



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 02:47 PM EDT

PDB ID : 7LZ8
Title : Tubulin-RB3_SLD-TTL in complex with compound 5t
Authors : White, S.W.; Yun, M.
Deposited on : 2021-03-09
Resolution : 2.92 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 : 2.23.1
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) : 2.23.1

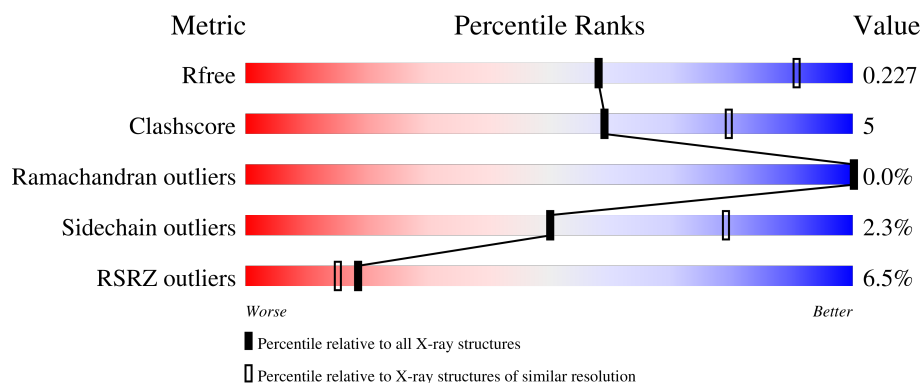
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	450	<div> <div>4%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
1	C	450	<div> <div>%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
2	B	445	<div> <div>4%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
2	D	445	<div> <div>7%</div> <div>76%</div> <div>17%</div> <div>•</div> <div>6%</div> </div>
3	E	143	<div> <div>7%</div> <div>69%</div> <div>15%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (15%), green (58%), yellow (8%), and grey (33%). The percentages are labeled below the bar segments.

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 16797 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
			3406	2155	581	649	21			
1	C	438	Total	C	N	O	S	0	0	0
			3428	2170	582	654	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3333	2093	571	643	26			
2	D	417	Total	C	N	O	S	0	0	0
			3278	2061	558	633	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			993	614	181	193	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	256	Total	C	N	O	S	0	0	0
			2095	1357	357	370	11			

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		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	2	Total	Ca	0	0
			2	2		

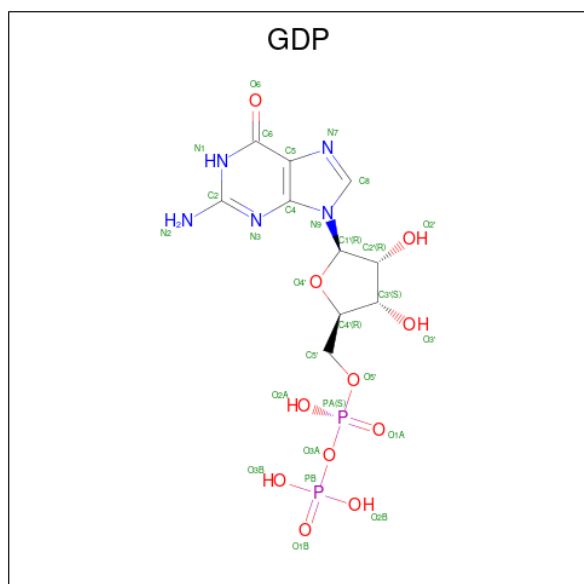
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



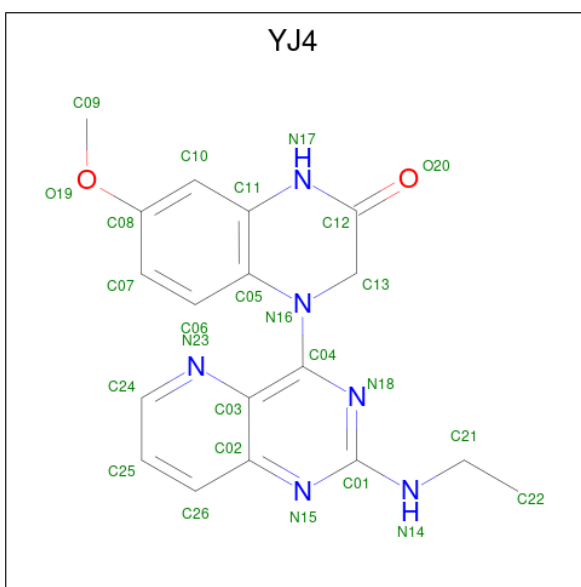
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 11 is 4-[2-(ethylamino)pyrido[3,2-d]pyrimidin-4-yl]-7-methoxy-3,4-dihydroquinolin-2(1H)-one (three-letter code: YJ4) (formula: C₁₈H₁₈N₆O₂) (labeled as "Ligand of Interest" by depositor).



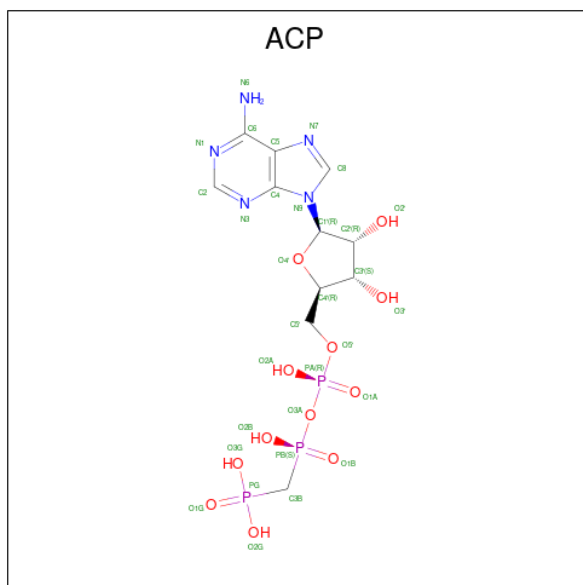
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O		0	0
			26	18	6	2			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			26	18	6	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	F	1	Total	C	N	O	0	0
			17	9	5	3		

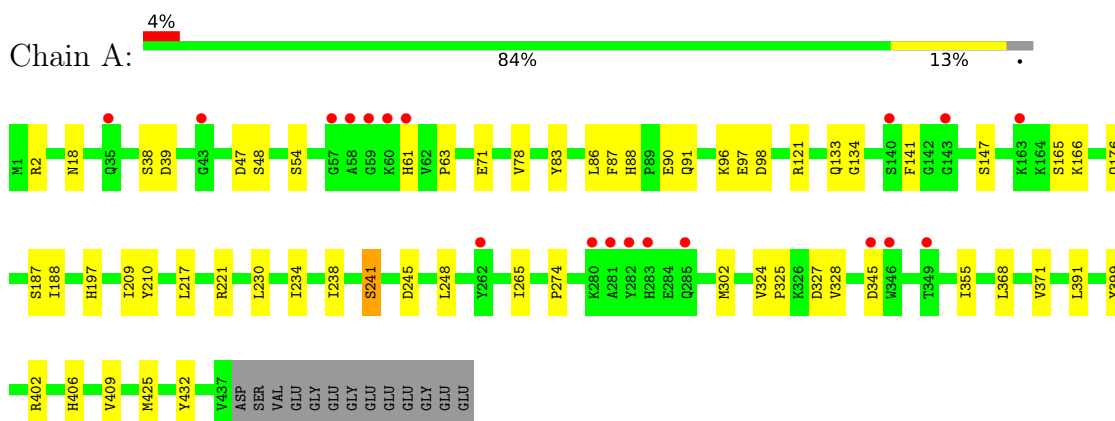
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	7	Total	O	0	0
			7	7		
13	B	10	Total	O	0	0
			10	10		
13	C	17	Total	O	0	0
			17	17		
13	D	3	Total	O	0	0
			3	3		

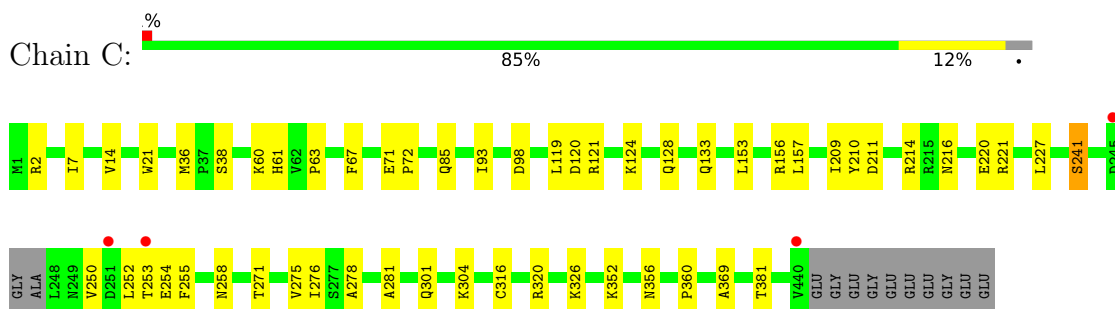
3 Residue-property plots [i](#)

