



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:54 PM UTC

PDB ID : 5XLZ / pdb_00005xlz
Title : The crystal structure of tubulin complexed with a benzylidene derivative of 9(10H)-anthracenone
Authors : Yu, Y.; Chen, Q.
Deposited on : 2017-05-12
Resolution : 2.30 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:

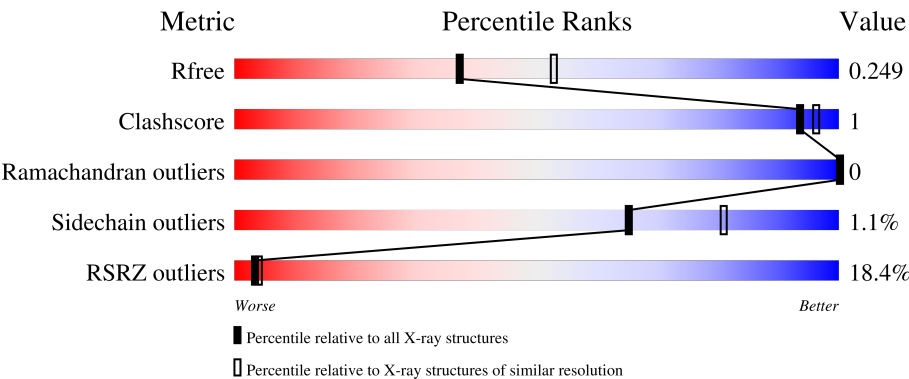
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	6% 95% • •
1	C	450	2% 95% • •
2	B	445	12% 91% • •
2	D	445	29% 90% 5% 5%
3	E	143	21% 83% • 15%

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Mol	Chain	Length	Quality of chain
4	F	384	40% 82% 5% 13%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 35306 atoms, of which 16927 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	H	N	O	S	0	7	0
			6791	2179	3345	586	657	24			
1	C	440	Total	C	H	N	O	S	0	4	0
			6806	2184	3351	587	659	25			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	4	0
			6629	2121	3248	581	653	26			
2	D	421	Total	C	H	N	O	S	0	1	0
			6510	2086	3190	566	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	2	0
			2031	623	1021	184	198	5			

There are 2 discrepancies between the modelled and reference sequences:

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

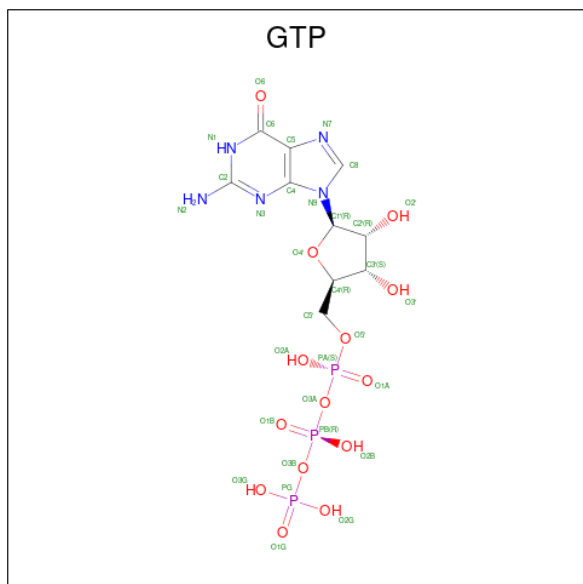
- Molecule 4 is a protein called Tubulin Tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	2	0
			5460	1766	2707	472	501	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 42	C 10	H 10	N 5	O 14	P 3	0	0
5	C	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0
5	D	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0

