



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:49 PM UTC

PDB ID : 5M8G / pdb_00005m8g
Title : Tubulin-MTD265 complex
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Deposited on : 2016-10-28
Resolution : 2.15 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:

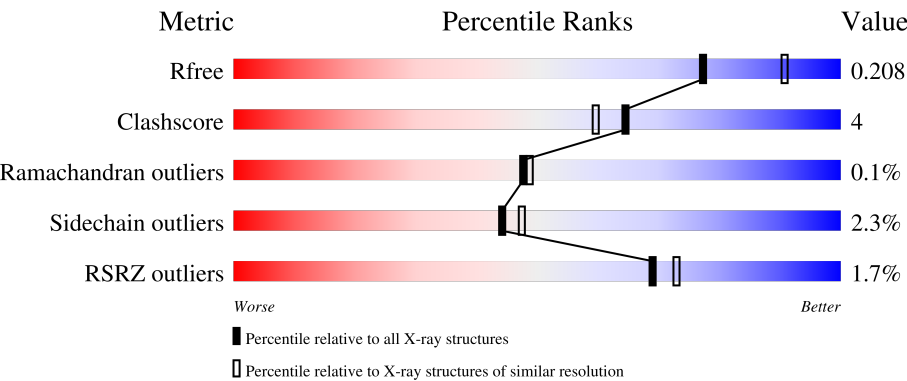
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	85%12%.
1	C	451	89%8%..
2	B	445	84%10%5%
2	D	445	81%15%.2%
3	E	143	75%11%14%3%

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Mol	Chain	Length	Quality of chain
4	F	384	3% 78% 7% • 14%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18016 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	440	Total	C	N	O	S	0	1	0
			3436	2172	584	657	23			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3331	2094	568	643	26			
2	D	427	Total	C	N	O	S	0	0	0
			3349	2101	572	650	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	0	0
			2724	1756	461	493	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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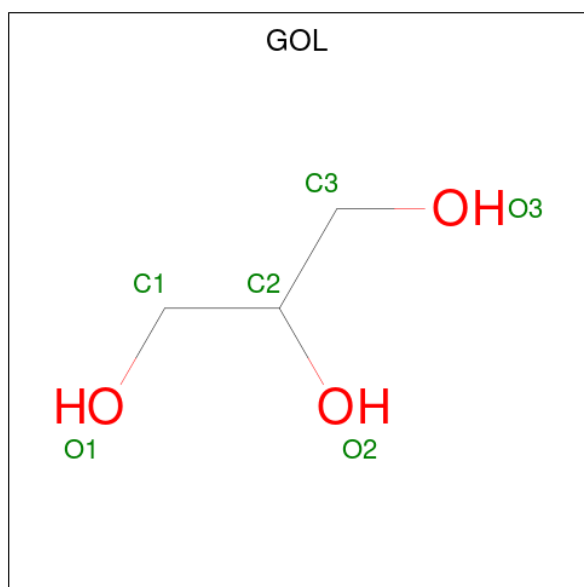
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

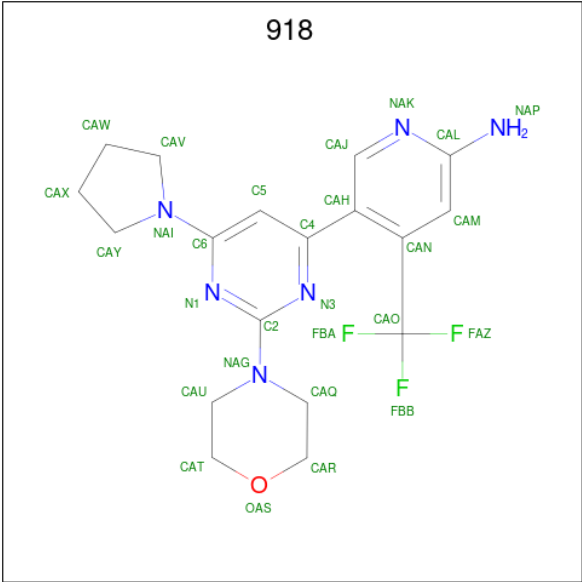
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

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



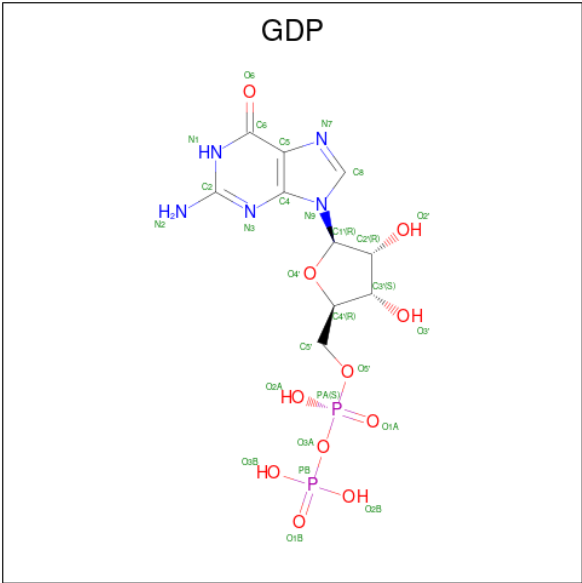
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 5-(2-morpholin-4-yl-6-pyrrolidin-1-yl-pyrimidin-4-yl)-4-(trifluoromethyl)pyridine-2-amine (CCD ID: 918) (formula: C₁₈H₂₁F₃N₆O).



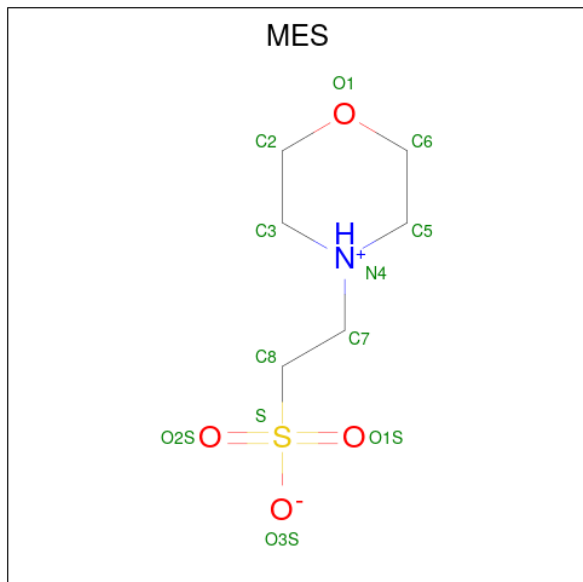
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	F	N	O	0	0
			28	18	3	6	1		
9	D	1	Total	C	F	N	O	0	0
			28	18	3	6	1		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



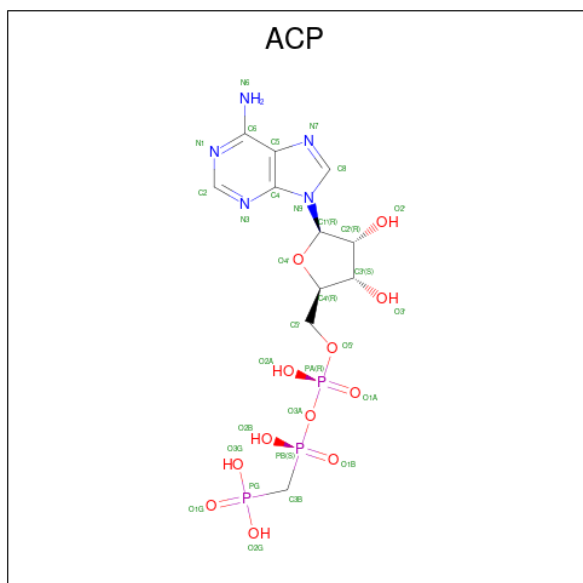
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
10	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

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



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

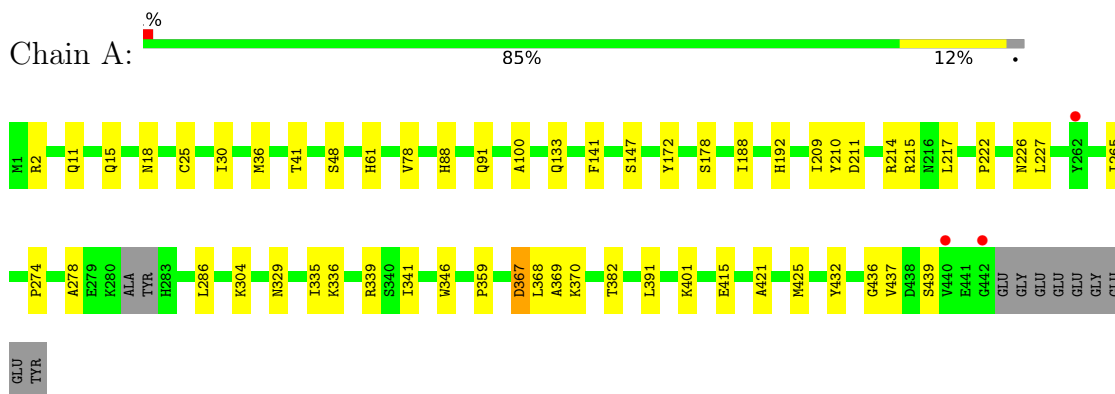
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	95	Total	O	0	0
			95	95		
13	B	93	Total	O	0	0
			93	93		
13	C	186	Total	O	0	0
			186	186		
13	D	51	Total	O	0	0
			51	51		
13	E	17	Total	O	0	0
			17	17		
13	F	36	Total	O	0	0
			36	36		

