0.58
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.49	0.57
4:F:13:VAL:HA	4:F:343:TYR:HE1	1.69	0.57
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.87	0.57
4:F:269:GLN:O	4:F:273:ASP:N	2.32	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.57
4:F:263:PHE:O	4:F:265:GLU:N	2.39	0.56
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.87	0.55
4:F:201:ILE:O	4:F:319:PHE:N	2.32	0.55
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.89	0.55
2:D:325:MET:HE2	2:D:355:VAL:HG21	1.88	0.54
2:B:416:MET:HE3	2:B:420:GLU:HG3	1.89	0.54
4:F:242:ASN:N	4:F:242:ASN:OD1	2.40	0.53
2:B:264:ARG:NE	2:B:431[A]:GLU:OE2	2.34	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.52
2:D:76:ASP:OD1	2:D:79:ARG:NH1	2.40	0.52
4:F:242:ASN:O	4:F:245:ILE:N	2.38	0.52
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.92	0.51
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.92	0.51
4:F:201:ILE:HB	4:F:319:PHE:HB2	1.92	0.51
2:D:215:ARG:NH1	12:D:652:HOH:O	2.40	0.51
1:A:97:GLU:HB2	2:B:1:MET:HG2	1.93	0.50
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.50
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.94	0.50
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.94	0.50
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.49
4:F:190:LEU:HB2	4:F:321:VAL:HG23	1.94	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ALA:HB2	2:B:304:ALA:N	2.26	0.49
2:D:120:ASP:O	2:D:124:LYS:HG2	2.12	0.49
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.94	0.49
2:B:305:CYS:O	2:B:307:PRO:HD3	2.11	0.49
2:B:300:ASN:O	12:B:798:HOH:O	2.20	0.49
4:F:61[A]:LEU:HD11	4:F:312:PHE:HD2	1.77	0.49
4:F:21:LEU:O	4:F:24:THR:OG1	2.28	0.48
1:A:308:ARG:HG2	1:A:340:SER:HB3	1.95	0.48
2:D:173:PRO:HG2	2:D:187:ALA:HB2	1.95	0.48
2:B:42:LEU:HB3	2:B:358:ILE:HD11	1.96	0.48
2:B:226:ASP:HA	2:B:278:ARG:HD2	1.95	0.48
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.53	0.48
2:B:297:ASP:OD1	10:B:503:POU:O2	2.28	0.48
2:B:304:ALA:N	12:B:616:HOH:O	2.46	0.48
1:C:360:PRO:HB2	12:C:787:HOH:O	2.12	0.48
4:F:213:ILE:HB	4:F:378:LEU:HB2	1.96	0.48
12:B:649:HOH:O	3:E:75:LYS:HD2	2.15	0.47
2:B:226:ASP:OD1	2:B:278:ARG:NH2	2.40	0.47
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.96	0.47
2:B:248:LEU:HD11	2:B:352:LYS:HB3	1.96	0.47
1:C:221:ARG:HD2	2:D:329:ASP:OD2	2.15	0.47
2:D:277:SER:O	2:D:278:ARG:HB3	2.14	0.47
2:D:269[A]:MET:HE2	2:D:305:CYS:HB2	1.97	0.47
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.15	0.47
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.30	0.46
1:C:381:THR:HG23	12:C:626:HOH:O	2.15	0.46
4:F:86:GLU:OE2	4:F:297:CYS:HA	2.15	0.46
4:F:257:GLU:HB2	4:F:260:ASN:HA	1.98	0.46
2:D:297:ASP:OD2	2:D:299:LYS:NZ	2.37	0.46
4:F:221:LEU:HD21	4:F:267:PHE:CG	2.50	0.46
4:F:80:LEU:O	4:F:84:SER:OG	2.22	0.46
10:D:503:POU:H27	10:D:503:POU:O15	2.16	0.45
10:D:503:POU:H46	10:D:503:POU:H40	1.80	0.45
3:E:128:LYS:HA	3:E:128:LYS:HD3	1.72	0.45
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.71	0.45
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.99	0.45
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.45
1:A:136[B]:LEU:HD23	1:A:169:PHE:HE2	1.82	0.44
1:A:221:ARG:HG3	2:B:325:MET:HB3	1.99	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.44
11:F:401:ACP:O2G	11:F:401:ACP:O2B	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:HE2	2:D:133:GLN:HA	1.99	0.44
4:F:192:LEU:HA	4:F:270:TYR:CZ	2.53	0.44
1:C:26:LEU:HD12	1:C:363[B]:VAL:HG12	2.00	0.44
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.17	0.44
4:F:61[B]:LEU:CD1	4:F:358:VAL:HG11	2.48	0.44
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
4:F:94:PHE:HA	4:F:95:PRO:HD2	1.88	0.43
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.00	0.43
2:B:33:THR:HG22	2:B:85:GLN:NE2	2.33	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.00	0.43
2:B:275:LEU:HD23	2:B:275:LEU:HA	1.88	0.43
2:D:172:MET:HA	2:D:173:PRO:HD3	1.85	0.43
2:D:305:CYS:SG	2:D:387:LEU:HB2	2.57	0.43
4:F:222:ARG:HB3	4:F:241:THR:OG1	2.17	0.43
2:B:2:ARG:HD2	2:B:130:ASP:HB3	2.00	0.43
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.99	0.43
4:F:61[B]:LEU:HD11	4:F:358:VAL:HG11	1.99	0.43
2:B:192:HIS:CE1	2:B:424:ASN:HD22	2.36	0.43
4:F:40:MET:HE1	4:F:48:PRO:HD2	2.01	0.43
4:F:82:LYS:HE3	4:F:82:LYS:HB2	1.71	0.43
10:B:503:POU:H40	10:B:503:POU:H46	1.91	0.43
4:F:8:ASP:OD2	4:F:44:ARG:NH1	2.52	0.43
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.00	0.43
1:C:209:ILE:HD11	1:C:302:MET:HG3	2.00	0.43
2:D:40:SER:OG	2:D:42:LEU:HB2	2.19	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.43
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.01	0.42
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.53	0.42
1:C:97:GLU:HG3	2:D:1:MET:HB2	2.02	0.42
1:C:107:HIS:O	3:E:105:MET:HE1	2.18	0.42
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.55	0.42
2:D:333:LEU:HG	12:D:642:HOH:O	2.20	0.42
1:C:347[A]:CYS:HA	1:C:348:PRO:HD3	1.93	0.42
4:F:320:MET:HB3	4:F:320:MET:HE2	1.69	0.42
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.50	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.19	0.42
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.02	0.42
2:D:150:GLY:O	2:D:154:ILE:HG12	2.20	0.42
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.55	0.42
1:A:298:PRO:HA	1:A:301:GLN:CD	2.45	0.42
2:B:2:ARG:HG3	2:B:3:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:330:ILE:H	4:F:330:ILE:HG13	1.64	0.42
1:C:194[B]:THR:HG21	12:C:617:HOH:O	2.19	0.42
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.02	0.42
1:A:311:LYS:HD3	1:A:344:VAL:HA	2.02	0.41
2:B:124:LYS:HB2	2:B:124:LYS:HE3	1.86	0.41
10:B:503:POU:H27	10:B:503:POU:O15	2.20	0.41
2:D:295:MET:HE3	2:D:295:MET:HB2	1.71	0.41
4:F:358:VAL:O	4:F:360:PRO:HD3	2.21	0.41
1:C:221:ARG:HD3	2:D:325:MET:SD	2.61	0.41
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.03	0.41
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.21	0.41
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.37	0.41
2:D:298:SER:OG	2:D:307:PRO:HD2	2.21	0.41
4:F:84:SER:OG	4:F:87:LEU:HB3	2.20	0.41
2:D:9:ALA:HA	2:D:68:VAL:O	2.21	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.04	0.40
10:B:503:POU:H32	10:B:503:POU:H8	1.89	0.40
4:F:183:GLN:HG2	4:F:184:LYS:N	2.36	0.40
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.21	0.40
2:B:369:ARG:HE	2:B:369:ARG:HB2	1.49	0.40
1:A:346:TRP:CD1	1:A:346:TRP:H	2.39	0.40
2:D:70:LEU:HD23	2:D:114:LEU:HD22	2.02	0.40
2:D:274:PRO:HB3	2:D:286:LEU:HD21	2.03	0.40
2:D:297:ASP:OD1	2:D:298:SER:N	2.55	0.40
4:F:318:ASP:HB2	4:F:330:ILE:O	2.21	0.40
4:F:307:LEU:HD13	4:F:309:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/451 (100%)	440 (98%)	9 (2%)	0	100	100
1	C	453/451 (100%)	441 (97%)	12 (3%)	0	100	100
2	B	438/445 (98%)	430 (98%)	8 (2%)	0	100	100
2	D	435/445 (98%)	421 (97%)	14 (3%)	0	100	100
3	E	125/143 (87%)	123 (98%)	2 (2%)	0	100	100
4	F	253/384 (66%)	239 (94%)	12 (5%)	2 (1%)	16	16
All	All	2153/2319 (93%)	2094 (97%)	57 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	264	PHE
4	F	189	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/379 (101%)	371 (97%)	11 (3%)	37	51
1	C	386/379 (102%)	382 (99%)	4 (1%)	68	81
2	B	382/383 (100%)	373 (98%)	9 (2%)	43	58
2	D	378/383 (99%)	368 (97%)	10 (3%)	40	55
3	E	116/127 (91%)	110 (95%)	6 (5%)	21	26
4	F	241/342 (70%)	210 (87%)	31 (13%)	4	4
All	All	1885/1993 (95%)	1814 (96%)	71 (4%)	28	40