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

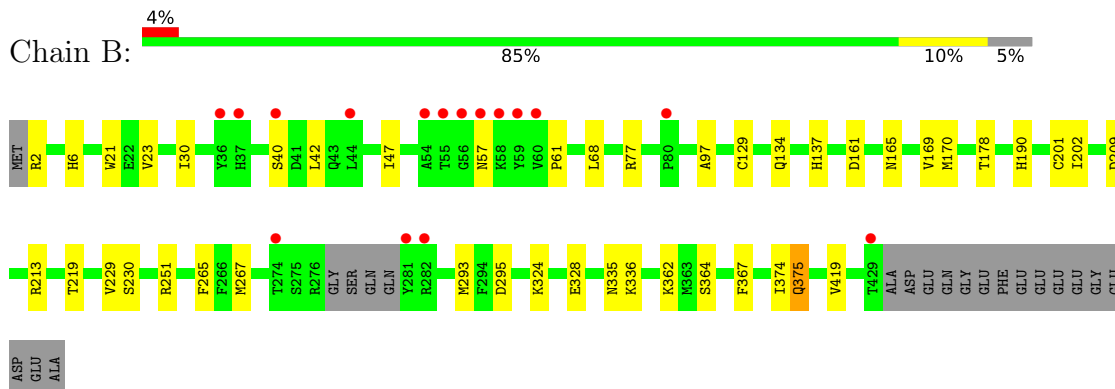
- Molecule 1: Tubulin alpha-1B chain



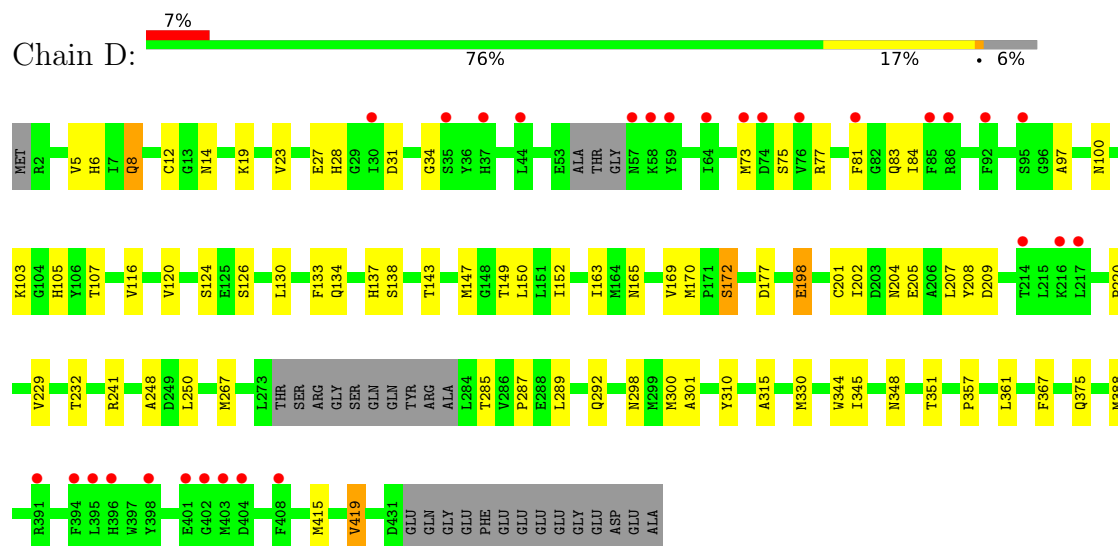
- Molecule 1: Tubulin alpha-1B chain



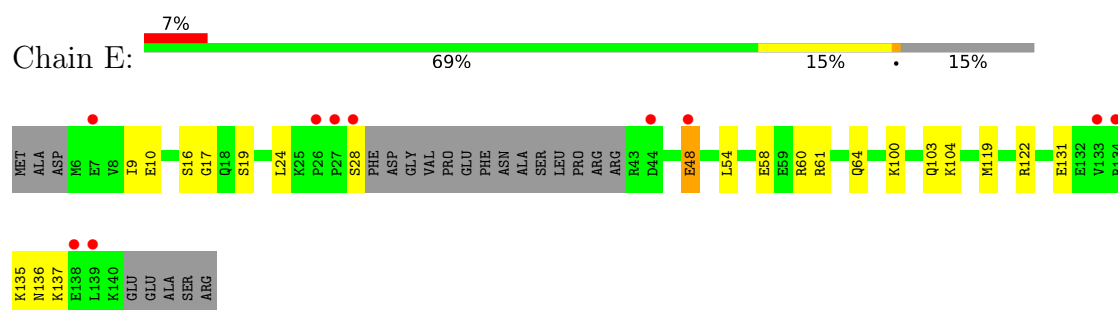
- Molecule 2: Tubulin beta-2B chain



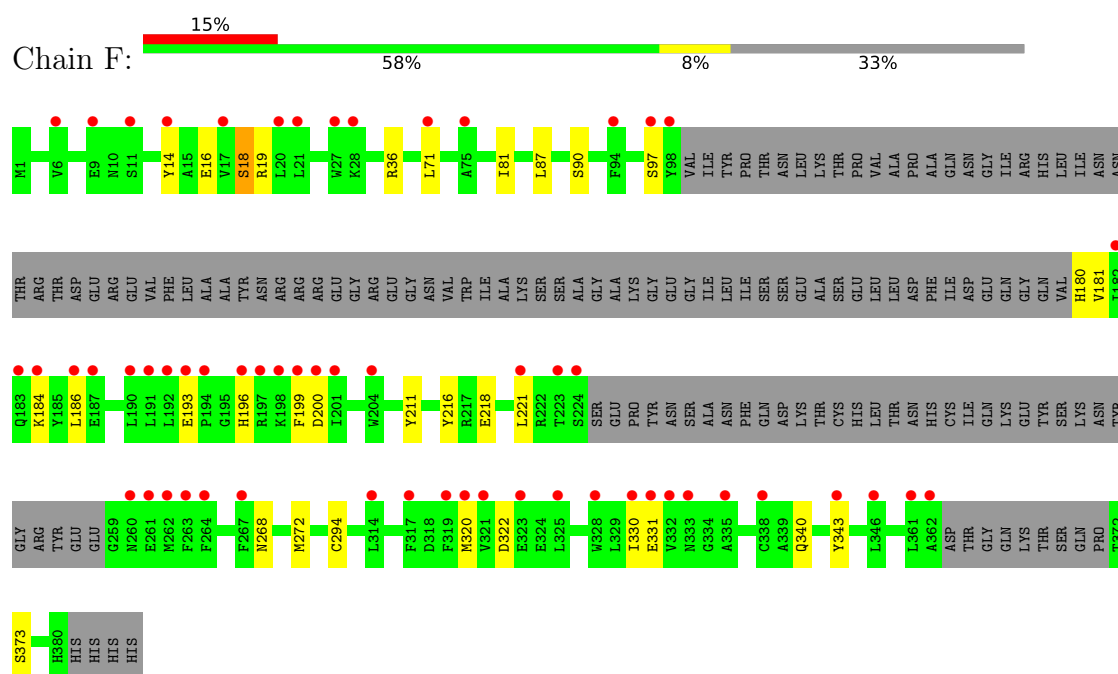
- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.57Å 155.04Å 182.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.36 – 2.92 49.77 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.36-2.92) 92.0 (49.77-2.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.184 , 0.228 0.185 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	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	0.94	EDS
Total number of atoms	16797	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: ACP, CA, MES, GDP, YJ4, MG, CL, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/3483	0.44	0/4729
1	C	0.27	0/3505	0.45	0/4757
2	B	0.26	0/3406	0.44	0/4613
2	D	0.26	0/3350	0.45	0/4537
3	E	0.25	0/1001	0.40	0/1328
4	F	0.25	0/2144	0.45	0/2897
All	All	0.26	0/16889	0.44	0/22861

