



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:26 PM UTC

PDB ID : 6QTN / pdb_00006qtn
Title : Tubulin-cyclostreptin complex
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Deposited on : 2019-02-25
Resolution : 1.90 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

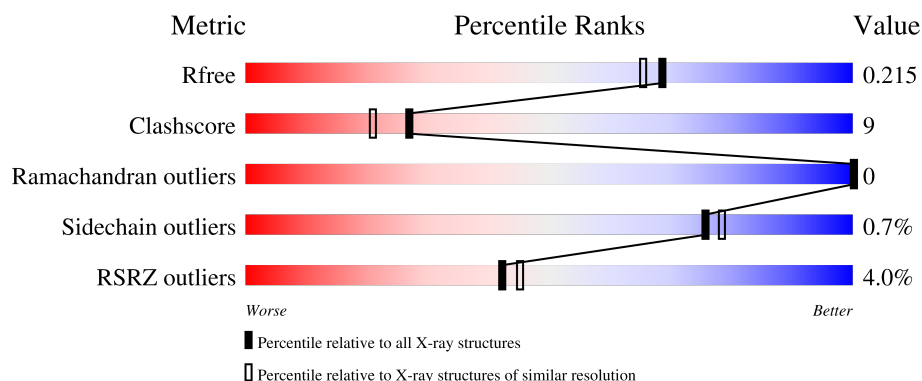
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



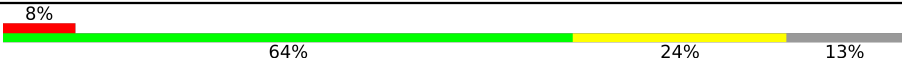
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	C	451	
2	B	445	
2	D	445	

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Mol	Chain	Length	Quality of chain
3	E	143	
4	F	384	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	GOL	B	505	-	X	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18338 atoms, of which 50 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	5	0
			3434	2178	581	651	24			
1	C	440	Total	C	N	O	S	0	6	0
			3467	2196	586	661	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	6	0
			3398	2133	579	659	27			
2	D	421	Total	C	N	O	S	0	2	0
			3315	2084	562	641	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	125	Total	C	N	O	S	0	0	0
			1031	634	188	204	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

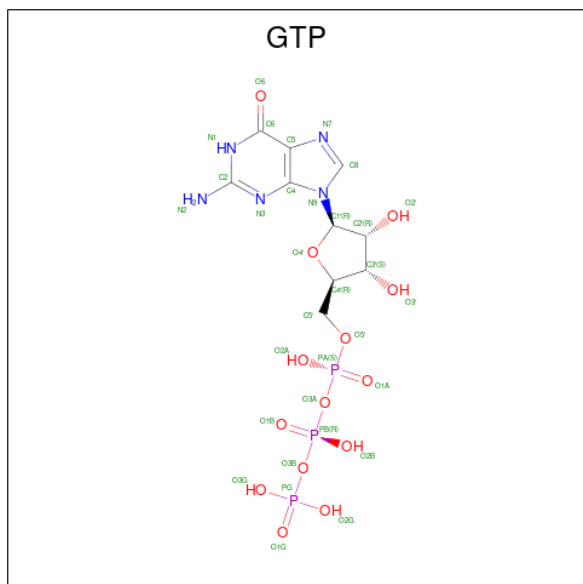
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	0	0
			2708	1743	460	491	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		

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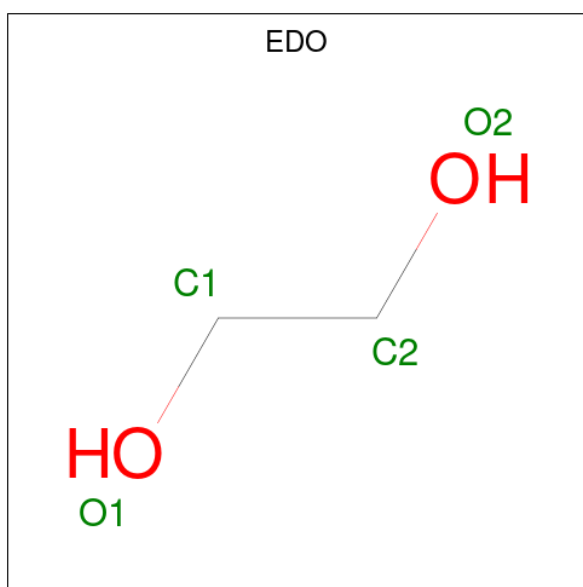
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

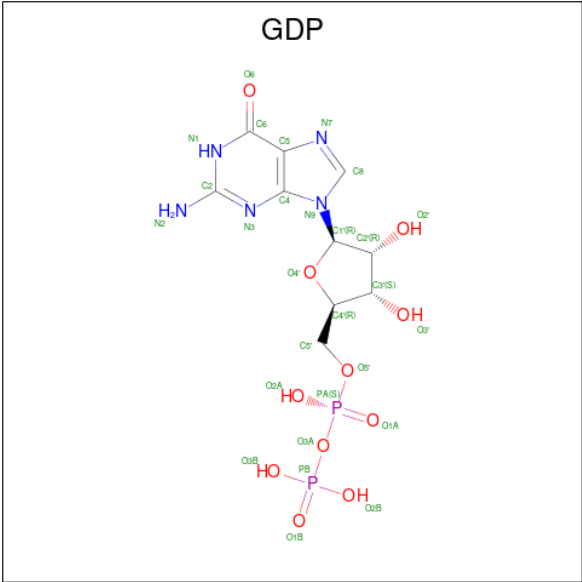
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



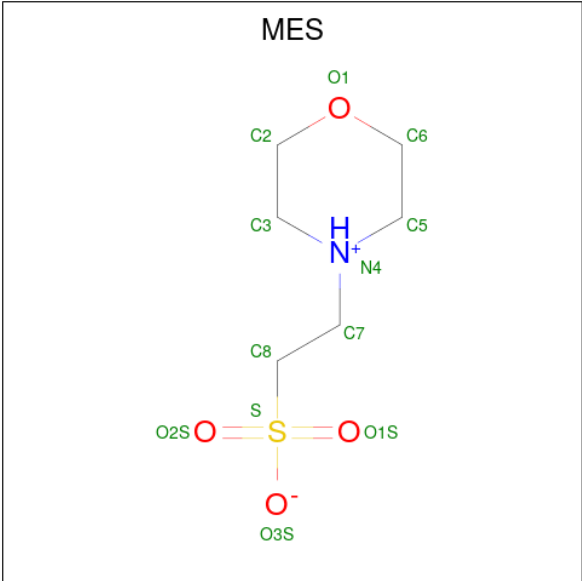
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	C	1	Total	C	H	O	0	0
			10	2	6	2		

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



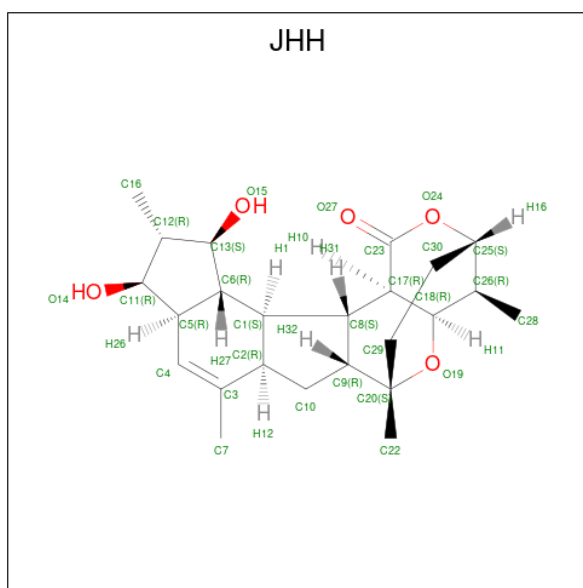
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



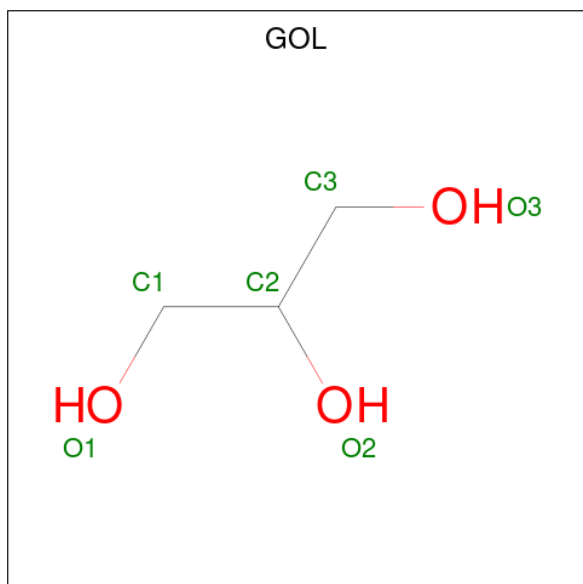
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is Cyclostreptin (CCD ID: JHH) (formula: $C_{24}H_{34}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			29	24	5		
11	D	1	Total	C	O	0	0
			29	24	5		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



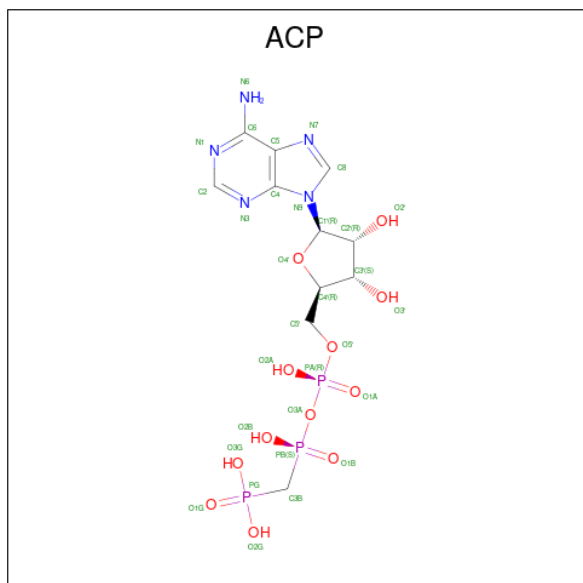
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	H	O	0	0
			14	3	8	3		
12	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

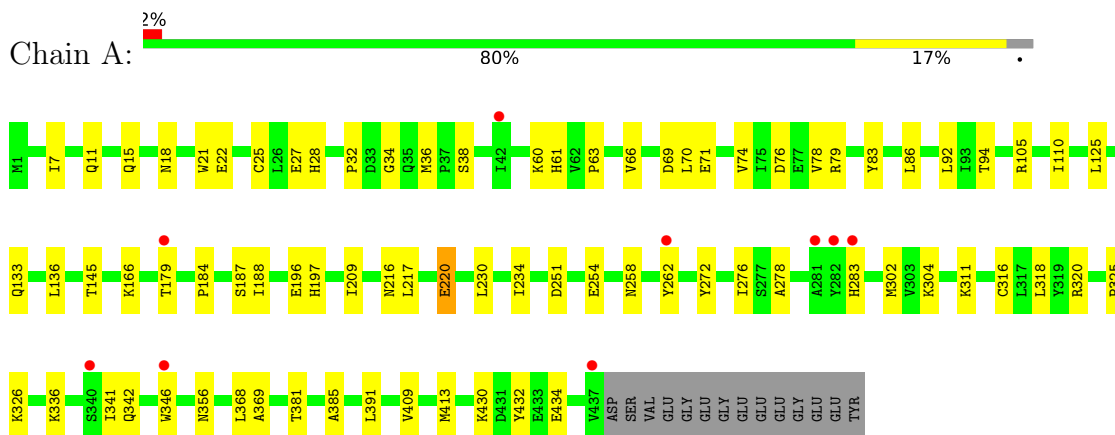
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	118	Total	O	0	0
			118	118		
14	B	141	Total	O	0	0
			141	141		
14	C	275	Total	O	0	0
			275	275		
14	D	70	Total	O	0	0
			70	70		
14	E	26	Total	O	0	0
			26	26		
14	F	51	Total	O	0	0
			51	51		