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

Mol	Chain	Res	Type
1	A	2	ARG
1	A	38	SER
1	A	41	THR

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Mol	Chain	Res	Type
1	A	47	ASP
1	A	88	HIS
1	A	90	GLU
1	A	124	LYS
1	A	188	ILE
1	A	234	ILE
1	A	336	LYS
1	A	381	THR
2	B	42	LEU
2	B	57	THR
2	B	177	VAL
2	B	200	GLU
2	B	298	SER
2	B	300	ASN
2	B	308	ARG
2	B	325	MET
2	B	369	ARG
1	C	215	ARG
1	C	221	ARG
1	C	297	GLU
1	C	384	ILE
2	D	1	MET
2	D	47	GLU
2	D	176	LYS
2	D	179	ASP
2	D	181	VAL
2	D	200	GLU
2	D	209	LEU
2	D	282	GLN
2	D	284	ARG
2	D	308	ARG
3	E	22	VAL
3	E	48	GLU
3	E	49	GLU
3	E	103	GLN
3	E	105	MET
3	E	135	LYS
4	F	33	ASP
4	F	70	LYS
4	F	71	LEU
4	F	80	LEU
4	F	183	GLN

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Mol	Chain	Res	Type
4	F	190	LEU
4	F	192	LEU
4	F	198	LYS
4	F	203	SER
4	F	213	ILE
4	F	217	ARG
4	F	223	THR
4	F	240	LEU
4	F	241	THR
4	F	242	ASN
4	F	244	CYS
4	F	245	ILE
4	F	264	PHE
4	F	275	LEU
4	F	285	LEU
4	F	288	LYS
4	F	299	GLU
4	F	308	HIS
4	F	320	MET
4	F	325	LEU
4	F	330	ILE
4	F	333	ASN
4	F	340	GLN
4	F	341	LYS
4	F	353	VAL
4	F	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	258	ASN
1	A	301	GLN
2	B	336	GLN
1	C	50	ASN
2	D	50	ASN
2	D	229	HIS
2	D	339	ASN
3	E	12	ASN
3	E	64	GLN
4	F	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GTP	C	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.50	9 (18%)
5	GTP	A	501	6	33,34,34	1.17	3 (9%)	50,54,54	1.51	10 (20%)
9	GDP	B	501	6	29,30,30	1.21	3 (10%)	45,47,47	1.82	8 (17%)
9	GDP	D	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.67	6 (13%)
10	POU	D	503	-	38,39,39	2.15	6 (15%)	44,57,57	1.96	9 (20%)
8	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.31	0
11	ACP	F	401	-	31,33,33	1.71	9 (29%)	47,52,52	1.96	12 (25%)
10	POU	B	503	-	38,39,39	2.31	8 (21%)	44,57,57	2.12	10 (22%)