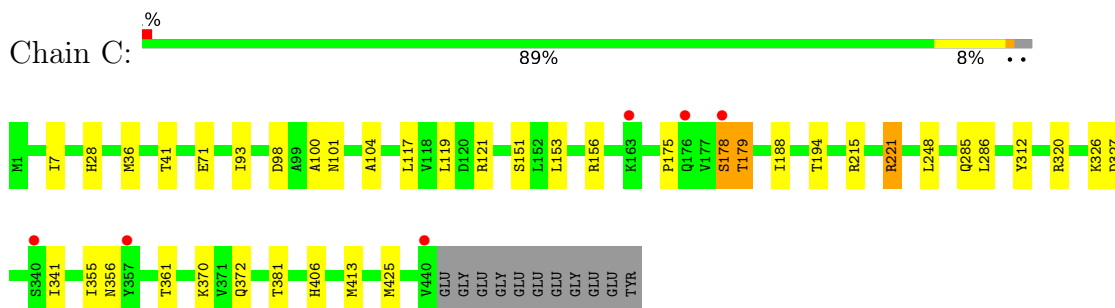
3 Residue-property plots

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

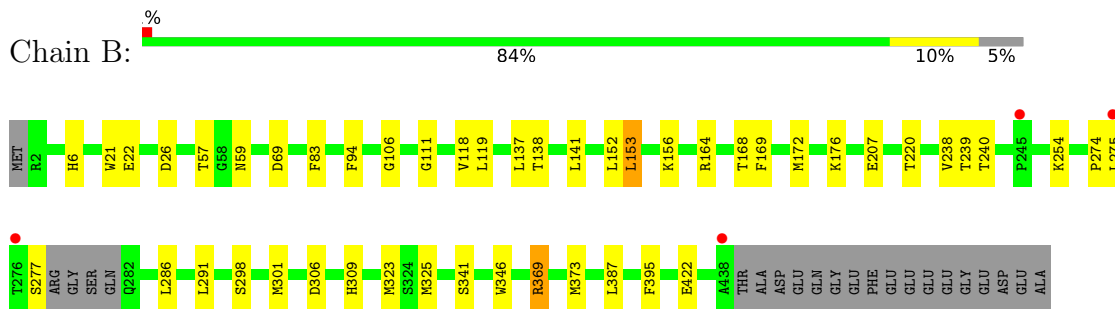
- Molecule 1: Tubulin alpha-1B chain



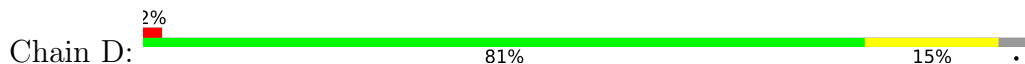
- Molecule 1: Tubulin alpha-1B chain

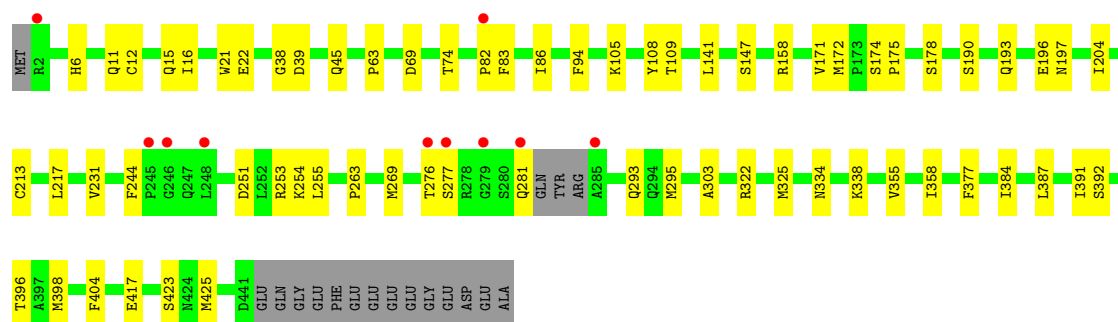


- Molecule 2: Tubulin beta-2B chain

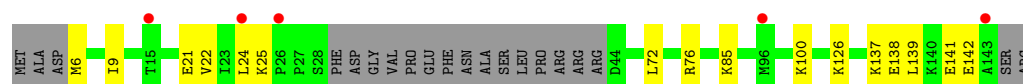
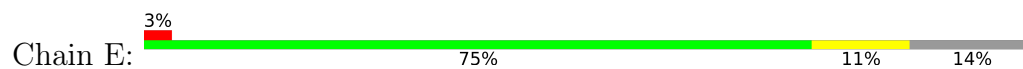


- Molecule 2: Tubulin beta-2B chain

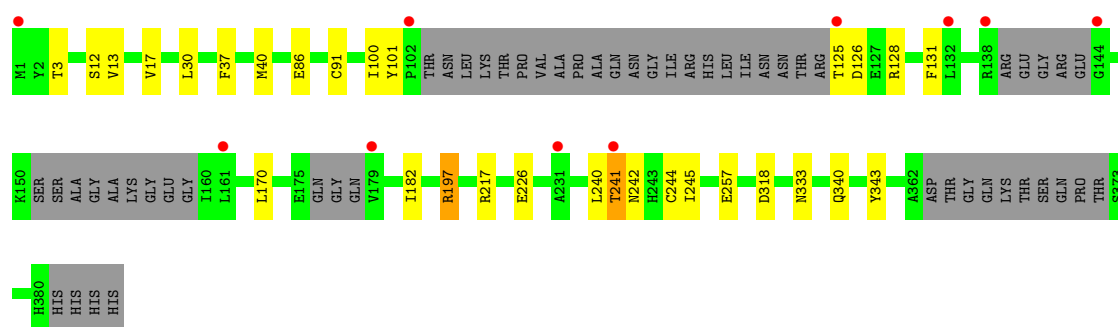
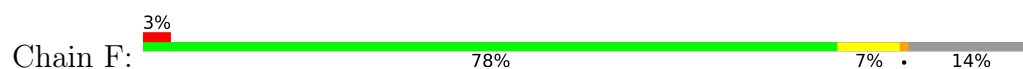




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.77Å 157.51Å 179.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.15 49.29 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-2.15) 99.7 (49.29-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.171 , 0.208 0.173 , 0.208	Depositor DCC
R_{free} test set	8071 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18016	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: CA, MES, GTP, ACP, 918, GOL, GDP, MG

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	0.32	0/3515	0.49	0/4769
1	C	0.39	0/3515	0.55	0/4772
2	B	0.35	0/3405	0.52	0/4612
2	D	0.29	0/3422	0.48	0/4635
3	E	0.30	0/1022	0.42	0/1356
4	F	0.24	0/2786	0.44	0/3763
All	All	0.32	0/17665	0.50	0/23907