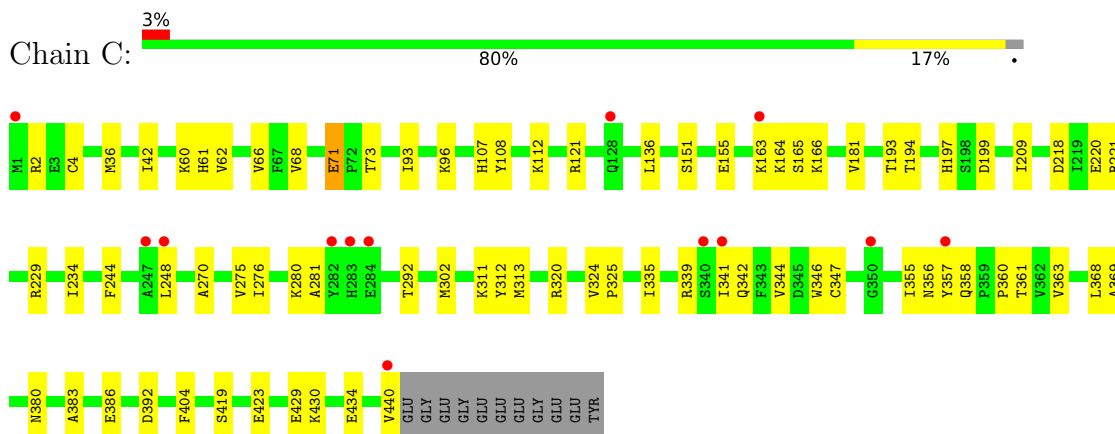
3 Residue-property plots [i](#)

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

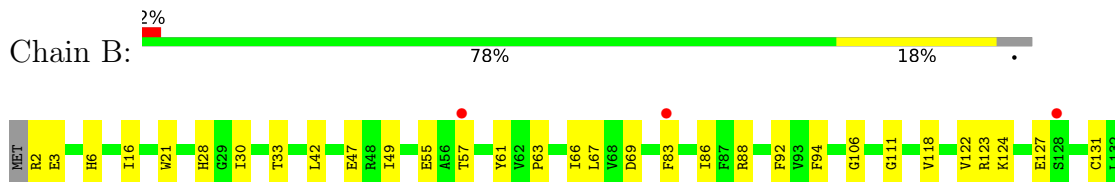
- Molecule 1: Tubulin alpha-1B chain

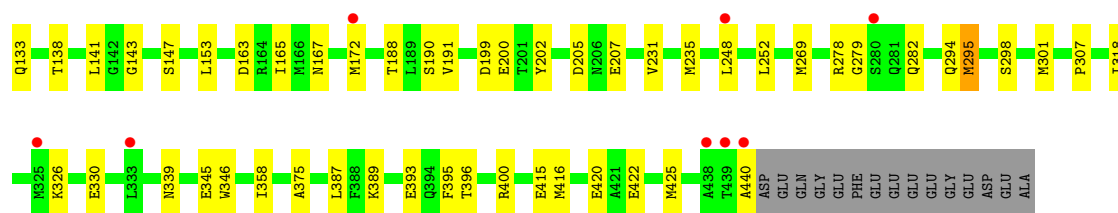


- Molecule 1: Tubulin alpha-1B chain

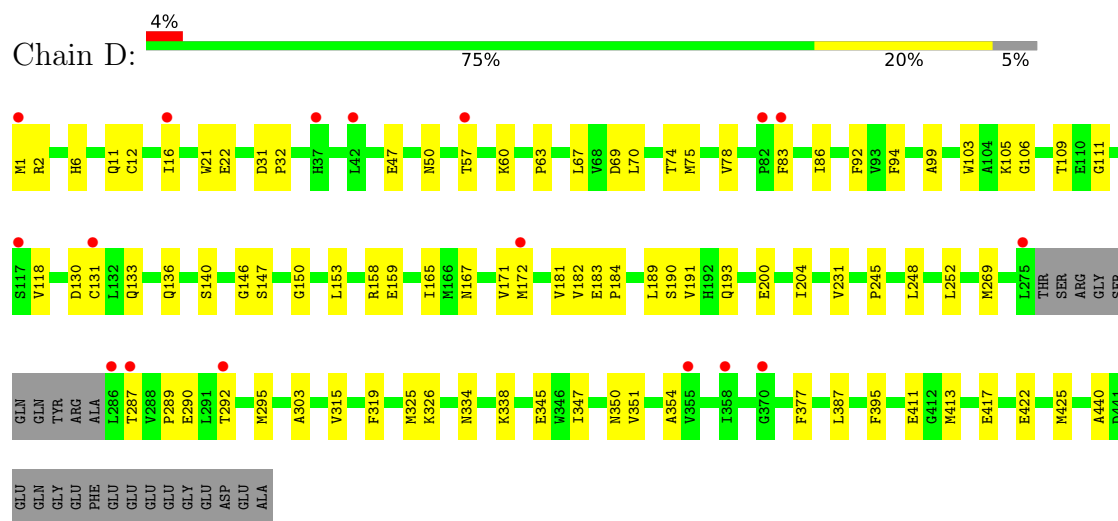


- Molecule 2: Tubulin beta-2B chain

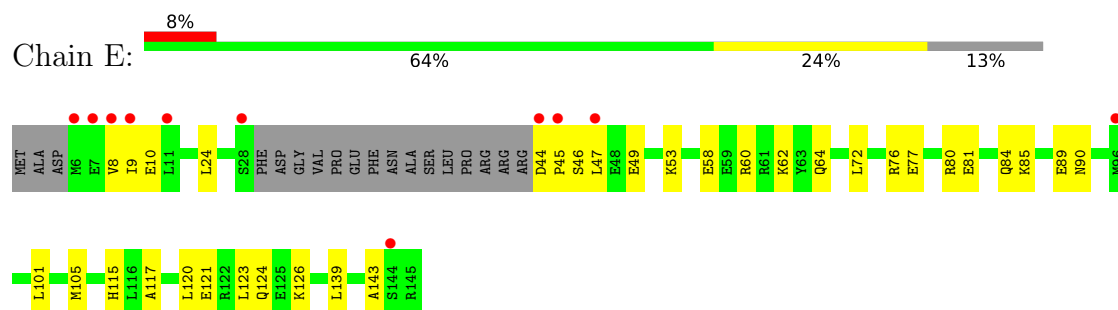




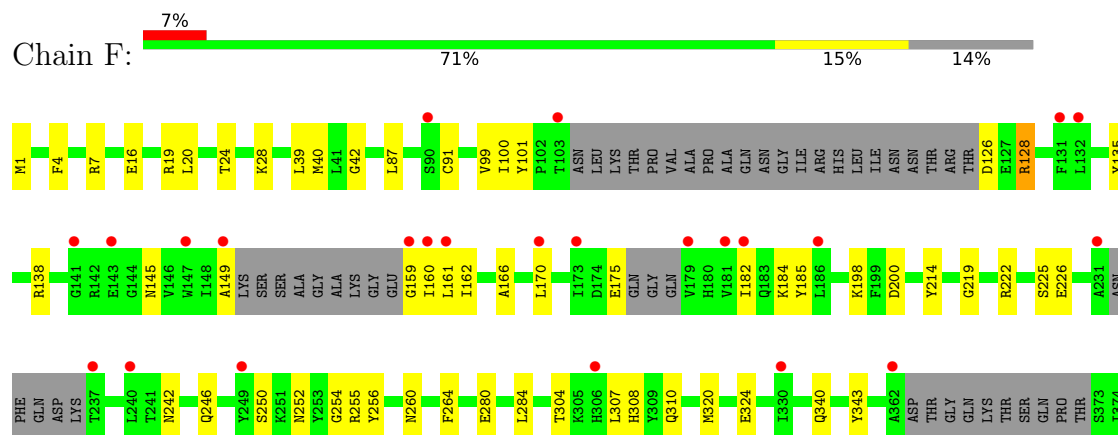
• Molecule 2: Tubulin beta-2B chain

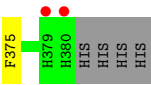


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.58Å 158.36Å 179.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 1.90 49.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.66-1.90) 100.0 (49.66-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.187 , 0.213 0.190 , 0.215	Depositor DCC
R_{free} test set	11839 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18338	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: EDO, MG, GOL, GDP, ACP, JHH, CA, MES, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/3527	0.35	0/4789
1	C	0.21	0/3557	0.42	0/4830
2	B	0.18	0/3488	0.37	0/4725
2	D	0.14	0/3394	0.32	0/4597
3	E	0.14	0/1039	0.29	0/1378
4	F	0.11	0/2769	0.32	0/3741
All	All	0.16	0/17774	0.35	0/24060