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
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
9	GDP	D	501	-	-	3/16/32/32	0/3/3/3
10	POU	D	503	-	-	7/54/76/76	0/1/2/2
8	GOL	A	504	-	-	4/4/4/4	-
11	ACP	F	401	-	-	10/19/38/38	0/3/3/3
10	POU	B	503	-	-	6/54/76/76	0/1/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	POU	C22-C21	10.46	1.56	1.33
10	D	503	POU	C22-C21	9.35	1.54	1.33
10	B	503	POU	C2-C1	-5.27	1.39	1.52
10	D	503	POU	C2-C1	-5.11	1.39	1.52
11	F	401	ACP	C5-C4	4.76	1.47	1.39
10	D	503	POU	C14-C15	4.37	1.60	1.53
5	A	501	GTP	PA-O3A	3.37	1.63	1.59
5	A	501	GTP	PB-O3A	3.08	1.62	1.59
9	D	501	GDP	C5-C4	3.04	1.47	1.38
11	F	401	ACP	PB-O3A	3.01	1.61	1.58
11	F	401	ACP	PG-O2G	2.99	1.61	1.55
9	B	501	GDP	C5-C4	2.97	1.46	1.38
10	D	503	POU	C14-C13	2.90	1.59	1.52
10	B	503	POU	O91-C9	2.87	1.44	1.39
10	D	503	POU	O91-C9	2.85	1.44	1.39
11	F	401	ACP	PG-O3G	2.84	1.61	1.55
11	F	401	ACP	C5-C6	2.72	1.48	1.41
11	F	401	ACP	PA-O3A	2.62	1.62	1.59
9	B	501	GDP	C6-N1	-2.61	1.34	1.38
10	B	503	POU	C23-C22	2.60	1.54	1.49
5	C	501	GTP	PB-O3B	2.56	1.62	1.59
9	B	501	GDP	PA-O3A	2.49	1.62	1.59
11	F	401	ACP	C8-N7	2.47	1.36	1.31
9	D	501	GDP	C6-N1	-2.34	1.34	1.38
10	B	503	POU	C14-C15	2.33	1.56	1.53
10	B	503	POU	C14-C13	2.29	1.57	1.52
10	D	503	POU	C23-C22	2.26	1.53	1.49
10	B	503	POU	O11-C11	2.20	1.47	1.43
11	F	401	ACP	C5-N7	-2.19	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O2B	2.16	1.61	1.56
10	B	503	POU	C9-C8	-2.10	1.51	1.53
5	A	501	GTP	C2-N3	2.06	1.38	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	POU	C13-C12-C11	-6.52	104.62	114.42
10	D	503	POU	C13-C12-C11	-6.28	104.98	114.42
9	B	501	GDP	C5-C4-N3	-6.19	118.54	128.39
11	F	401	ACP	C5-C4-N3	-5.78	118.76	126.72
10	B	503	POU	C15-O15-C1	5.76	126.93	116.58
9	D	501	GDP	C5-C4-N3	-5.52	119.60	128.39
10	B	503	POU	O9-C9-C8	5.20	112.89	105.25
9	B	501	GDP	C2-N3-C4	4.99	120.89	112.30
10	D	503	POU	O9-C9-C8	4.78	112.27	105.25
9	B	501	GDP	N9-C4-N3	4.74	135.42	125.95
11	F	401	ACP	C2'-C1'-N9	-4.62	101.83	113.30
9	D	501	GDP	C2-N3-C4	4.59	120.21	112.30
10	D	503	POU	C15-O15-C1	4.57	124.79	116.58
5	C	501	GTP	C5-C4-N3	-4.25	121.63	128.39
11	F	401	ACP	N3-C4-N9	4.24	134.38	127.17
5	C	501	GTP	C2-N3-C4	4.18	119.50	112.30
9	D	501	GDP	N9-C4-N3	4.13	134.21	125.95
11	F	401	ACP	C4-C5-N7	-3.79	106.25	110.58
5	A	501	GTP	C5-C4-N3	-3.77	122.39	128.39
10	B	503	POU	O15-C15-C21	3.70	119.58	109.59
5	A	501	GTP	C2-N3-C4	3.67	118.62	112.30
11	F	401	ACP	C2-N3-C4	3.62	120.67	111.83
10	D	503	POU	C3-C4-C5	-3.54	106.62	114.70
10	D	503	POU	O15-C15-C14	3.45	113.87	106.65
9	D	501	GDP	C6-C5-N7	3.43	136.54	130.29
9	B	501	GDP	C6-C5-N7	3.31	136.31	130.29
11	F	401	ACP	N3-C2-N1	-3.30	123.58	128.58
5	A	501	GTP	N9-C8-N7	-3.21	107.45	113.40
11	F	401	ACP	PB-O3A-PA	-3.19	121.97	132.37
10	B	503	POU	O15-C15-C14	3.08	113.09	106.65
10	B	503	POU	C3-C4-C5	-3.05	107.72	114.70
5	C	501	GTP	C2-N1-C6	-2.90	119.85	125.11
11	F	401	ACP	C5-N7-C8	2.68	107.66	103.45
10	D	503	POU	O15-C15-C21	2.67	116.81	109.59
5	C	501	GTP	O6-C6-C5	-2.65	119.54	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C8-N7-C5	2.64	108.97	104.26
5	C	501	GTP	N9-C4-N3	2.64	131.23	125.95
9	B	501	GDP	C4-C5-N7	-2.63	106.50	110.67
9	D	501	GDP	C4-C5-N7	-2.61	106.53	110.67
5	C	501	GTP	N9-C8-N7	-2.58	108.62	113.40
5	A	501	GTP	O2G-PG-O3B	2.57	113.25	104.64
10	D	503	POU	O91-C9-O9	-2.53	103.20	109.47
5	C	501	GTP	O2A-PA-O3A	2.50	114.04	107.27
5	C	501	GTP	C5-C6-N1	2.48	119.58	113.25
5	A	501	GTP	O5'-PA-O1A	-2.44	99.27	108.94
5	A	501	GTP	N9-C4-N3	2.39	130.74	125.95
11	F	401	ACP	C6-C5-N7	2.39	136.70	132.09
10	B	503	POU	C4-C3-C2	-2.33	108.00	113.26
10	B	503	POU	C25-C21-C22	-2.32	117.60	123.56
9	B	501	GDP	O2A-PA-O3A	2.31	113.51	107.27
10	B	503	POU	O91-C9-O9	-2.23	103.94	109.47
11	F	401	ACP	O4'-C1'-N9	2.22	112.35	108.09
11	F	401	ACP	C4-N9-C8	2.19	108.04	105.74
9	B	501	GDP	O6-C6-C5	-2.19	120.75	126.53
10	B	503	POU	O9-C5-C6	2.17	112.84	109.02
11	F	401	ACP	C2'-C3'-C4'	-2.16	98.44	102.61
10	D	503	POU	O9-C5-C6	2.15	112.80	109.02
5	A	501	GTP	O2B-PB-O3A	2.12	112.99	107.27
9	D	501	GDP	O6-C6-C5	-2.11	120.97	126.53
5	A	501	GTP	C2-N1-C6	-2.10	121.30	125.11
9	B	501	GDP	C8-N7-C5	2.06	107.92	104.26
5	C	501	GTP	O2B-PB-O3A	2.06	112.83	107.27
5	A	501	GTP	C5-C6-N1	2.05	118.48	113.25
10	D	503	POU	C13-C14-C15	-2.04	109.87	114.49

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
8	A	504	GOL	O1-C1-C2-O2
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	C1-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O3A