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	3406	0	3316	32	0
1	C	3428	0	3339	33	0
2	B	3333	0	3213	24	0
2	D	3278	0	3148	45	0
3	E	993	0	1012	14	0
4	F	2095	0	2097	16	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
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	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
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	0	12	0	0
10	B	24	0	24	1	0
11	B	26	0	0	0	0
11	D	26	0	0	1	0
12	F	17	0	8	3	0
13	A	7	0	0	0	0
13	B	10	0	0	0	0
13	C	17	0	0	0	0
13	D	3	0	0	0	0
All	All	16797	0	16205	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)
2:B:178:THR:HG22	1:C:258:ASN:HD21	1.53	0.74
2:D:375:GLN:HB2	2:D:419:VAL:HG23	1.72	0.71
1:C:252:LEU:HA	1:C:255:PHE:HD2	1.62	0.65
2:D:330:MET:HG3	2:D:351:THR:HG21	1.78	0.64
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.81	0.63
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.82	0.61
2:B:219:THR:HG21	1:C:326:LYS:HA	1.83	0.60
3:E:100:LYS:HA	3:E:103:GLN:HG2	1.83	0.60
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.83	0.60
2:B:202:ILE:HD13	2:B:229:VAL:HG13	1.83	0.59
4:F:81:ILE:HD13	4:F:87:LEU:HD13	1.84	0.59
2:D:31:ASP:OD1	2:D:34:GLY:N	2.34	0.59
2:D:170:MET:HE3	2:D:201:CYS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:O	1:A:91:GLN:HG2	2.04	0.57
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.86	0.56
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.69	0.56
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.86	0.56
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.87	0.56
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.71	0.55
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
3:E:60:ARG:O	3:E:64:GLN:HG2	2.07	0.54
4:F:186:LEU:HD11	4:F:322:ASP:HB3	1.90	0.54
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.43	0.54
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.90	0.54
2:D:232:THR:HG21	2:D:300:MET:HG3	1.90	0.54
2:D:12:CYS:SG	2:D:138:SER:HB3	2.49	0.53
2:B:375:GLN:HB2	2:B:419:VAL:HG13	1.90	0.53
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.91	0.53
1:C:214:ARG:NH1	1:C:220:GLU:O	2.42	0.52
2:D:100:ASN:HD22	2:D:103:LYS:HG3	1.75	0.52
4:F:184:LYS:O	12:F:401:ACP:N6	2.42	0.52
1:A:399:TYR:O	1:A:402:ARG:NH1	2.41	0.51
2:B:2:ARG:HA	2:B:129:CYS:O	2.11	0.51
2:D:172:SER:OG	2:D:205:GLU:N	2.44	0.51
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.46	0.51
2:D:134:GLN:HA	2:D:165:ASN:O	2.11	0.51
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.76	0.50
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.50
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.42	0.50
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.93	0.50
4:F:330:ILE:HD13	12:F:401:ACP:H3'	1.94	0.50
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.94	0.49
2:B:209:ASP:O	2:B:213:ARG:HG2	2.12	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.49
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.95	0.48
2:B:161:ASP:O	2:B:251:ARG:NH2	2.46	0.48
4:F:320:MET:HB3	4:F:330:ILE:HD11	1.93	0.48
1:C:210:TYR:OH	1:C:221:ARG:HD2	2.14	0.48
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.95	0.48
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.48	0.48
1:A:325:PRO:O	1:A:328:VAL:HG22	2.14	0.48
2:D:105:HIS:O	2:D:150:LEU:HD22	2.14	0.48
1:C:276:ILE:HG23	1:C:369:ALA:HB3	1.96	0.48
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:THR:HG23	2:D:287:PRO:HD2	1.96	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.47
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.95	0.47
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.80	0.47
2:B:267:MET:HG2	2:B:374:ILE:HD13	1.96	0.47
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.97	0.47
2:B:293:MET:CG	2:B:367:PHE:HB2	2.44	0.47
2:D:292:GLN:HG2	2:D:298:ASN:HD21	1.79	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.14	0.47
2:B:335:ASN:OD1	4:F:36:ARG:HD3	2.14	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.47
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.80	0.47
1:C:252:LEU:HA	1:C:255:PHE:CD2	2.46	0.46
2:D:6:HIS:NE2	2:D:8:GLN:HG2	2.31	0.46
2:D:107:THR:HG21	3:E:137:LYS:NZ	2.30	0.46
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.30	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.46
2:B:134:GLN:HA	2:B:165:ASN:O	2.16	0.46
1:A:241:SER:HB3	1:A:248:LEU:O	2.16	0.46
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.98	0.46
2:D:116:VAL:O	2:D:120:VAL:HG13	2.16	0.46
1:A:406:HIS:HA	1:A:409:VAL:HG22	1.98	0.46
2:B:169:VAL:HA	2:B:202:ILE:O	2.16	0.46
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.97	0.45
1:C:216:ASN:HB3	1:C:275:VAL:O	2.17	0.45
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.34	0.45
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.97	0.45
2:B:324:LYS:NZ	2:B:328:GLU:OE1	2.47	0.45
3:E:103:GLN:HG3	3:E:104:LYS:N	2.31	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.45
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.57	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.44
1:A:324:VAL:O	1:A:327:ASP:HB2	2.17	0.44
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.99	0.44
1:A:245:ASP:O	3:E:16:SER:OG	2.31	0.44
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.81	0.44
1:A:141:PHE:O	1:A:147:SER:HB3	2.18	0.44
3:E:135:LYS:HA	3:E:135:LYS:HD3	1.73	0.44
2:B:295:ASP:HA	10:B:503:MES:O3S	2.18	0.44
1:C:255:PHE:CE1	1:C:316:CYS:HB3	2.53	0.44
1:C:250:VAL:HG11	1:C:352:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.33	0.44
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.49	0.43
3:E:48:GLU:H	3:E:48:GLU:HG3	1.47	0.43
2:B:30:ILE:HD11	2:B:47:ILE:HD11	2.00	0.43
3:E:9:ILE:HG22	3:E:10:GLU:HG2	1.99	0.43
1:A:54:SER:O	1:A:61:HIS:HA	2.18	0.43
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.99	0.43
2:D:149:THR:HA	2:D:152:ILE:HG12	2.01	0.43
1:C:271:THR:HG22	1:C:301:GLN:HG2	2.00	0.43
1:A:355:ILE:O	3:E:17:GLY:HA3	2.18	0.43
2:D:165:ASN:HD22	2:D:198:GLU:HB2	1.84	0.43
4:F:16:GLU:HA	4:F:19:ARG:HD2	2.01	0.43
1:C:2:ARG:HB3	1:C:133:GLN:NE2	2.33	0.43
2:D:124:SER:HB2	2:D:130:LEU:HD22	2.01	0.43
2:D:208:TYR:HE1	2:D:220:PRO:HD2	1.82	0.43
2:B:293:MET:HE3	2:B:293:MET:HB3	1.93	0.43
1:C:120:ASP:O	1:C:124:LYS:HG2	2.19	0.43
1:A:96:LYS:HG3	1:A:97:GLU:H	1.84	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.19	0.42
2:D:415:MET:O	2:D:419:VAL:HG12	2.18	0.42
2:D:81:PHE:O	2:D:84:ILE:HG22	2.20	0.42
2:D:100:ASN:ND2	2:D:103:LYS:HG3	2.34	0.42
1:C:60:LYS:HB3	1:C:60:LYS:HE2	1.74	0.42
2:D:28:HIS:NE2	2:D:241:ARG:HB3	2.35	0.42
1:A:63:PRO:HG2	1:A:87:PHE:CE2	2.55	0.42
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.01	0.42
4:F:186:LEU:HB3	12:F:401:ACP:H2	2.02	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
4:F:14:TYR:O	4:F:18:SER:OG	2.36	0.42
4:F:193:GLU:HG3	4:F:196:HIS:H	1.85	0.42
2:B:40:SER:OG	2:B:42:LEU:HB2	2.19	0.41
2:D:19:LYS:O	2:D:23:VAL:HG12	2.19	0.41
2:D:204:ASN:HA	2:D:207:LEU:HD12	2.02	0.41
1:A:90:GLU:O	1:A:121:ARG:HD3	2.20	0.41
2:B:23:VAL:HG21	2:B:230:SER:HB2	2.02	0.41
1:C:241:SER:HB3	1:C:250:VAL:O	2.21	0.41
1:C:320:ARG:HD3	1:C:360:PRO:HB3	2.03	0.41
4:F:180:HIS:HB3	4:F:181:VAL:H	1.74	0.41
1:A:210:TYR:OH	1:A:221:ARG:NH1	2.51	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLN:H	1:C:85:GLN:HG2	1.49	0.41
2:D:344:TRP:CE3	2:D:345:ILE:HG13	2.55	0.41
1:C:276:ILE:HG12	1:C:281:ALA:HB2	2.02	0.41
1:A:234:ILE:O	1:A:238:ILE:HG13	2.20	0.41
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.89	0.41
2:D:73:MET:O	2:D:77:ARG:HG3	2.20	0.41
2:D:357:PRO:HB2	2:D:361:LEU:O	2.20	0.41
2:D:5:VAL:HB	2:D:133:PHE:CD2	2.57	0.41
2:D:23:VAL:O	2:D:27:GLU:HG3	2.21	0.41
2:B:178:THR:HG22	1:C:258:ASN:ND2	2.28	0.40
2:D:97:ALA:HB3	5:D:501:GTP:O3G	2.20	0.40
2:D:289:LEU:HD12	2:D:289:LEU:HA	1.92	0.40
2:D:292:GLN:HG2	2:D:298:ASN:ND2	2.36	0.40
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.03	0.40
4:F:268:ASN:O	4:F:272:MET:HG3	2.21	0.40
2:D:143:THR:HB	2:D:147:MET:HE2	2.04	0.40
2:D:248:ALA:HB1	11:D:504:YJ4:N14	2.37	0.40
3:E:54:LEU:HD23	3:E:54:LEU:HA	1.95	0.40
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.95	0.40
3:E:119:MET:O	3:E:122:ARG:HG2	2.21	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	435/450 (97%)	422 (97%)	13 (3%)	0	100	100
1	C	434/450 (96%)	423 (98%)	11 (2%)	0	100	100
2	B	420/445 (94%)	413 (98%)	7 (2%)	0	100	100
2	D	411/445 (92%)	401 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	248/384 (65%)	236 (95%)	11 (4%)	1 (0%)	34	65
All	All	2065/2317 (89%)	2011 (97%)	53 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	373	SER

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	366/378 (97%)	361 (99%)	5 (1%)	67	88
1	C	371/378 (98%)	366 (99%)	5 (1%)	69	89
2	B	366/383 (96%)	357 (98%)	9 (2%)	47	77
2	D	360/383 (94%)	349 (97%)	11 (3%)	40	72
3	E	107/127 (84%)	102 (95%)	5 (5%)	26	58
4	F	230/342 (67%)	224 (97%)	6 (3%)	46	76
All	All	1800/1991 (90%)	1759 (98%)	41 (2%)	50	79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	47	ASP
1	A	48	SER
1	A	176	GLN
1	A	241	SER
2	B	57	ASN
2	B	77	ARG
2	B	137	HIS
2	B	170	MET

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Mol	Chain	Res	Type
2	B	190	HIS
2	B	336	LYS
2	B	362	LYS
2	B	364	SER
2	B	375	GLN
1	C	38	SER
1	C	128	GLN
1	C	241	SER
1	C	253	THR
1	C	381	THR
2	D	8	GLN
2	D	75	SER
2	D	83	GLN
2	D	126	SER
2	D	137	HIS
2	D	172	SER
2	D	177	ASP
2	D	198	GLU
2	D	209	ASP
2	D	388	MET
2	D	419	VAL
3	E	19	SER
3	E	24	LEU
3	E	48	GLU
3	E	131	GLU
3	E	136	ASN
4	F	18	SER
4	F	90	SER
4	F	97	SER
4	F	200	ASP
4	F	211	TYR
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	99	ASN
1	C	133	GLN
2	D	8	GLN
2	D	100	ASN
2	D	165	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 10 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$
5	GTP	D	501	7	26,34,34	1.04	1 (3%)	33,54,54	1.78	7 (21%)
12	ACP	F	401	-	16,19,33	1.65	3 (18%)	15,28,52	2.00	3 (20%)
11	YJ4	B	506	-	28,29,29	1.02	2 (7%)	35,41,41	1.83	6 (17%)
5	GTP	A	501	7	26,34,34	1.02	1 (3%)	33,54,54	1.76	8 (24%)
9	GDP	B	501	-	24,30,30	1.18	2 (8%)	31,47,47	1.89	7 (22%)
11	YJ4	D	504	-	28,29,29	1.01	2 (7%)	35,41,41	1.74	9 (25%)
5	GTP	C	501	7	26,34,34	1.03	1 (3%)	33,54,54	1.81	8 (24%)
10	MES	B	502	-	12,12,12	2.28	1 (8%)	14,16,16	2.02	4 (28%)
10	MES	B	503	-	12,12,12	2.26	1 (8%)	14,16,16	1.91	5 (35%)