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3434	0	3365	57	0
1	C	3467	0	3387	61	0
2	B	3398	0	3282	69	0
2	D	3315	0	3199	66	0
3	E	1031	0	1047	23	0
4	F	2708	0	2674	58	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	4	6	6	0	0
8	C	4	6	6	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	12	1	0
11	B	29	0	0	0	0
11	D	29	0	0	0	0
12	B	6	8	8	0	0
12	C	12	16	16	0	0
13	F	31	14	14	1	0
14	A	118	0	0	5	0
14	B	141	0	0	5	0
14	C	275	0	0	5	0
14	D	70	0	0	4	0
14	E	26	0	0	0	0
14	F	51	0	0	2	0
All	All	18288	50	17064	320	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 (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:THR:HA	2:B:425:MET:HE1	1.33	1.03
1:C:220:GLU:HG2	2:D:326:LYS:HD2	1.51	0.92
1:A:220:GLU:HG2	2:B:326:LYS:HD2	1.54	0.88
2:B:269:MET:HE2	2:B:301:MET:HE3	1.59	0.85
4:F:149:ALA:HA	4:F:182:ILE:HD13	1.59	0.84
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.60	0.82
2:B:269:MET:CE	2:B:301:MET:HE3	2.10	0.82
4:F:16:GLU:OE1	4:F:19:ARG:NH2	2.12	0.82
2:B:422:GLU:HG3	14:B:616:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.60	0.81
2:B:172:MET:HE2	2:B:387:LEU:HD21	1.64	0.80
2:B:42:LEU:HD22	2:B:358:ILE:HD11	1.65	0.77
2:D:1:MET:HG3	2:D:50:ASN:HD22	1.50	0.76
2:B:88:ARG:HH22	2:B:124:LYS:HE3	1.50	0.76
3:E:9:ILE:HG22	3:E:10:GLU:HG3	1.68	0.76
2:D:287:THR:HG23	2:D:290:GLU:H	1.50	0.75
1:C:276:ILE:CD1	1:C:369:ALA:HB3	2.16	0.75
1:C:218:ASP:OD2	1:C:280:LYS:NZ	2.20	0.74
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.27	0.74
1:C:361:THR:HG23	14:C:771:HOH:O	1.90	0.72
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.23	0.71
2:B:191:VAL:HB	2:B:425:MET:HE2	1.73	0.71
3:E:120:LEU:O	3:E:124:GLN:HG2	1.90	0.71
4:F:7:ARG:CD	4:F:40:MET:HE3	2.21	0.71
1:A:38:SER:O	14:A:601:HOH:O	2.09	0.70
2:B:269:MET:HE3	14:B:673:HOH:O	1.91	0.70
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.74	0.69
1:A:326:LYS:HE2	1:A:326:LYS:H	1.56	0.69
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.75	0.69
2:B:188:THR:HA	2:B:425:MET:CE	2.20	0.68
1:A:209:ILE:HD11	1:A:302:MET:SD	2.32	0.68
1:C:276:ILE:HD13	1:C:281:ALA:HB2	1.75	0.68
1:A:304:LYS:HE3	4:F:308:HIS:HB3	1.76	0.68
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.75	0.67
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.76	0.67
2:D:106:GLY:O	2:D:111:GLY:HA3	1.95	0.67
2:B:294:GLN:OE1	14:B:601:HOH:O	2.12	0.67
1:C:324:VAL:HG22	1:C:325:PRO:HD2	1.77	0.66
1:C:163:LYS:HG3	3:E:90:ASN:OD1	1.95	0.66
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.60	0.66
2:B:83:PHE:O	2:B:86:ILE:HG22	1.95	0.65
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.79	0.65
2:D:136:GLN:HA	2:D:167:ASN:O	1.97	0.64
2:D:147:SER:HB2	2:D:190:SER:OG	1.97	0.64
2:B:163:ASP:OD1	14:B:602:HOH:O	2.15	0.64
1:C:276:ILE:HD12	1:C:276:ILE:O	1.98	0.64
2:D:57:THR:O	2:D:60:LYS:HE2	1.98	0.64
2:D:105:LYS:HA	2:D:109:THR:OG1	1.98	0.63
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.32	0.63
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:246:GLN:O	4:F:250:SER:HB2	1.98	0.63
1:C:220:GLU:CG	2:D:326:LYS:HD2	2.28	0.63
4:F:310:GLN:HA	4:F:310:GLN:HE21	1.63	0.63
2:D:2:ARG:NH2	14:D:601:HOH:O	2.32	0.62
1:C:430:LYS:NZ	1:C:434:GLU:OE1	2.27	0.62
2:D:1:MET:HG3	2:D:50:ASN:ND2	2.14	0.62
2:B:295:MET:HE3	2:B:375:ALA:HB1	1.80	0.62
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.81	0.62
2:B:165:ILE:HD13	10:B:503:MES:H82	1.82	0.62
1:A:430:LYS:O	1:A:434:GLU:HG2	2.00	0.61
1:C:209:ILE:HD11	1:C:302:MET:CE	2.30	0.61
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.81	0.61
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.82	0.61
1:C:181[B]:VAL:HG12	14:D:625:HOH:O	1.99	0.61
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.81	0.61
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.01	0.60
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.82	0.60
4:F:170:LEU:O	4:F:170:LEU:HD23	2.02	0.60
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG23	1.84	0.60
2:B:345:GLU:HG2	2:B:440:ALA:HB3	1.85	0.59
3:E:44:ASP:HB3	3:E:45:PRO:HD3	1.83	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.59
2:D:191:VAL:HG11	2:D:425:MET:HE2	1.83	0.59
1:A:105:ARG:NH1	1:A:110:ILE:HD11	2.17	0.59
2:B:295:MET:CE	2:B:375:ALA:HB1	2.32	0.59
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.03	0.59
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.02	0.59
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.85	0.59
4:F:100:ILE:HG23	4:F:128:ARG:HB2	1.85	0.59
2:B:346:TRP:HB3	2:B:440:ALA:HB2	1.85	0.58
1:C:270:ALA:O	1:C:302:MET:HG2	2.03	0.58
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.86	0.57
4:F:138:ARG:HB2	4:F:145:ASN:HD22	1.68	0.57
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.34	0.57
2:B:106:GLY:O	2:B:111:GLY:HA3	2.05	0.57
2:D:334:ASN:OD1	2:D:338:LYS:HE2	2.04	0.57
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.85	0.57
4:F:225:SER:HB3	4:F:252:ASN:HB2	1.87	0.57
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.22	0.57
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.45	0.57
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:O	2:D:94:PHE:HA	2.05	0.56
4:F:7:ARG:NE	4:F:40:MET:HE3	2.20	0.56
1:A:220:GLU:HG2	2:B:326:LYS:CD	2.29	0.56
2:B:279:GLY:O	2:B:282:GLN:HG2	2.06	0.56
4:F:126:ASP:N	14:F:501:HOH:O	2.38	0.56
4:F:99:VAL:O	4:F:100:ILE:HD13	2.07	0.55
4:F:184:LYS:HD3	4:F:185:TYR:N	2.21	0.55
2:B:69:ASP:O	2:B:94:PHE:HA	2.06	0.55
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.42	0.55
3:E:46:SER:OG	3:E:49:GLU:HG3	2.05	0.55
2:B:188:THR:HG23	2:B:425:MET:HE3	1.88	0.55
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.71	0.55
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.36	0.55
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.72	0.54
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.41	0.54
1:A:70:LEU:HD12	1:A:145:THR:OG1	2.07	0.54
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.08	0.54
2:B:298:SER:HA	2:B:301:MET:HG3	1.89	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.88	0.53
2:D:191:VAL:HB	2:D:425:MET:CE	2.37	0.53
1:C:320:ARG:HA	1:C:356:ASN:O	2.08	0.53
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	0.53
2:B:269:MET:HE1	2:B:301:MET:HE3	1.88	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
4:F:149:ALA:O	4:F:160:ILE:HG23	2.08	0.53
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.43	0.53
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.89	0.53
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.74	0.53
2:B:345:GLU:OE1	2:B:345:GLU:N	2.35	0.52
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.91	0.52
1:A:304:LYS:HE3	4:F:308:HIS:CB	2.40	0.52
1:A:184:PRO:O	1:A:188:ILE:HD13	2.10	0.52
4:F:246:GLN:HA	4:F:250:SER:OG	2.09	0.51
1:A:7:ILE:HG12	1:A:66[B]:VAL:CG2	2.40	0.51
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.45	0.51
4:F:40:MET:HE2	4:F:42:GLY:HA2	1.92	0.51
4:F:20:LEU:O	4:F:24:THR:HG23	2.10	0.51
2:B:301:MET:HE2	2:B:307:PRO:HG3	1.92	0.51
2:D:74:THR:HB	14:D:617:HOH:O	2.10	0.51
1:C:280:LYS:HE2	14:C:616:HOH:O	2.10	0.51
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.41	0.50
4:F:138:ARG:HB2	4:F:145:ASN:ND2	2.26	0.50
2:B:123:ARG:O	2:B:127:GLU:HG3	2.10	0.50
1:A:74:VAL:HB	14:A:607:HOH:O	2.12	0.50
1:A:276:ILE:HD12	1:A:283:HIS:CD2	2.47	0.50
1:C:324:VAL:HG22	14:C:785:HOH:O	2.12	0.50
2:D:287:THR:HG22	2:D:290:GLU:CG	2.41	0.49
3:E:72:LEU:O	3:E:76:ARG:HG2	2.11	0.49
3:E:101:LEU:O	3:E:105:MET:HG2	2.12	0.49
4:F:128:ARG:CZ	4:F:170:LEU:HD11	2.42	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.49
1:C:151:SER:HA	1:C:194[B]:THR:HG22	1.92	0.49
1:C:419:SER:O	1:C:423:GLU:HG3	2.11	0.49
1:C:107:HIS:HE1	1:C:155:GLU:OE1	1.95	0.49
4:F:40:MET:HE2	4:F:42:GLY:CA	2.43	0.49
4:F:101:TYR:CD1	4:F:126:ASP:HB2	2.47	0.49
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	3.00	0.49
2:D:292:THR:HG22	2:D:319:PHE:CZ	2.48	0.49
2:B:2:ARG:HA	2:B:131:CYS:O	2.13	0.49
4:F:226:GLU:OE2	4:F:250:SER:HB3	2.12	0.49
2:B:3:GLU:OE2	2:B:3:GLU:N	2.42	0.49
2:D:158:ARG:HD3	14:D:631:HOH:O	2.12	0.49
4:F:254:GLY:H	4:F:260:ASN:HD21	1.61	0.49
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.95	0.49
1:A:311:LYS:HE3	1:A:342:GLN:HE21	1.77	0.48
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.48
3:E:80:ARG:O	3:E:84:GLN:HG2	2.14	0.48
1:C:383:ALA:O	1:C:386[A]:GLU:HB2	2.13	0.48
3:E:8:VAL:O	3:E:9:ILE:HD13	2.14	0.48
4:F:87:LEU:O	4:F:91:CYS:HB2	2.13	0.48
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.78	0.48
1:A:311:LYS:HG2	1:A:342:GLN:HG2	1.96	0.48
2:B:191:VAL:HB	2:B:425:MET:CE	2.42	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.48
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.95	0.48
1:A:216:ASN:ND2	14:A:604:HOH:O	2.47	0.48
2:D:83:PHE:O	2:D:86:ILE:HG22	2.14	0.48
2:D:395:PHE:CE1	2:D:422:GLU:HB2	2.49	0.48
1:A:336:LYS:NZ	1:A:341:ILE:O	2.47	0.47
2:D:287:THR:HG22	2:D:290:GLU:OE2	2.14	0.47
4:F:138:ARG:CB	4:F:145:ASN:HD22	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:162:ILE:HD13	4:F:185:TYR:CE1	2.49	0.47
1:C:42:ILE:HD12	1:C:42:ILE:N	2.30	0.47
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.47	0.47
1:C:165:SER:HA	1:C:199:ASP:OD2	2.14	0.47
1:A:234:ILE:HD12	1:A:272:TYR:HB2	1.97	0.47
4:F:160:ILE:HG22	4:F:161:LEU:N	2.30	0.47
1:A:32:PRO:HA	1:A:83:TYR:CD2	2.50	0.47
4:F:1:MET:CE	4:F:28:LYS:HB2	2.45	0.47
4:F:242:ASN:ND2	13:F:401:ACP:O2B	2.47	0.47
1:C:71:GLU:OE2	1:C:73:THR:HG23	2.15	0.47
1:A:69:ASP:O	1:A:94:THR:HA	2.15	0.46
2:B:30:ILE:HD12	2:B:30:ILE:N	2.30	0.46
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.98	0.46
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.97	0.46
4:F:161:LEU:C	4:F:161:LEU:HD12	2.40	0.46
2:B:141:LEU:HD12	2:B:172:MET:SD	2.56	0.46
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.51	0.46
3:E:117:ALA:O	3:E:121:GLU:HG3	2.14	0.46
2:D:16:ILE:HD12	2:D:231:VAL:HG11	1.97	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.46
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.98	0.46
2:B:138[A]:THR:HG21	2:B:235:MET:HE1	1.98	0.46
2:B:88:ARG:NH2	2:B:124:LYS:HE3	2.27	0.46
2:B:318:ILE:N	2:B:318:ILE:HD12	2.31	0.46
2:D:183:GLU:N	2:D:184:PRO:HD2	2.31	0.46
3:E:49:GLU:O	3:E:53:LYS:HG3	2.15	0.46
1:A:409:VAL:HA	1:A:413:MET:O	2.16	0.46
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.98	0.46
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.99	0.45
1:C:2:ARG:HA	1:C:2:ARG:NE	2.32	0.45
4:F:100:ILE:HD12	4:F:128:ARG:CA	2.44	0.45
2:B:205:ASP:OD1	2:B:207[B]:GLU:HB3	2.15	0.45
4:F:255:ARG:NH1	14:F:505:HOH:O	2.49	0.45
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.99	0.45
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.99	0.45
2:D:109:THR:HG21	2:D:411:GLU:OE1	2.17	0.45
2:D:295:MET:CG	2:D:377:PHE:HB2	2.46	0.45
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.90	0.45
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.99	0.45
1:A:179:THR:HA	2:B:248:LEU:HD11	1.98	0.45
1:C:234:ILE:HG12	1:C:302:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:47:LEU:HD23	3:E:47:LEU:O	2.16	0.45
1:A:196:GLU:HG2	14:A:638:HOH:O	2.17	0.45
2:D:287:THR:CG2	2:D:290:GLU:HG3	2.47	0.45
1:A:356:ASN:HB2	14:A:648:HOH:O	2.17	0.45
2:B:326:LYS:O	2:B:330:GLU:HG3	2.17	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.44
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.52	0.44
2:B:172:MET:HE3	2:B:172:MET:HB3	1.81	0.44
4:F:4:PHE:HA	4:F:39:LEU:O	2.17	0.44
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.18	0.44
1:C:108:TYR:O	1:C:112:LYS:HG2	2.18	0.44
3:E:60:ARG:O	3:E:64:GLN:HG3	2.16	0.44
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.98	0.44
1:C:276:ILE:HD12	1:C:369:ALA:HB3	1.95	0.44
3:E:85:LYS:O	3:E:89:GLU:HG3	2.17	0.44
1:C:440:VAL:HG22	1:C:440:VAL:O	2.16	0.44
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.82	0.44
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.00	0.44
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.52	0.44
2:B:33:THR:HG22	2:B:33:THR:O	2.17	0.44
1:A:325:PRO:HD2	1:A:326:LYS:NZ	2.33	0.43
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.52	0.43
1:A:136:LEU:HD12	1:A:136:LEU:N	2.33	0.43
2:B:278:ARG:HD2	2:B:278:ARG:N	2.32	0.43
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	2.00	0.43
2:D:1:MET:CG	2:D:50:ASN:HD22	2.26	0.43
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.99	0.43
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.34	0.43
1:C:276:ILE:HD13	1:C:369:ALA:HB3	1.97	0.43
4:F:161:LEU:HD12	4:F:161:LEU:O	2.18	0.43
1:A:11:GLN:O	1:A:15:GLN:HG3	2.17	0.43
2:D:287:THR:CG2	2:D:290:GLU:H	2.23	0.43
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.53	0.43
1:C:151:SER:HB2	1:C:193:THR:CG2	2.48	0.43
2:D:74:THR:O	2:D:78:VAL:HG23	2.19	0.43
2:D:193:GLN:HE22	3:E:126:LYS:NZ	2.16	0.43
2:D:248:LEU:HD23	2:D:354:ALA:HB2	2.01	0.43
4:F:225:SER:OG	4:F:260:ASN:ND2	2.49	0.43
1:A:28:HIS:O	1:A:36:MET:HE3	2.18	0.43
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.48	0.42
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.42
4:F:135:TYR:CD2	4:F:166:ALA:HB2	2.54	0.42
3:E:81:GLU:HA	3:E:84:GLN:HG2	2.02	0.42
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.42
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.28	0.42
1:A:66[A]:VAL:HG23	1:A:125:LEU:HD12	2.01	0.42
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.54	0.42
2:B:415:GLU:OE2	14:B:603:HOH:O	2.21	0.42
2:D:413:MET:HE3	2:D:417:GLU:CD	2.44	0.42
3:E:124:GLN:HA	3:E:124:GLN:NE2	2.35	0.42
2:B:167:ASN:HD21	2:B:202:TYR:HE2	1.66	0.42
4:F:254:GLY:H	4:F:260:ASN:ND2	2.17	0.42
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.02	0.42
2:D:118:VAL:HG11	2:D:153:LEU:HD11	2.02	0.42
1:C:392:ASP:OD2	1:C:429:GLU:OE1	2.37	0.41
1:C:181[B]:VAL:HG11	1:C:404:PHE:CZ	2.55	0.41
4:F:138:ARG:HH21	4:F:184:LYS:HZ1	1.67	0.41
4:F:159:GLY:C	4:F:160:ILE:HG13	2.46	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.55	0.41
2:B:55:GLU:HG3	2:B:61:TYR:CE1	2.55	0.41
2:B:88:ARG:HH22	2:B:124:LYS:CE	2.25	0.41
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.41
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.03	0.41
1:C:164:LYS:HE2	1:C:164:LYS:HB2	1.83	0.41
2:D:146:GLY:O	2:D:150:GLY:HA3	2.20	0.41
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.02	0.41
1:A:326:LYS:H	1:A:326:LYS:CE	2.29	0.41
2:B:416:MET:HE3	2:B:420:GLU:HG3	2.01	0.41
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.03	0.41
1:C:234:ILE:HD12	1:C:234:ILE:N	2.35	0.41
2:D:11:GLN:HA	2:D:74:THR:HG21	2.02	0.41
2:D:159:GLU:HG3	3:E:123:LEU:HD13	2.01	0.41
2:B:28:HIS:HB3	2:B:49:ILE:HD13	2.01	0.41
1:C:311:LYS:HG2	1:C:342:GLN:NE2	2.35	0.41
1:C:313:MET:HE3	1:C:380:ASN:CG	2.46	0.41
14:C:644:HOH:O	3:E:115:HIS:HE1	2.03	0.41
2:B:199:ASP:C	2:B:200:GLU:HG3	2.46	0.41
2:B:295:MET:HE3	2:B:375:ALA:CB	2.49	0.41
2:D:181:VAL:HG13	2:D:182:VAL:HG13	2.03	0.41
4:F:175:GLU:OE1	4:F:175:GLU:N	2.54	0.41
4:F:255:ARG:HG3	4:F:256:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:THR:O	2:B:400:ARG:HG2	2.21	0.41
1:C:60:LYS:HG2	1:C:62:VAL:CG2	2.51	0.41
1:C:324:VAL:HG22	1:C:325:PRO:CD	2.47	0.41
4:F:135:TYR:C	4:F:135:TYR:CD1	2.98	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.56	0.41
1:A:66[B]:VAL:HG13	1:A:125:LEU:HD12	2.03	0.40
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.02	0.40
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.61	0.40
2:B:42:LEU:HD22	2:B:358:ILE:CD1	2.44	0.40
2:B:345:GLU:H	2:B:345:GLU:CD	2.26	0.40
1:C:229:ARG:HD2	14:C:610:HOH:O	2.20	0.40
2:D:287:THR:HG22	2:D:290:GLU:HG3	2.03	0.40
2:B:389:LYS:O	2:B:393:GLU:HG3	2.21	0.40
1:C:229:ARG:NE	1:C:363:VAL:HG21	2.37	0.40
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.03	0.40
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.03	0.40
3:E:139:LEU:O	3:E:143:ALA:HB3	2.21	0.40
1:A:70:LEU:HD22	1:A:110:ILE:CG2	2.50	0.40
1:A:346:TRP:CD1	1:A:346:TRP:H	2.39	0.40
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.40
4:F:1:MET:HE3	4:F:28:LYS:CB	2.51	0.40
1:C:368:LEU:HD23	1:C:368:LEU:HA	1.95	0.40
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.52	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	440/451 (98%)	434 (99%)	6 (1%)	0	100	100
1	C	444/451 (98%)	433 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	433/445 (97%)	428 (99%)	5 (1%)	0	100	100
2	D	419/445 (94%)	412 (98%)	7 (2%)	0	100	100
3	E	121/143 (85%)	121 (100%)	0	0	100	100
4	F	319/384 (83%)	305 (96%)	14 (4%)	0	100	100
All	All	2176/2319 (94%)	2133 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	373/379 (98%)	370 (99%)	3 (1%)	73	75
1	C	377/379 (100%)	374 (99%)	3 (1%)	73	75
2	B	376/383 (98%)	372 (99%)	4 (1%)	65	67
2	D	366/383 (96%)	365 (100%)	1 (0%)	86	88
3	E	112/127 (88%)	111 (99%)	1 (1%)	70	73
4	F	296/342 (86%)	294 (99%)	2 (1%)	76	78
All	All	1900/1993 (95%)	1886 (99%)	14 (1%)	76	78