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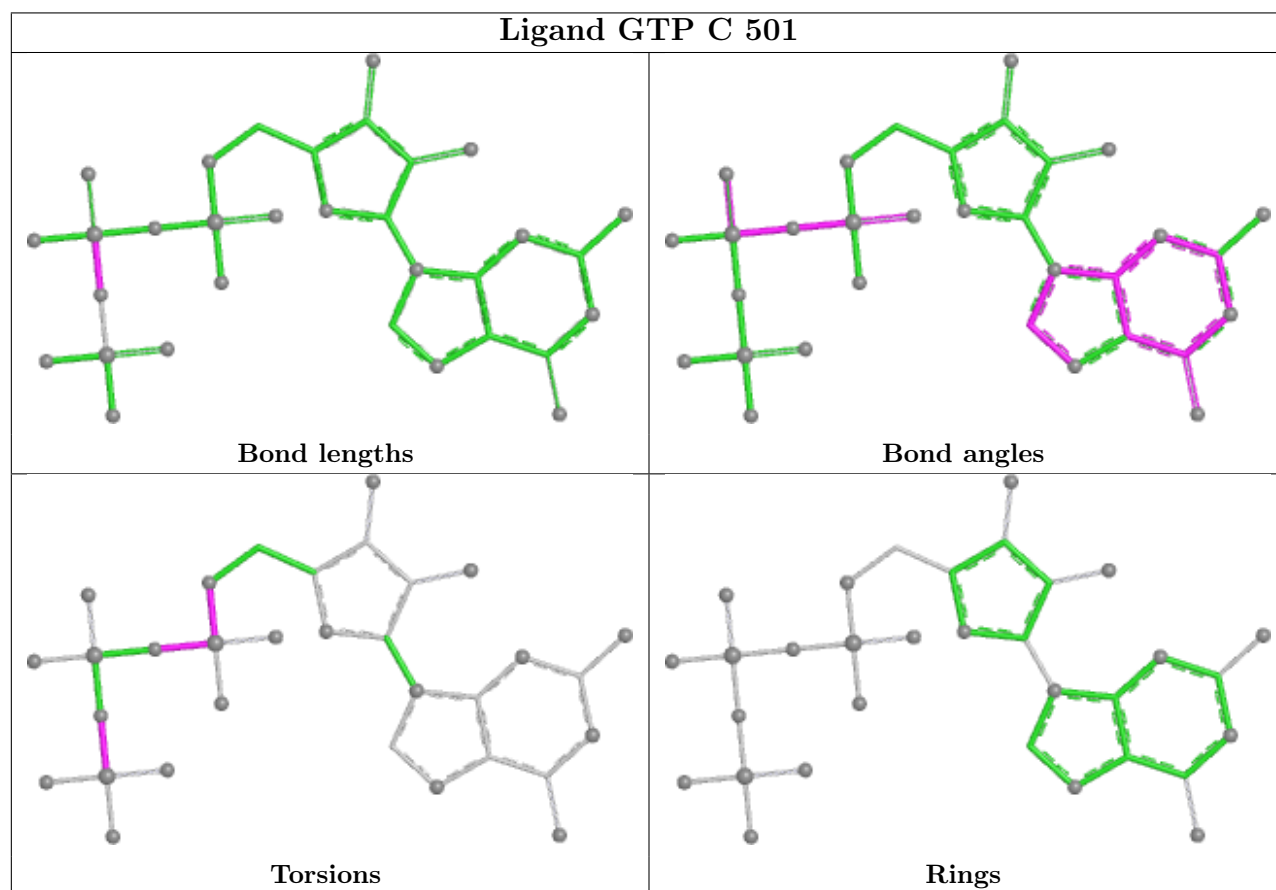
Mol	Chain	Res	Type	Atoms
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
10	B	503	POU	C15-C21-C22-C23
10	D	503	POU	C15-C21-C22-C23
8	A	504	GOL	O2-C2-C3-O3
10	B	503	POU	C25-C21-C22-C23
10	D	503	POU	C25-C21-C22-C23
10	B	503	POU	C8-C7-O7-C17
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
10	D	503	POU	C6-C7-O7-C17
10	D	503	POU	C8-C7-O7-C17
10	D	503	POU	C21-C15-O15-C1
5	A	501	GTP	PB-O3B-PG-O1G
10	B	503	POU	C14-C13-O13-C20
10	D	503	POU	C12-C13-O13-C20
10	B	503	POU	C2-C3-O3-C16
10	D	503	POU	C2-C3-O3-C16
9	B	501	GDP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	503	POU	C6-C7-O7-C17
5	C	501	GTP	PB-O3A-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'

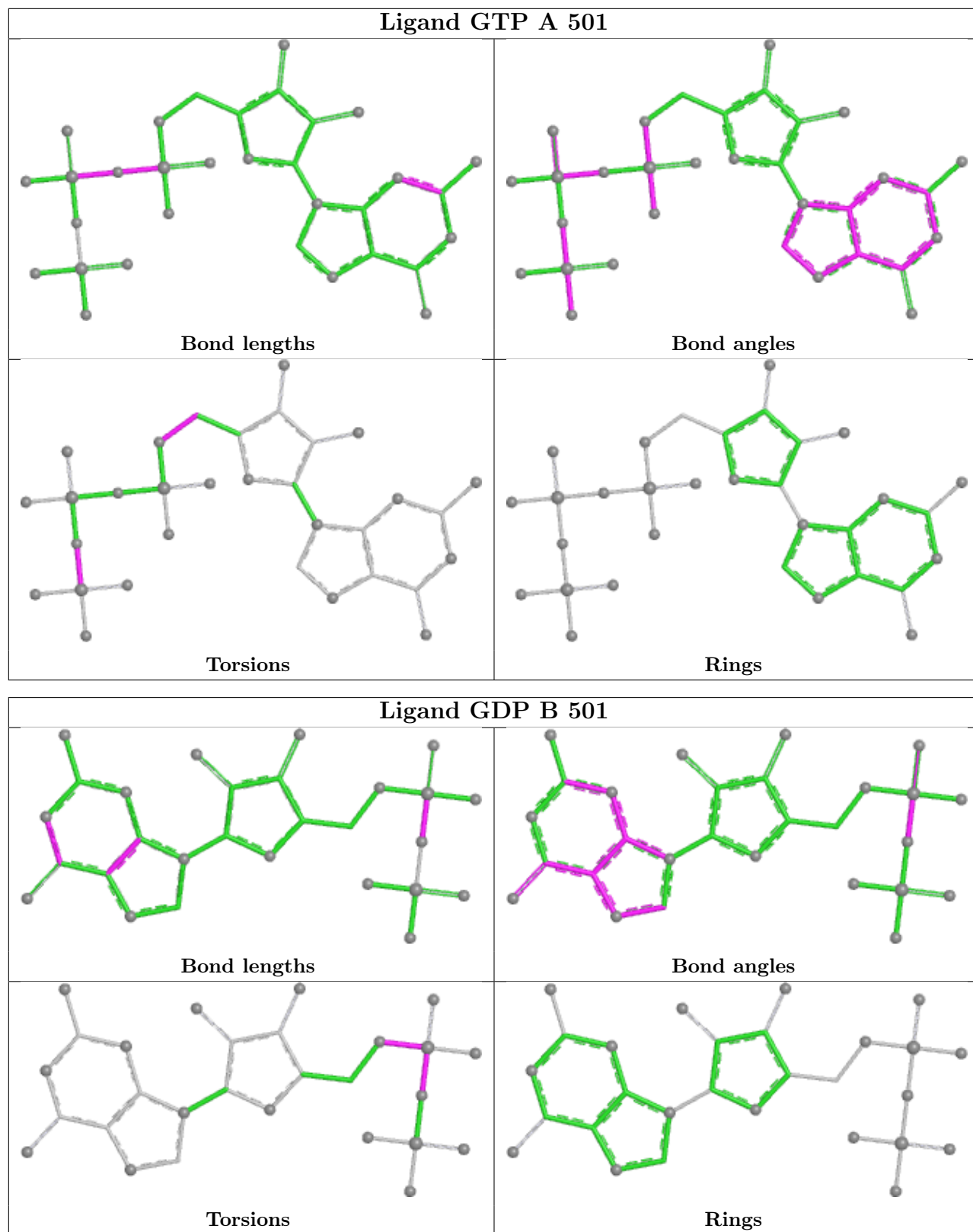
There are no ring outliers.