- 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		

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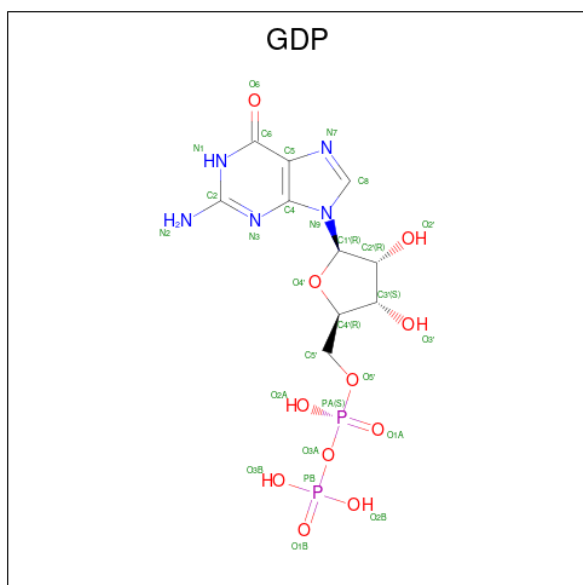
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

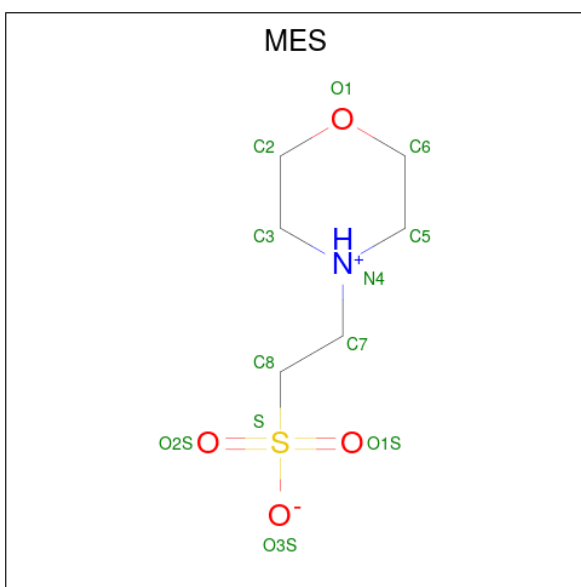
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



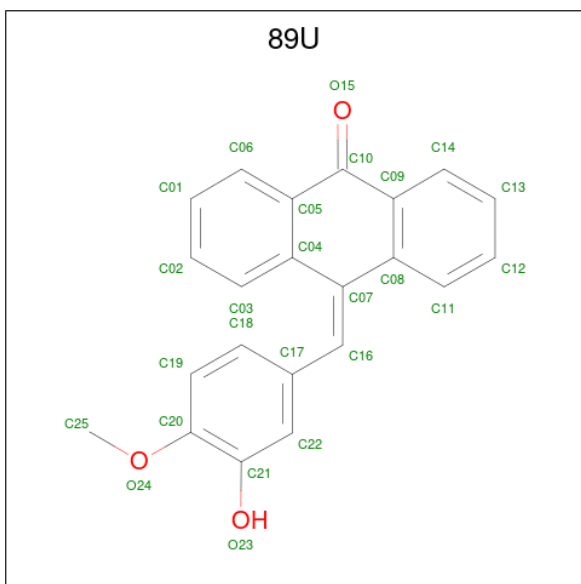
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		
9	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 10 is 10-[(4-methoxy-3-oxidanyl-phenyl)methylidene]anthracen-9-one (CCD ID: 89U) (formula: C₂₂H₁₆O₃).



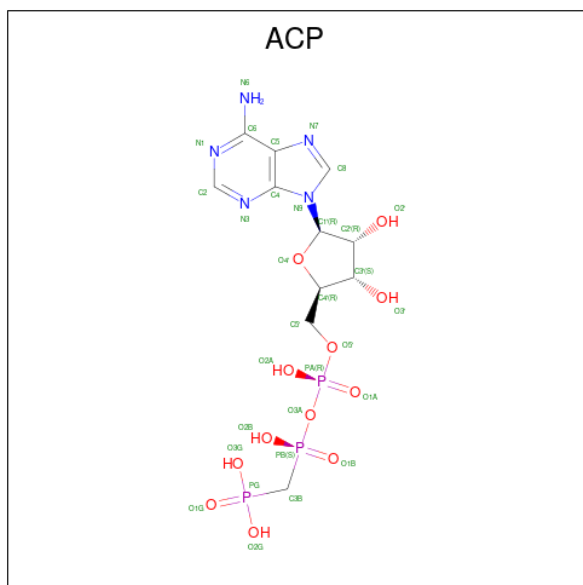
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			25	22	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			25	22	3		