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	220	GLU
1	A	381	THR
2	B	47	GLU
2	B	57	THR
2	B	295	MET
2	B	339	ASN
1	C	71	GLU
1	C	339	ARG

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Mol	Chain	Res	Type
1	C	347	CYS
2	D	200	GLU
3	E	77	GLU
4	F	128	ARG
4	F	324	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
2	B	167	ASN
2	B	349	ASN
1	C	342	GLN
1	C	356	ASN
2	D	11	GLN
2	D	37	HIS
2	D	50	ASN
2	D	300	ASN
3	E	12	ASN
3	E	124	GLN
4	F	145	ASN
4	F	252	ASN
4	F	260	ASN
4	F	306	HIS
4	F	310	GLN
4	F	333	ASN
4	F	340	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 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	GOL	C	504	-	5,5,5	1.23	1 (20%)	5,5,5	1.47	1 (20%)
10	MES	B	503	-	12,12,12	2.03	1 (8%)	15,16,16	1.71	3 (20%)
8	EDO	A	504	-	3,3,3	0.44	0	2,2,2	0.39	0
5	GTP	A	501	6	33,34,34	0.93	2 (6%)	50,54,54	1.51	8 (16%)
9	GDP	B	501	6	29,30,30	1.11	3 (10%)	45,47,47	1.63	6 (13%)
11	JHH	B	504	2	34,34,34	0.91	1 (2%)	36,57,57	1.61	5 (13%)
12	GOL	B	505	-	5,5,5	1.34	1 (20%)	5,5,5	1.27	1 (20%)
8	EDO	C	506	-	3,3,3	0.51	0	2,2,2	0.17	0
5	GTP	C	501	6	33,34,34	0.93	1 (3%)	50,54,54	1.47	10 (20%)
9	GDP	D	501	6	29,30,30	1.15	2 (6%)	45,47,47	1.72	6 (13%)
11	JHH	D	503	2	34,34,34	0.93	1 (2%)	36,57,57	1.64	5 (13%)
13	ACP	F	401	6	31,33,33	1.40	4 (12%)	47,52,52	2.09	10 (21%)
12	GOL	C	505	-	5,5,5	0.91	0	5,5,5	1.04	0