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	D	501	7	-	3/18/38/38	0/3/3/3
12	ACP	F	401	-	-	0/0/17/38	0/3/3/3
11	YJ4	B	506	-	-	2/8/21/21	0/4/4/4
5	GTP	A	501	7	-	6/18/38/38	0/3/3/3
9	GDP	B	501	-	-	4/12/32/32	0/3/3/3
11	YJ4	D	504	-	-	2/8/21/21	0/4/4/4
5	GTP	C	501	7	-	5/18/38/38	0/3/3/3
10	MES	B	502	-	-	4/6/14/14	0/1/1/1
10	MES	B	503	-	-	0/6/14/14	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	502	MES	C8-S	-7.66	1.66	1.77
10	B	503	MES	C8-S	-7.56	1.66	1.77
9	B	501	GDP	C6-C5	4.18	1.48	1.41
5	A	501	GTP	C6-N1	3.41	1.39	1.33
5	C	501	GTP	C6-N1	3.40	1.38	1.33
12	F	401	ACP	O3'-C3'	-3.38	1.36	1.43
5	D	501	GTP	C6-N1	3.36	1.38	1.33
12	F	401	ACP	C6-N6	3.15	1.45	1.34
12	F	401	ACP	C5-C4	-2.56	1.34	1.40
11	D	504	YJ4	C13-N16	2.42	1.49	1.46
11	B	506	YJ4	C05-N16	2.41	1.44	1.40
11	B	506	YJ4	C13-N16	2.41	1.49	1.46
9	B	501	GDP	C5-C4	2.31	1.47	1.40
11	D	504	YJ4	C05-N16	2.26	1.44	1.40

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	506	YJ4	O20-C12-N17	-5.89	116.23	121.43
11	D	504	YJ4	O20-C12-N17	-5.62	116.47	121.43
5	C	501	GTP	N3-C2-N1	-5.54	119.83	127.22
5	A	501	GTP	N3-C2-N1	-5.44	119.97	127.22
5	D	501	GTP	N3-C2-N1	-5.29	120.16	127.22
12	F	401	ACP	N3-C2-N1	-5.16	120.61	128.68
9	B	501	GDP	C2-N3-C4	4.98	121.05	115.36
5	A	501	GTP	C2-N3-C4	4.81	120.85	115.36
5	C	501	GTP	C2-N3-C4	4.56	120.57	115.36
10	B	503	MES	C5-N4-C3	4.44	118.83	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	C2-N3-C4	4.33	120.30	115.36
10	B	502	MES	C5-N4-C3	4.32	118.56	108.83
11	B	506	YJ4	C21-N14-C01	-4.12	118.77	123.85
9	B	501	GDP	C5-C6-N1	-3.95	118.03	123.43
9	B	501	GDP	C6-N1-C2	3.92	122.15	115.93
9	B	501	GDP	C6-C5-C4	-3.79	117.18	120.80
11	B	506	YJ4	C09-O19-C08	3.78	125.71	117.51
11	D	504	YJ4	C09-O19-C08	3.55	125.22	117.51
12	F	401	ACP	C5-C6-N6	3.52	125.70	120.35
5	D	501	GTP	PB-O3B-PG	-3.43	121.05	132.83
9	B	501	GDP	N3-C2-N1	-3.27	122.86	127.22
10	B	502	MES	O1S-S-C8	3.23	110.80	106.92
5	D	501	GTP	PA-O3A-PB	-3.19	121.89	132.83
11	B	506	YJ4	C13-C12-N17	3.04	119.91	116.13
5	C	501	GTP	PB-O3B-PG	-2.95	122.69	132.83
9	B	501	GDP	C4-C5-N7	-2.95	106.32	109.40
5	A	501	GTP	PB-O3B-PG	-2.91	122.85	132.83
11	D	504	YJ4	C13-C12-N17	2.89	119.73	116.13
9	B	501	GDP	PA-O3A-PB	-2.82	123.15	132.83
10	B	503	MES	O1S-S-C8	2.66	110.11	106.92
5	D	501	GTP	C5-C6-N1	-2.63	119.83	123.43
5	C	501	GTP	PA-O3A-PB	-2.63	123.82	132.83
5	C	501	GTP	C5-C6-N1	-2.50	120.01	123.43
11	D	504	YJ4	C21-N14-C01	-2.49	120.77	123.85
10	B	502	MES	C6-C5-N4	-2.49	106.33	110.10
10	B	502	MES	O3S-S-C8	2.46	109.75	105.77
11	B	506	YJ4	C24-N23-C03	2.46	120.36	117.30
12	F	401	ACP	C3'-C2'-C1'	2.44	104.69	101.04
5	C	501	GTP	C6-N1-C2	2.42	119.78	115.93
5	A	501	GTP	PA-O3A-PB	-2.42	124.51	132.83
11	D	504	YJ4	C24-N23-C03	2.36	120.24	117.30
11	D	504	YJ4	N14-C01-N18	-2.35	113.13	117.19
5	C	501	GTP	N2-C2-N1	2.34	120.89	117.25
11	D	504	YJ4	C11-N17-C12	-2.34	121.60	124.49
11	B	506	YJ4	C11-N17-C12	-2.31	121.63	124.49
11	D	504	YJ4	N18-C04-N16	-2.31	113.82	116.26
10	B	503	MES	O3S-S-C8	2.27	109.45	105.77
5	D	501	GTP	C6-N1-C2	2.27	119.54	115.93
10	B	503	MES	C7-N4-C5	2.22	116.92	111.23
5	A	501	GTP	N2-C2-N1	2.21	120.69	117.25
5	C	501	GTP	O3G-PG-O3B	2.19	111.98	104.64
10	B	503	MES	O2S-S-C8	2.19	109.55	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	-2.19	120.44	123.43
5	D	501	GTP	N2-C2-N1	2.18	120.65	117.25
5	A	501	GTP	C6-N1-C2	2.14	119.33	115.93
11	D	504	YJ4	C22-C21-N14	-2.13	104.22	111.42
5	A	501	GTP	O2G-PG-O3B	2.07	111.59	104.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

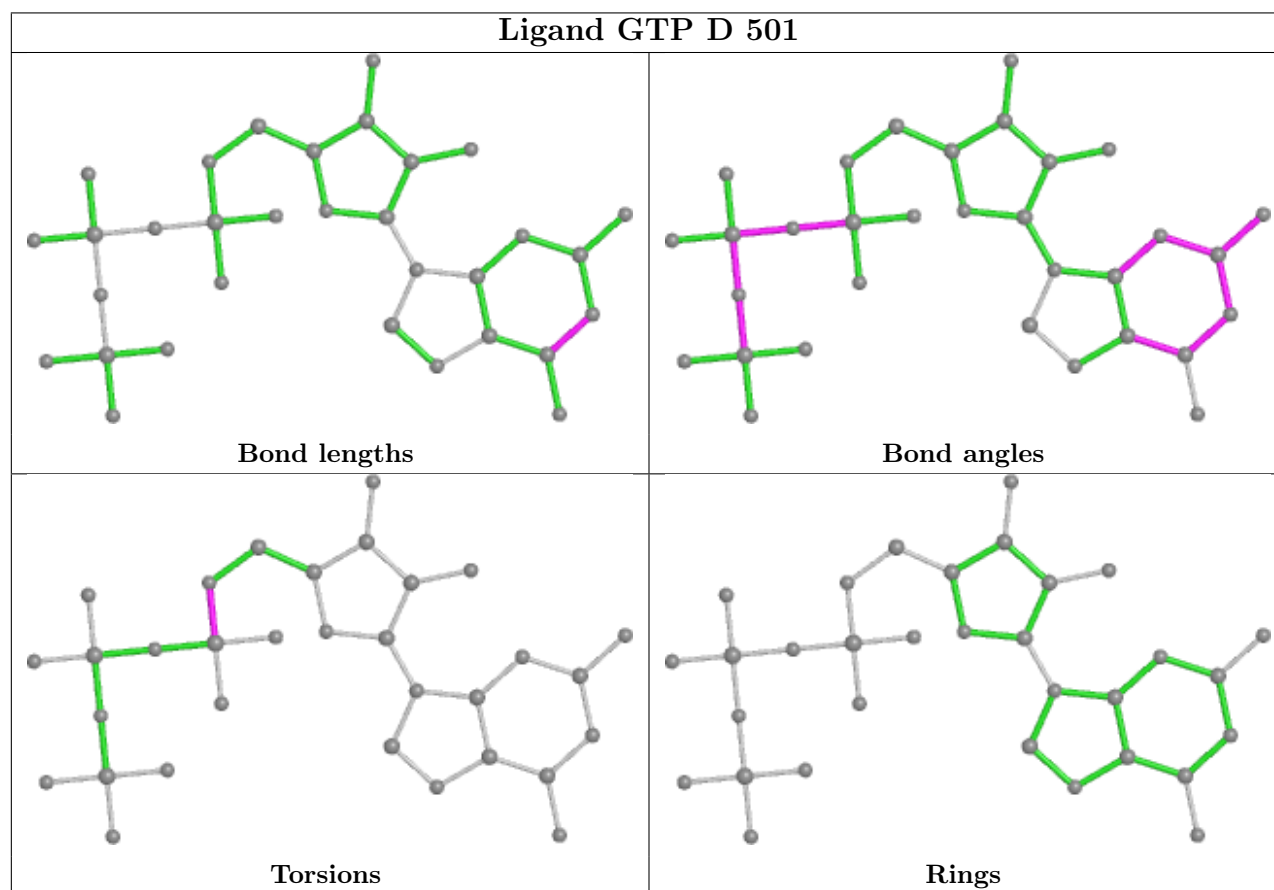
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	502	MES	C7-C8-S-O2S
10	B	502	MES	C7-C8-S-O3S
11	B	506	YJ4	C03-C04-N16-C13
11	D	504	YJ4	C03-C04-N16-C13
11	D	504	YJ4	N18-C04-N16-C13
11	B	506	YJ4	N18-C04-N16-C13
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	PB-O3A-PA-O1A
10	B	502	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
10	B	502	MES	C8-C7-N4-C3