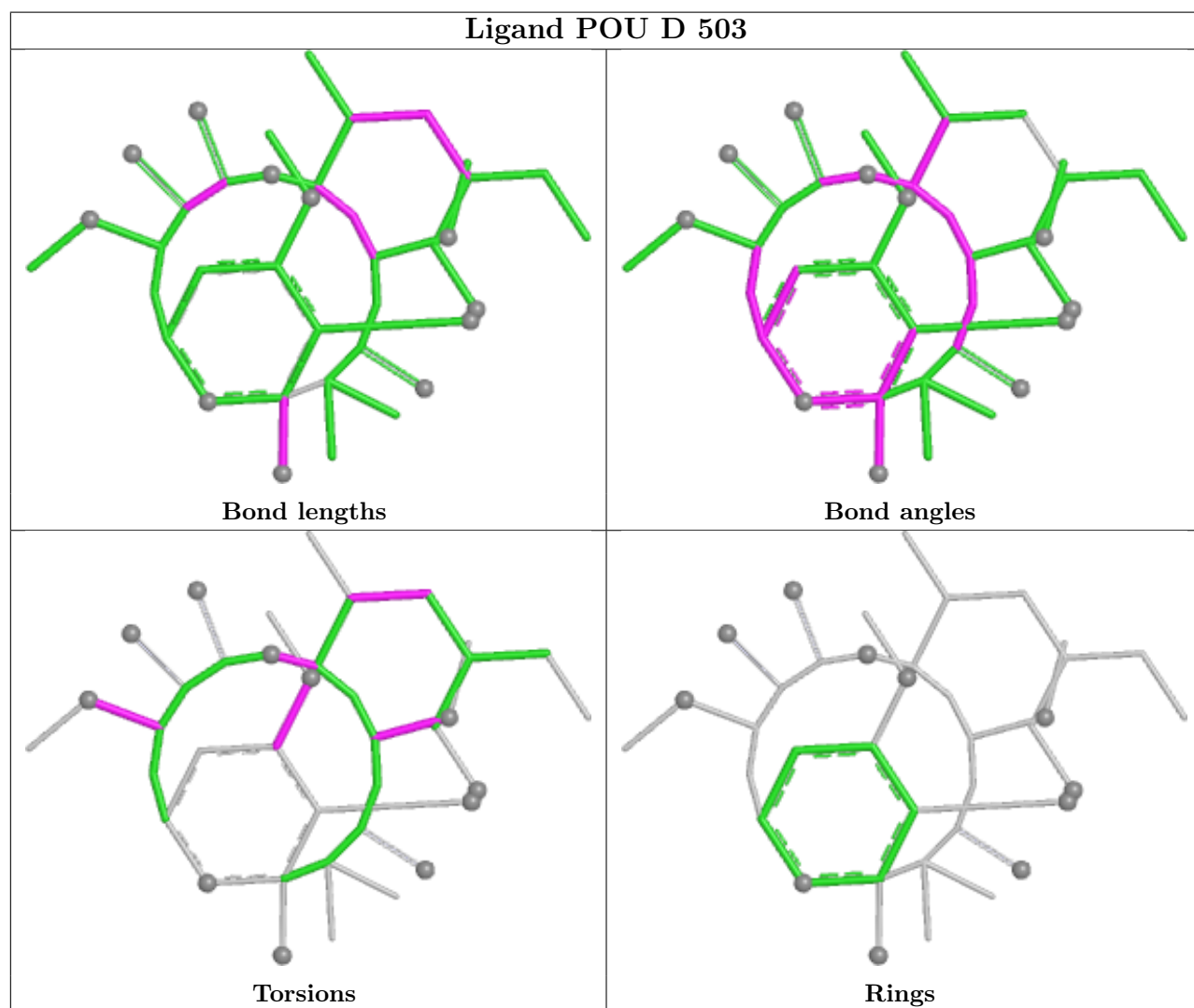
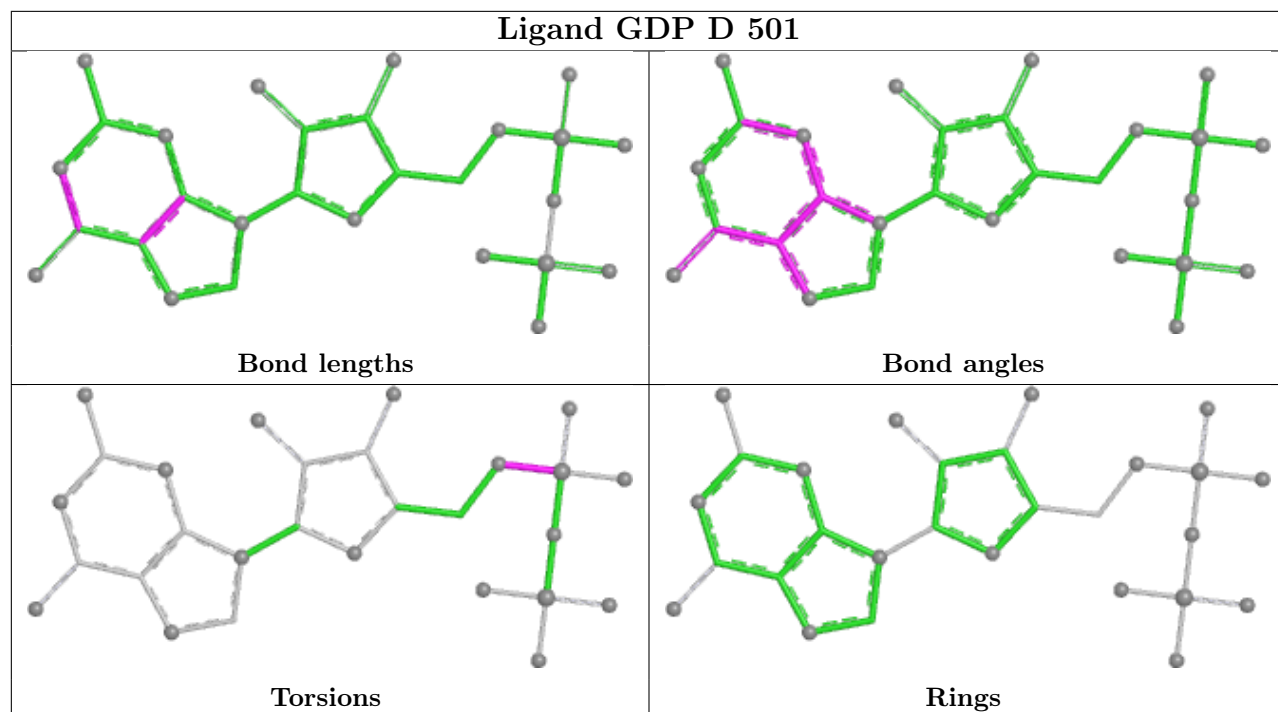
4 monomers are involved in 8 short contacts:

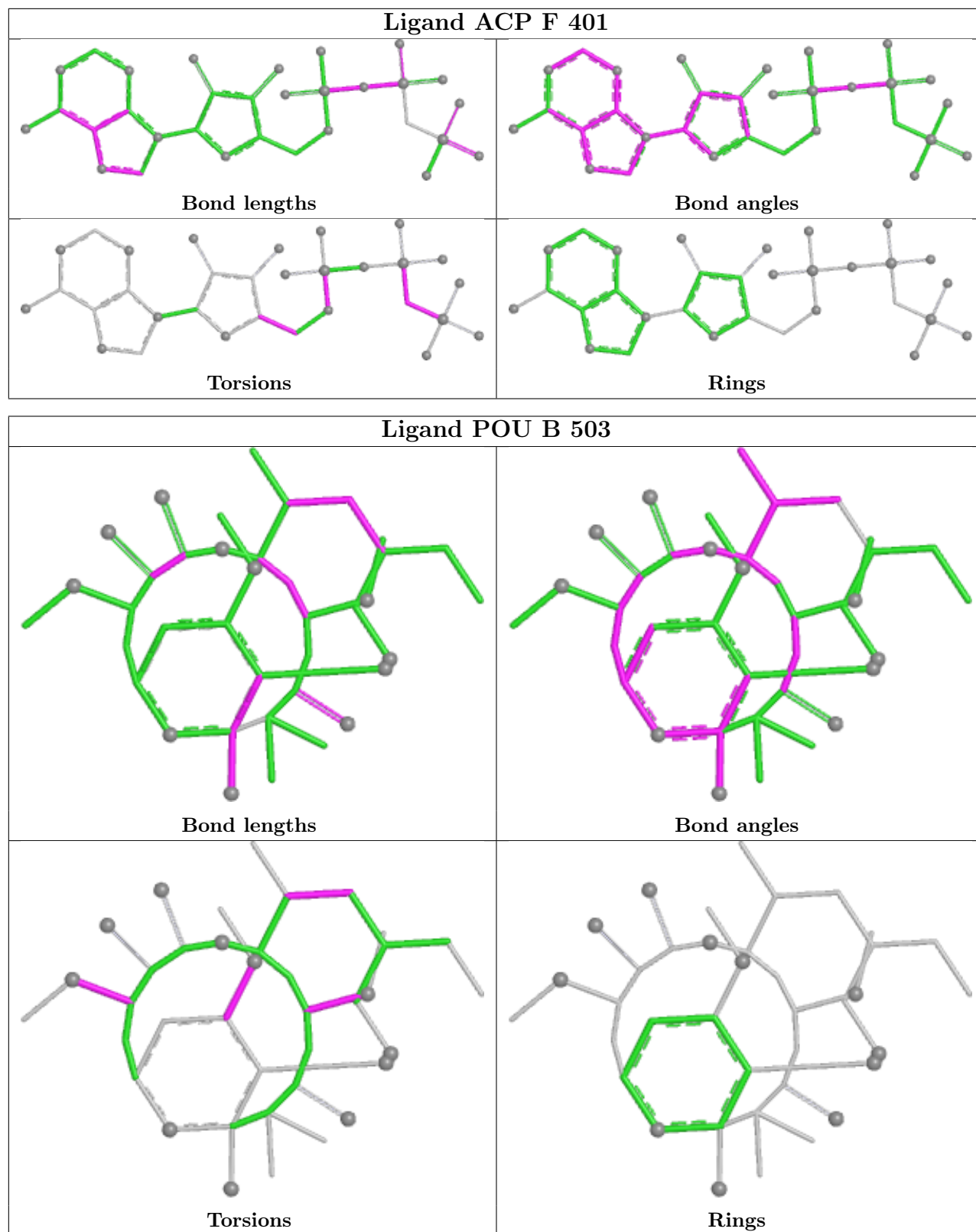
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
10	D	503	POU	2	0
11	F	401	ACP	1	0
10	B	503	POU	4	0

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	439/451 (97%)	-0.29	7 (1%) 70 67	15, 32, 66, 112	12 (2%)
1	C	440/451 (97%)	-0.59	8 (1%) 67 64	10, 22, 45, 68	15 (3%)
2	B	428/445 (96%)	-0.36	7 (1%) 70 67	11, 27, 58, 112	14 (3%)
2	D	431/445 (96%)	0.11	16 (3%) 45 42	18, 44, 77, 102	12 (2%)
3	E	123/143 (86%)	0.29	6 (4%) 35 31	18, 44, 85, 121	6 (4%)
4	F	265/384 (69%)	2.16	136 (51%) 0 0	34, 79, 123, 153	1 (0%)
All	All	2126/2319 (91%)	0.06	180 (8%) 16 14	10, 35, 92, 153	60 (2%)

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	7.5
2	D	1	MET	6.0
3	E	143	ALA	5.8
4	F	271	LEU	5.4
4	F	275	LEU	5.4
4	F	179	VAL	5.3
4	F	191	LEU	5.1
4	F	375	PHE	5.1
4	F	337	ALA	5.0
1	A	282	TYR	5.0
4	F	321	VAL	5.0
4	F	330	ILE	5.0
4	F	285	LEU	5.0
4	F	199	PHE	4.9
4	F	186	LEU	4.8
4	F	203	SER	4.7
4	F	291	ILE	4.5
4	F	319	PHE	4.4
4	F	213	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	4.4
4	F	240	LEU	4.4
4	F	280	GLU	4.4
4	F	241	THR	4.3
4	F	256	TYR	4.3
4	F	97	SER	4.3
4	F	362	ALA	4.3
4	F	254	GLY	4.1
4	F	290	ILE	4.1
4	F	374	ILE	4.1
4	F	264	PHE	4.0
4	F	327	VAL	4.0
4	F	192	LEU	4.0
4	F	189	PRO	3.9
4	F	354	ALA	3.9
4	F	329	LEU	3.8
2	B	438	ALA	3.8
1	A	281	ALA	3.7
4	F	183	GLN	3.7
4	F	296	MET	3.7
4	F	350	ILE	3.7
4	F	267	PHE	3.6
4	F	205	VAL	3.6
4	F	287	ILE	3.6
4	F	201	ILE	3.6
2	B	282	GLN	3.5
4	F	338	CYS	3.5
2	B	1	MET	3.5
4	F	230	SER	3.5
4	F	216	TYR	3.5
4	F	190	LEU	3.5
4	F	90	SER	3.4
4	F	325	LEU	3.4
4	F	270	TYR	3.4
4	F	181	VAL	3.4
4	F	78	VAL	3.4
4	F	268	ASN	3.3
4	F	298	ILE	3.3
4	F	346	LEU	3.3
2	D	276	THR	3.3
4	F	377	LYS	3.3
1	C	440	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	320	MET	3.2
4	F	75	ALA	3.2
4	F	211	TYR	3.2
4	F	344	ALA	3.2
4	F	77	LEU	3.1
4	F	245	ILE	3.1
4	F	198	LYS	3.1
2	B	281	GLN	3.1
4	F	185	TYR	3.1
4	F	255	ARG	3.1
4	F	228	TYR	3.0
4	F	94	PHE	3.0
4	F	204	TRP	3.0
4	F	243	HIS	3.0
4	F	260	ASN	3.0
4	F	266	GLU	3.0
4	F	87	LEU	2.9
4	F	238	CYS	2.9
2	D	283	TYR	2.9
2	D	58	GLY	2.9
4	F	263	PHE	2.9
4	F	328	TRP	2.9
4	F	376	ILE	2.9
4	F	184	LYS	2.9
4	F	5	VAL	2.9
4	F	341	LYS	2.8
4	F	214	TYR	2.8
4	F	315	PHE	2.8
4	F	200	ASP	2.8
3	E	28	SER	2.8
4	F	215	LEU	2.8
4	F	239	HIS	2.8
2	D	404	PHE	2.8
4	F	219	GLY	2.8
2	D	407	TRP	2.7
4	F	360	PRO	2.7
4	F	262	MET	2.7
4	F	378	LEU	2.7
4	F	317	PHE	2.7
4	F	306	HIS	2.7
2	D	279	GLY	2.7
1	A	283	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	349	GLY	2.7
4	F	44	ARG	2.7
4	F	333	ASN	2.6
4	F	223	THR	2.6
4	F	272	MET	2.6
4	F	289	HIS	2.6
4	F	217	ARG	2.6
2	D	82	PRO	2.6
4	F	93	TRP	2.6
4	F	373	SER	2.6
1	C	285	GLN	2.5
4	F	86	GLU	2.5
4	F	187	GLU	2.5
4	F	259	GLY	2.5
1	A	262	TYR	2.5
4	F	227	PRO	2.5
2	D	277	SER	2.5
4	F	353	VAL	2.5
4	F	207	VAL	2.4
4	F	332	VAL	2.4
4	F	286	GLN	2.4
4	F	188	LYS	2.4
4	F	80	LEU	2.4
4	F	210	LEU	2.4
1	C	245	ASP	2.4
2	D	390	ARG	2.4
4	F	218	GLU	2.4
1	C	43	GLY	2.4
4	F	361	LEU	2.4
2	D	81	GLY	2.4
3	E	139	LEU	2.4
4	F	91	CYS	2.3
1	A	439	SER	2.3
3	E	6	MET	2.3
4	F	225	SER	2.3
4	F	81	ILE	2.3
4	F	20	LEU	2.3
4	F	295	LEU	2.3
4	F	27	TRP	2.3
2	D	441	ASP	2.2
4	F	96	GLU	2.2
4	F	180	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	163	LYS	2.2
2	D	57	THR	2.2
4	F	274	ALA	2.2
1	C	357	TYR	2.2
4	F	220	VAL	2.2
4	F	45	ASN	2.2
4	F	310	GLN	2.2
2	B	280	SER	2.2
4	F	92	THR	2.2
4	F	343	TYR	2.2
4	F	69	ASP	2.2
4	F	82	LYS	2.2
2	D	282	GLN	2.2
4	F	334	GLY	2.2
2	D	305	CYS	2.2
4	F	314	LEU	2.1
2	D	179	ASP	2.1
4	F	294	CYS	2.1
4	F	31	ARG	2.1
4	F	79	LYS	2.1
3	E	7	GLU	2.1
4	F	6	VAL	2.1
2	B	58	GLY	2.1
4	F	293	SER	2.1
1	A	284	GLU	2.1
1	C	46	ASP	2.1
4	F	269	GLN	2.1
3	E	27	PRO	2.1
4	F	85	PRO	2.1
4	F	72	CYS	2.0
2	B	284	ARG	2.0
4	F	195	GLY	2.0
1	C	340	SER	2.0
4	F	257	GLU	2.0
1	A	329	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

