



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:26 AM UTC

PDB ID : 8CLD / pdb_00008cld
Title : Ansamitocin P3 bound to tubulin (T2R-TTL) complex
Authors : Wranik, M.; Kepa, M.W.; Bertrand, Q.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on : 2023-02-16
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

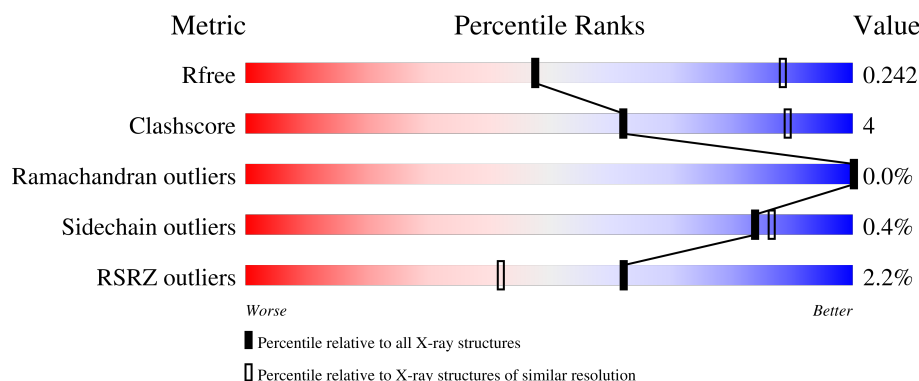
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	% 90% 7% .
1	C	451	2% 91% 6% .
2	B	445	% 90% 6% .
2	D	445	% 83% 11% 5%
3	E	189	4% 62% .. 36%

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Mol	Chain	Length	Quality of chain
4	F	384	5% 73% 13% • 12%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17497 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	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	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			1010	623	184	198	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	336	Total	C	N	O	S	0	0	0
			2761	1773	473	501	14			

There are 6 discrepancies between the modelled and reference sequences:

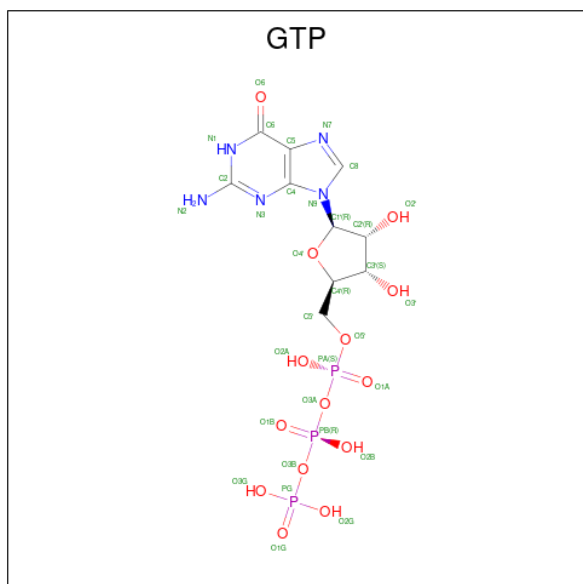
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1
F	381	HIS	-	expression tag	UNP A0A8C9FGJ1
F	382	HIS	-	expression tag	UNP A0A8C9FGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP A0A8C9FGJ1
F	384	HIS	-	expression tag	UNP A0A8C9FGJ1

- 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		

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

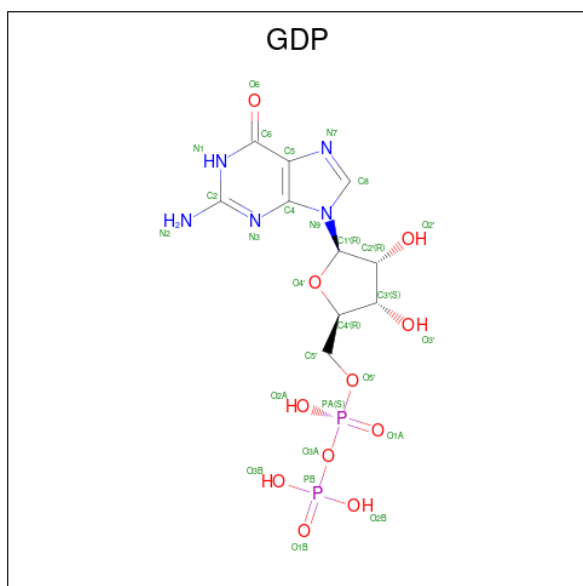
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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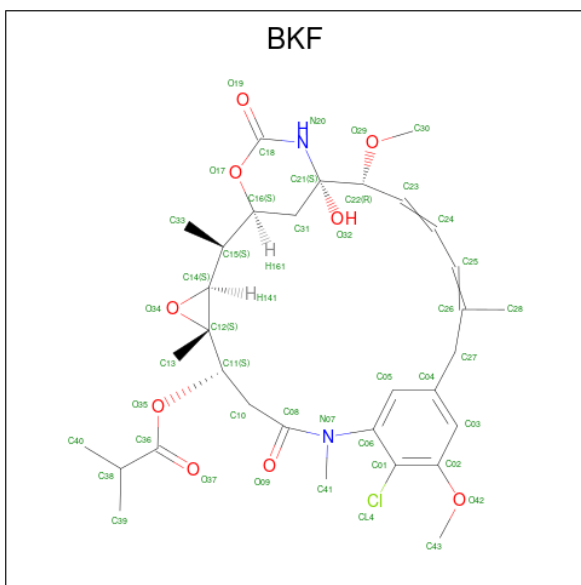
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

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



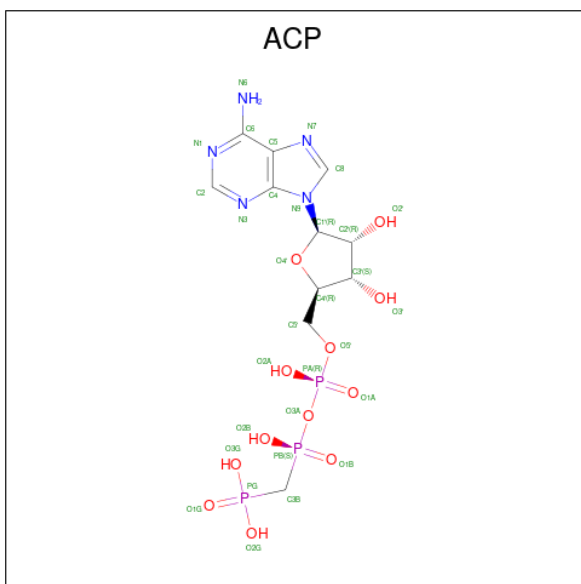
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is (1S,2S,3S,5S,6S,16Z,18Z,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxo-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5] hexacosa-10(26),11,13,16,18-pentaen-6-yl 2-methylpropanoate (CCD ID: BKF) (formula: $C_{32}H_{43}ClN_2O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total 44	C 32	Cl 1	N 2	O 9	0	0

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

- Molecule 11 is water.