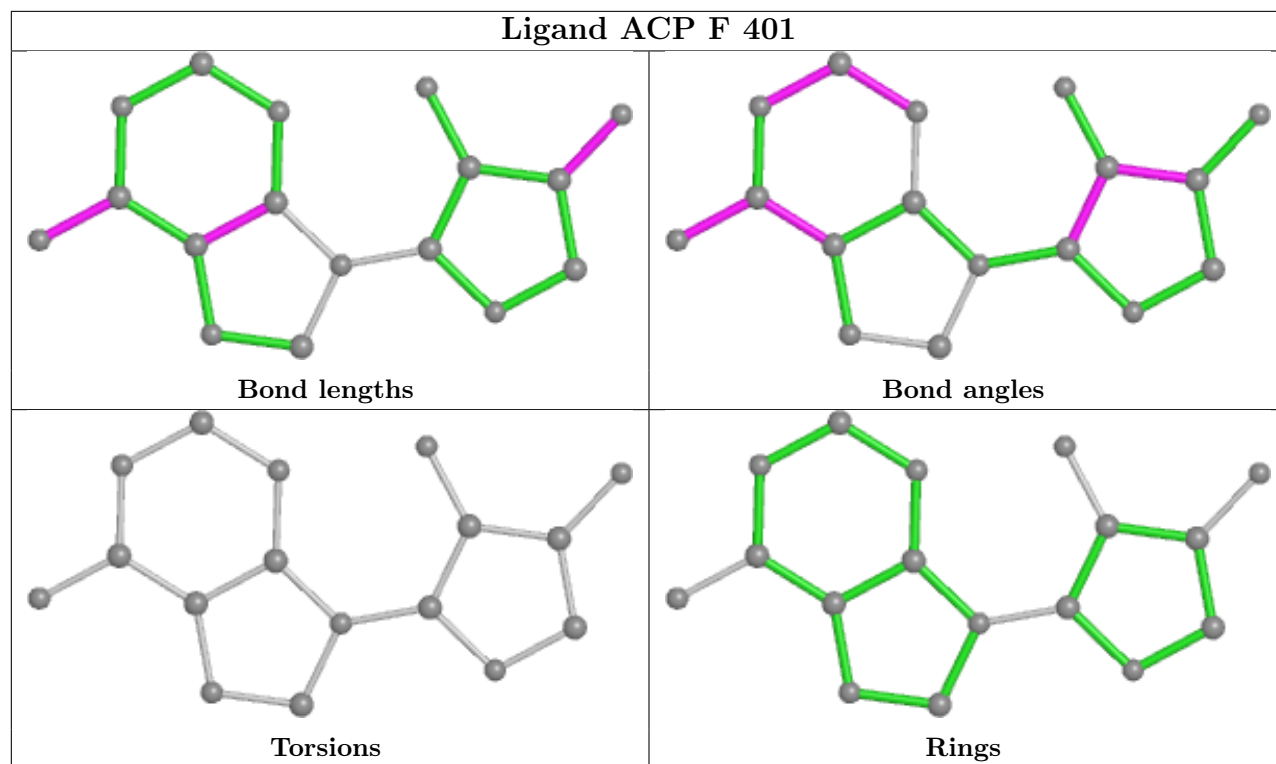
There are no ring outliers.

4 monomers are involved in 6 short contacts:

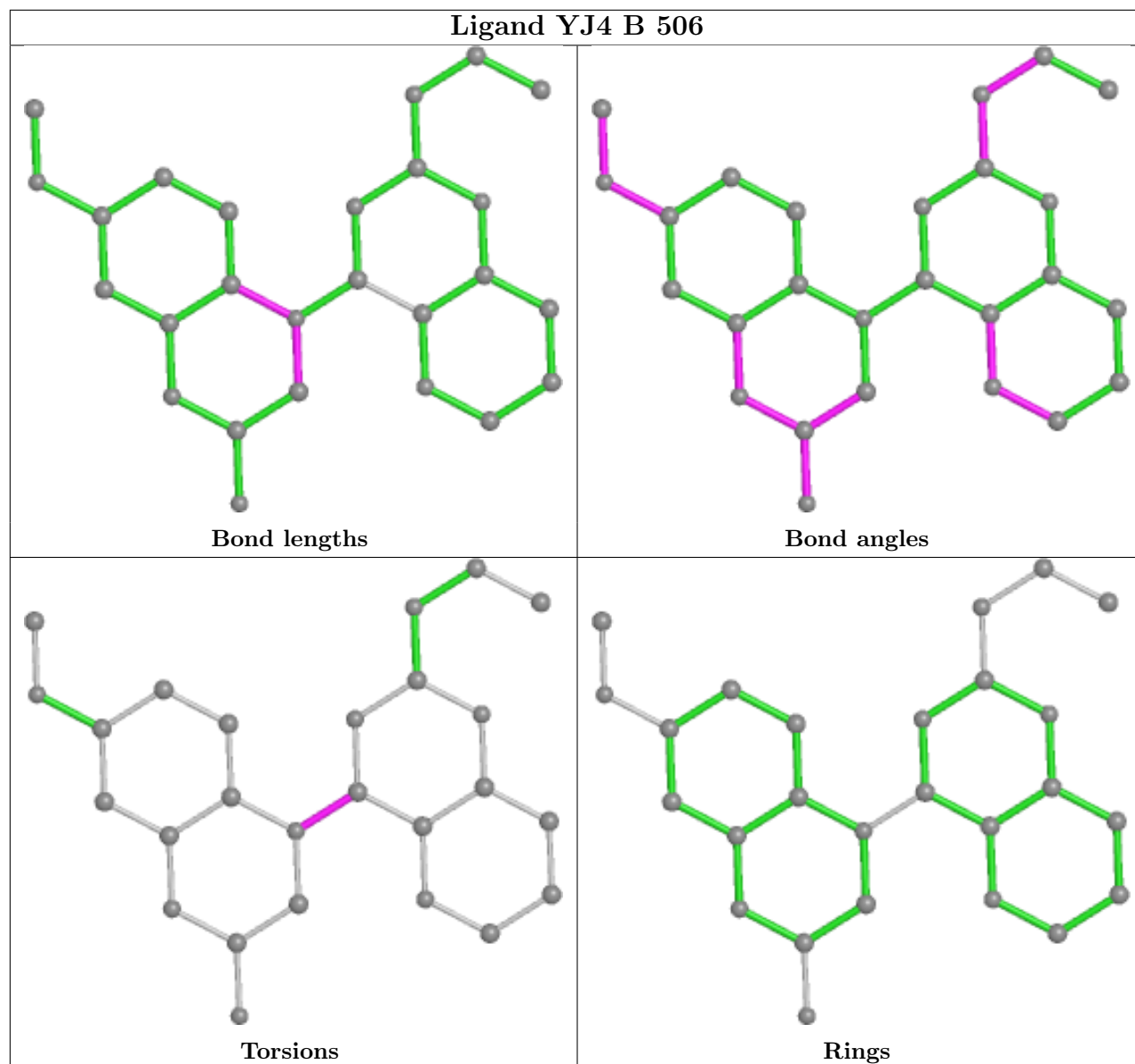
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	GTP	1	0
12	F	401	ACP	3	0
11	D	504	YJ4	1	0
10	B	503	MES	1	0