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	3436	0	3348	31	0
1	C	3437	0	3349	20	0
2	B	3331	0	3208	27	0
2	D	3349	0	3223	38	0
3	E	1014	0	1029	11	0
4	F	2724	0	2698	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
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	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	0	0	0
9	D	28	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	12	0	12	0	0
11	D	12	0	12	1	0
12	F	31	0	14	1	0
13	A	95	0	0	0	0
13	B	93	0	0	2	0
13	C	186	0	0	1	0
13	D	51	0	0	1	0
13	E	17	0	0	1	0
13	F	36	0	0	0	0
All	All	18016	0	16949	134	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 4.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ARG:NH1	2:D:197:ASN:OD1	2.22	0.73
4:F:318:ASP:OD2	12:F:402:ACP:O3G	2.06	0.72
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.65
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.79	0.64
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.81	0.63
4:F:101:TYR:O	4:F:128:ARG:NH2	2.33	0.62
2:D:253:ARG:NH1	11:D:504:MES:O3S	2.33	0.62
2:D:11:GLN:HA	2:D:74:THR:HG21	1.83	0.61
2:B:152:LEU:HD11	2:B:156:LYS:HZ3	1.67	0.60
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.84	0.60
1:A:88:HIS:N	1:A:91:GLN:OE1	2.27	0.59
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.85	0.59
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.84	0.58
3:E:6:MET:HE3	3:E:22:VAL:HG11	1.85	0.58
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.85	0.58
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.84	0.58
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.37	0.58
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.57
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.57
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.85	0.56
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.40	0.56
1:C:221:ARG:HD2	2:D:325:MET:HB3	1.87	0.56
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.88	0.55
3:E:137:LYS:O	3:E:141:GLU:HG2	2.07	0.55
2:B:323:MET:HB3	2:B:373:MET:HE1	1.89	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.88	0.55
3:E:139:LEU:O	3:E:142:GLU:HG2	2.08	0.54
3:E:85:LYS:NZ	13:E:201:HOH:O	2.28	0.54
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.43	0.54
2:D:325:MET:SD	2:D:355:VAL:HG21	2.48	0.53
1:C:175:PRO:HA	1:C:179:THR:OG1	2.08	0.53
2:B:220:THR:O	13:B:601:HOH:O	2.19	0.53
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.44	0.53
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.08	0.52
2:D:193:GLN:OE1	3:E:126:LYS:HE2	2.09	0.52
2:D:16:ILE:HD13	2:D:231:VAL:HG11	1.91	0.52
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.46	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
2:D:325:MET:HE1	2:D:355:VAL:HG21	1.93	0.50
2:B:118:VAL:HG11	2:B:153:LEU:HD21	1.94	0.49
2:D:12:CYS:HB2	10:D:502:GDP:C8	2.47	0.49
1:C:101:ASN:ND2	2:D:254:LYS:HE2	2.26	0.49
1:A:346:TRP:CD1	1:A:346:TRP:H	2.30	0.49
1:A:336:LYS:NZ	1:A:341:ILE:O	2.46	0.49
3:E:24:LEU:O	3:E:25:LYS:HD2	2.13	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.28	0.48
4:F:241:THR:O	4:F:241:THR:OG1	2.30	0.48
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.48	0.48
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.95	0.48
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.48
2:B:323:MET:HE2	2:B:373:MET:HE2	1.96	0.48
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.95	0.48
1:C:327:ASP:OD2	13:C:601:HOH:O	2.19	0.47
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.97	0.47
3:E:72:LEU:O	3:E:76:ARG:HG2	2.15	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.95	0.47
1:A:359:PRO:HB2	1:A:370:LYS:HE2	1.96	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.46
2:D:325:MET:CE	2:D:355:VAL:HG21	2.45	0.46
2:D:398:MET:HE3	2:D:404:PHE:HD2	1.81	0.46
4:F:240:LEU:HB3	4:F:242:ASN:HD22	1.80	0.46
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.50	0.46
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.98	0.46
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.42	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.51	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.16	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.97	0.45
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.48	0.45
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.99	0.44
2:D:82:PRO:O	2:D:83:PHE:HB2	2.18	0.44
4:F:128:ARG:HH11	4:F:170:LEU:HD23	1.82	0.44
1:A:211:ASP:HB3	1:A:215:ARG:NH2	2.32	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.44
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.98	0.44
2:D:174:SER:O	2:D:178:SER:N	2.51	0.44
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.18	0.44
2:B:141:LEU:HD12	2:B:172:MET:SD	2.57	0.44
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.53	0.44
2:B:176:LYS:HD3	2:B:207:GLU:CG	2.47	0.44
2:B:298:SER:HA	2:B:301:MET:HG3	2.00	0.43
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.00	0.43
1:A:11:GLN:O	1:A:15:GLN:HG3	2.18	0.43
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.00	0.43
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.54	0.43
4:F:240:LEU:HB3	4:F:242:ASN:ND2	2.34	0.43
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.43
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:SER:HA	1:C:194:THR:HG22	2.01	0.43
2:D:392:SER:O	2:D:396:THR:HG22	2.19	0.43
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.54	0.42
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.54	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.42
2:D:391:ILE:HG22	2:D:425:MET:HE1	2.01	0.42
2:B:373:MET:HE2	2:B:373:MET:HB3	1.42	0.42
2:D:251:ASP:O	2:D:255:LEU:HG	2.18	0.42
2:D:105:LYS:HA	2:D:109:THR:OG1	2.20	0.42
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.42
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.87	0.42
2:D:22:GLU:OE1	2:D:82:PRO:HG2	2.19	0.42
3:E:100:LYS:HE3	3:E:100:LYS:HB2	1.85	0.42
4:F:126:ASP:OD2	4:F:128:ARG:HB2	2.19	0.42
2:D:175:PRO:HA	2:D:178:SER:HB3	2.02	0.42
1:A:25:CYS:HB3	1:A:30:ILE:O	2.19	0.42
1:C:28:HIS:O	1:C:36:MET:HE3	2.20	0.42
1:A:211:ASP:HB3	1:A:215:ARG:HH22	1.85	0.42
2:B:238:VAL:HG23	2:B:239:THR:HG23	2.01	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.20	0.41
4:F:13:VAL:O	4:F:17:VAL:HG23	2.20	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.41
1:A:329:ASN:HB3	3:E:6:MET:HE2	2.02	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.55	0.41
2:D:334:ASN:HD21	2:D:338:LYS:NZ	2.18	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.41
1:A:382:THR:HG21	1:A:436:GLY:HA3	2.01	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.55	0.41
2:B:164:ARG:HD2	13:B:685:HOH:O	2.20	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.03	0.41
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.33	0.41
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.41
2:D:39:ASP:OD1	2:D:39:ASP:N	2.54	0.41
2:D:281:GLN:NE2	13:D:602:HOH:O	2.39	0.40
4:F:3:THR:HB	4:F:30:LEU:HD11	2.02	0.40
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.20	0.40
2:D:141:LEU:HD12	2:D:172:MET:SD	2.62	0.40
2:B:286:LEU:HD23	2:B:291:LEU:HG	2.04	0.40
1:C:286:LEU:HD23	1:C:286:LEU:HA	1.80	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/451 (97%)	427 (98%)	9 (2%)	1 (0%)	43	42
1	C	438/451 (97%)	431 (98%)	6 (1%)	1 (0%)	43	42
2	B	419/445 (94%)	409 (98%)	10 (2%)	0	100	100
2	D	423/445 (95%)	416 (98%)	7 (2%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	319/384 (83%)	314 (98%)	5 (2%)	0	100	100
All	All	2155/2319 (93%)	2115 (98%)	38 (2%)	2 (0%)	48	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
1	C	178	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/379 (98%)	366 (98%)	6 (2%)	55	61
1	C	371/379 (98%)	362 (98%)	9 (2%)	43	45
2	B	366/383 (96%)	357 (98%)	9 (2%)	42	44
2	D	368/383 (96%)	359 (98%)	9 (2%)	43	45
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	77
4	F	300/342 (88%)	291 (97%)	9 (3%)	36	37
All	All	1887/1993 (95%)	1844 (98%)	43 (2%)	44	47

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	367	ASP
1	A	415	GLU
1	A	437	VAL
1	A	439	SER
2	B	57	THR
2	B	59	ASN
2	B	153	LEU
2	B	240	THR
2	B	275	LEU
2	B	277	SER
2	B	325	MET
2	B	341	SER
2	B	369	ARG
1	C	41	THR
1	C	178	SER
1	C	179	THR
1	C	215	ARG
1	C	221	ARG
1	C	326	LYS
1	C	361	THR
1	C	370	LYS
1	C	381	THR
2	D	15	GLN
2	D	86	ILE
2	D	196	GLU
2	D	276	THR
2	D	277	SER
2	D	293	GLN

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Mol	Chain	Res	Type
2	D	322	ARG
2	D	384	ILE
2	D	423	SER
3	E	138	GLU
4	F	12	SER
4	F	86	GLU
4	F	91	CYS
4	F	125	THR
4	F	197	ARG
4	F	217	ARG
4	F	226	GLU
4	F	241	THR
4	F	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
2	B	37	HIS
2	B	91	ASN
2	B	192	HIS
2	B	385	GLN
2	B	436	GLN
1	C	15	GLN
1	C	176	GLN
1	C	393	HIS
2	D	8	GLN
2	D	96	GLN
2	D	136	GLN
3	E	71	HIS
4	F	242	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	A	501	6	33,34,34	0.86	1 (3%)	50,54,54	1.41	8 (16%)
12	ACP	F	402	6	31,33,33	1.96	10 (32%)	47,52,52	1.87	11 (23%)
5	GTP	C	501	6	33,34,34	0.89	1 (3%)	50,54,54	1.56	9 (18%)
10	GDP	B	502	6	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
8	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.41	0
9	918	D	501	-	31,31,31	1.26	3 (9%)	42,45,45	2.28	11 (26%)
10	GDP	D	502	6	29,30,30	1.23	3 (10%)	45,47,47	1.80	8 (17%)
9	918	B	501	-	31,31,31	1.32	3 (9%)	42,45,45	2.18	13 (30%)
11	MES	B	506	-	12,12,12	1.93	1 (8%)	15,16,16	1.85	3 (20%)
11	MES	D	504	-	12,12,12	2.16	1 (8%)	15,16,16	1.76	3 (20%)

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	A	501	6	-	9/22/38/38	0/3/3/3
12	ACP	F	402	6	-	5/19/38/38	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
10	GDP	B	502	6	-	5/16/32/32	0/3/3/3
8	GOL	A	505	-	-	2/4/4/4	-
9	918	D	501	-	-	0/18/33/33	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GDP	D	502	6	-	4/16/32/32	0/3/3/3
9	918	B	501	-	-	0/18/33/33	0/4/4/4
11	MES	B	506	-	-	0/6/14/14	0/1/1/1
11	MES	D	504	-	-	1/6/14/14	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	504	MES	C8-S	-7.20	1.67	1.77
11	B	506	MES	C8-S	-6.30	1.68	1.77
12	F	402	ACP	C5-C4	4.71	1.47	1.39
12	F	402	ACP	PB-O1B	4.13	1.61	1.51
9	D	501	918	CAO-CAN	-3.99	1.41	1.50
12	F	402	ACP	PB-O3A	3.76	1.62	1.58
9	B	501	918	CAO-CAN	-3.73	1.42	1.50
9	B	501	918	CAH-C4	-3.41	1.40	1.48
9	D	501	918	CAH-C4	-3.28	1.40	1.48
9	B	501	918	C6-NAI	-3.26	1.30	1.37
10	D	502	GDP	C5-C4	3.13	1.47	1.38
12	F	402	ACP	PA-O3A	3.08	1.62	1.59
12	F	402	ACP	PB-O2B	-3.05	1.48	1.56
12	F	402	ACP	PG-O2G	2.99	1.61	1.55
12	F	402	ACP	PG-O3G	2.79	1.61	1.55
12	F	402	ACP	C5-C6	2.75	1.48	1.41
10	D	502	GDP	C6-N1	-2.70	1.33	1.38
10	D	502	GDP	PA-O3A	2.69	1.62	1.59
10	B	502	GDP	C5-C4	2.57	1.45	1.38
5	C	501	GTP	PA-O3A	2.55	1.62	1.59
10	B	502	GDP	C6-N1	-2.53	1.34	1.38
5	A	501	GTP	PA-O3A	2.41	1.62	1.59
12	F	402	ACP	C8-N7	2.38	1.36	1.31
9	D	501	918	CAJ-NAK	2.31	1.39	1.34
12	F	402	ACP	C5-N7	-2.16	1.35	1.39
10	B	502	GDP	C5-N7	-2.02	1.35	1.39