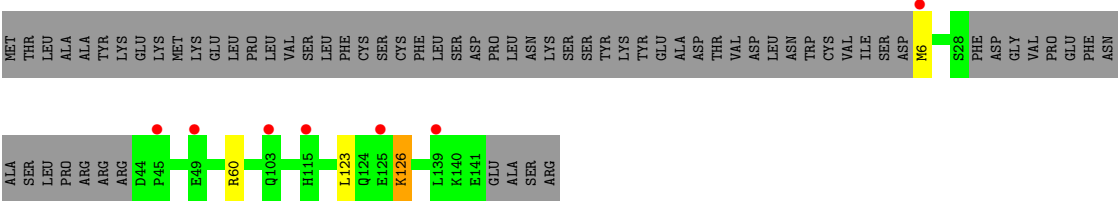
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total 1	O 1	0	0
11	C	1	Total 1	O 1	0	0
11	E	1	Total 1	O 1	0	0

- Molecule 1: Detyrosinated tubulin alpha-1B chain

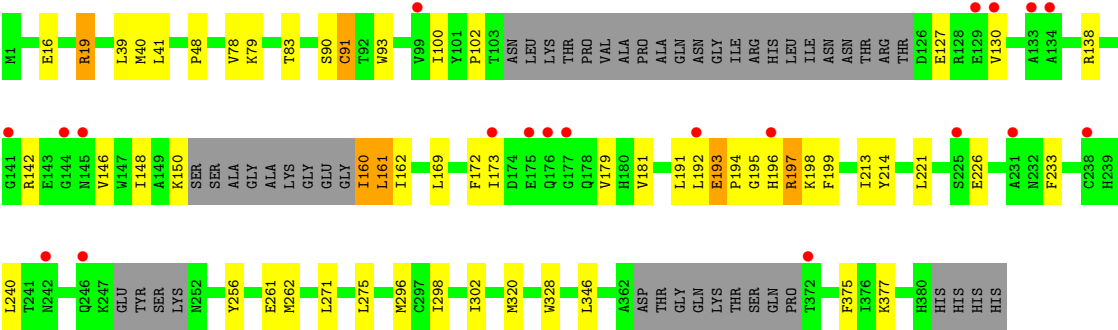




• Molecule 3: Stathmin-4



• 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	106.06Å 159.61Å 180.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.10 – 3.20 15.10 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.10-3.20) 98.9 (15.10-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.200 , 0.241 0.207 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 113.4	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	0.89	EDS
Total number of atoms	17497	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 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, GDP, MG, BKF, CA, 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	0.22	0/3494	0.47	0/4743
1	C	0.24	1/3515 (0.0%)	0.44	0/4772
2	B	0.20	0/3436	0.43	0/4654
2	D	0.22	0/3382	0.48	0/4581
3	E	0.16	0/1019	0.47	1/1352 (0.1%)
4	F	0.30	0/2823	0.55	0/3813
All	All	0.23	1/17669 (0.0%)	0.47	1/23915 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2
4	F	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	325	PRO	C-O	-5.04	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	126	LYS	N-CA-C	-5.50	106.41	113.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	156	ARG	Sidechain
2	D	359	ARG	Sidechain
4	F	19	ARG	Sidechain
4	F	193	GLU	Peptide
4	F	197	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3330	22	0
1	C	3437	0	3348	18	0
2	B	3361	0	3238	17	0
2	D	3309	0	3189	29	0
3	E	1010	0	1024	6	0
4	F	2761	0	2733	52	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	D	44	0	0	1	0
10	F	31	0	14	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
11	E	1	0	0	0	0
All	All	17497	0	16924	141	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 (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ILE:HD12	4:F:173:ILE:HD13	1.55	0.89
1:A:42:ILE:HD12	1:A:42:ILE:O	1.86	0.75
4:F:192:LEU:HD23	4:F:193:GLU:N	2.05	0.72
4:F:192:LEU:HD22	4:F:197:ARG:NE	2.07	0.68
4:F:161:LEU:C	4:F:161:LEU:HD12	2.20	0.65
4:F:90:SER:O	4:F:91:CYS:C	2.40	0.64
1:A:293:ASN:ND2	1:A:339:ARG:HH21	1.97	0.63
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.81	0.63
4:F:192:LEU:HD23	4:F:192:LEU:C	2.23	0.63
4:F:161:LEU:HD23	4:F:172:PHE:CD2	2.35	0.62
4:F:160:ILE:HG21	4:F:240:LEU:HD21	1.82	0.60
4:F:161:LEU:HD12	4:F:162:ILE:N	2.17	0.59
4:F:377:LYS:HD2	4:F:377:LYS:H	1.67	0.59
2:B:356:ILE:HD12	2:B:356:ILE:H	1.68	0.58
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.85	0.58
4:F:192:LEU:HD21	4:F:194:PRO:HD2	1.85	0.57
4:F:240:LEU:HD12	4:F:240:LEU:N	2.20	0.56
1:A:187:SER:CB	1:A:391:LEU:HD21	2.34	0.56
1:C:381:THR:HG22	1:C:383:ALA:H	1.70	0.56
2:D:57:ASN:ND2	2:D:57:ASN:O	2.38	0.56
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.42	0.54
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.88	0.54
2:D:215:LEU:HB3	2:D:217:LEU:HD23	1.90	0.54
4:F:213:ILE:HD11	4:F:296:MET:CE	2.37	0.53
1:A:414:GLU:OE2	3:E:60:ARG:NH2	2.42	0.53
4:F:197:ARG:HH22	4:F:256:TYR:CB	2.22	0.53
2:D:332:ASN:OD1	2:D:336:LYS:HE3	2.09	0.53
2:D:33:THR:C	2:D:58:LYS:HZ1	2.17	0.52
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.90	0.52
2:D:239:CYS:SG	2:D:316:ILE:HD12	2.50	0.52
1:A:274:PRO:HD3	1:A:374:ALA:HA	1.90	0.52
2:D:107:THR:OG1	2:D:108:GLU:N	2.43	0.52
3:E:6:MET:HA	3:E:6:MET:HE2	1.90	0.52
3:E:6:MET:HE2	3:E:6:MET:N	2.25	0.52
3:E:6:MET:HE2	3:E:6:MET:CA	2.40	0.51
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.45	0.51
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.93	0.51
4:F:161:LEU:HD21	4:F:169:LEU:HD23	1.92	0.51
2:D:306:ARG:NH2	2:D:337:ASN:OD1	2.44	0.50
2:B:135:LEU:HG	2:B:137:HIS:ND1	2.27	0.50
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.92	0.50
4:F:162:ILE:N	4:F:162:ILE:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TRP:CZ2	1:A:435:VAL:HG13	2.46	0.50
2:D:215:LEU:CB	2:D:217:LEU:HD23	2.42	0.49
1:A:412:GLY:O	3:E:60:ARG:NH1	2.46	0.49
2:D:36:TYR:CE2	2:D:44:LEU:HD11	2.48	0.49
1:C:68:VAL:HG21	1:C:118:VAL:HG21	1.93	0.49
4:F:79:LYS:O	4:F:83:THR:HG23	2.12	0.49
2:D:189:VAL:HG11	2:D:415:MET:HE2	1.94	0.49
2:B:301:ALA:O	2:B:303:CYS:N	2.43	0.48
2:D:318:ARG:HA	2:D:354:CYS:O	2.14	0.48
4:F:346:LEU:C	4:F:346:LEU:HD13	2.38	0.48
2:B:42:LEU:HD13	2:B:356:ILE:HD11	1.96	0.48
4:F:197:ARG:HH22	4:F:256:TYR:HB2	1.78	0.48
2:D:67:ASP:HB3	2:D:73:MET:HE2	1.96	0.48
2:D:323:MET:HE1	2:D:353:VAL:HB	1.95	0.47
4:F:146:VAL:HG11	4:F:233:PHE:CE1	2.49	0.47
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.47	0.47
4:F:192:LEU:HD11	4:F:262:MET:CE	2.44	0.47
4:F:161:LEU:HD23	4:F:172:PHE:HD2	1.79	0.47
2:B:219:THR:HG21	1:C:326:LYS:HA	1.97	0.47
2:D:232:THR:OG1	2:D:300:MET:HE3	2.15	0.47
4:F:127:GLU:HB2	4:F:130:VAL:CG1	2.45	0.47
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.49	0.47
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.50	0.46
4:F:160:ILE:CG2	4:F:240:LEU:HD21	2.46	0.46
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.97	0.46
1:C:181:VAL:HG11	1:C:404:PHE:CZ	2.51	0.46
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.46	0.46
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.44	0.46
2:D:285:THR:HB	2:D:287:PRO:HD2	1.98	0.46
2:B:356:ILE:HD12	2:B:356:ILE:N	2.31	0.46
2:D:152:ILE:HG23	2:D:164:MET:HG2	1.97	0.45
4:F:16:GLU:OE2	4:F:19:ARG:CZ	2.65	0.45
1:A:39:ASP:OD2	1:A:61:HIS:HE1	2.00	0.45
4:F:198:LYS:HE2	4:F:320:MET:HE1	1.99	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.32	0.45
2:D:67:ASP:CB	2:D:73:MET:HE2	2.47	0.45
4:F:148:ILE:HD11	4:F:160:ILE:HD12	1.97	0.45
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.99	0.45
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.99	0.45
4:F:191:LEU:HD13	4:F:196:HIS:CE1	2.52	0.44
1:A:136:LEU:HD12	1:A:136:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:502:BKF:C41	9:D:502:BKF:CL4	3.02	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.44
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.99	0.44
4:F:271:LEU:HD23	4:F:275:LEU:HD12	1.99	0.44
2:B:135:LEU:HD23	2:B:137:HIS:CE1	2.52	0.44
1:C:72:PRO:O	1:C:76:ASP:CG	2.61	0.44
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.53	0.44
2:D:172:SER:OG	2:D:205:GLU:OE1	2.30	0.44
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.99	0.44
4:F:150:LYS:HG2	4:F:160:ILE:HD11	1.99	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.52	0.43
4:F:226:GLU:OE1	4:F:226:GLU:N	2.51	0.43
4:F:78:VAL:HG21	4:F:181:VAL:HG21	2.00	0.43
4:F:102:PRO:HD2	4:F:179:VAL:HA	2.00	0.43
4:F:161:LEU:HD11	4:F:169:LEU:HD23	1.99	0.43
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.49	0.43
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.12	0.43
2:B:189:VAL:HG11	2:B:415:MET:HE2	2.01	0.43
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.43
4:F:192:LEU:C	4:F:192:LEU:CD2	2.92	0.42
1:A:324:VAL:CG2	1:A:325:PRO:HD2	2.48	0.42
1:A:324:VAL:HG23	1:A:325:PRO:HD2	2.01	0.42
2:D:238:THR:HB	2:D:316:ILE:HD13	2.02	0.42
4:F:39:LEU:HD21	4:F:41:LEU:HD21	2.00	0.42
4:F:192:LEU:HD11	4:F:262:MET:HE1	2.00	0.42
2:B:316:ILE:HG23	2:B:366:THR:HB	2.01	0.42
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.42
2:D:161:ASP:C	2:D:162:ARG:HE	2.28	0.42
4:F:221:LEU:O	4:F:261:GLU:HA	2.19	0.42
2:B:2:ARG:HA	2:B:129:CYS:O	2.20	0.42
2:D:46:ARG:NH2	2:D:248:ALA:O	2.52	0.42
4:F:198:LYS:CE	4:F:320:MET:HE1	2.50	0.41
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.41
4:F:240:LEU:N	4:F:240:LEU:CD1	2.82	0.41
2:B:317:PHE:O	2:B:353:VAL:HA	2.20	0.41
1:C:320:ARG:HA	1:C:356:ASN:O	2.20	0.41
2:D:94:GLN:OE1	2:D:94:GLN:N	2.47	0.41
4:F:40:MET:HE1	4:F:48:PRO:HD2	2.02	0.41
4:F:298:ILE:HD12	4:F:302:ILE:HD13	2.02	0.41
1:C:370:LYS:C	1:C:370:LYS:HD3	2.45	0.41
4:F:213:ILE:CD1	4:F:296:MET:CE	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:195:GLY:O	4:F:196:HIS:C	2.63	0.41
4:F:138:ARG:O	4:F:142:ARG:N	2.53	0.41
1:C:71:GLU:HG2	1:C:72:PRO:HD2	2.03	0.41
4:F:148:ILE:HD11	4:F:160:ILE:CD1	2.51	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
1:C:69:ASP:O	1:C:94:THR:HA	2.21	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.40
4:F:256:TYR:CD1	4:F:256:TYR:N	2.89	0.40
2:B:134:GLN:HA	2:B:165:ASN:O	2.20	0.40
4:F:93:TRP:O	4:F:328:TRP:HA	2.22	0.40
1:C:324:VAL:O	1:C:325:PRO:C	2.63	0.40
4:F:161:LEU:HD11	4:F:169:LEU:CD2	2.51	0.40
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.40
1:A:134:GLY:HA3	1:A:165:SER:O	2.22	0.40
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.55	0.40
2:D:76:VAL:HG23	2:D:77:ARG:N	2.37	0.40
2:D:375:GLN:HB2	2:D:419:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	422 (97%)	13 (3%)	0	100	100
1	C	438/451 (97%)	426 (97%)	12 (3%)	0	100	100
2	B	425/445 (96%)	416 (98%)	9 (2%)	0	100	100
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	118/189 (62%)	116 (98%)	2 (2%)	0	100	100
4	F	326/384 (85%)	309 (95%)	16 (5%)	1 (0%)	36	68
All	All	2159/2365 (91%)	2096 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	91	CYS