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



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

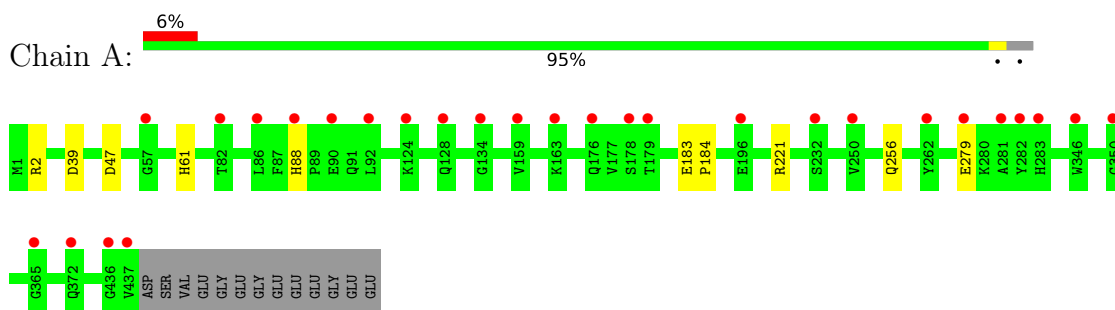
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	150	Total	O	0	0
			150	150		
12	B	153	Total	O	0	0
			153	153		
12	C	286	Total	O	0	0
			286	286		
12	D	85	Total	O	0	0
			85	85		
12	E	36	Total	O	0	0
			36	36		
12	F	69	Total	O	0	0
			69	69		

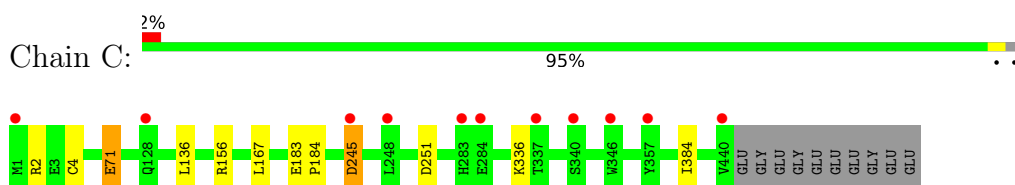
3 Residue-property plots [i](#)

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.