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	GOL	C	504	-	-	0/4/4/4	-
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
8	EDO	A	504	-	-	0/1/1/1	-
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
12	GOL	B	505	-	-	4/4/4/4	-
11	JHH	B	504	2	-	-	0/6/6/6
8	EDO	C	506	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
9	GDP	D	501	6	-	3/16/32/32	0/3/3/3
11	JHH	D	503	2	-	-	0/6/6/6
13	ACP	F	401	6	-	2/19/38/38	0/3/3/3
12	GOL	C	505	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-6.72	1.68	1.77
13	F	401	ACP	PB-O3A	3.45	1.62	1.58
9	D	501	GDP	C5-C4	3.11	1.47	1.38
13	F	401	ACP	PG-O2G	3.03	1.61	1.55
13	F	401	ACP	PG-O3G	2.81	1.61	1.55
9	B	501	GDP	C5-C4	2.73	1.46	1.38
13	F	401	ACP	PA-O3A	2.66	1.62	1.59
11	D	503	JHH	O24-C25	-2.54	1.43	1.46
11	B	504	JHH	O24-C25	-2.45	1.43	1.46
5	C	501	GTP	PA-O3A	2.35	1.62	1.59
9	D	501	GDP	C6-N1	-2.34	1.34	1.38
5	A	501	GTP	PA-O3A	2.34	1.62	1.59
9	B	501	GDP	C6-N1	-2.27	1.34	1.38
9	B	501	GDP	C4-N9	-2.13	1.32	1.38
5	A	501	GTP	C2-N3	2.10	1.38	1.33
12	B	505	GOL	O2-C2	-2.05	1.37	1.43
12	C	504	GOL	O2-C2	-2.02	1.37	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	503	JHH	C22-C20-C29	-6.37	102.80	110.79
11	B	504	JHH	C22-C20-C29	-6.33	102.84	110.79
13	F	401	ACP	C5-C4-N3	-5.90	118.59	126.72
9	D	501	GDP	C5-C4-N3	-5.85	119.08	128.39
13	F	401	ACP	PB-O3A-PA	-5.46	114.55	132.37
13	F	401	ACP	N3-C4-N9	5.09	135.83	127.17
9	B	501	GDP	C5-C4-N3	-4.97	120.48	128.39
9	D	501	GDP	C2-N3-C4	4.96	120.85	112.30
5	A	501	GTP	C5-C4-N3	-4.64	121.01	128.39
10	B	503	MES	C5-N4-C3	4.50	118.54	108.84
5	A	501	GTP	C2-N3-C4	4.48	120.01	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C2-N3-C4	4.42	119.90	112.30
5	C	501	GTP	C2-N3-C4	4.41	119.90	112.30
5	C	501	GTP	C5-C4-N3	-4.31	121.53	128.39
9	D	501	GDP	N9-C4-N3	4.11	134.17	125.95
13	F	401	ACP	C5-N7-C8	4.04	109.81	103.45
9	B	501	GDP	N9-C4-N3	3.88	133.71	125.95
13	F	401	ACP	N3-C2-N1	-3.64	123.07	128.58
9	D	501	GDP	C6-C5-N7	3.57	136.78	130.29
13	F	401	ACP	C2-N3-C4	3.52	120.43	111.83
11	D	503	JHH	C16-C12-C13	-3.19	110.21	113.96
13	F	401	ACP	C5'-C4'-C3'	-3.16	103.84	115.21
12	C	504	GOL	C3-C2-C1	-3.10	100.42	111.80
9	B	501	GDP	C6-C5-N7	3.09	135.92	130.29
13	F	401	ACP	C4-C5-N7	-3.04	107.11	110.58
11	B	504	JHH	C16-C12-C13	-2.99	110.44	113.96
10	B	503	MES	O1S-S-C8	2.92	111.15	106.73
13	F	401	ACP	N9-C8-N7	-2.90	109.82	113.94
11	D	503	JHH	C16-C12-C11	-2.89	110.56	113.96
5	C	501	GTP	N9-C8-N7	-2.81	108.19	113.40
9	B	501	GDP	O6-C6-C5	-2.76	119.26	126.53
9	D	501	GDP	C4-C5-N7	-2.75	106.31	110.67
5	C	501	GTP	N9-C4-N3	2.68	131.31	125.95
11	B	504	JHH	C5-C6-C13	-2.64	100.08	103.66
11	D	503	JHH	C5-C6-C1	-2.63	107.70	117.93
5	A	501	GTP	N9-C8-N7	-2.58	108.62	113.40
5	A	501	GTP	C8-N7-C5	2.53	108.77	104.26
5	A	501	GTP	C2-N1-C6	-2.51	120.55	125.11
12	B	505	GOL	C3-C2-C1	-2.47	102.73	111.80
5	A	501	GTP	N9-C4-N3	2.47	130.89	125.95
11	B	504	JHH	C16-C12-C11	-2.46	111.06	113.96
11	B	504	JHH	C5-C6-C1	-2.44	108.46	117.93
10	B	503	MES	O3S-S-C8	2.38	110.66	106.00
11	D	503	JHH	C10-C2-C1	-2.34	100.56	104.62
5	C	501	GTP	C8-N7-C5	2.33	108.42	104.26
5	C	501	GTP	C5-C6-N1	2.30	119.11	113.25
5	A	501	GTP	C5-C6-N1	2.26	119.00	113.25
5	C	501	GTP	N1-C2-N3	-2.13	119.42	123.32
5	C	501	GTP	C2-N1-C6	-2.12	121.27	125.11
5	A	501	GTP	C4-C5-N7	-2.10	107.34	110.67
5	C	501	GTP	O6-C6-C5	-2.07	121.08	126.53
9	B	501	GDP	O4'-C1'-N9	-2.02	103.78	108.36
5	C	501	GTP	O2A-PA-O3A	2.02	112.73	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	401	ACP	C3'-C2'-C1'	2.01	105.27	101.46
9	D	501	GDP	O6-C6-C5	-2.01	121.23	126.53

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
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
12	B	505	GOL	C1-C2-C3-O3
13	F	401	ACP	O4'-C4'-C5'-O5'
13	F	401	ACP	C3'-C4'-C5'-O5'
12	B	505	GOL	O1-C1-C2-C3
12	B	505	GOL	O2-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O2G
12	B	505	GOL	O1-C1-C2-O2
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
9	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A

There are no ring outliers.

3 monomers are involved in 3 short contacts:

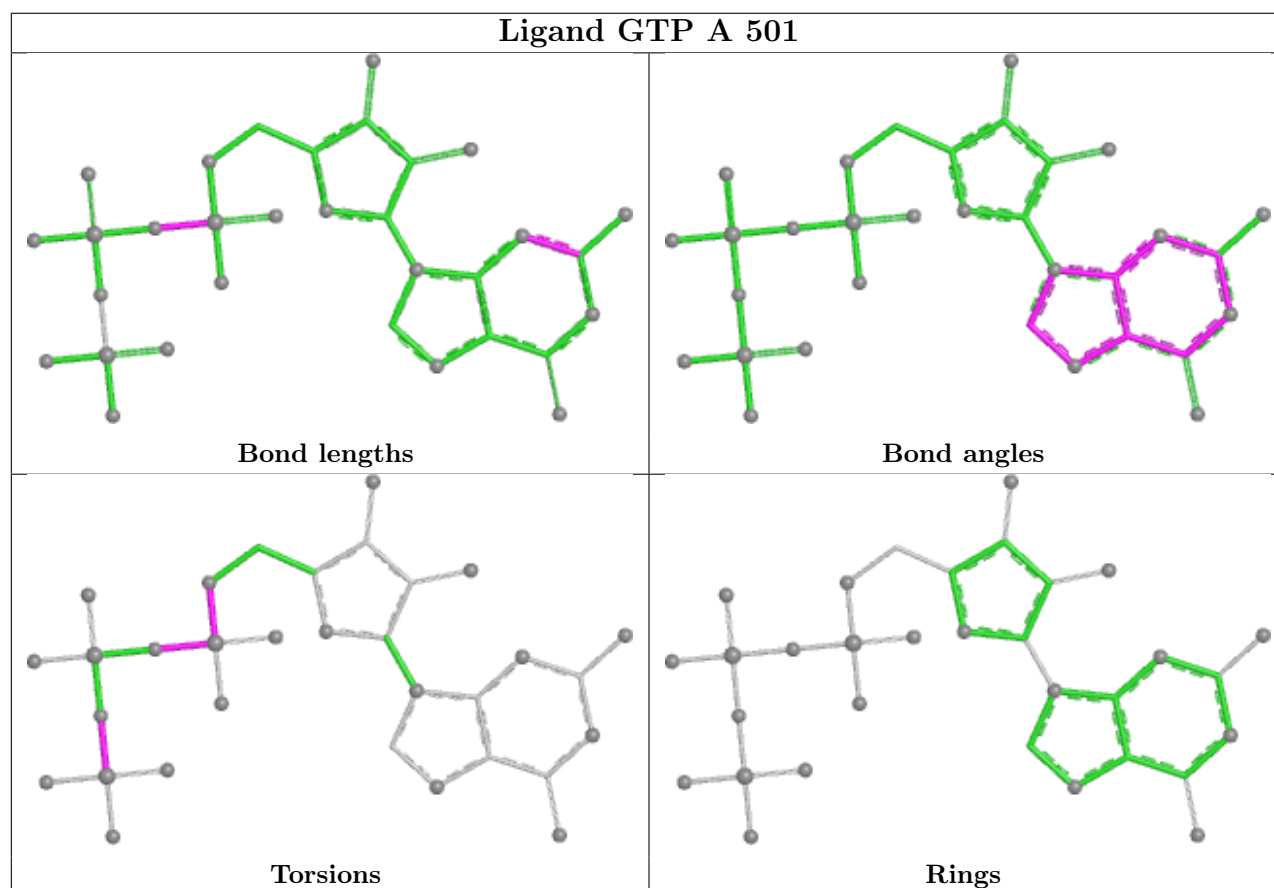
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	1	0