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	368/379 (97%)	366 (100%)	2 (0%)	81	85
1	C	371/379 (98%)	370 (100%)	1 (0%)	86	88
2	B	369/383 (96%)	368 (100%)	1 (0%)	86	88
2	D	364/383 (95%)	364 (100%)	0	100	100
3	E	110/171 (64%)	109 (99%)	1 (1%)	70	81
4	F	303/342 (89%)	301 (99%)	2 (1%)	76	83
All	All	1885/2037 (92%)	1878 (100%)	7 (0%)	84	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	274	PRO
2	B	316	ILE
1	C	71	GLU
3	E	126	LYS
4	F	160	ILE
4	F	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
4	F	380	HIS

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
10	ACP	F	401	-	31,33,33	0.68	1 (3%)	47,52,52	1.21	2 (4%)
5	GTP	A	501	6	33,34,34	0.63	0	50,54,54	0.60	0
5	GTP	C	501	6	33,34,34	0.62	0	50,54,54	0.59	0
8	GDP	B	501	6	29,30,30	0.59	0	45,47,47	0.45	0
8	GDP	D	501	-	29,30,30	0.62	0	45,47,47	0.63	1 (2%)
9	BKF	D	502	-	45,47,47	3.02	15 (33%)	53,71,71	3.07	26 (49%)

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
10	ACP	F	401	-	-	7/19/38/38	0/3/3/3
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
8	GDP	D	501	-	-	4/16/32/32	0/3/3/3
9	BKF	D	502	-	-	19/50/76/76	0/2/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	502	BKF	C08-N07	8.26	1.51	1.35
9	D	502	BKF	C10-C11	7.32	1.62	1.52
9	D	502	BKF	C12-C14	7.02	1.56	1.47
9	D	502	BKF	C06-N07	6.90	1.52	1.44
9	D	502	BKF	C15-C16	6.86	1.69	1.53
9	D	502	BKF	C27-C26	-5.31	1.48	1.52
9	D	502	BKF	C06-C01	4.81	1.45	1.40
9	D	502	BKF	C41-N07	4.07	1.53	1.46
9	D	502	BKF	C21-N20	3.81	1.52	1.45
9	D	502	BKF	C10-C08	3.59	1.57	1.51
10	F	401	ACP	PB-O3A	3.39	1.62	1.58
9	D	502	BKF	C18-N20	2.53	1.40	1.34
9	D	502	BKF	C02-C01	2.43	1.44	1.40
9	D	502	BKF	O42-C02	2.35	1.41	1.37
9	D	502	BKF	O35-C11	-2.32	1.42	1.46
9	D	502	BKF	O19-C18	2.10	1.25	1.21