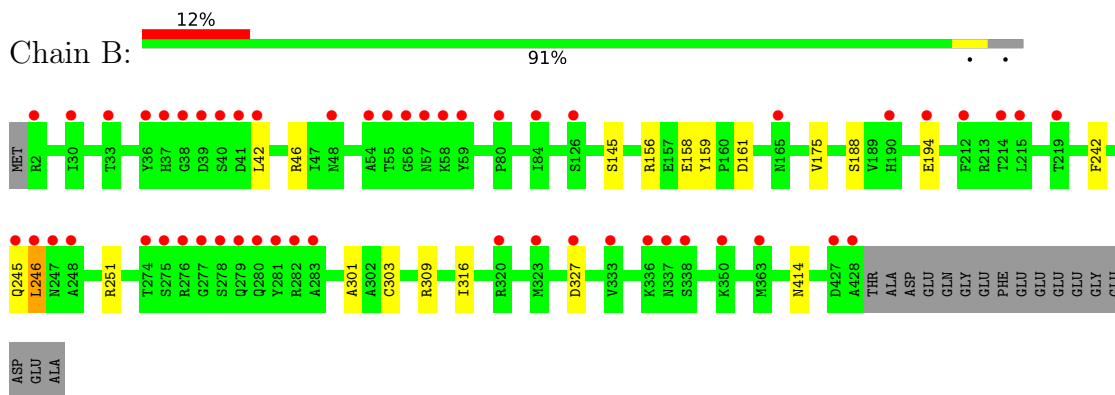
- Molecule 1: Tubulin alpha-1B chain



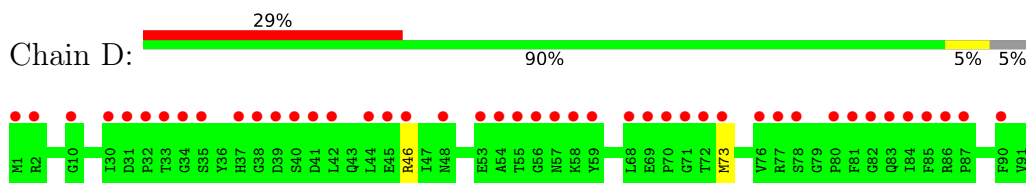
- Molecule 1: Tubulin alpha-1B chain

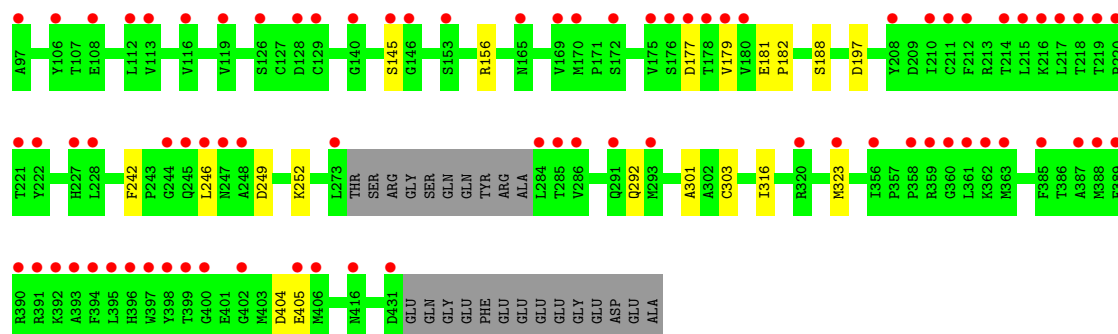


- Molecule 2: Tubulin beta-2B chain

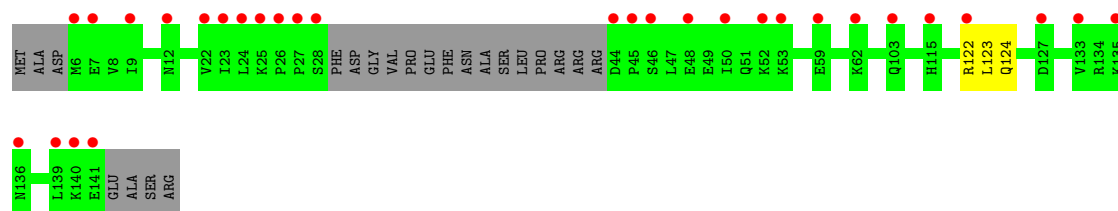
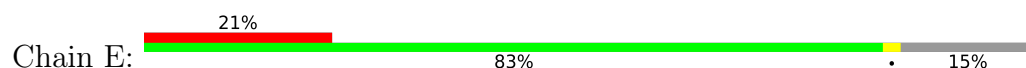