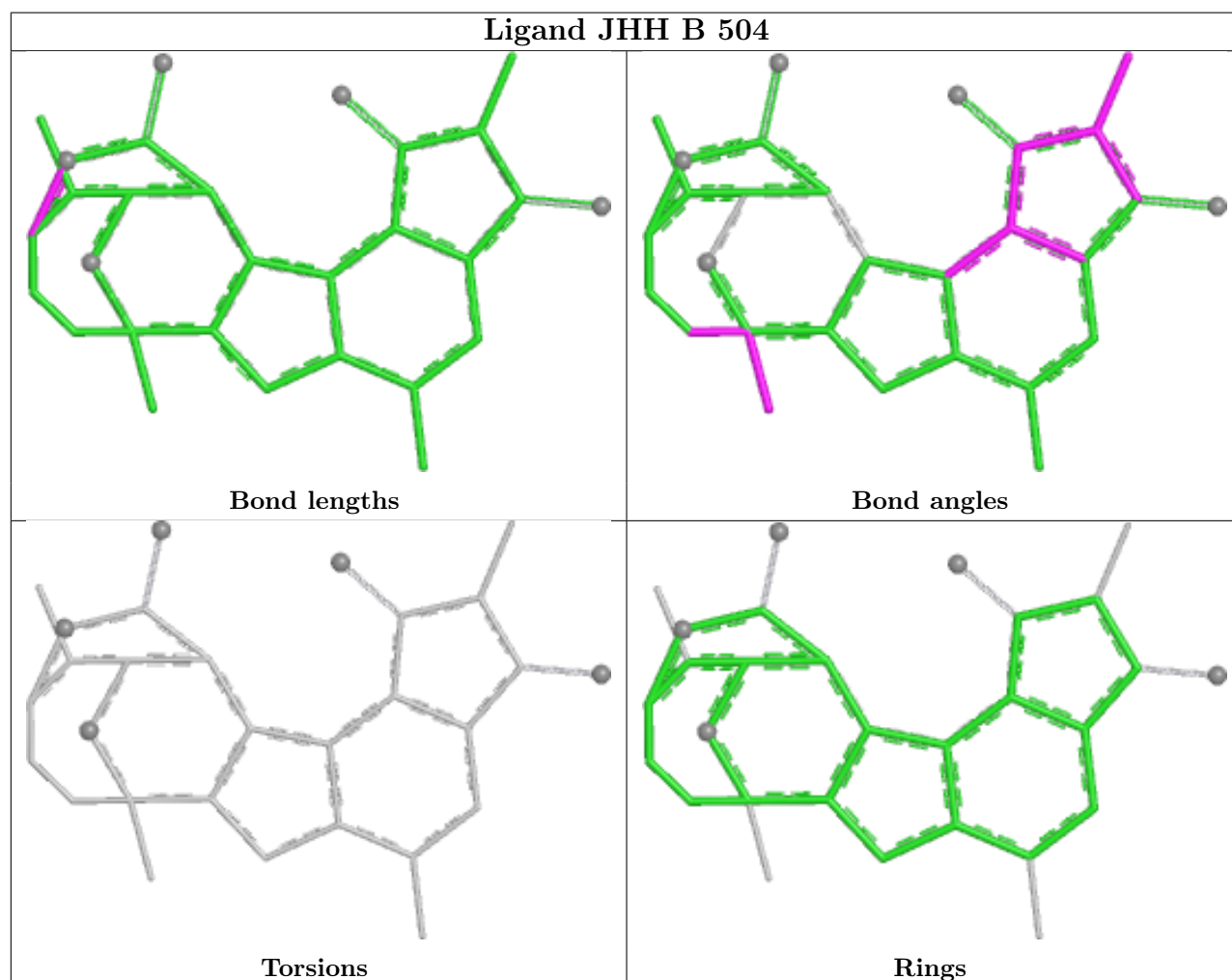
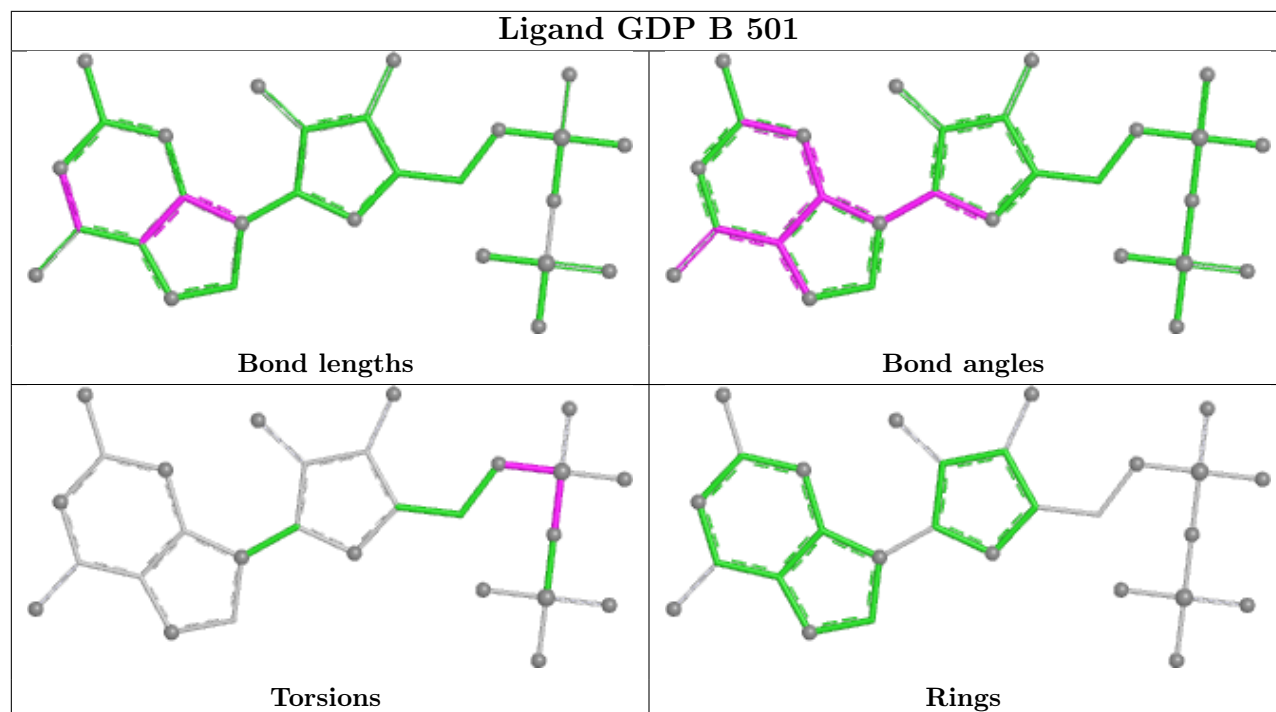
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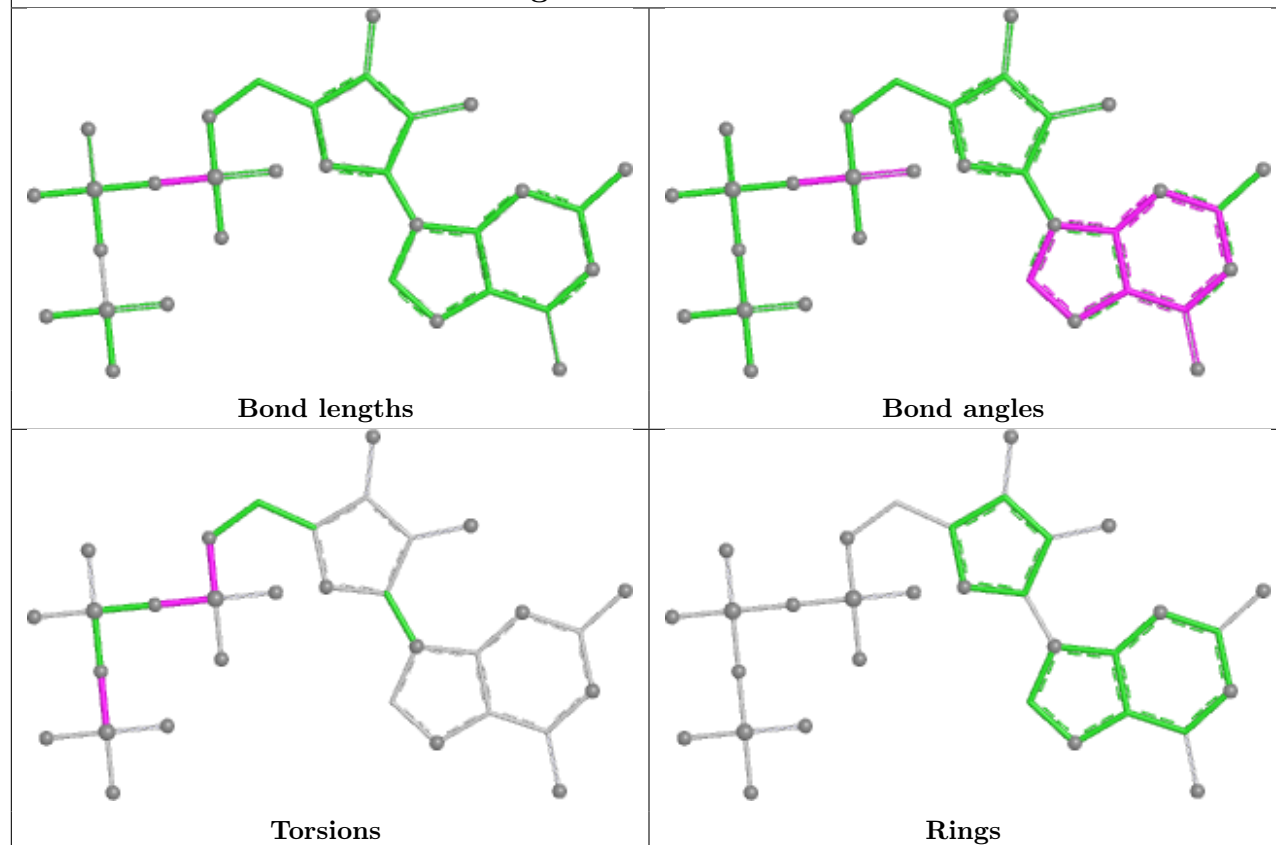
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
13	F	401	ACP	1	0