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	BKF	C05-C06-C01	-8.70	111.98	122.54
9	D	502	BKF	C12-O34-C14	7.06	64.81	60.81
10	F	401	ACP	PB-O3A-PA	-6.84	110.06	132.37
9	D	502	BKF	O35-C36-C38	5.96	122.14	111.14
9	D	502	BKF	O09-C08-C10	-5.77	111.30	122.07
9	D	502	BKF	O35-C36-O37	-5.63	113.78	123.95
9	D	502	BKF	O42-C02-C01	4.66	120.55	115.44
9	D	502	BKF	O34-C14-C15	4.53	122.84	117.41
9	D	502	BKF	C28-C26-C25	-4.52	102.95	122.50
9	D	502	BKF	C06-C05-C04	4.25	126.91	120.28
9	D	502	BKF	C28-C26-C27	-4.13	112.06	115.53
9	D	502	BKF	C43-O42-C02	3.90	123.24	117.51
9	D	502	BKF	C41-N07-C08	-3.54	113.46	119.14
9	D	502	BKF	C33-C15-C16	3.33	116.23	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	BKF	O34-C12-C14	-3.24	57.33	59.38
9	D	502	BKF	C11-O35-C36	3.22	123.83	118.20
9	D	502	BKF	O09-C08-N07	-3.20	116.53	121.94
9	D	502	BKF	C13-C12-C11	3.13	122.82	114.62
9	D	502	BKF	O34-C14-C12	-2.89	57.86	59.82
9	D	502	BKF	C02-C01-CL4	-2.89	114.95	120.27
9	D	502	BKF	C03-C02-C01	-2.56	117.92	120.99
9	D	502	BKF	O32-C21-C31	-2.44	103.19	109.98
9	D	502	BKF	O29-C22-C23	-2.30	104.47	111.08
8	D	501	GDP	O2B-PB-O1B	2.23	119.53	110.83
9	D	502	BKF	O35-C11-C10	2.23	109.39	105.09
9	D	502	BKF	C16-C15-C14	2.15	116.71	111.19
9	D	502	BKF	O17-C18-N20	2.12	122.72	118.78
9	D	502	BKF	O17-C16-C15	2.10	109.71	105.68
10	F	401	ACP	O2'-C2'-C3'	-2.01	105.39	111.82

There are no chirality outliers.

All (43) 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-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	B	501	GDP	PA-O3A-PB-O3B
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	D	502	BKF	C08-C10-C11-C12
9	D	502	BKF	O34-C14-C15-C33
9	D	502	BKF	C33-C15-C16-O17
9	D	502	BKF	C33-C15-C16-C31
9	D	502	BKF	C21-C22-C23-C24
9	D	502	BKF	C21-C22-O29-C30
9	D	502	BKF	C22-C23-C24-C25
9	D	502	BKF	C23-C24-C25-C26
9	D	502	BKF	C24-C25-C26-C27
9	D	502	BKF	C28-C26-C27-C04
9	D	502	BKF	C01-C06-N07-C08

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Mol	Chain	Res	Type	Atoms
9	D	502	BKF	C01-C06-N07-C41
9	D	502	BKF	C05-C06-N07-C08
9	D	502	BKF	C05-C06-N07-C41
9	D	502	BKF	O37-C36-O35-C11
9	D	502	BKF	C38-C36-O35-C11
10	F	401	ACP	PB-C3B-PG-O1G
10	F	401	ACP	PB-C3B-PG-O3G
10	F	401	ACP	PG-C3B-PB-O1B
10	F	401	ACP	PG-C3B-PB-O3A
10	F	401	ACP	O4'-C4'-C5'-O5'
10	F	401	ACP	C3'-C4'-C5'-O5'
9	D	502	BKF	O29-C22-C23-C24
5	C	501	GTP	C4'-C5'-O5'-PA
10	F	401	ACP	PG-C3B-PB-O2B
5	A	501	GTP	C4'-C5'-O5'-PA
8	D	501	GDP	C4'-C5'-O5'-PA
9	D	502	BKF	O37-C36-C38-C40
5	A	501	GTP	PA-O3A-PB-O2B
9	D	502	BKF	O35-C36-C38-C40
5	C	501	GTP	PA-O3A-PB-O2B
5	C	501	GTP	PA-O3A-PB-O1B

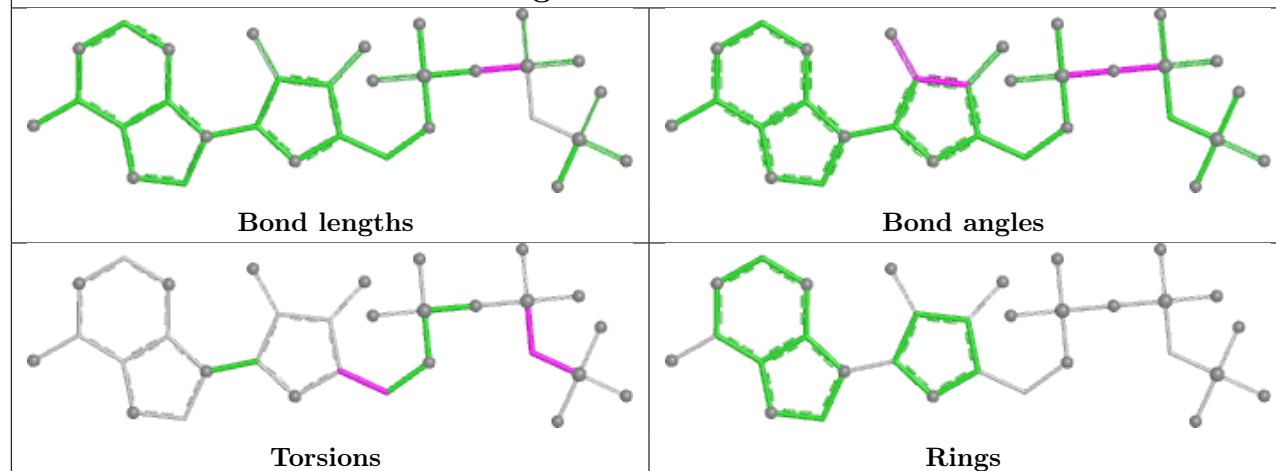
There are no ring outliers.

2 monomers are involved in 2 short contacts:

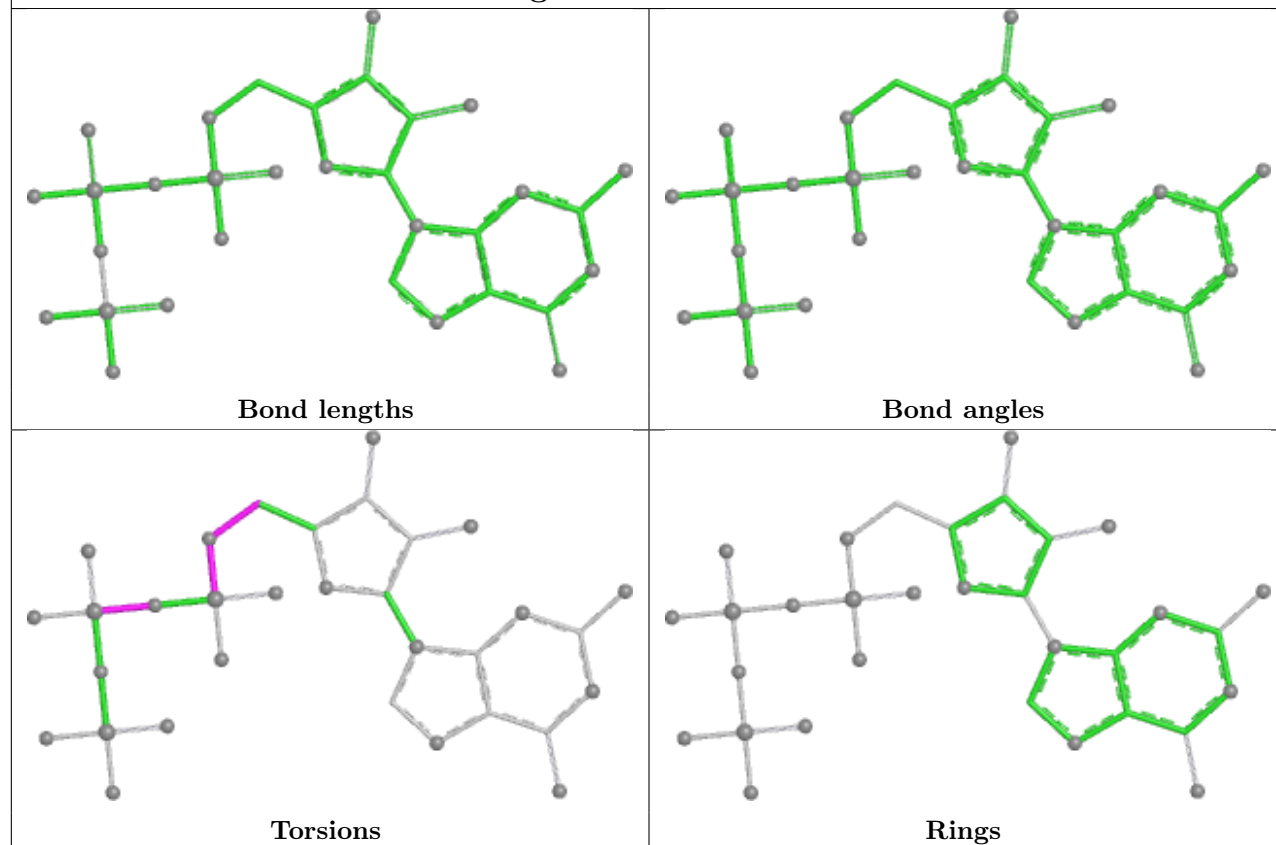
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
9	D	502	BKF	1	0

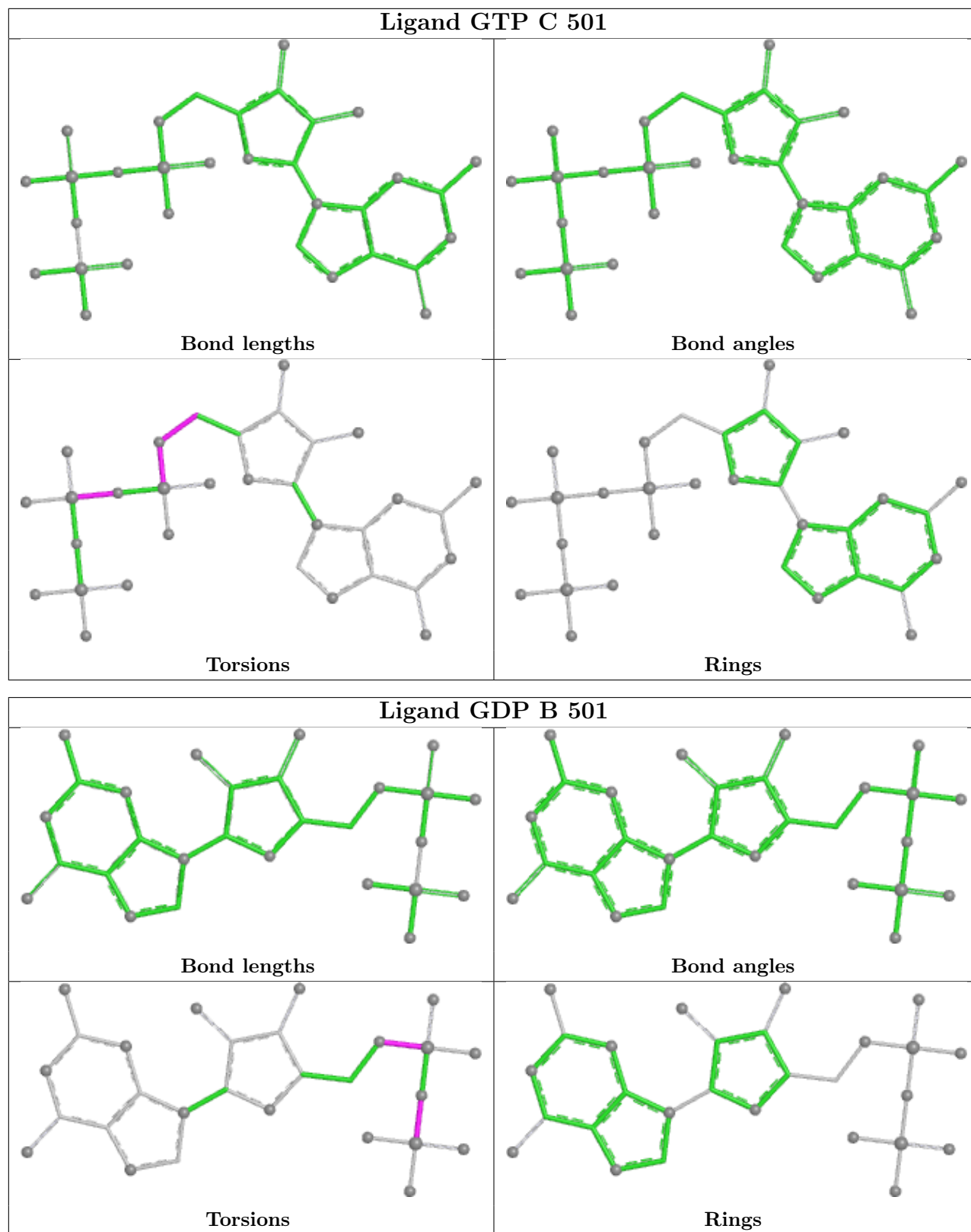
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