- Molecule 2: Tubulin beta-2B chain

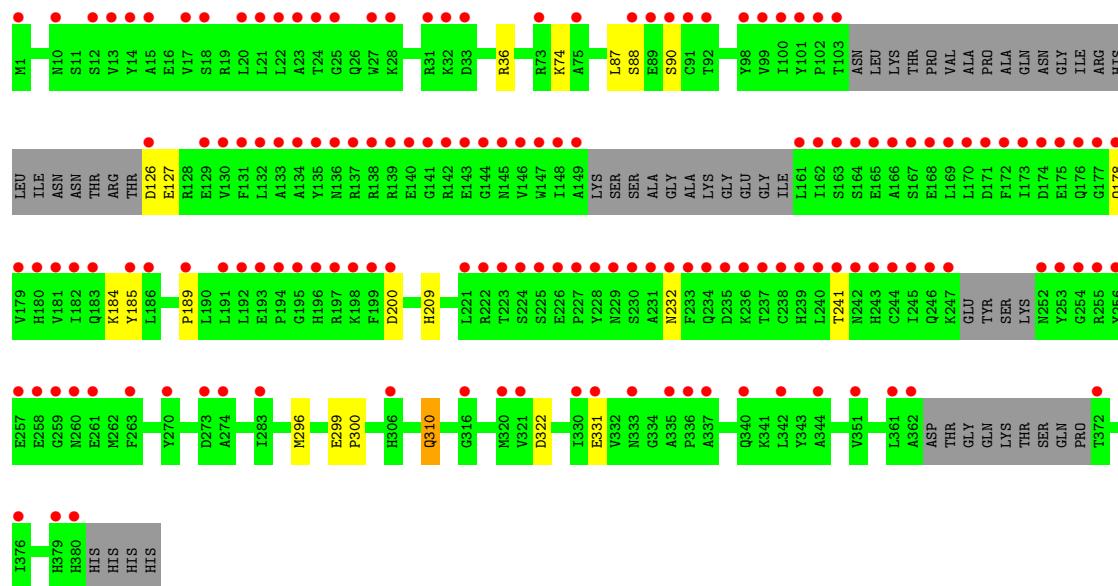
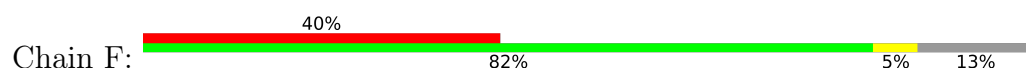




• Molecule 3: Stathmin-4



• 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	105.47Å 158.44Å 181.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.67 – 2.30 42.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.67-2.30) 98.0 (42.67-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.216 , 0.247 0.223 , 0.249	Depositor DCC
R_{free} test set	1343 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35306	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 89U, MG, MES, CA, ACP, GDP, 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	0.30	0/3548	0.62	0/4815
1	C	0.29	0/3539	0.61	0/4805
2	B	0.29	0/3473	0.65	2/4702 (0.0%)
2	D	0.29	0/3393	0.62	0/4595
3	E	0.27	0/1027	0.58	0/1363
4	F	0.25	0/2821	0.58	0/3811
All	All	0.29	0/17801	0.61	2/24091 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	246	LEU	CA-C-N	9.76	140.18	121.54
2	B	246	LEU	C-N-CA	9.76	140.18	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3446	3345	3322	6	0
1	C	3455	3351	3357	7	0
2	B	3381	3248	3238	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3320	3190	3201	11	0
3	E	1010	1021	1014	2	0
4	F	2753	2707	2712	13	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
9	B	24	25	25	0	0
10	B	25	0	0	0	0
10	D	25	0	0	0	0
11	F	31	0	14	1	0
12	A	150	0	0	2	0
12	B	153	0	0	5	0
12	C	286	0	0	3	0
12	D	85	0	0	2	0
12	E	36	0	0	0	0
12	F	69	0	0	3	0
All	All	18379	16927	16931	49	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 1.