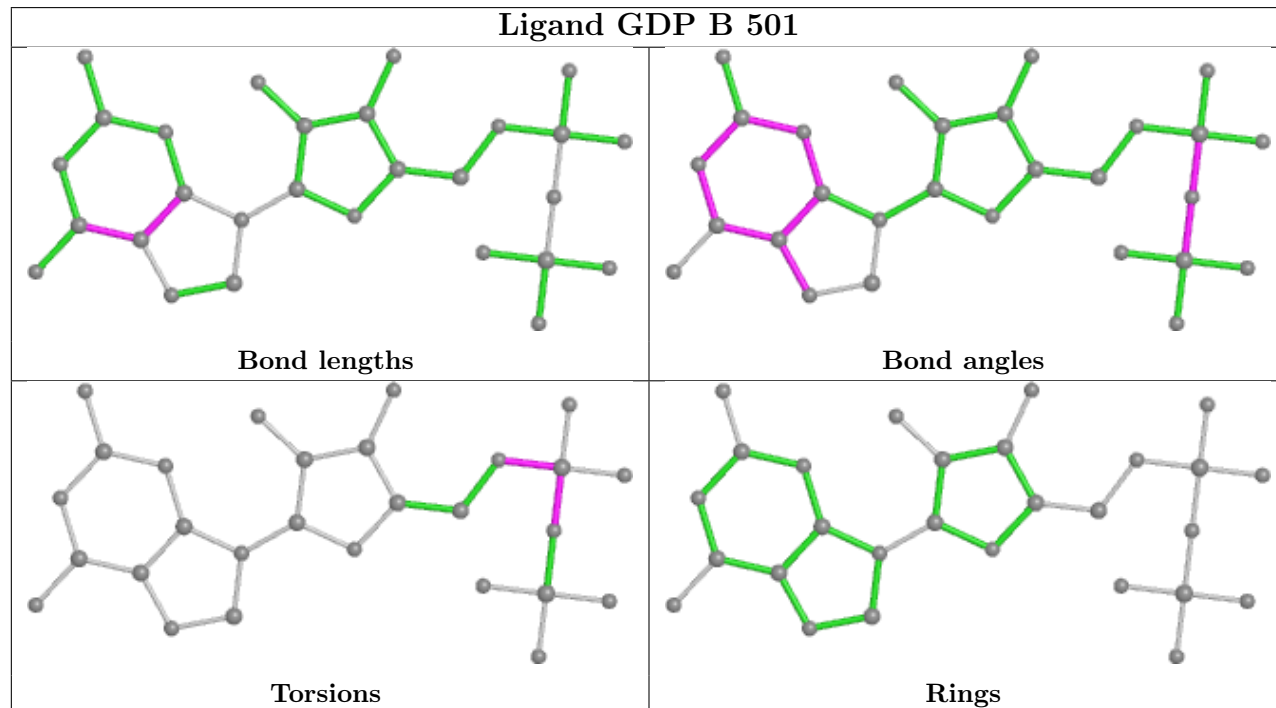
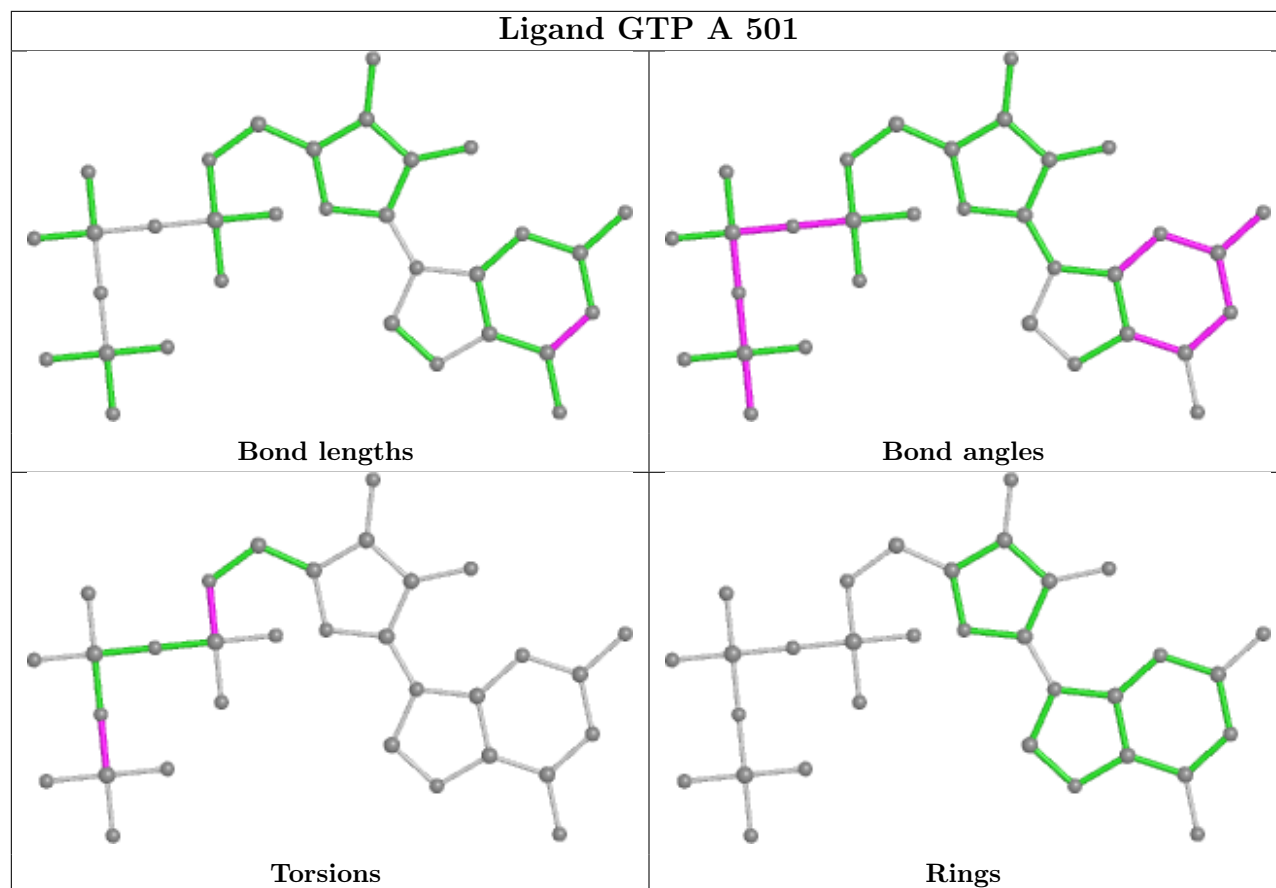
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