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

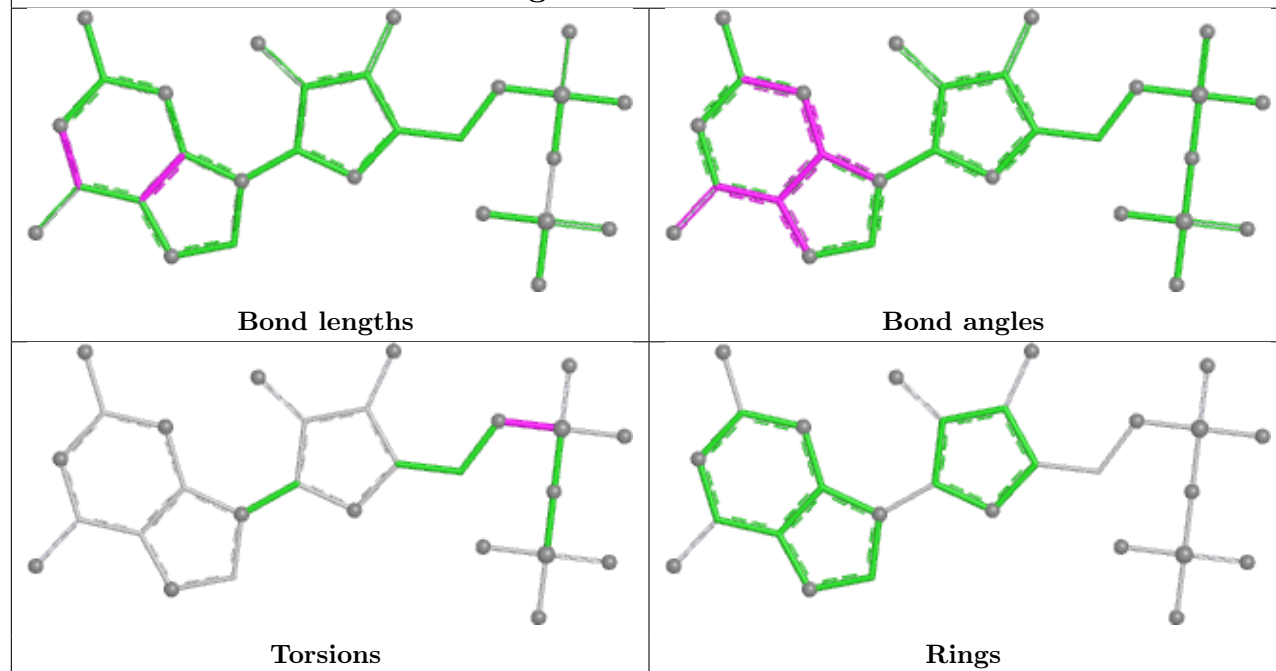


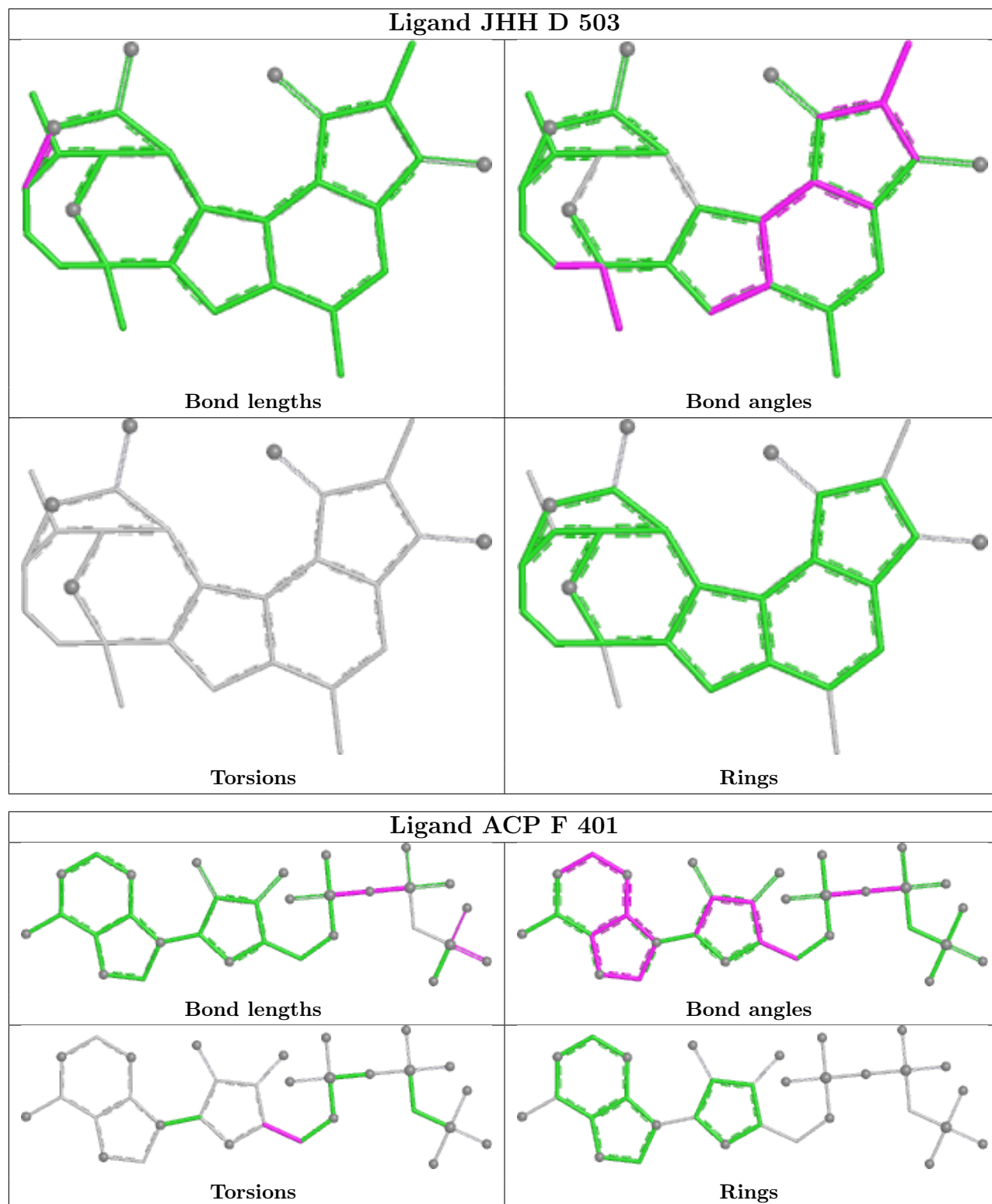


Ligand GTP C 501



Ligand GDP D 501





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%)	0.34	9 (2%) 63 67	31, 56, 90, 140	5 (1%)
1	C	440/451 (97%)	0.03	13 (2%) 52 56	18, 43, 71, 108	6 (1%)
2	B	429/445 (96%)	0.20	11 (2%) 57 61	21, 50, 89, 121	6 (1%)
2	D	421/445 (94%)	0.45	17 (4%) 42 45	34, 65, 96, 128	2 (0%)
3	E	125/143 (87%)	0.71	11 (8%) 15 16	40, 71, 114, 142	0
4	F	331/384 (86%)	0.72	26 (7%) 18 20	45, 76, 139, 172	0
All	All	2183/2319 (94%)	0.35	87 (3%) 42 45	18, 57, 105, 172	19 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	5.4
1	C	440	VAL	4.9
4	F	149	ALA	4.8
1	A	437	VAL	4.5
1	A	179	THR	4.0
4	F	103	THR	4.0
4	F	179	VAL	4.0
2	B	248	LEU	3.8
3	E	45	PRO	3.7
4	F	380	HIS	3.6
4	F	159	GLY	3.6
2	B	439	THR	3.6
1	C	283	HIS	3.5
1	C	357	TYR	3.5
2	D	172	MET	3.5
2	B	438	ALA	3.4
1	A	262	TYR	3.3
4	F	330	ILE	3.3
2	D	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.2
4	F	143	GLU	3.2
1	A	282	TYR	3.2
1	C	163	LYS	3.2
4	F	240	LEU	3.2
2	B	280	SER	3.2
4	F	237	THR	3.1
4	F	90	SER	3.1
2	D	286	LEU	3.1
4	F	131	PHE	3.0
3	E	9	ILE	3.0
4	F	186	LEU	3.0
1	A	42	ILE	3.0
4	F	170	LEU	2.9
4	F	160	ILE	2.9
1	C	350	GLY	2.9
4	F	362	ALA	2.8
1	C	248	LEU	2.8
4	F	181	VAL	2.8
1	C	247	ALA	2.7
2	B	440	ALA	2.7
4	F	379	HIS	2.7
2	D	370	GLY	2.7
2	D	82	PRO	2.7
4	F	231	ALA	2.7
4	F	141	GLY	2.6
2	D	83	PHE	2.6
3	E	6	MET	2.6
2	B	128	SER	2.6
2	B	333	LEU	2.5
2	D	358	ILE	2.5
4	F	132	LEU	2.5
1	A	281	ALA	2.5
2	D	287	THR	2.5
1	C	340	SER	2.4
3	E	8	VAL	2.4
4	F	182	ILE	2.4
2	D	42	LEU	2.4
1	A	283	HIS	2.4
3	E	47	LEU	2.3
2	D	131	CYS	2.3
1	C	284	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	355	VAL	2.3
2	B	325	MET	2.3
1	A	340	SER	2.3
3	E	7	GLU	2.3
2	D	275	LEU	2.3
2	B	83	PHE	2.2
4	F	306	HIS	2.2
2	D	292	THR	2.2
2	D	37	HIS	2.2
2	D	117	SER	2.2
3	E	144	SER	2.2
2	B	57	THR	2.2
3	E	28	SER	2.2
3	E	96	MET	2.1
1	C	341	ILE	2.1
4	F	173	ILE	2.1
1	A	346	TRP	2.1
1	C	282	TYR	2.1
2	B	172	MET	2.1
1	C	128	GLN	2.1
2	D	16	ILE	2.0
4	F	249	TYR	2.0
2	D	57	THR	2.0
3	E	11	LEU	2.0
4	F	147	TRP	2.0
3	E	44	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

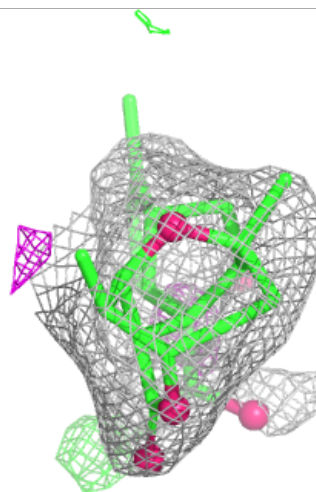
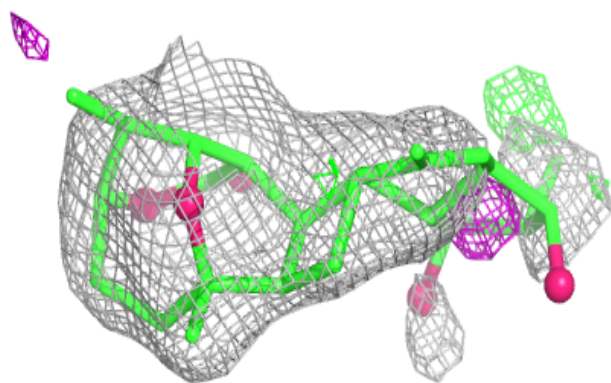
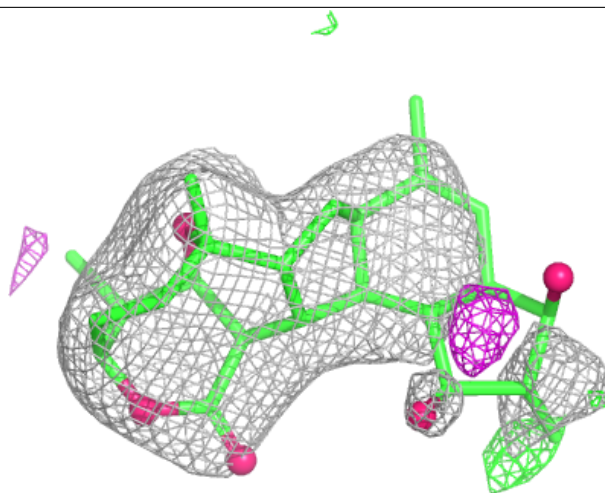
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
8	EDO	C	506	4/4	0.80	0.24	56,82,92,99	0
8	EDO	A	504	4/4	0.87	0.14	72,86,92,94	0
12	GOL	B	505	6/6	0.87	0.14	42,78,96,96	0
11	JHH	D	503	29/29	0.88	0.14	59,86,117,117	0
11	JHH	B	504	29/29	0.88	0.16	49,77,118,119	0
12	GOL	C	504	6/6	0.88	0.12	55,80,100,109	0
13	ACP	F	401	31/31	0.89	0.09	78,103,126,141	0
12	GOL	C	505	6/6	0.90	0.13	66,84,101,101	0
6	MG	D	502	1/1	0.93	0.07	62,62,62,62	0
10	MES	B	503	12/12	0.93	0.10	37,48,58,66	0
9	GDP	D	501	28/28	0.94	0.09	51,55,64,70	0
6	MG	F	402	1/1	0.94	0.06	67,67,67,67	0
7	CA	A	503	1/1	0.97	0.05	68,68,68,68	0
9	GDP	B	501	28/28	0.98	0.05	31,35,39,42	0
5	GTP	C	501	32/32	0.98	0.05	28,33,36,39	0
5	GTP	A	501	32/32	0.98	0.05	30,38,43,45	0
7	CA	C	503	1/1	0.99	0.04	52,52,52,52	0
6	MG	A	502	1/1	0.99	0.03	38,38,38,38	0
6	MG	B	502	1/1	0.99	0.05	27,27,27,27	0
6	MG	C	502	1/1	0.99	0.02	33,33,33,33	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.