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	918	C4-N3-C2	8.66	122.37	115.88
9	D	501	918	C4-N3-C2	8.22	122.03	115.88
12	F	402	ACP	C5-C4-N3	-6.05	118.39	126.72
10	D	502	GDP	C5-C4-N3	-5.68	119.35	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	502	GDP	C5-C4-N3	-5.45	119.71	128.39
11	B	506	MES	C5-N4-C3	5.44	120.56	108.84
10	B	502	GDP	C2-N3-C4	5.13	121.14	112.30
12	F	402	ACP	N3-C4-N9	4.86	135.43	127.17
9	D	501	918	CAJ-CAH-C4	-4.60	114.16	121.24
11	D	504	MES	C5-N4-C3	4.52	118.58	108.84
5	C	501	GTP	C2-N3-C4	4.51	120.06	112.30
10	D	502	GDP	C2-N3-C4	4.50	120.05	112.30
9	B	501	918	CAU-NAG-CAQ	4.34	121.33	111.57
9	B	501	918	CAJ-CAH-C4	-4.27	114.67	121.24
5	C	501	GTP	C5-C4-N3	-4.25	121.62	128.39
9	D	501	918	CAU-NAG-CAQ	4.08	120.75	111.57
10	B	502	GDP	N9-C4-N3	3.99	133.94	125.95
10	D	502	GDP	N9-C4-N3	3.90	133.75	125.95
5	A	501	GTP	C5-C4-N3	-3.85	122.26	128.39
10	B	502	GDP	C6-C5-N7	3.80	137.21	130.29
9	B	501	918	CAY-NAI-C6	3.79	128.17	123.58
12	F	402	ACP	C4-C5-N7	-3.75	106.30	110.58
9	D	501	918	CAY-NAI-C6	3.72	128.09	123.58
10	D	502	GDP	C6-C5-N7	3.69	137.01	130.29
9	B	501	918	N3-C2-N1	-3.65	119.78	126.27
12	F	402	ACP	C2-N3-C4	3.64	120.72	111.83
5	A	501	GTP	C2-N3-C4	3.59	118.47	112.30
9	D	501	918	N3-C2-N1	-3.55	119.96	126.27
9	D	501	918	C2-N1-C6	3.39	121.70	115.02
9	D	501	918	C5-C4-N3	-3.30	118.52	122.34
5	C	501	GTP	N9-C8-N7	-3.18	107.51	113.40
12	F	402	ACP	C4-N9-C8	3.06	108.95	105.74
9	D	501	918	C4-CAH-CAN	3.03	127.33	123.07
12	F	402	ACP	N3-C2-N1	-2.98	124.07	128.58
10	D	502	GDP	C4-C5-N7	-2.95	106.00	110.67
5	A	501	GTP	O2B-PB-O3A	2.91	115.15	107.27
11	B	506	MES	O1S-S-C8	2.86	111.06	106.73
12	F	402	ACP	C5-N7-C8	2.85	107.94	103.45
9	D	501	918	CAT-CAU-NAG	2.84	115.31	109.93
9	D	501	918	N3-C2-NAG	2.84	121.16	117.12
9	B	501	918	C5-C4-N3	-2.74	119.16	122.34
5	C	501	GTP	C8-N7-C5	2.69	109.05	104.26
9	B	501	918	C2-N1-C6	2.65	120.25	115.02
5	C	501	GTP	N9-C4-N3	2.64	131.23	125.95
10	B	502	GDP	C4-C5-N7	-2.59	106.56	110.67
5	A	501	GTP	N9-C8-N7	-2.57	108.64	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C8-N7-C5	2.47	108.66	104.26
12	F	402	ACP	C3'-C2'-C1'	2.45	106.10	101.46
11	D	504	MES	O1S-S-C8	2.40	110.35	106.73
10	D	502	GDP	O2B-PB-O3A	2.36	112.56	104.64
12	F	402	ACP	N9-C8-N7	-2.33	110.63	113.94
11	B	506	MES	O3S-S-O1S	-2.31	105.62	111.40
12	F	402	ACP	PB-O3A-PA	-2.31	124.83	132.37
10	B	502	GDP	O6-C6-C5	-2.31	120.44	126.53
5	A	501	GTP	C4-C5-N7	-2.29	107.04	110.67
11	D	504	MES	O3S-S-C8	2.28	110.46	106.00
9	B	501	918	CAM-CAN-CAH	-2.27	117.18	119.85
9	B	501	918	CAV-NAI-C6	-2.24	120.87	123.58
5	C	501	GTP	C5-C6-N1	2.19	118.84	113.25
5	C	501	GTP	O2A-PA-O3A	2.18	113.18	107.27
5	C	501	GTP	C2-N1-C6	-2.17	121.18	125.11
9	B	501	918	CAH-CAJ-NAK	-2.13	121.15	124.53
10	D	502	GDP	C8-N7-C5	2.13	108.05	104.26
9	B	501	918	N1-C2-NAG	2.12	120.14	117.12
9	B	501	918	C4-CAH-CAN	2.11	126.03	123.07
9	B	501	918	N3-C2-NAG	2.07	120.07	117.12
12	F	402	ACP	C6-C5-N7	2.05	136.05	132.09
9	D	501	918	C5-C6-N1	-2.04	119.40	123.34
5	A	501	GTP	N9-C4-N3	2.02	130.00	125.95
10	D	502	GDP	O4'-C1'-N9	-2.02	103.78	108.36
5	A	501	GTP	O2A-PA-O3A	2.01	112.72	107.27
10	B	502	GDP	C5-C6-N1	2.00	118.36	113.25
5	C	501	GTP	C4-C5-N7	-2.00	107.50	110.67

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	505	GOL	O1-C1-C2-O2
8	A	505	GOL	O1-C1-C2-C3
10	B	502	GDP	C5'-O5'-PA-O3A
10	B	502	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	B	502	GDP	C5'-O5'-PA-O2A
10	D	502	GDP	C5'-O5'-PA-O3A
10	D	502	GDP	C5'-O5'-PA-O1A
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O2B
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
11	D	504	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3B-PG-O1G
10	D	502	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O3G
12	F	402	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
10	B	502	GDP	PB-O3A-PA-O1A
10	B	502	GDP	PB-O3A-PA-O2A
10	D	502	GDP	PB-O3A-PA-O2A

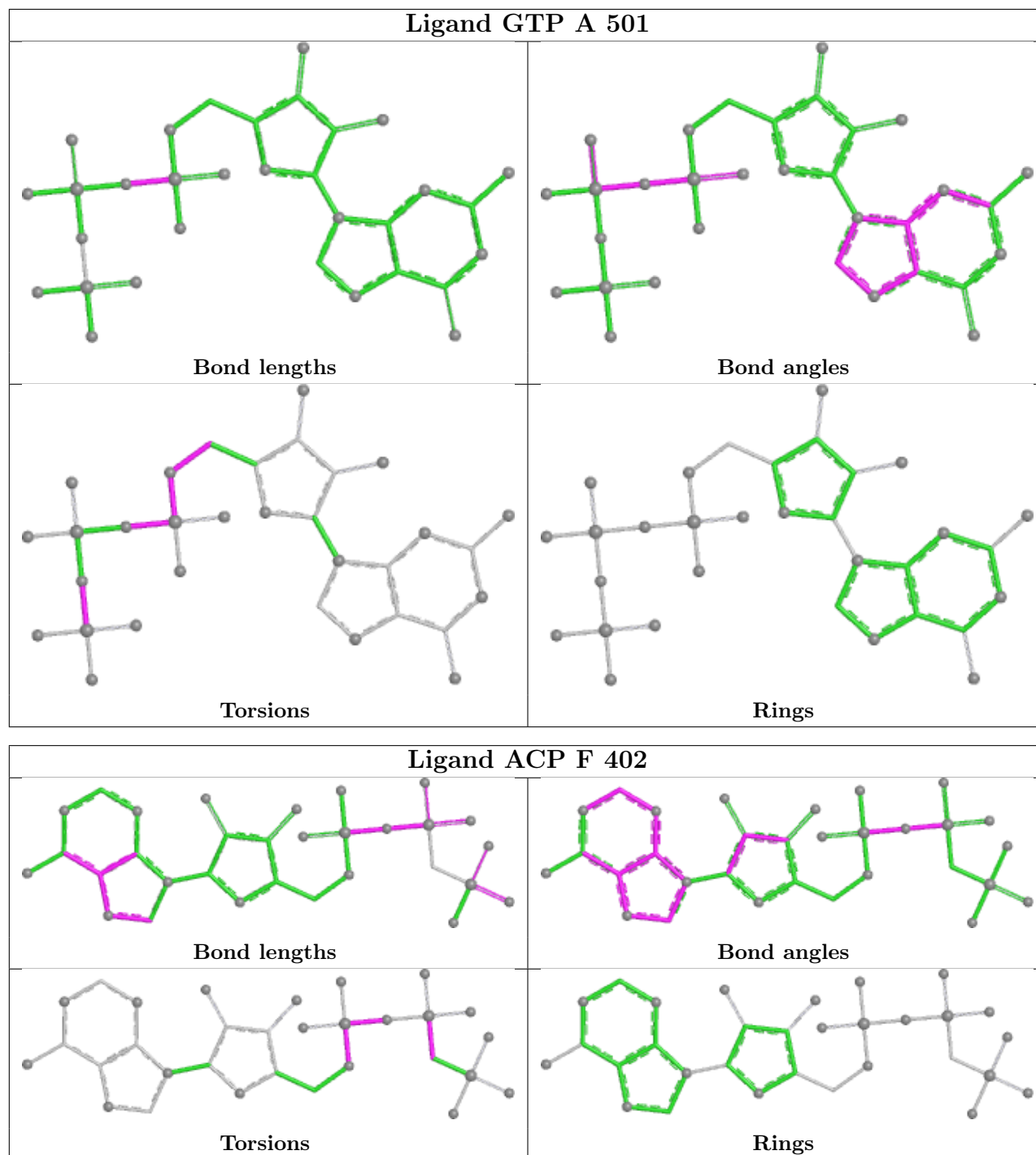
There are no ring outliers.