All (49) 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:159:TYR:N	12:B:601:HOH:O	2.07	0.88
2:B:414:ASN:ND2	12:B:602:HOH:O	2.18	0.75
2:B:161:ASP:O	2:B:251[B]:ARG:NH2	2.27	0.67
1:C:156:ARG:NH1	12:C:607:HOH:O	2.28	0.66
1:A:221:ARG:NH2	2:B:327:ASP:OD2	2.30	0.65
2:D:292:GLN:NE2	12:D:604:HOH:O	2.30	0.63
12:D:601:HOH:O	3:E:122:ARG:NH2	2.34	0.61
2:B:145:SER:HG	2:B:188:SER:HG	1.50	0.59
4:F:126:ASP:N	12:F:505:HOH:O	2.36	0.59
2:B:158:GLU:N	12:B:601:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:ASP:OD1	2:D:405:GLU:N	2.36	0.58
4:F:331:GLU:OE2	11:F:401:ACP:H3B2	2.03	0.58
2:B:145:SER:OG	2:B:188:SER:OG	2.21	0.57
1:C:245:ASP:N	1:C:245:ASP:OD1	2.38	0.57
4:F:184:LYS:NZ	4:F:185:TYR:O	2.38	0.56
4:F:178:GLN:N	4:F:178:GLN:OE1	2.40	0.55
2:D:46:ARG:NH1	2:D:242:PHE:O	2.41	0.54
1:C:336:LYS:NZ	12:C:621:HOH:O	2.40	0.53
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.41	0.52
4:F:126:ASP:OD1	4:F:127:GLU:N	2.43	0.52
2:B:309:ARG:NH1	12:B:617:HOH:O	2.42	0.52
1:A:2:ARG:NH2	12:A:619:HOH:O	2.43	0.51
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.26	0.51
1:C:71:GLU:O	12:C:601:HOH:O	2.20	0.50
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.42	0.49
2:B:156:ARG:NH1	2:B:194[A]:GLU:O	2.46	0.49
1:A:88:HIS:NE2	12:A:609:HOH:O	2.35	0.48
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.53	0.48
4:F:232:ASN:O	12:F:501:HOH:O	2.20	0.47
2:B:156:ARG:C	12:B:601:HOH:O	2.57	0.47
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.34	0.47
2:D:145:SER:HG	2:D:188:SER:HG	1.64	0.46
2:D:177:ASP:OD1	2:D:177:ASP:N	2.51	0.44
2:D:181:GLU:N	2:D:182:PRO:HD2	2.33	0.43
4:F:36:ARG:NH2	12:F:510:HOH:O	2.51	0.43
4:F:209:HIS:HB2	4:F:310[A]:GLN:HG2	2.02	0.42
2:D:301:ALA:O	2:D:303:CYS:N	2.53	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
2:D:73:MET:HG3	2:D:92:PHE:HB3	2.03	0.41
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.03	0.41
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.03	0.41
2:B:46:ARG:NH1	2:B:242:PHE:O	2.54	0.40
2:B:301:ALA:O	2:B:303:CYS:N	2.50	0.40
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	0.40
2:D:249:ASP:OD1	2:D:252:LYS:N	2.46	0.40
4:F:189:PRO:HA	4:F:322:ASP:HA	2.01	0.40
1:A:47:ASP:N	1:A:47:ASP:OD1	2.54	0.40
4:F:87:LEU:O	4:F:88:SER:OG	2.26	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	442/450 (98%)	427 (97%)	15 (3%)	0	100	100
1	C	442/450 (98%)	433 (98%)	9 (2%)	0	100	100
2	B	429/445 (96%)	414 (96%)	15 (4%)	0	100	100
2	D	418/445 (94%)	410 (98%)	8 (2%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	326/384 (85%)	318 (98%)	8 (2%)	0	100	100
All	All	2176/2317 (94%)	2121 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/378 (99%)	372 (99%)	3 (1%)	73	86
1	C	375/378 (99%)	370 (99%)	5 (1%)	61	77
2	B	373/383 (97%)	368 (99%)	5 (1%)	61	77
2	D	365/383 (95%)	361 (99%)	4 (1%)	65	81
3	E	111/127 (87%)	110 (99%)	1 (1%)	70	84
4	F	303/342 (89%)	299 (99%)	4 (1%)	61	77
All	All	1902/1991 (96%)	1880 (99%)	22 (1%)	65	79

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	279[A]	GLU
1	A	279[B]	GLU
2	B	42	LEU
2	B	175	VAL
2	B	245	GLN
2	B	246	LEU
2	B	316	ILE
1	C	2	ARG
1	C	71	GLU
1	C	245	ASP
1	C	251	ASP
1	C	384	ILE
2	D	179	VAL
2	D	246	LEU
2	D	316	ILE
2	D	323	MET
3	E	124	GLN
4	F	90	SER
4	F	296	MET
4	F	310[A]	GLN
4	F	310[B]	GLN

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

Mol	Chain	Res	Type
1	A	301	GLN
2	B	8	GLN
2	B	134	GLN
2	B	227	HIS
2	B	245	GLN
2	B	347	ASN
2	B	426	GLN
1	C	293	ASN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	11	GLN
2	D	48	ASN
2	D	347	ASN
3	E	78	HIS