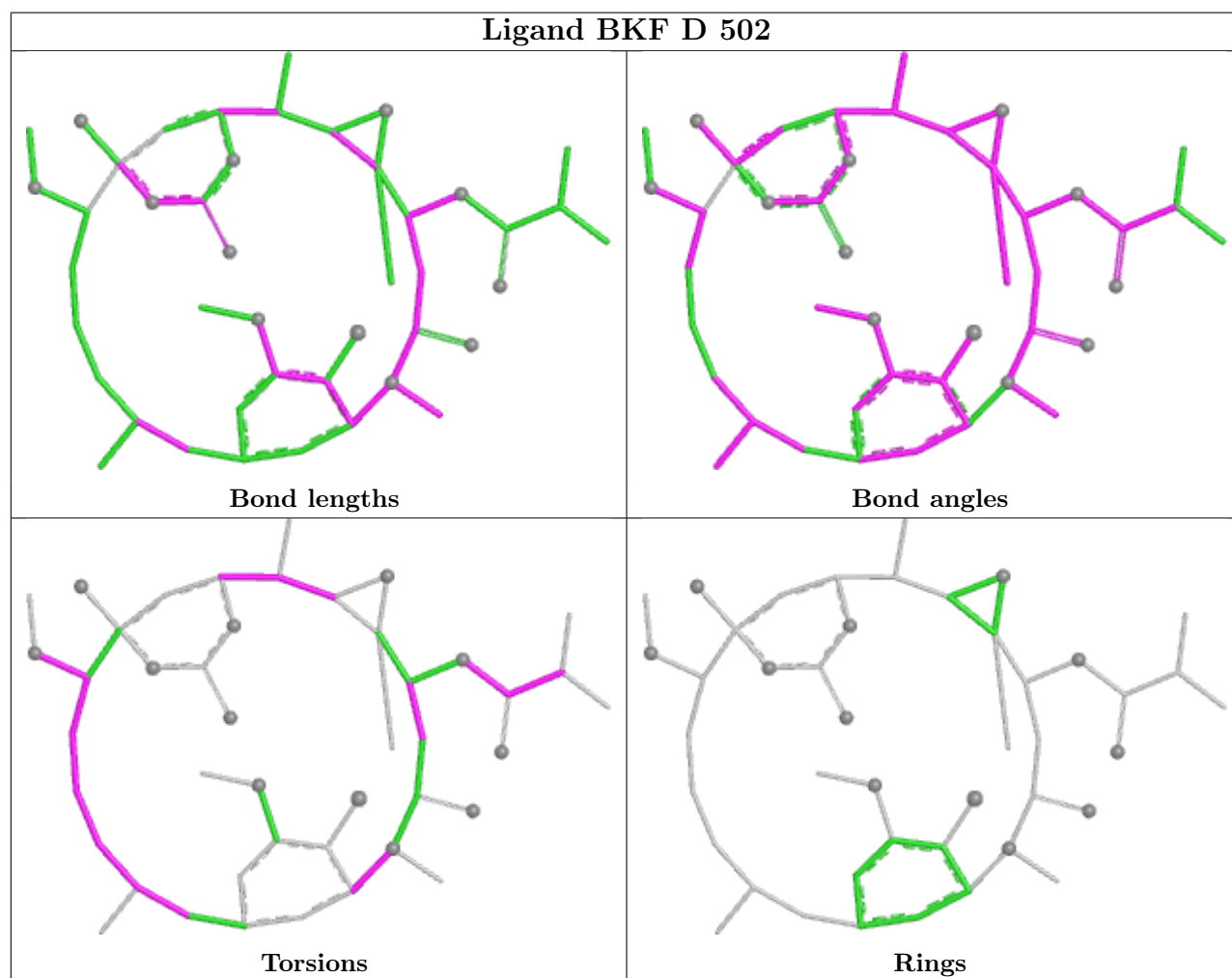
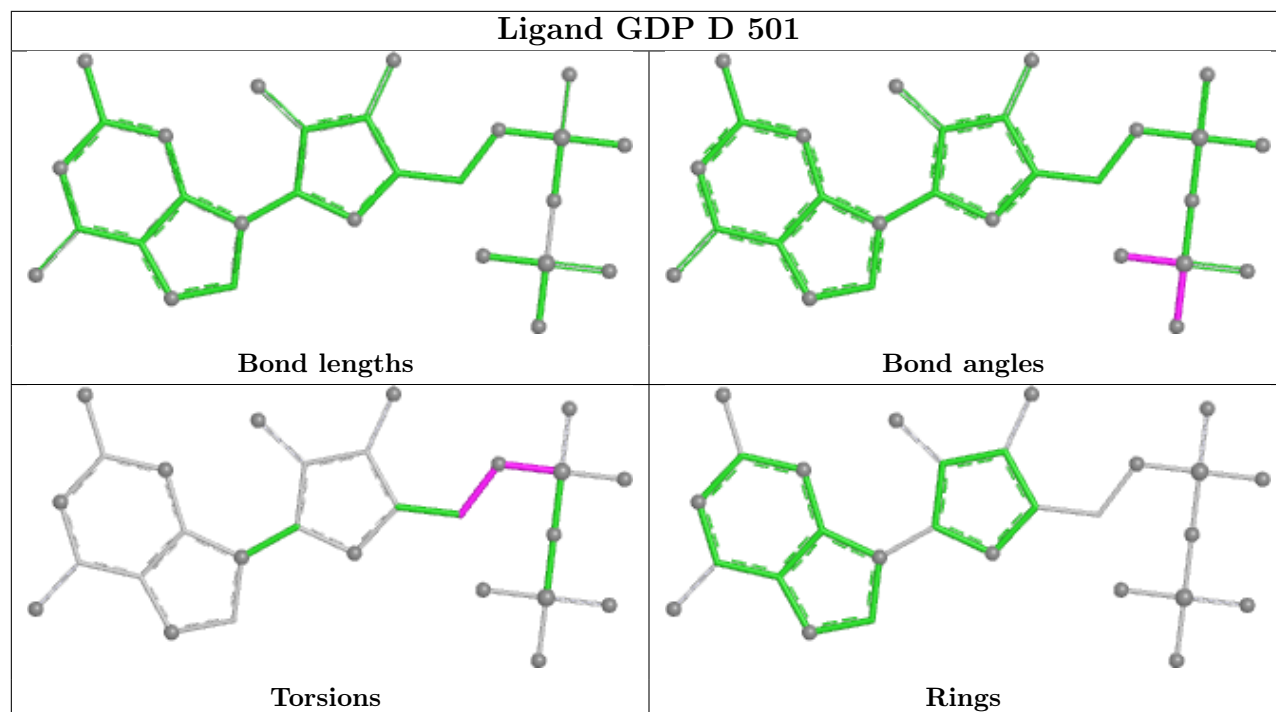
Ligand ACP F 401



Ligand GTP A 501







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	437/451 (96%)	-0.08	3 (0%) 84 69	31, 54, 93, 164	0
1	C	440/451 (97%)	-0.18	8 (1%) 67 48	23, 44, 80, 113	0
2	B	427/445 (95%)	-0.09	5 (1%) 76 58	24, 50, 93, 185	0
2	D	421/445 (94%)	0.06	4 (0%) 79 63	33, 65, 102, 139	0
3	E	121/189 (64%)	0.31	7 (5%) 29 18	32, 67, 111, 158	1 (0%)
4	F	336/384 (87%)	0.43	20 (5%) 27 17	43, 83, 161, 195	0
All	All	2182/2365 (92%)	0.02	47 (2%) 62 42	23, 59, 114, 195	1 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	133	ALA	4.5
4	F	238	CYS	4.2
4	F	141	GLY	3.7
4	F	372	THR	3.7
4	F	177	GLY	3.6
4	F	144	GLY	3.5
4	F	134	ALA	3.4
3	E	139	LEU	3.2
2	B	78	SER	3.2
4	F	173	ILE	3.1
2	B	291	GLN	3.0
1	C	356	ASN	3.0
4	F	175	GLU	2.8
1	C	249	ASN	2.7
1	C	251	ASP	2.7
3	E	45	PRO	2.7
2	D	37	HIS	2.7
2	D	386	THR	2.6
4	F	176	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	2.5
2	B	125	GLU	2.5
4	F	145	ASN	2.5
1	C	232	SER	2.5
4	F	196	HIS	2.4
1	A	284	GLU	2.3
4	F	225	SER	2.3
4	F	242	ASN	2.3
1	A	256	GLN	2.3
4	F	130	VAL	2.3
4	F	246	GLN	2.2
4	F	99	VAL	2.2
2	B	332	ASN	2.2
2	D	57	ASN	2.2
1	A	162	GLY	2.1
3	E	115[A]	HIS	2.1
4	F	192	LEU	2.1
2	D	73	MET	2.1
1	C	90	GLU	2.1
4	F	129	GLU	2.1
3	E	6	MET	2.0
1	C	350	GLY	2.0
3	E	49	GLU	2.0
3	E	125	GLU	2.0
1	C	236	SER	2.0
2	B	48	ASN	2.0
3	E	103	GLN	2.0
1	C	308	ARG	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.