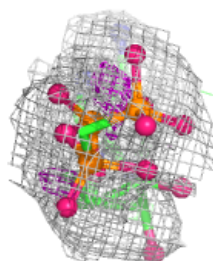
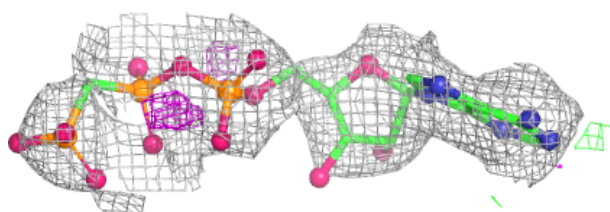
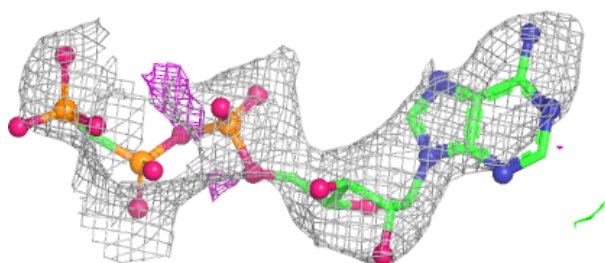
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ACP	F	401	31/31	0.70	0.15	67,106,145,166	0
6	MG	D	502	1/1	0.73	0.28	67,67,67,67	0
8	GOL	A	504	6/6	0.83	0.17	57,60,60,62	0
10	POU	D	503	38/38	0.84	0.14	35,59,74,77	0
10	POU	B	503	38/38	0.85	0.13	23,44,77,81	0
7	CA	A	503	1/1	0.87	0.11	68,68,68,68	0
9	GDP	D	501	28/28	0.95	0.08	27,36,45,53	0
6	MG	C	502	1/1	0.96	0.04	18,18,18,18	0
5	GTP	A	501	32/32	0.98	0.05	10,17,22,41	0
6	MG	A	502	1/1	0.99	0.02	14,14,14,14	0
6	MG	B	502	1/1	0.99	0.02	9,9,9,9	0
5	GTP	C	501	32/32	0.99	0.03	4,13,19,30	0
9	GDP	B	501	28/28	0.99	0.04	11,16,20,22	0

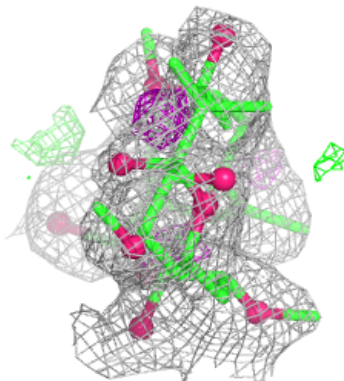
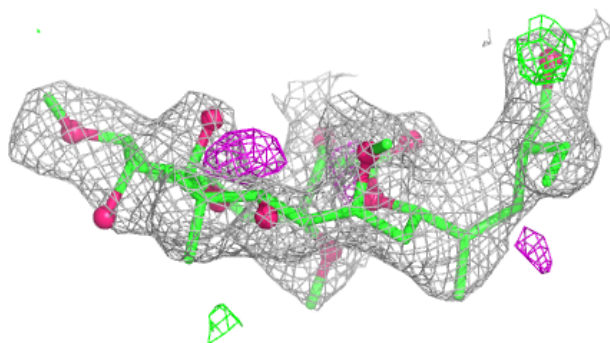
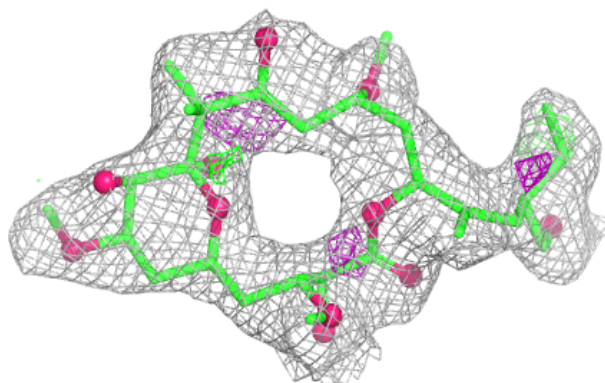
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

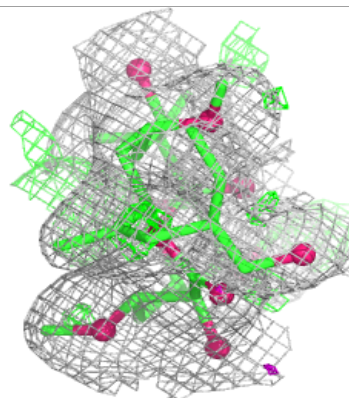
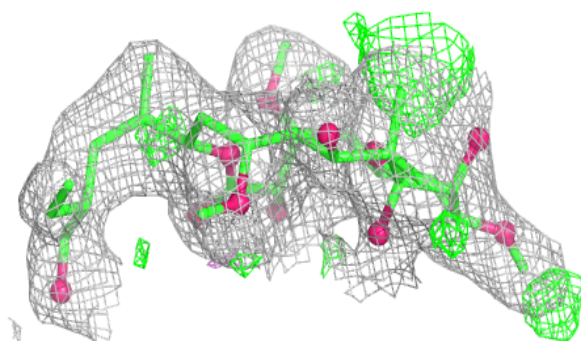
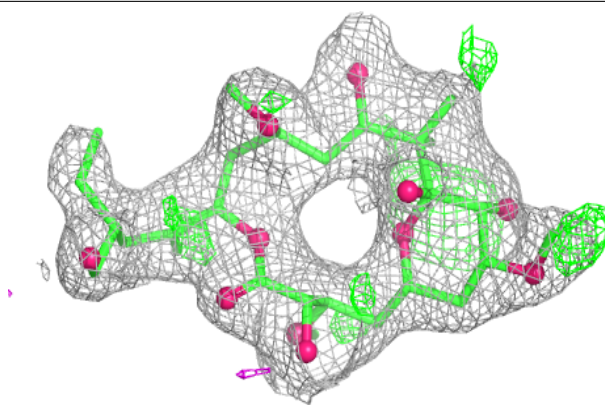
**Electron density around POU D 503:**