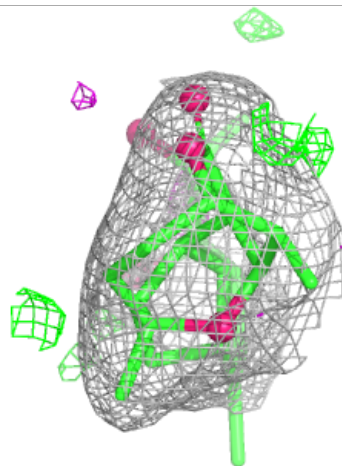
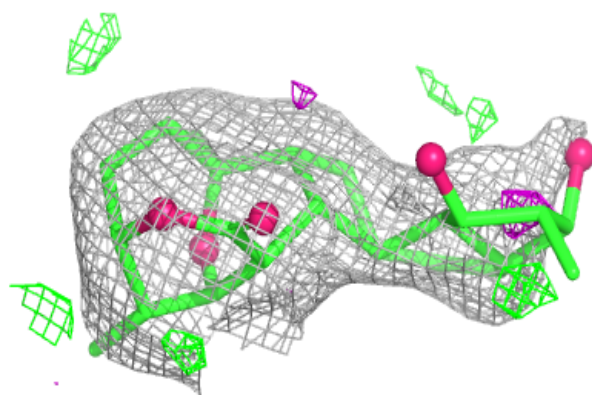
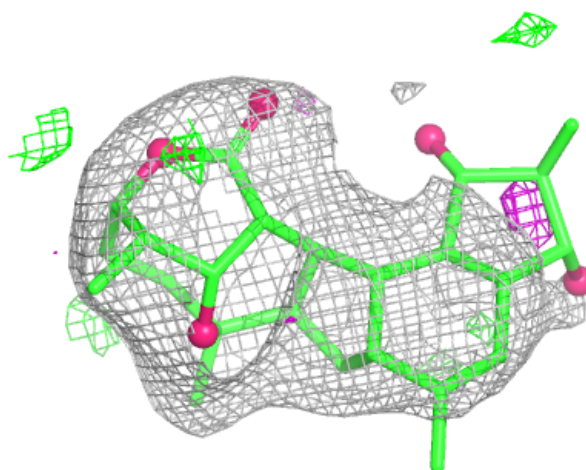
Electron density around JHH D 503:

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



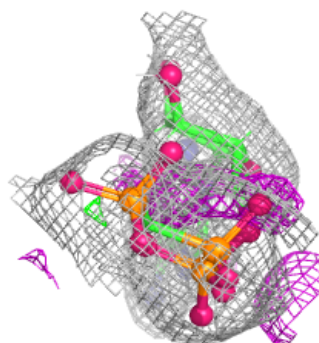
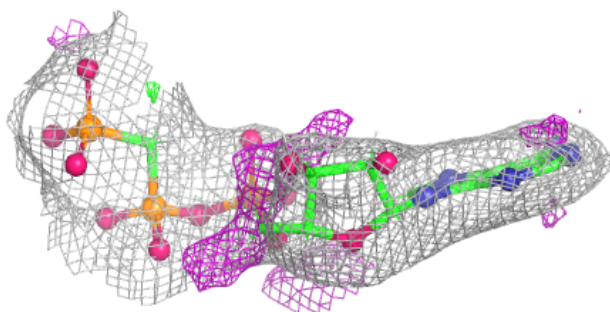
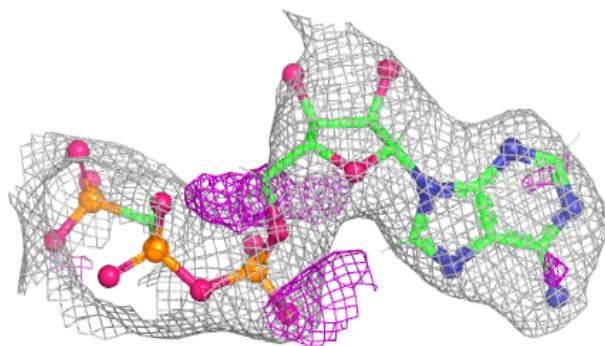
Electron density around JHH B 504:

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

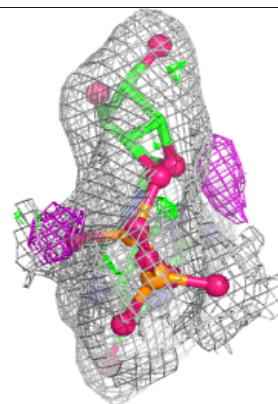
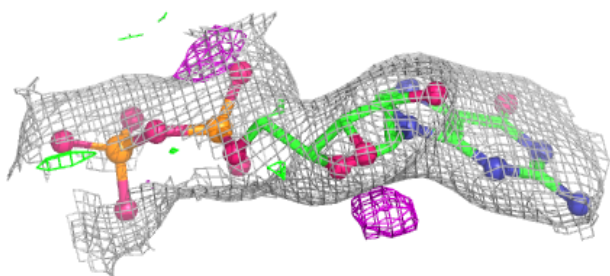
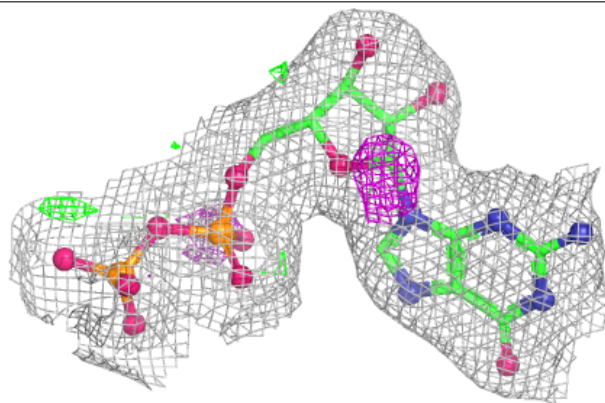


Electron density around ACP F 401:

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

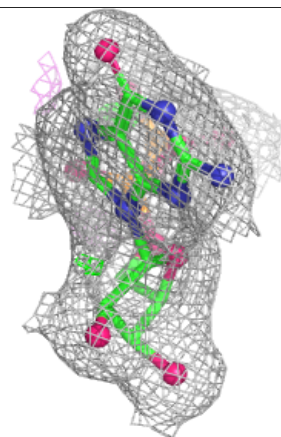
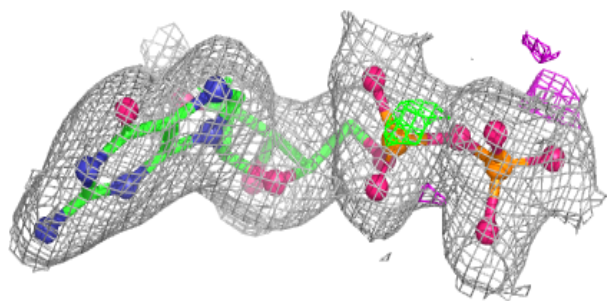
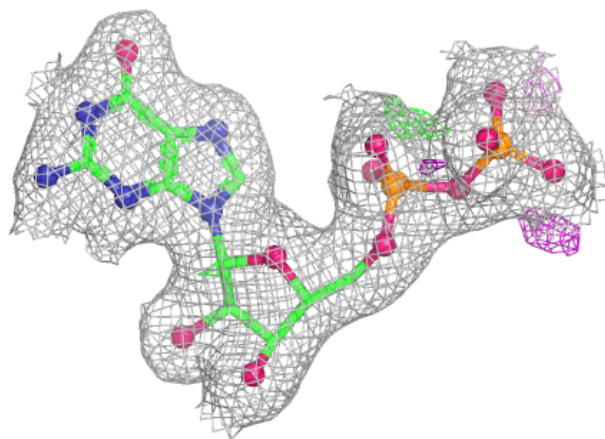
**Electron density around GDP D 501:**

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



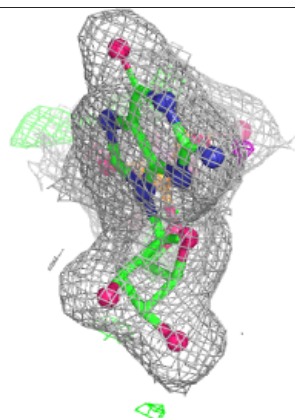
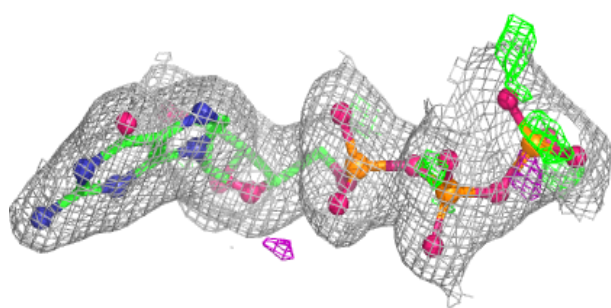
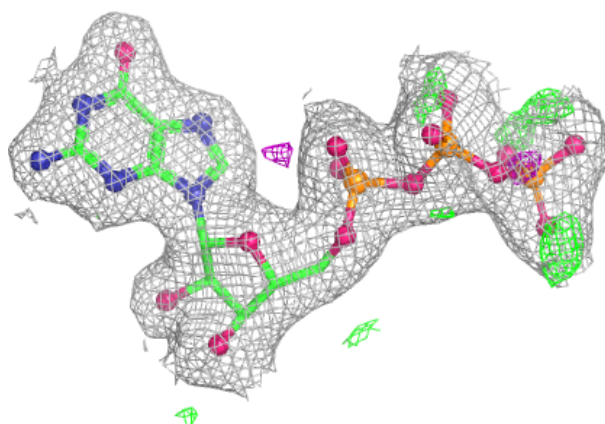
Electron density around GDP B 501:

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

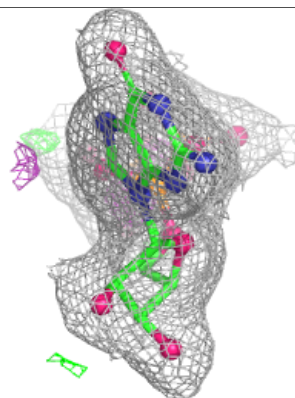
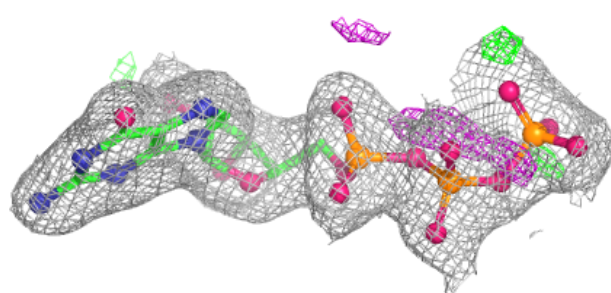
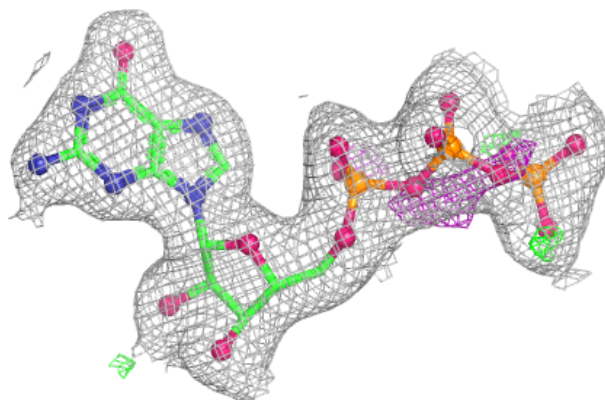


Electron density around GTP C 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.