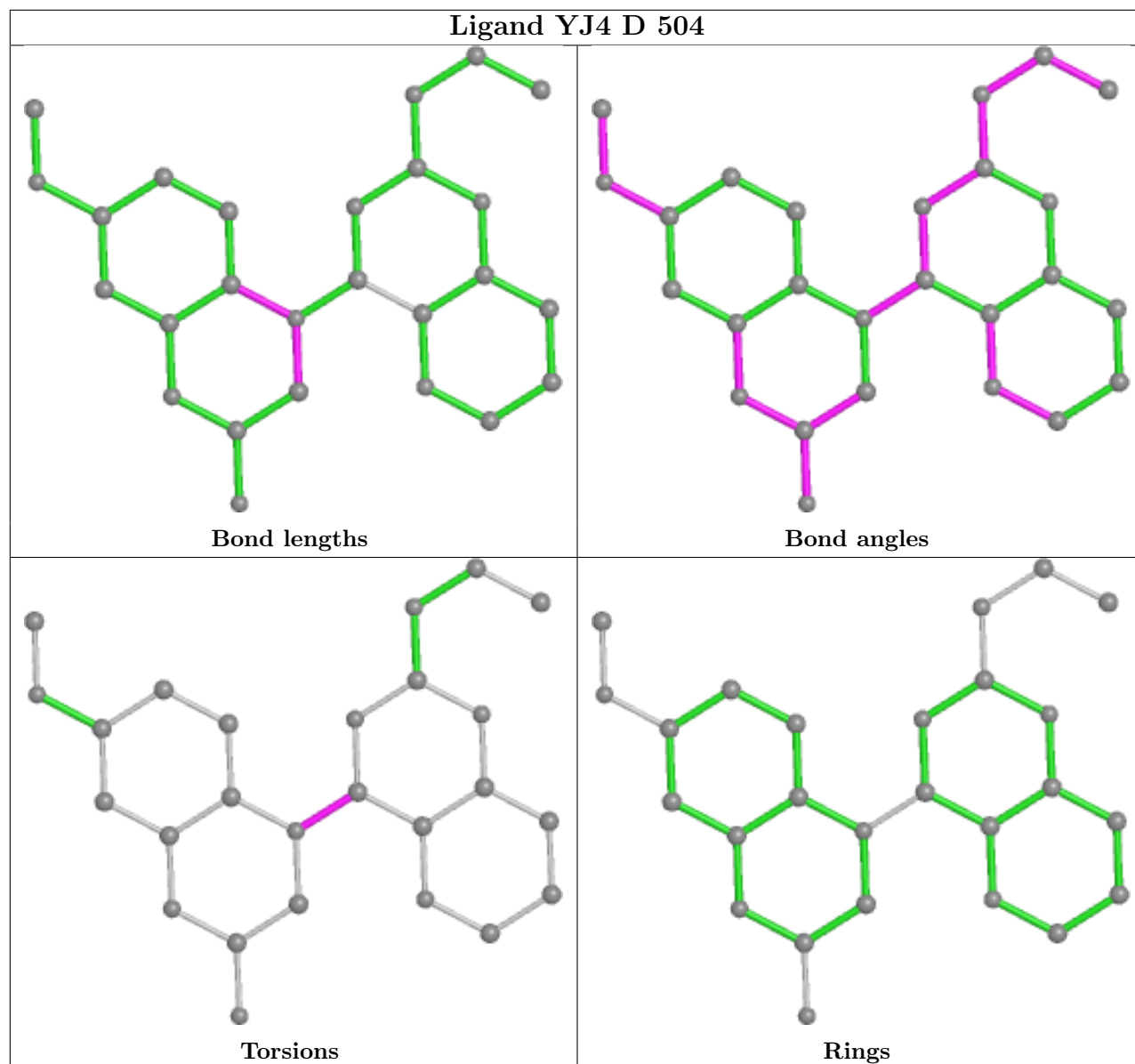


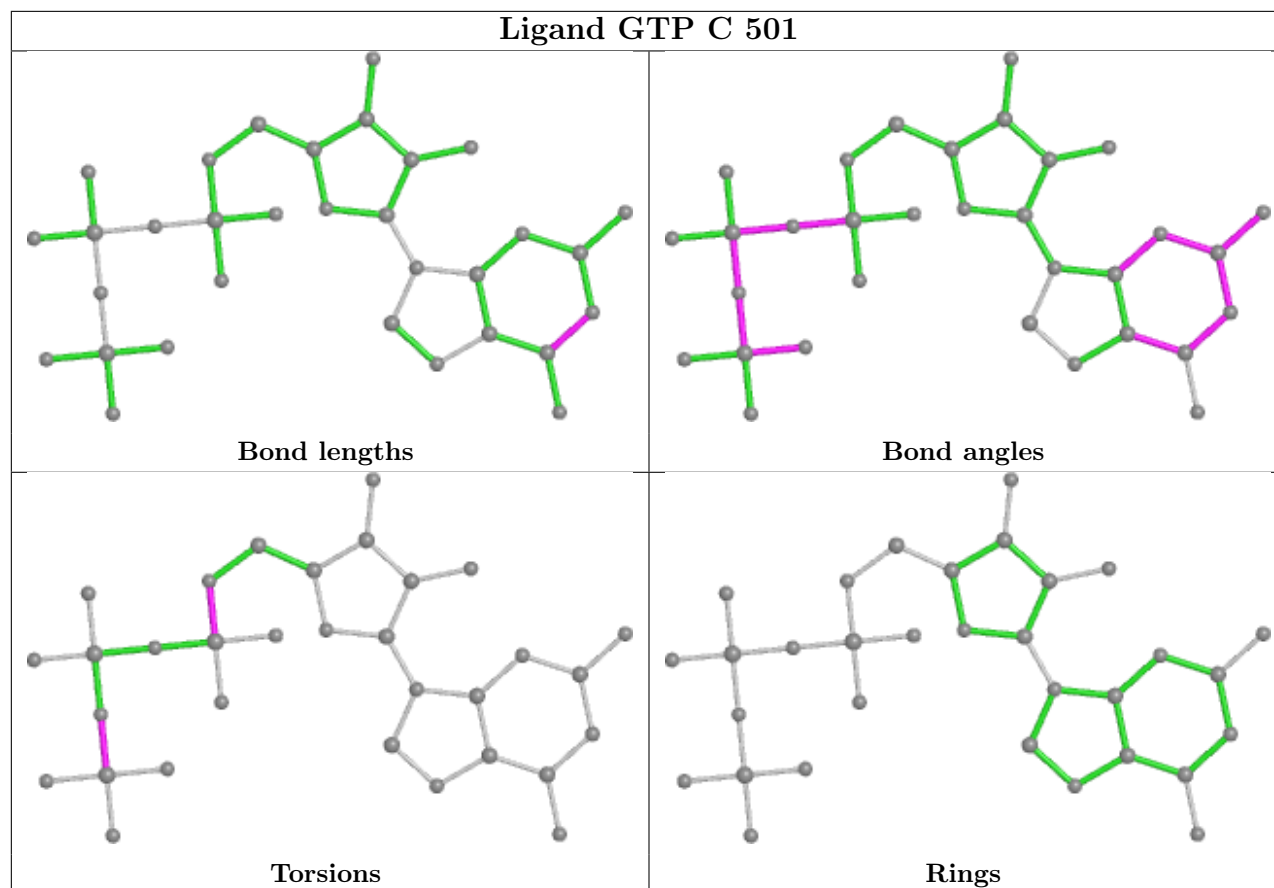
Ligand YJ4 B 506





Ligand YJ4 D 504





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	0.30	19 (4%) 35 32	57, 81, 121, 164	0
1	C	438/450 (97%)	0.00	4 (0%) 84 84	50, 66, 99, 147	0
2	B	424/445 (95%)	0.20	16 (3%) 40 37	48, 68, 111, 153	0
2	D	417/445 (93%)	0.45	29 (6%) 16 13	61, 95, 131, 156	0
3	E	121/143 (84%)	0.42	10 (8%) 11 9	57, 94, 136, 167	0
4	F	256/384 (66%)	1.07	58 (22%) 0 0	65, 103, 146, 177	0
All	All	2093/2317 (90%)	0.35	136 (6%) 18 15	48, 82, 128, 177	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	GLY	4.5
4	F	183	GLN	4.5
4	F	196	HIS	4.3
4	F	362	ALA	4.1
2	B	57	ASN	4.1
4	F	221	LEU	4.1
4	F	9	GLU	4.1
1	C	440	VAL	4.0
2	B	55	THR	4.0
4	F	197	ARG	4.0
4	F	263	PHE	3.9
3	E	133	VAL	3.9
4	F	223	THR	3.8
4	F	261	GLU	3.7
1	A	43	GLY	3.7
2	D	394	PHE	3.7
4	F	320	MET	3.7
4	F	319	PHE	3.7
3	E	27	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	224	SER	3.6
2	D	403	MET	3.6
4	F	98	TYR	3.6
2	D	396	HIS	3.6
3	E	139	LEU	3.5
4	F	198	LYS	3.5
4	F	204	TRP	3.5
1	A	280	LYS	3.5
4	F	335	ALA	3.4
1	A	59	GLY	3.4
2	D	74	ASP	3.4
3	E	28	SER	3.3
4	F	192	LEU	3.3
2	D	95	SER	3.3
4	F	264	PHE	3.3
1	A	283	HIS	3.3
4	F	184	LYS	3.2
2	B	59	TYR	3.2
2	D	76	VAL	3.2
2	B	281	TYR	3.2
4	F	193	GLU	3.2
4	F	267	PHE	3.1
4	F	11	SER	3.1
4	F	200	ASP	3.1
3	E	44	ASP	3.0
4	F	262	MET	3.0
4	F	328	TRP	3.0
2	B	54	ALA	3.0
2	D	214	THR	3.0
4	F	191	LEU	3.0
2	D	408	PHE	3.0
2	B	56	GLY	3.0
1	A	282	TYR	2.9
1	A	281	ALA	2.9
2	D	92	PHE	2.9
2	B	282	ARG	2.9
2	D	59	TYR	2.9
4	F	361	LEU	2.9
4	F	321	VAL	2.9
2	D	44	LEU	2.9
4	F	186	LEU	2.9
4	F	97	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	349	THR	2.8
4	F	323	GLU	2.8
1	A	60	LYS	2.8
4	F	17	VAL	2.8
4	F	75	ALA	2.8
2	D	398	TYR	2.8
3	E	48	GLU	2.7
4	F	14	TYR	2.7
2	B	44	LEU	2.7
4	F	187	GLU	2.7
1	A	140	SER	2.6
4	F	330	ILE	2.6
1	A	285	GLN	2.6
2	D	64	ILE	2.6
2	B	37	HIS	2.6
2	D	57	ASN	2.6
4	F	346	LEU	2.5
2	D	85	PHE	2.5
4	F	190	LEU	2.5
1	A	346	TRP	2.5
2	B	60	VAL	2.5
2	D	404	ASP	2.5
1	A	163	LYS	2.5
4	F	201	ILE	2.5
4	F	332	VAL	2.5
2	D	402	GLY	2.5
2	D	58	LYS	2.5
1	C	251	ASP	2.4
1	C	253	THR	2.4
2	D	30	ILE	2.4
4	F	20	LEU	2.4
4	F	199	PHE	2.4
4	F	182	ILE	2.4
4	F	343	TYR	2.4
2	D	216	LYS	2.3
2	D	35	SER	2.3
4	F	333	ASN	2.3
4	F	28	LYS	2.3
3	E	26	PRO	2.3
4	F	314	LEU	2.3
1	A	61	HIS	2.3
1	C	245	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.3
2	B	58	LYS	2.3
3	E	7	GLU	2.3
2	D	217	LEU	2.3
3	E	138	GLU	2.3
2	D	37	HIS	2.2
1	A	143	GLY	2.2
4	F	71	LEU	2.2
4	F	94	PHE	2.2
4	F	317	PHE	2.2
2	B	429	THR	2.2
2	B	274	THR	2.2
2	D	86	ARG	2.2
4	F	194	PRO	2.2
2	B	36	TYR	2.2
4	F	331	GLU	2.1
1	A	345	ASP	2.1
1	A	58	ALA	2.1
4	F	338	CYS	2.1
2	D	395	LEU	2.1
2	D	73	MET	2.1
2	D	391	ARG	2.1
2	D	401	GLU	2.1
2	B	80	PRO	2.1
4	F	325	LEU	2.1
4	F	6	VAL	2.1
2	B	40	SER	2.0
4	F	260	ASN	2.0
1	A	35	GLN	2.0
4	F	27	TRP	2.0
3	E	134	ARG	2.0
4	F	21	LEU	2.0
2	D	81	PHE	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

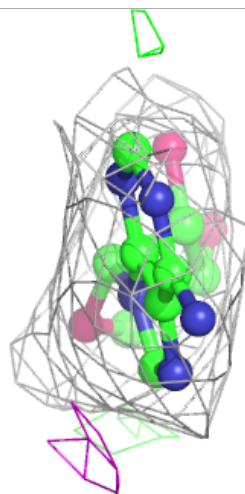
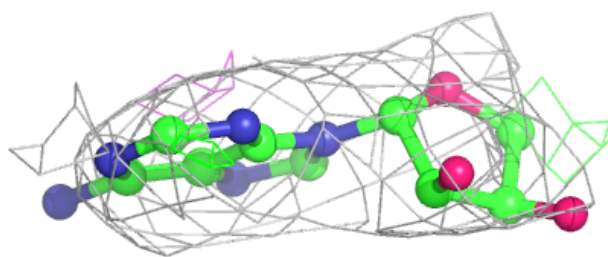
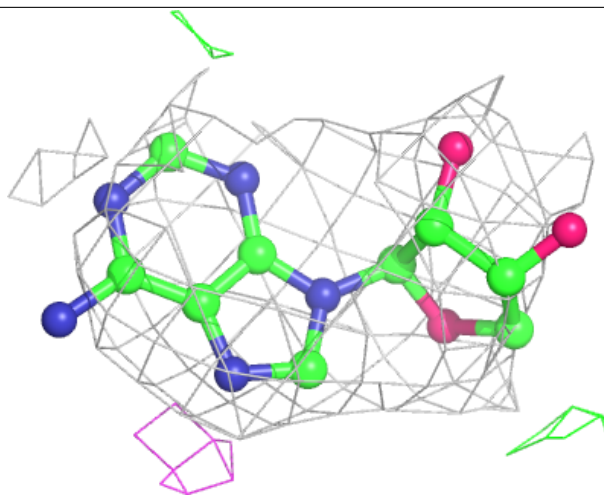
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CA	B	505	1/1	0.74	0.37	120,120,120,120	0
6	CA	C	504	1/1	0.81	0.30	124,124,124,124	0
12	ACP	F	401	17/31	0.84	0.32	119,132,155,166	0
8	CL	D	503	1/1	0.85	0.66	86,86,86,86	0
6	CA	A	502	1/1	0.86	0.15	133,133,133,133	0
7	MG	B	504	1/1	0.93	0.26	109,109,109,109	0
7	MG	D	502	1/1	0.93	0.09	104,104,104,104	0
8	CL	A	504	1/1	0.94	0.13	102,102,102,102	0
10	MES	B	503	12/12	0.95	0.24	89,103,134,147	0
10	MES	B	502	12/12	0.96	0.19	61,73,90,103	0
6	CA	C	502	1/1	0.96	0.14	97,97,97,97	0
7	MG	A	503	1/1	0.96	0.20	58,58,58,58	0
7	MG	C	503	1/1	0.97	0.16	62,62,62,62	0
5	GTP	D	501	32/32	0.97	0.12	80,99,115,120	0
11	YJ4	D	504	26/26	0.97	0.20	58,69,89,93	0
9	GDP	B	501	28/28	0.97	0.24	47,56,64,81	0
11	YJ4	B	506	26/26	0.98	0.20	50,63,78,81	0
5	GTP	A	501	32/32	0.98	0.29	56,60,75,83	0
5	GTP	C	501	32/32	0.98	0.19	54,58,77,82	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.