3 monomers are involved in 3 short contacts:

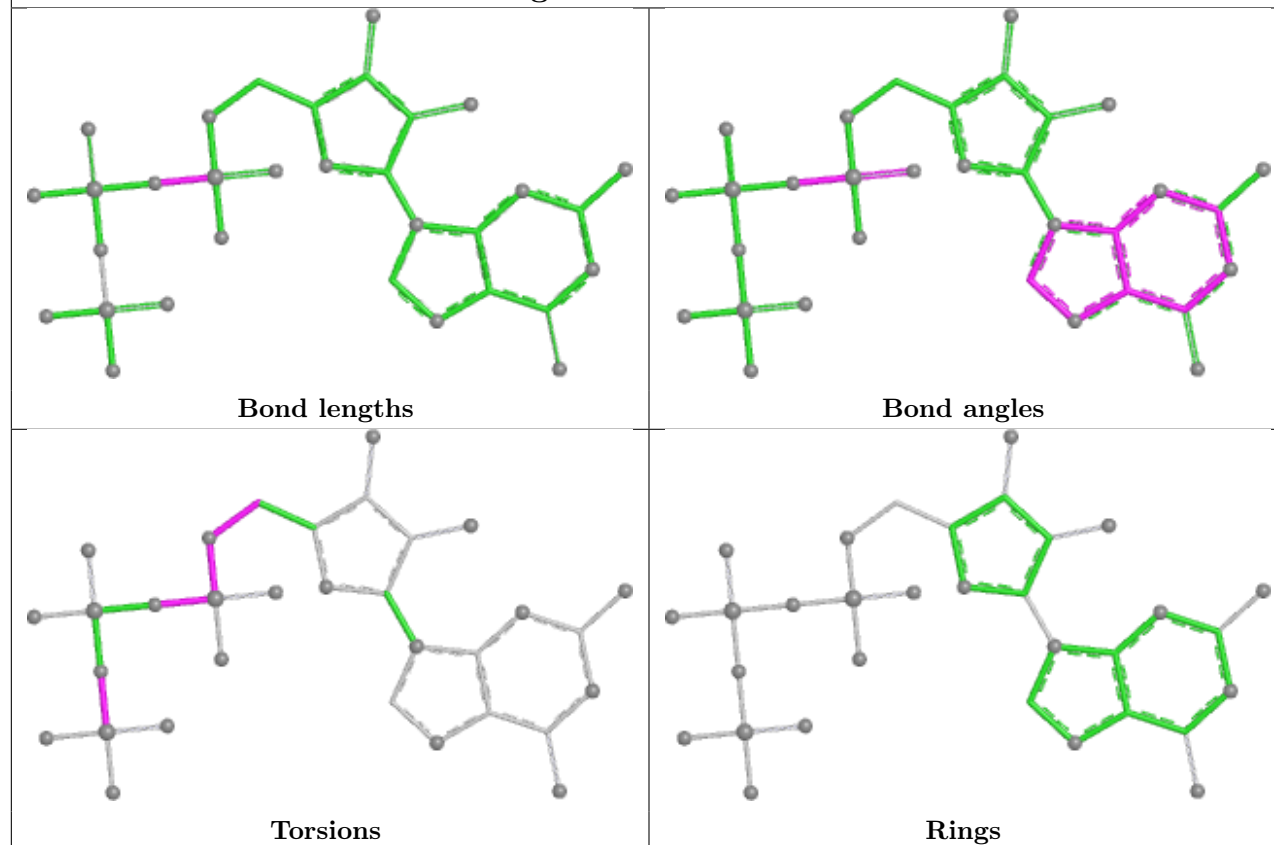
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	402	ACP	1	0
10	D	502	GDP	1	0
11	D	504	MES	1	0

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

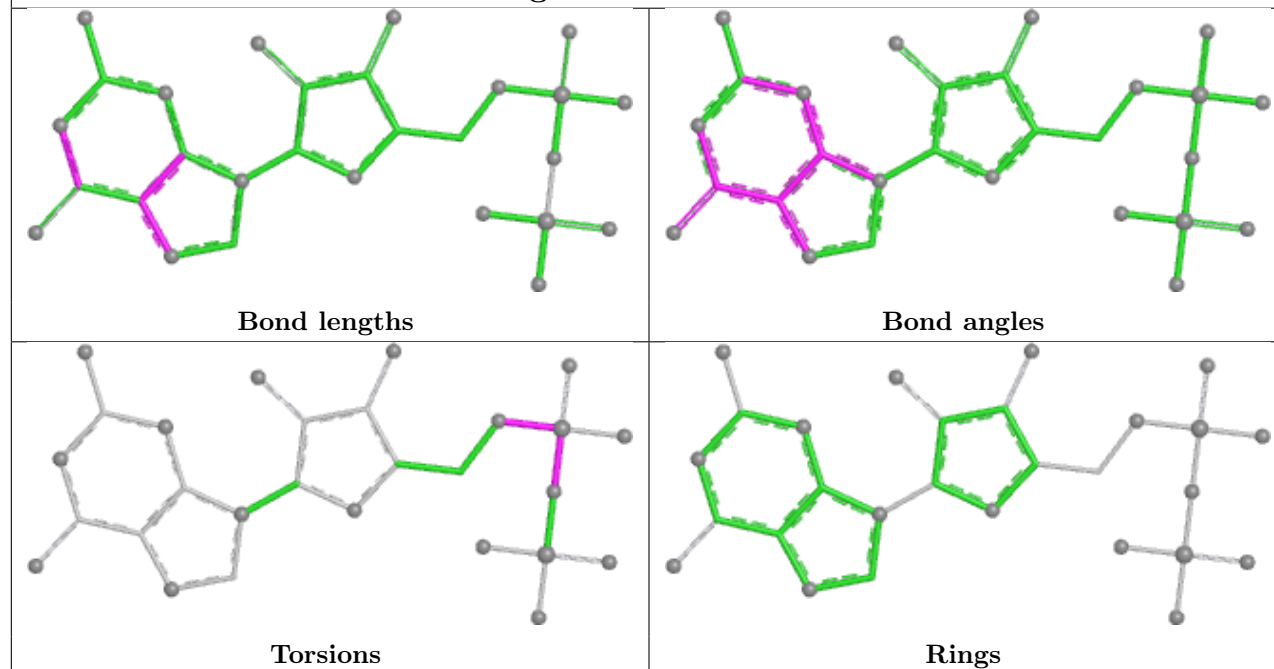
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