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Mol	Chain	Res	Type
3	E	92	ASN
4	F	180	HIS
4	F	269	GLN
4	F	333	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 6 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
10	89U	B	504	-	28,28,28	1.33	7 (25%)	40,40,40	1.13	5 (12%)
9	MES	B	505	-	12,12,12	2.31	1 (8%)	15,16,16	1.47	2 (13%)
5	GTP	C	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.49	8 (16%)
8	GDP	B	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.67	6 (13%)
5	GTP	A	501	6	33,34,34	0.96	1 (3%)	50,54,54	1.49	8 (16%)
11	ACP	F	401	-	31,33,33	3.33	14 (45%)	47,52,52	4.38	24 (51%)
5	GTP	D	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.50	8 (16%)
10	89U	D	502	-	28,28,28	1.26	6 (21%)	40,40,40	1.21	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MES	B	503	-	12,12,12	2.32	1 (8%)	15,16,16	2.43	5 (33%)

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	89U	B	504	-	-	2/6/22/22	0/4/4/4
9	MES	B	505	-	-	5/6/14/14	0/1/1/1
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	10/22/38/38	0/3/3/3
11	ACP	F	401	-	-	8/19/38/38	0/3/3/3
5	GTP	D	501	6	-	8/22/38/38	0/3/3/3
10	89U	D	502	-	-	2/6/22/22	0/4/4/4
9	MES	B	503	-	-	1/6/14/14	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PA-O3A	10.83	1.71	1.59
11	F	401	ACP	PB-O3A	8.05	1.67	1.58
9	B	503	MES	C8-S	-7.78	1.66	1.77
9	B	505	MES	C8-S	-7.75	1.66	1.77
11	F	401	ACP	PB-O1B	6.27	1.66	1.51
11	F	401	ACP	PG-O3G	4.33	1.64	1.55
11	F	401	ACP	O4'-C1'	3.90	1.51	1.42
11	F	401	ACP	C2-N3	3.51	1.40	1.33
11	F	401	ACP	C2-N1	3.38	1.39	1.33
11	F	401	ACP	C5-N7	-3.27	1.33	1.39
11	F	401	ACP	C5-C4	-3.23	1.33	1.39
8	B	501	GDP	C5-C4	3.03	1.47	1.38
11	F	401	ACP	C5-C6	-2.90	1.32	1.41
8	B	501	GDP	C6-N1	-2.81	1.33	1.38
11	F	401	ACP	PG-O2G	2.72	1.61	1.55
10	D	502	89U	C08-C07	2.51	1.53	1.47
10	B	504	89U	C09-C10	2.48	1.53	1.48
10	B	504	89U	C08-C07	2.43	1.53	1.47
10	B	504	89U	C04-C07	2.42	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	89U	C09-C10	2.42	1.53	1.48
10	D	502	89U	C04-C07	2.40	1.53	1.47
5	C	501	GTP	PA-O3A	2.39	1.62	1.59
10	D	502	89U	C05-C10	2.36	1.53	1.48
10	B	504	89U	C05-C10	2.36	1.53	1.48
11	F	401	ACP	C4-N9	-2.32	1.32	1.37
10	B	504	89U	O24-C20	2.29	1.40	1.37
8	B	501	GDP	C5-N7	-2.24	1.34	1.39
11	F	401	ACP	C8-N9	-2.21	1.33	1.37
10	B	504	89U	O15-C10	-2.19	1.18	1.22
10	B	504	89U	O23-C21	2.16	1.40	1.36
5	D	501	GTP	C2-N3	2.16	1.38	1.33
5	A	501	GTP	C2-N3	2.12	1.38	1.33
10	D	502	89U	O15-C10	-2.11	1.19	1.22
10	D	502	89U	O23-C21	2.09	1.40	1.36
5	C	501	GTP	C2-N3	2.08	1.38	1.33
11	F	401	ACP	PA-O5'	2.01	1.67	1.59