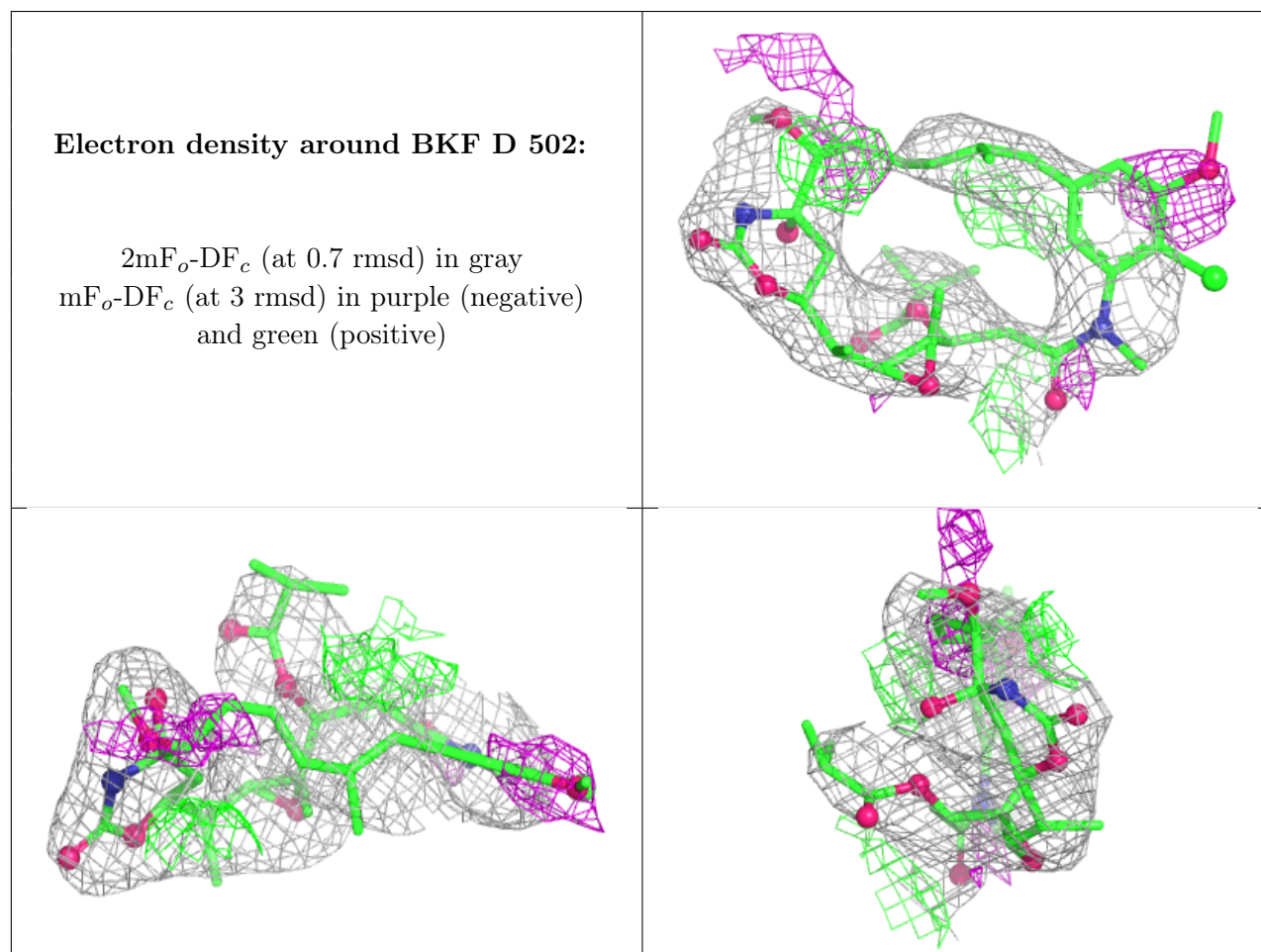
6.4 Ligands [i](#)

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.

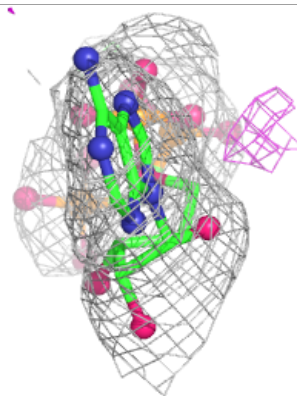
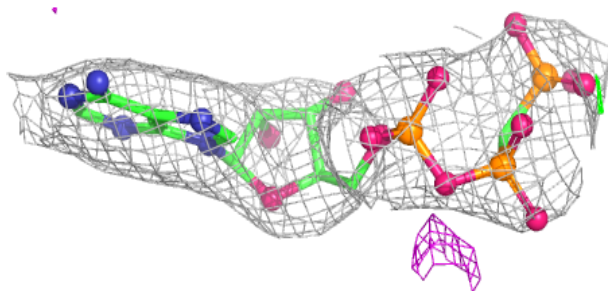
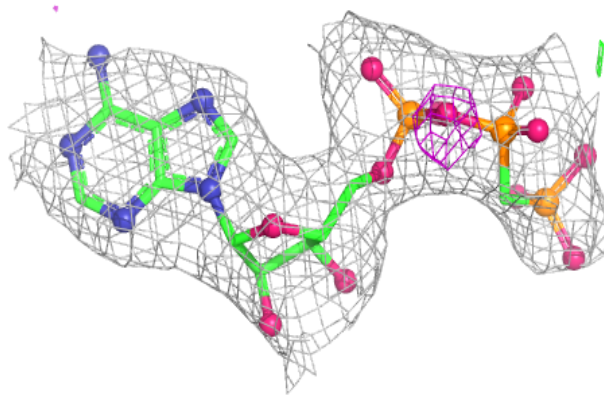
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	C	502	1/1	0.66	0.20	29,29,29,29	0
9	BKF	D	502	44/44	0.69	0.16	51,71,84,149	0
10	ACP	F	401	31/31	0.82	0.11	81,95,113,120	0
8	GDP	D	501	28/28	0.85	0.13	48,60,72,84	0
6	MG	B	502	1/1	0.89	0.20	39,39,39,39	0
6	MG	A	502	1/1	0.91	0.24	36,36,36,36	0
5	GTP	A	501	32/32	0.91	0.11	33,42,50,52	0
8	GDP	B	501	28/28	0.92	0.11	28,38,46,53	0
7	CA	A	503	1/1	0.92	0.10	79,79,79,79	0
5	GTP	C	501	32/32	0.93	0.11	30,37,45,51	0
7	CA	C	503	1/1	0.93	0.07	64,64,64,64	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.

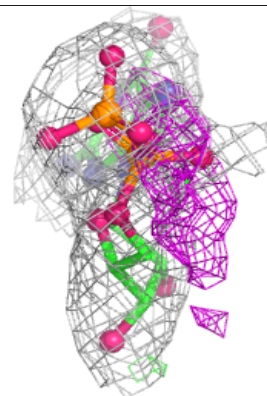
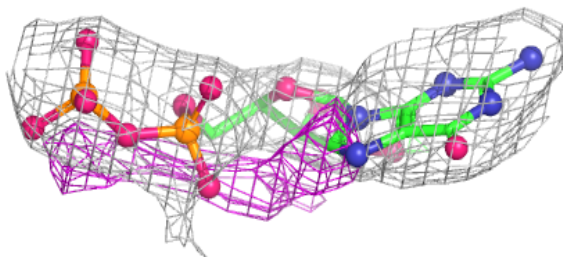
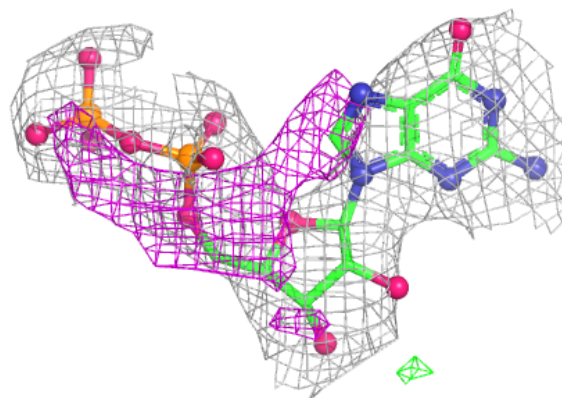


Electron density around ACP F 401:

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

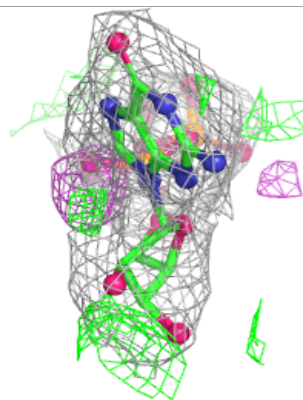
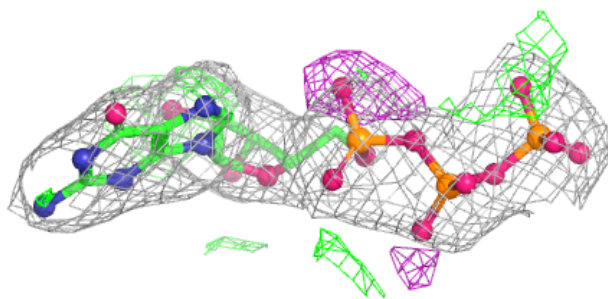
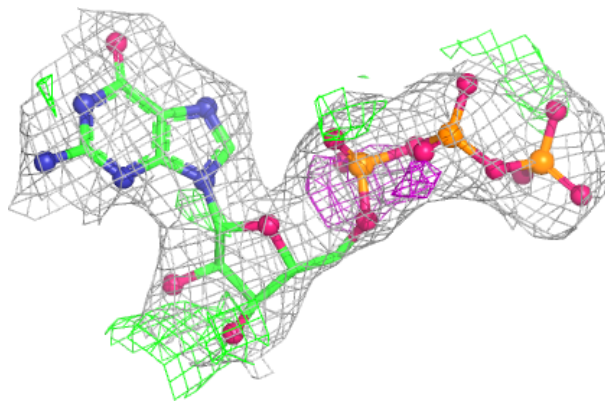
**Electron density around GDP D 501:**

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



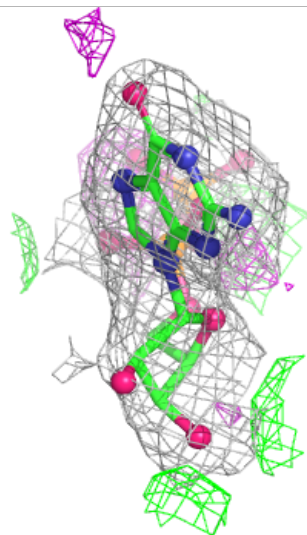
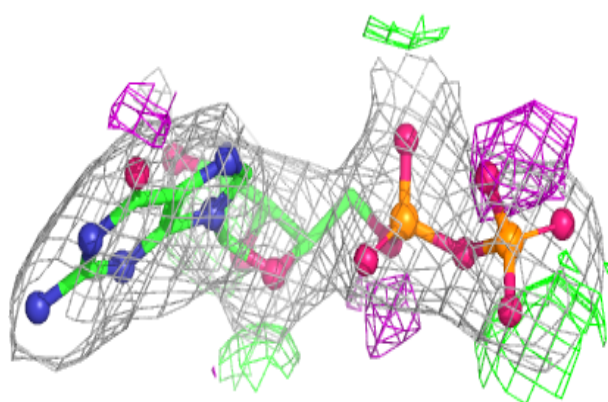
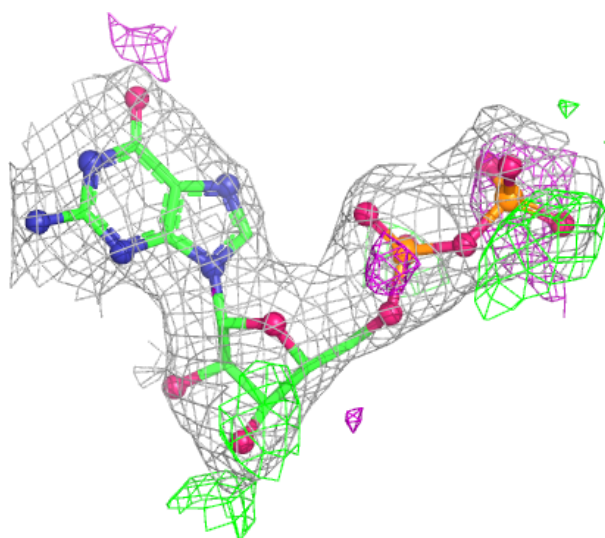
Electron density around GTP A 501:

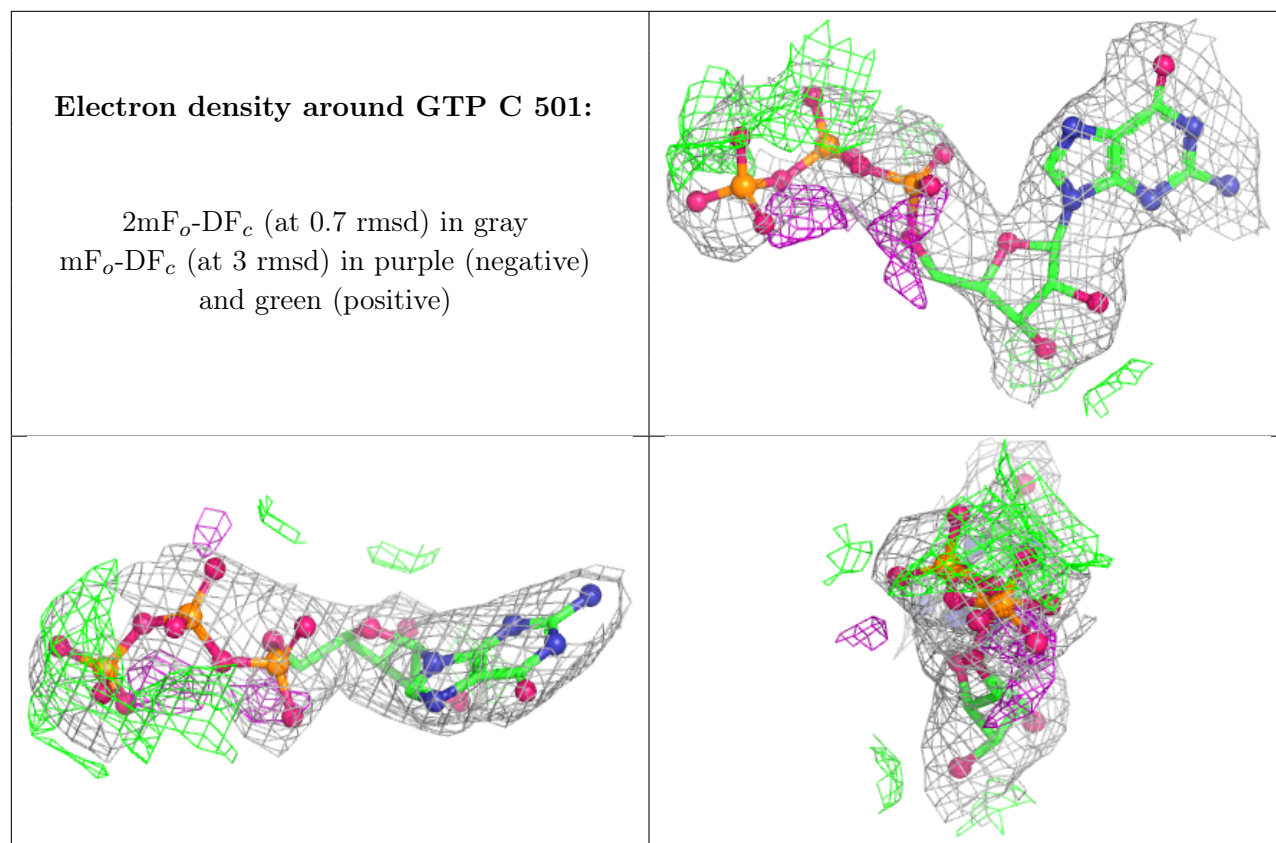
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.