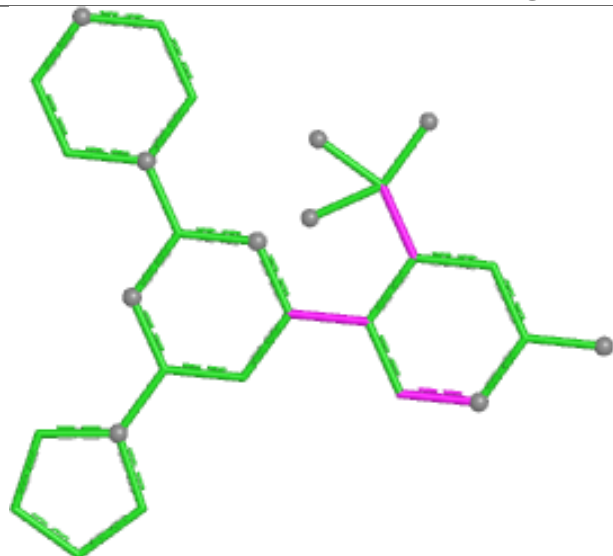
Ligand GTP C 501



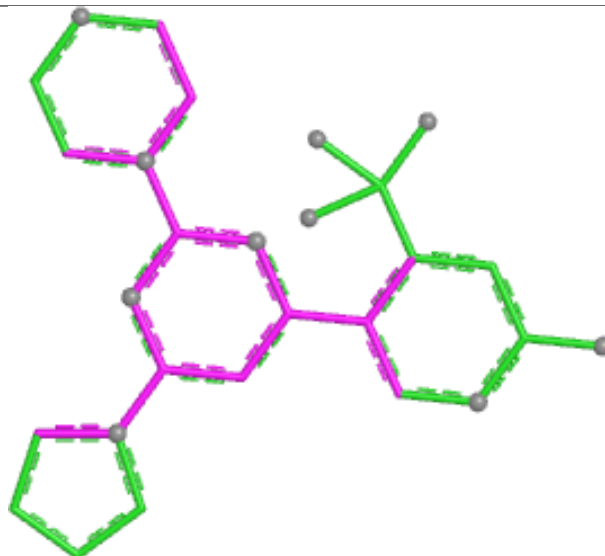
Ligand GDP B 502



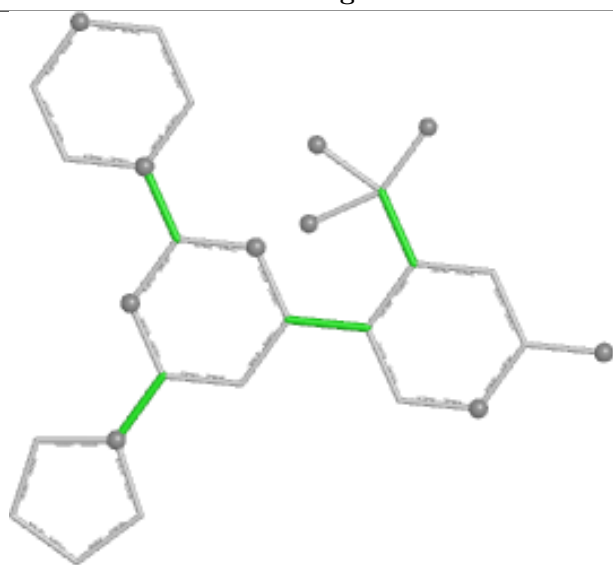
Ligand 918 D 501



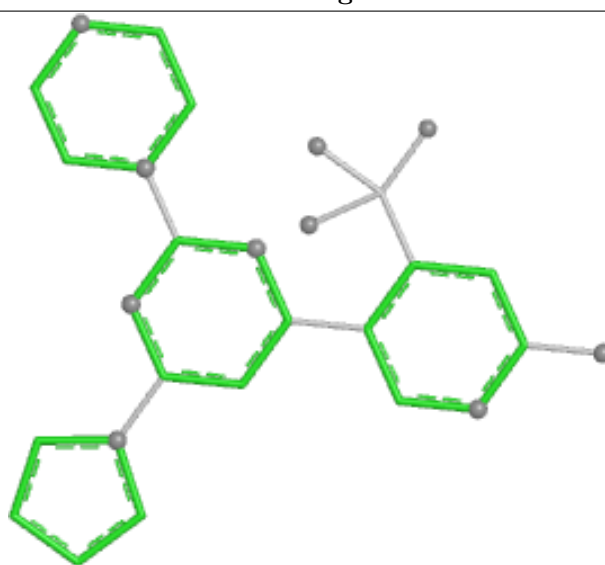
Bond lengths



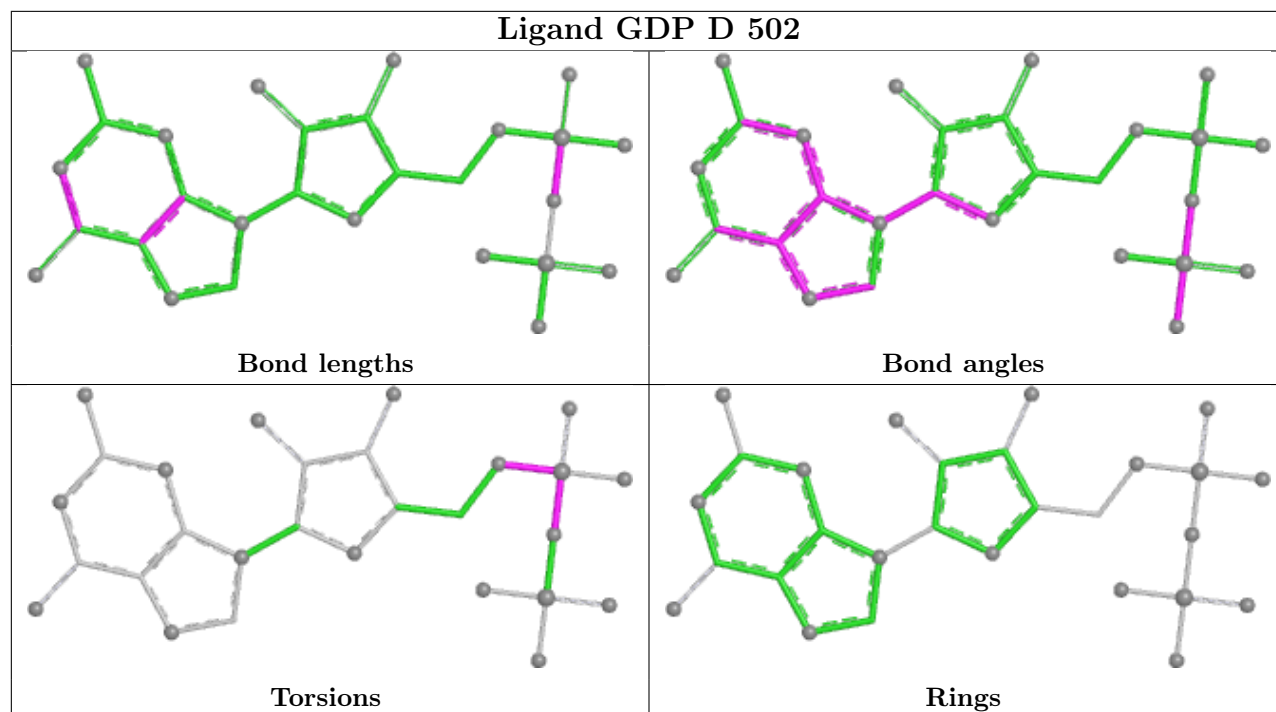
Bond angles

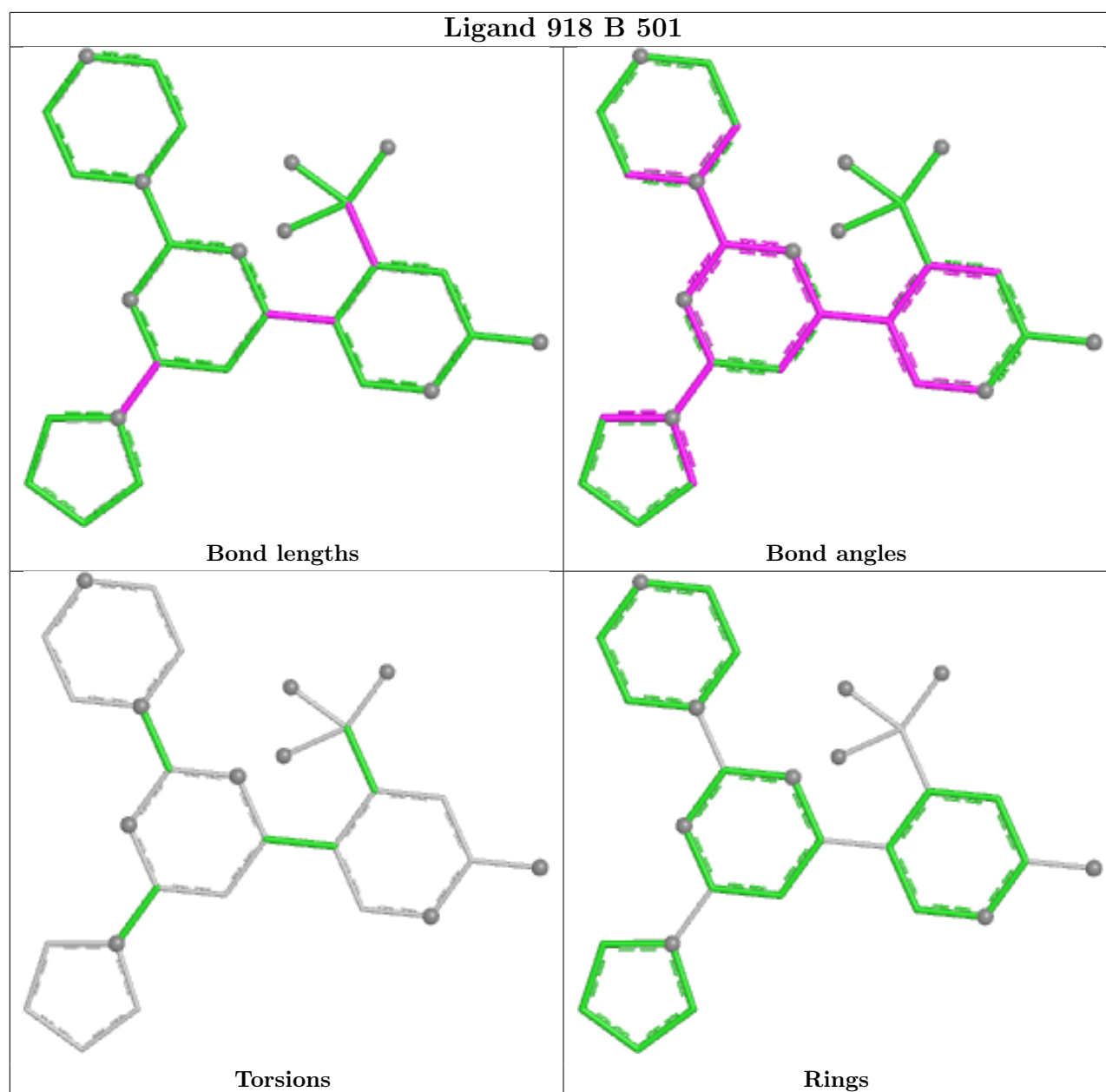


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/451 (97%)	-0.20	3 (0%) 84 86	34, 56, 95, 136	1 (0%)
1	C	440/451 (97%)	-0.41	6 (1%) 73 77	31, 44, 77, 119	0
2	B	423/445 (95%)	-0.22	4 (0%) 81 84	32, 52, 88, 132	2 (0%)
2	D	427/445 (95%)	0.02	10 (2%) 61 65	38, 65, 100, 132	4 (0%)
3	E	123/143 (86%)	0.21	5 (4%) 41 46	40, 70, 113, 131	0
4	F	331/384 (86%)	0.24	10 (3%) 52 56	47, 83, 141, 168	0
All	All	2184/2319 (94%)	-0.11	38 (1%) 69 73	31, 59, 110, 168	7 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	438	ALA	4.0
2	B	245	PRO	3.7
2	D	276	THR	3.4
2	D	279	GLY	3.4
3	E	143	ALA	3.3
2	B	276	THR	3.3
4	F	179	VAL	3.3
2	D	245	PRO	3.2
3	E	15	THR	3.1
2	D	2	ARG	3.1
1	C	357	TYR	2.8
2	D	285	ALA	2.8
4	F	102	PRO	2.7
3	E	96	MET	2.7
1	A	440	VAL	2.7
1	C	340	SER	2.6
1	C	440	VAL	2.6
2	D	246	GLY	2.5
3	E	26	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	125	THR	2.5
1	C	178	SER	2.5
1	C	163	LYS	2.5
2	B	275	LEU	2.4
1	C	176	GLN	2.3
3	E	24	LEU	2.3
4	F	161	LEU	2.2
2	D	277	SER	2.2
4	F	138	ARG	2.2
4	F	241	THR	2.2
2	D	281	GLN	2.2
4	F	1	MET	2.2
2	D	82	PRO	2.1
2	D	248	LEU	2.1
1	A	262	TYR	2.1
1	A	442	GLY	2.1
4	F	144	GLY	2.1
4	F	231	ALA	2.0