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



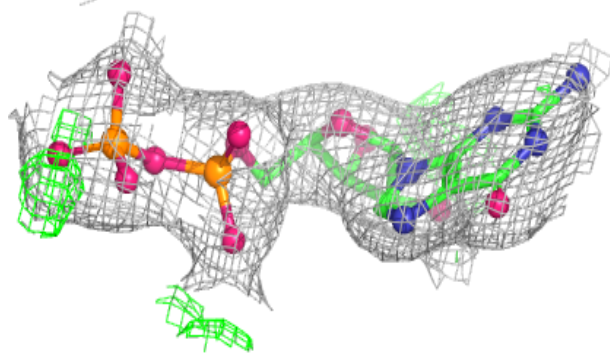
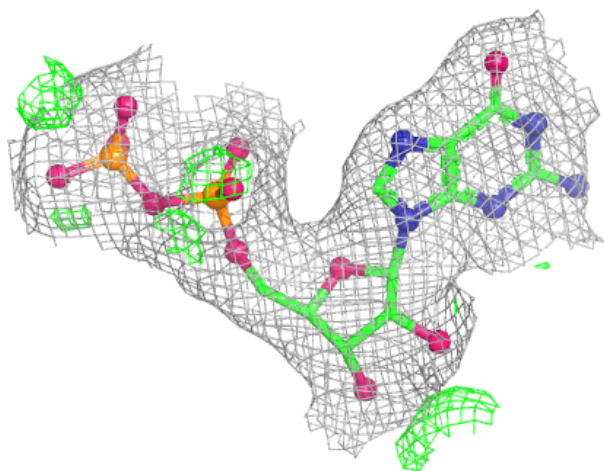
Electron density around POU B 503:

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



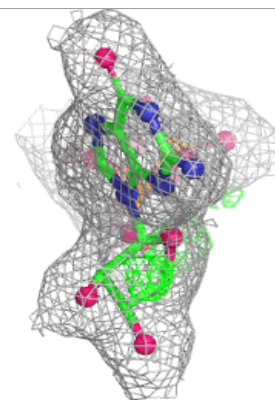
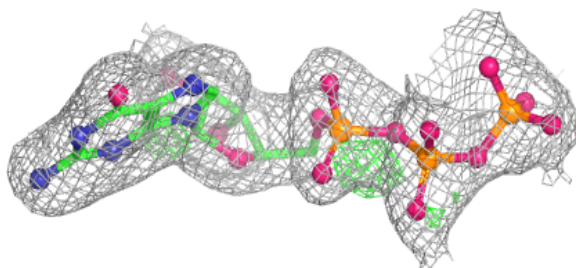
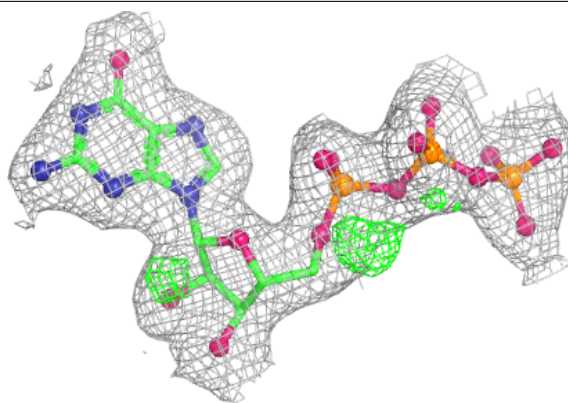
Electron density around GDP D 501:

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

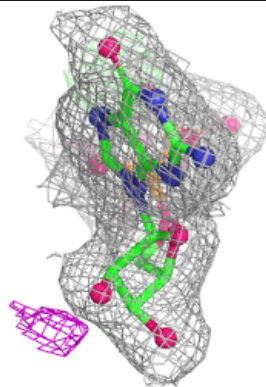
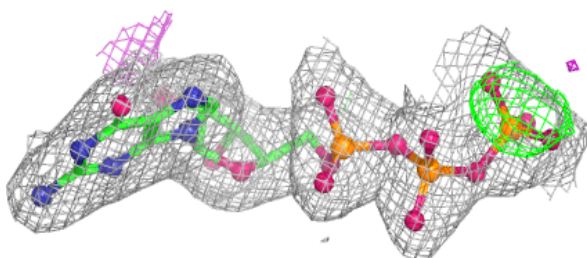
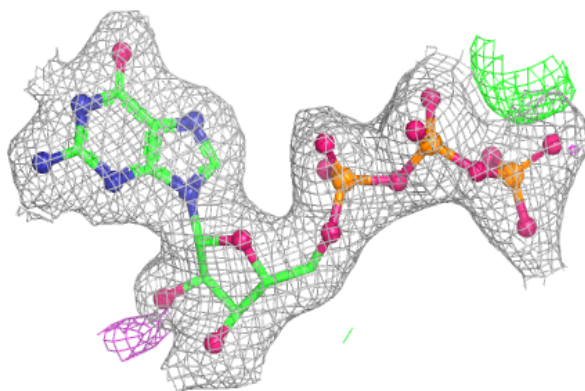


Electron density around GTP A 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

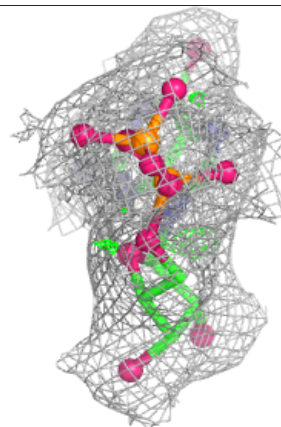
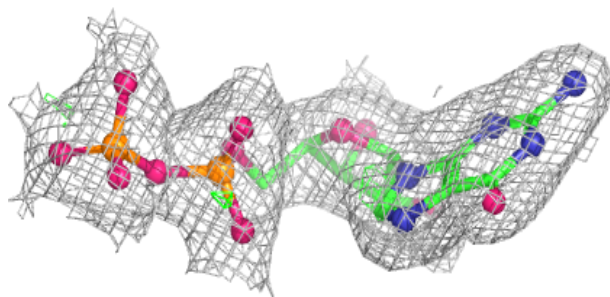
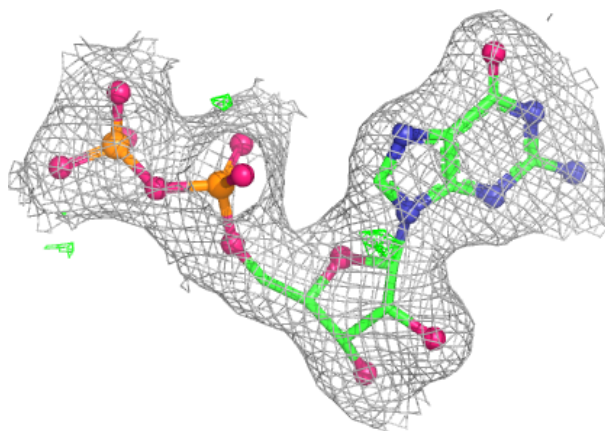
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.