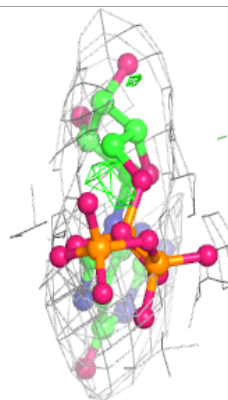
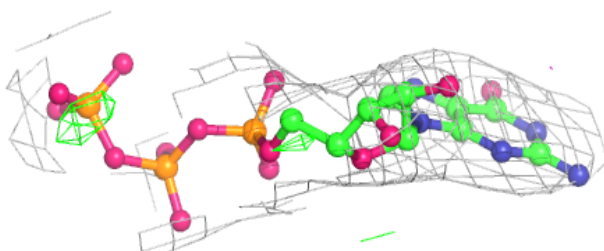
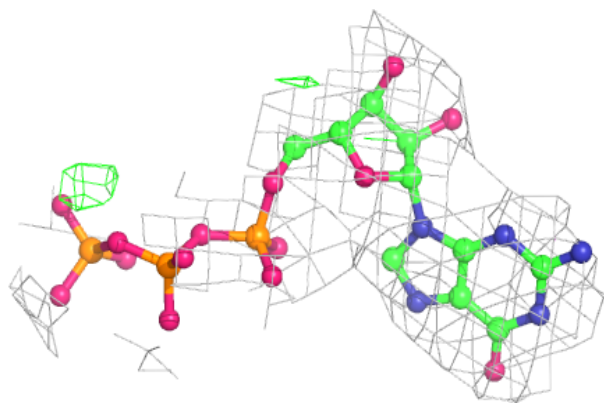
Electron density around ACP F 401:

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

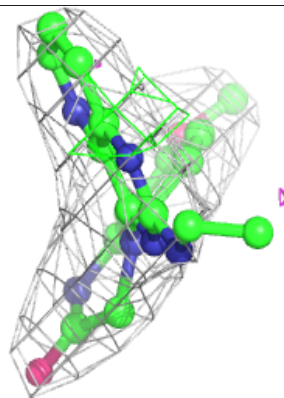
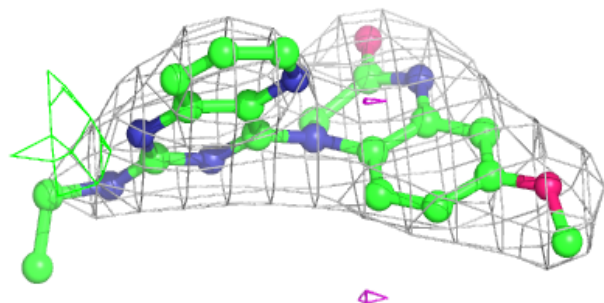
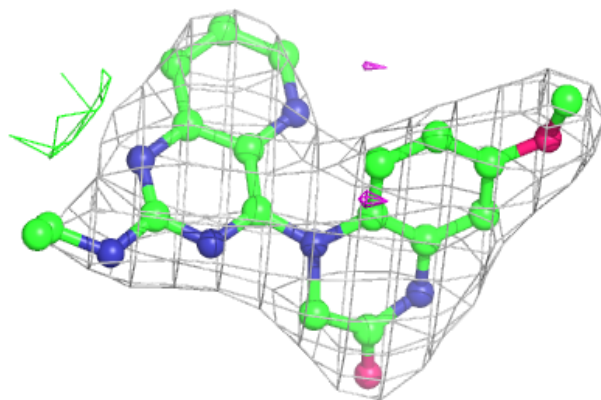


Electron density around GTP D 501:

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

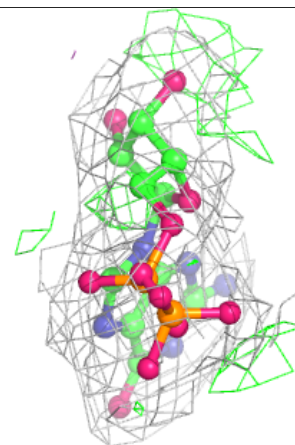
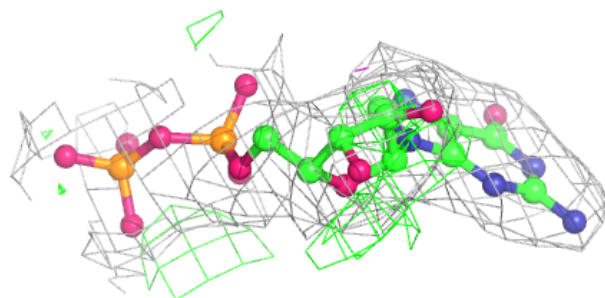
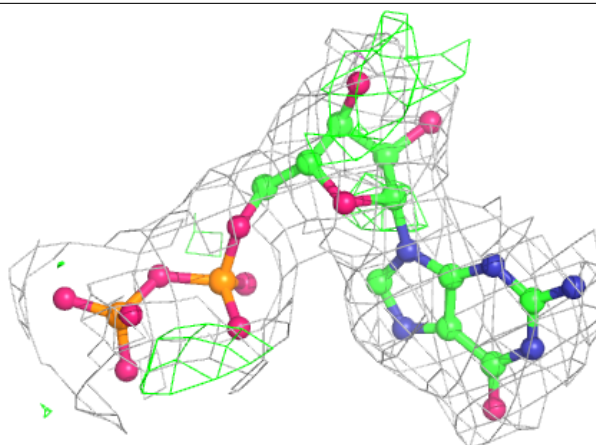
**Electron density around YJ4 D 504:**

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

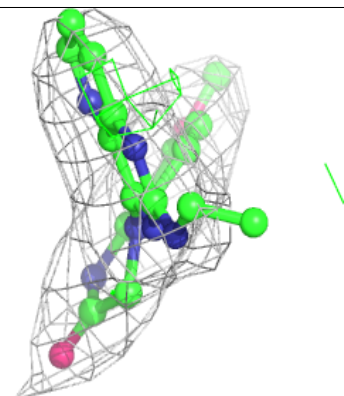
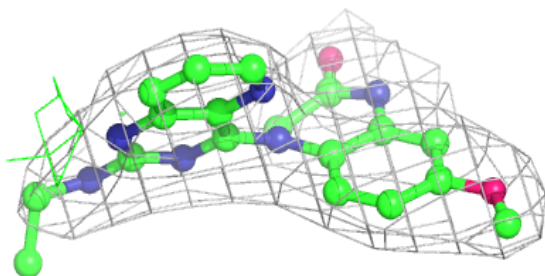
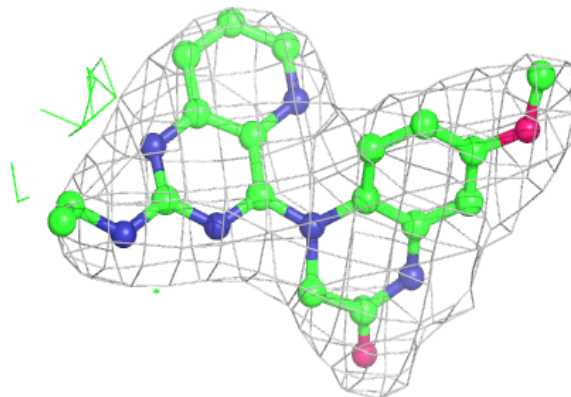


Electron density around GDP B 501:

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

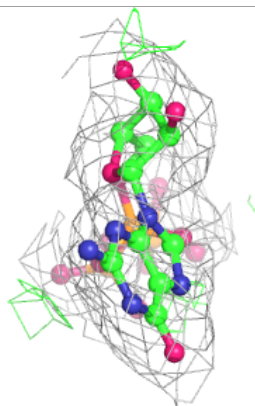
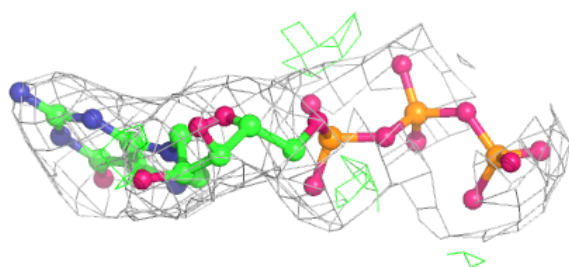
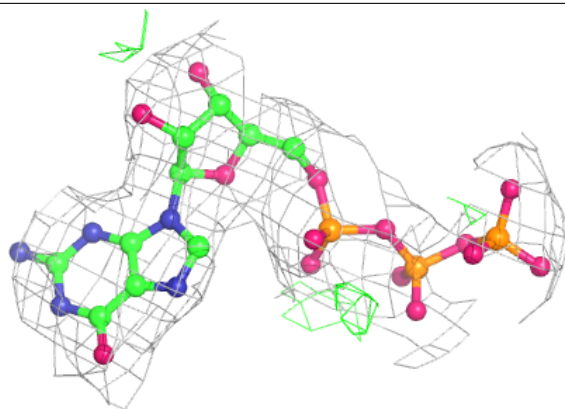
**Electron density around YJ4 B 506:**

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

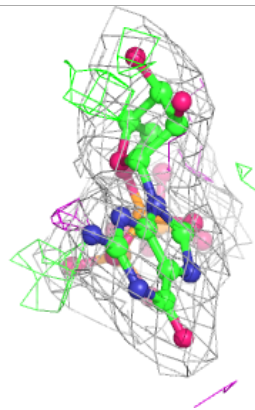
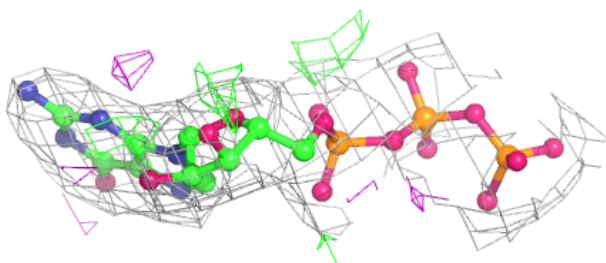
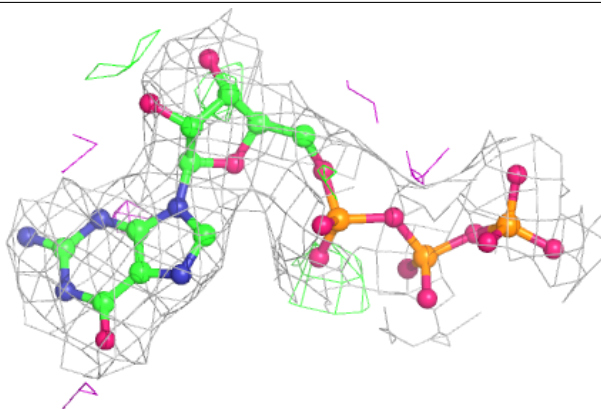


Electron density around GTP A 501:

$2mF_o - DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.