4	F	132	LEU	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
7	CA	B	504	1/1	0.87	0.16	112,112,112,112	0
11	MES	D	504	12/12	0.88	0.17	89,100,103,107	0
8	GOL	A	505	6/6	0.89	0.14	78,81,88,89	0
7	CA	A	504	1/1	0.90	0.10	114,114,114,114	0

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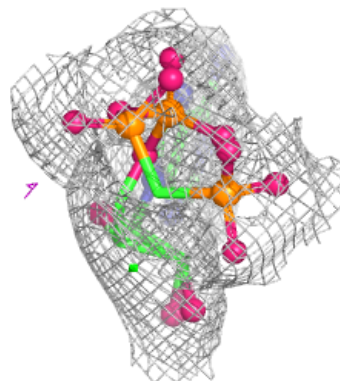
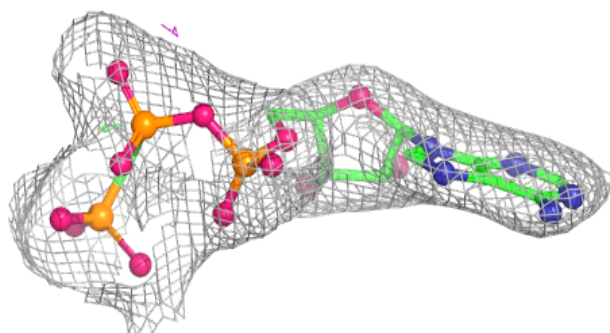
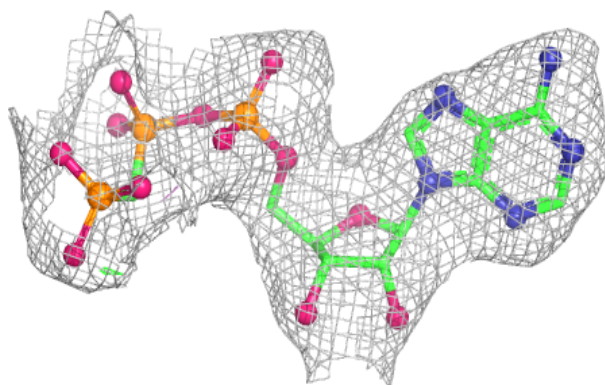
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	B	505	1/1	0.91	0.12	92,92,92,92	0
11	MES	B	506	12/12	0.94	0.09	36,47,67,75	0
12	ACP	F	402	31/31	0.94	0.07	82,96,119,130	0
10	GDP	D	502	28/28	0.95	0.08	46,56,66,72	0
6	MG	F	401	1/1	0.95	0.06	71,71,71,71	0
9	918	D	501	28/28	0.96	0.08	44,50,57,60	0
9	918	B	501	28/28	0.97	0.06	34,44,55,60	0
6	MG	D	503	1/1	0.97	0.04	61,61,61,61	0
5	GTP	A	501	32/32	0.99	0.04	32,40,44,54	0
5	GTP	C	501	32/32	0.99	0.04	27,34,40,44	0
7	CA	A	503	1/1	0.99	0.05	75,75,75,75	0
10	GDP	B	502	28/28	0.99	0.04	31,37,43,43	0
6	MG	A	502	1/1	1.00	0.02	38,38,38,38	0
6	MG	B	503	1/1	1.00	0.06	30,30,30,30	0
6	MG	C	502	1/1	1.00	0.02	39,39,39,39	0
7	CA	C	503	1/1	1.00	0.03	59,59,59,59	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.

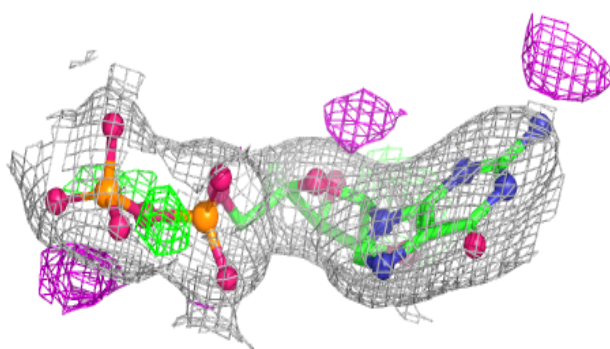
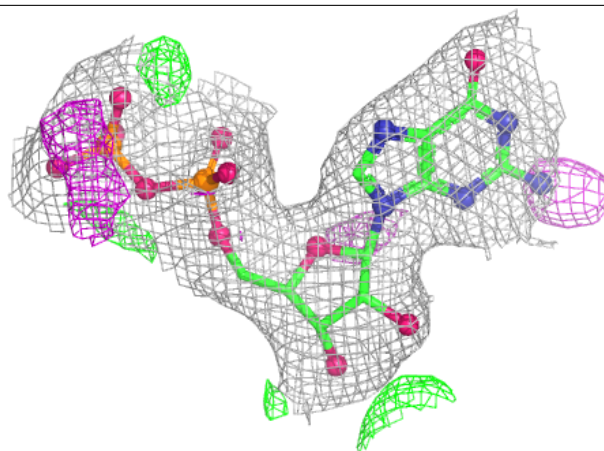
Electron density around ACP F 402:

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



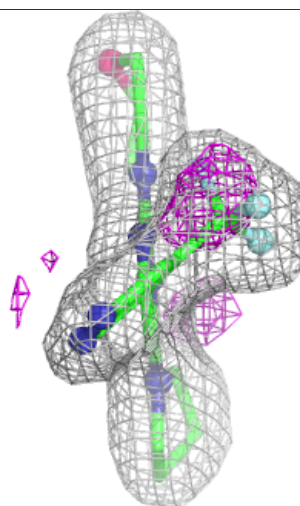
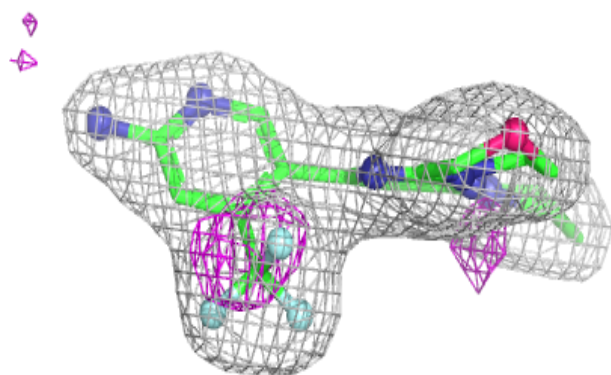
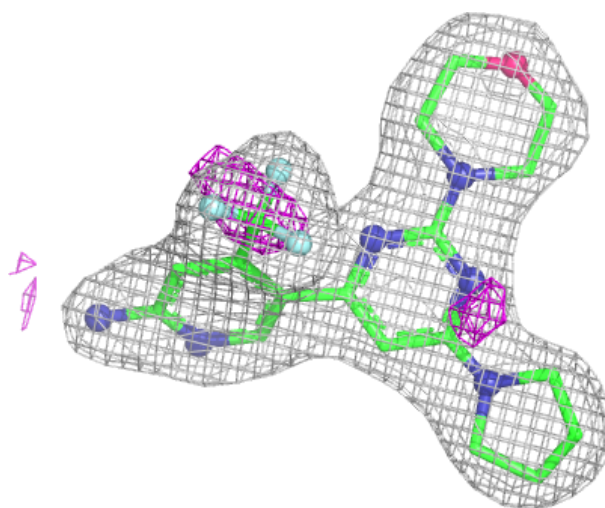
Electron density around GDP D 502:

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



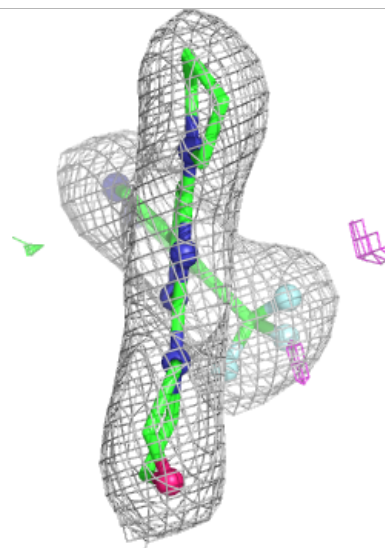
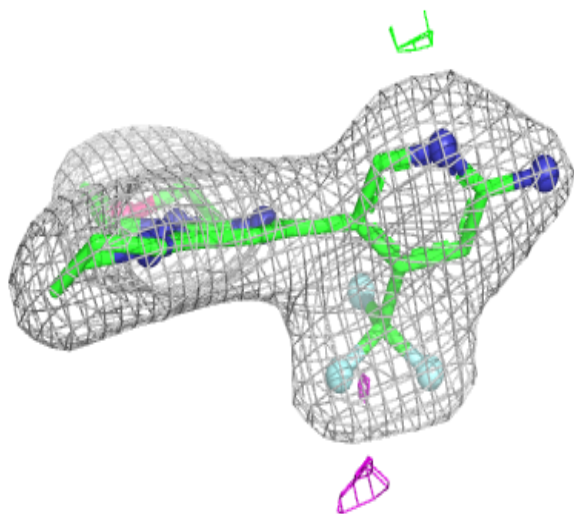
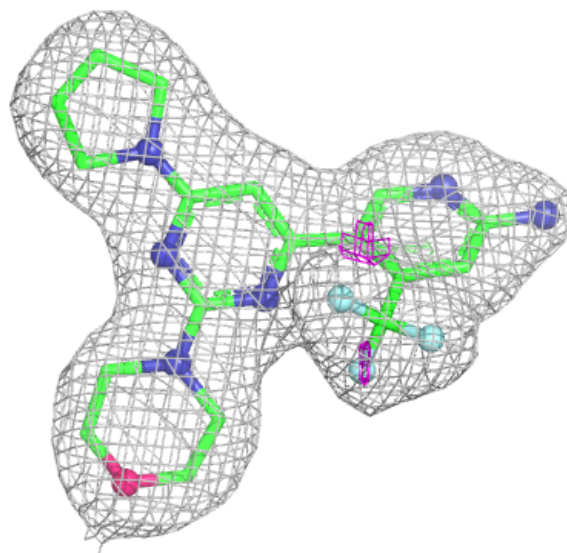
Electron density around 918 D 501:

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



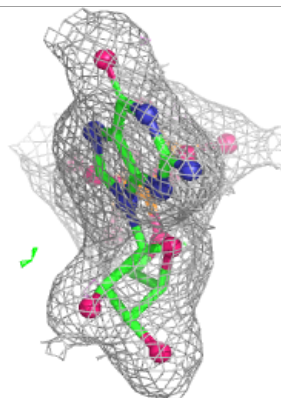
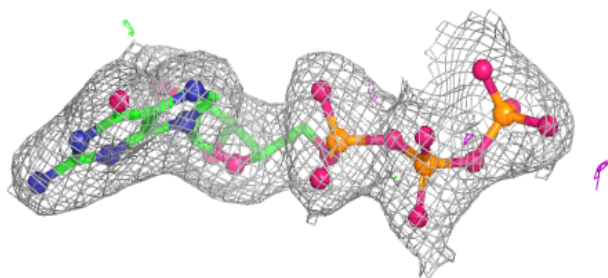
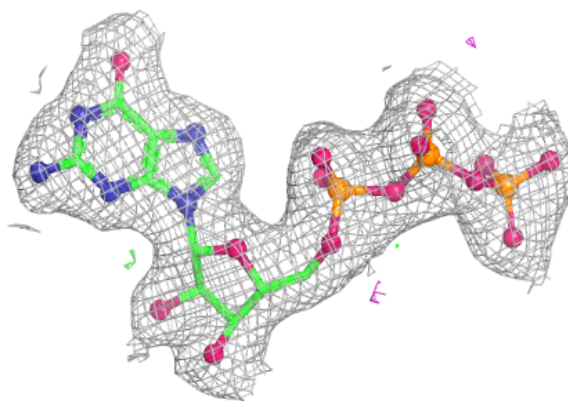
Electron density around 918 B 501:

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

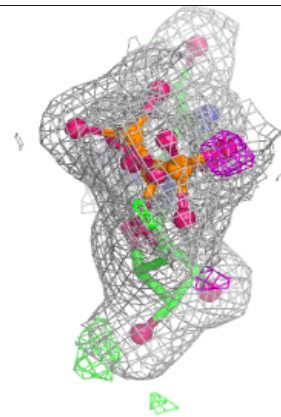
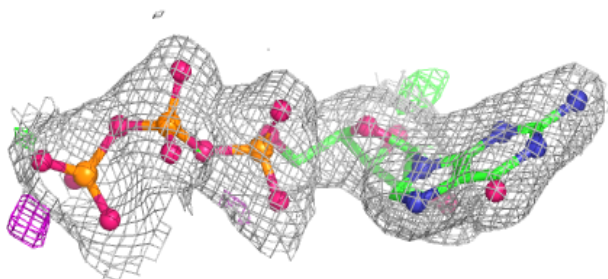
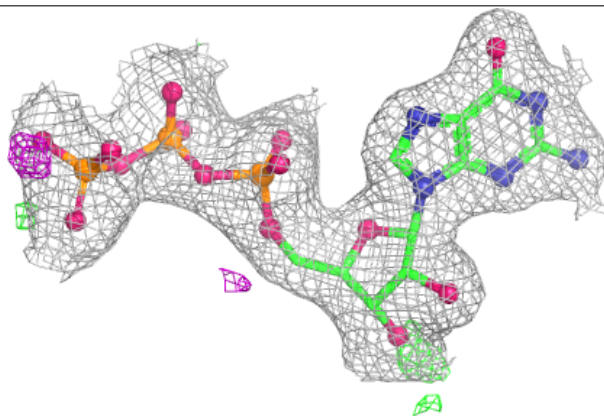


Electron density around GTP A 501:

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

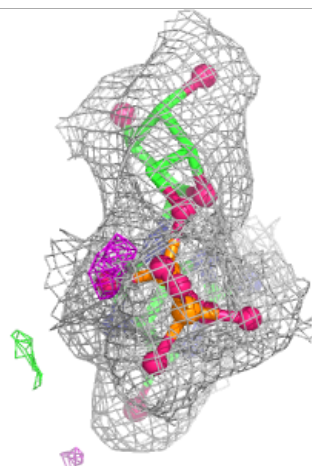
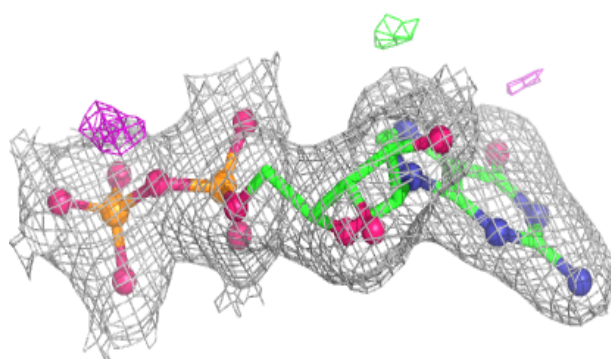
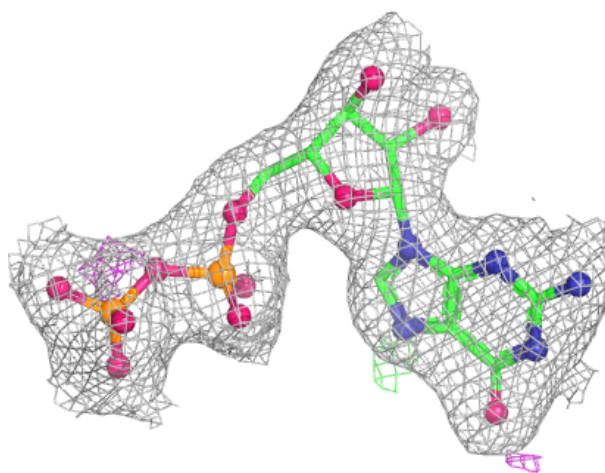
**Electron density around GTP C 501:**

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



Electron density around GDP B 502:

$2mF_o-DF_c$ (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.