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	O4'-C4'-C3'	-14.89	75.60	105.15
11	F	401	ACP	O4'-C1'-N9	-14.63	80.00	108.09
11	F	401	ACP	C2'-C1'-N9	8.73	135.01	113.30
11	F	401	ACP	O4'-C1'-C2'	-8.46	88.52	106.62
11	F	401	ACP	N3-C2-N1	-6.85	118.21	128.58
11	F	401	ACP	O5'-C5'-C4'	6.25	130.29	108.99
8	B	501	GDP	C5-C4-N3	-5.58	119.50	128.39
11	F	401	ACP	C2'-C3'-C4'	-5.52	91.94	102.61
5	C	501	GTP	C5-C4-N3	-4.83	120.70	128.39
5	D	501	GTP	C5-C4-N3	-4.83	120.71	128.39
5	A	501	GTP	C5-C4-N3	-4.81	120.73	128.39
9	B	503	MES	C7-N4-C5	4.81	124.05	111.24
8	B	501	GDP	C2-N3-C4	4.68	120.36	112.30
9	B	503	MES	C5-N4-C3	4.62	118.78	108.84
11	F	401	ACP	C4-N9-C1'	-4.60	115.87	126.63
9	B	503	MES	C6-C5-N4	-4.57	103.17	110.12
11	F	401	ACP	N9-C8-N7	-4.55	107.48	113.94
5	D	501	GTP	C2-N3-C4	4.52	120.09	112.30
11	F	401	ACP	O2B-PB-C3B	4.50	125.38	106.73
5	A	501	GTP	C2-N3-C4	4.47	120.00	112.30
5	C	501	GTP	C2-N3-C4	4.47	119.99	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	N9-C4-N3	4.20	134.35	125.95
11	F	401	ACP	C5-C4-N3	-3.98	121.23	126.72
11	F	401	ACP	C1'-N9-C8	3.89	135.72	127.09
9	B	505	MES	C5-N4-C3	3.68	116.78	108.84
10	B	504	89U	O24-C20-C21	3.59	119.94	114.55
8	B	501	GDP	C6-C5-N7	3.49	136.63	130.29
11	F	401	ACP	C5-C6-N6	-3.14	115.50	123.29
10	D	502	89U	O24-C20-C21	3.10	119.19	114.55
5	D	501	GTP	N9-C4-N3	3.08	132.11	125.95
11	F	401	ACP	C2-N3-C4	3.06	119.31	111.83
5	C	501	GTP	N9-C4-N3	3.04	132.03	125.95
5	A	501	GTP	N9-C4-N3	3.04	132.03	125.95
11	F	401	ACP	O2A-PA-O3A	2.95	115.26	107.27
11	F	401	ACP	C5-N7-C8	2.88	107.98	103.45
10	D	502	89U	C25-O24-C20	-2.83	113.36	117.51
5	C	501	GTP	C2-N1-C6	-2.79	120.05	125.11
10	D	502	89U	C08-C07-C04	2.77	120.00	114.81
5	A	501	GTP	C2-N1-C6	-2.77	120.09	125.11
10	B	504	89U	C08-C07-C04	2.75	119.97	114.81
5	D	501	GTP	C2-N1-C6	-2.69	120.23	125.11
5	D	501	GTP	N9-C8-N7	-2.67	108.44	113.40
5	C	501	GTP	N9-C8-N7	-2.63	108.52	113.40
11	F	401	ACP	O2G-PG-C3B	-2.62	100.05	106.40
5	A	501	GTP	N9-C8-N7	-2.61	108.56	113.40
11	F	401	ACP	O1G-PG-C3B	2.53	116.89	111.37
5	C	501	GTP	C8-N7-C5	2.51	108.74	104.26
5	D	501	GTP	C8-N7-C5	2.49	108.70	104.26
10	B	504	89U	C11-C08-C07	-2.49	117.76	122.68
11	F	401	ACP	C4-N9-C8	2.49	108.35	105.74
11	F	401	ACP	C6-C5-C4	2.48	120.57	117.18
10	D	502	89U	C11-C08-C07	-2.48	117.79	122.68
5	A	501	GTP	C8-N7-C5	2.45	108.63	104.26
8	B	501	GDP	C4-C5-N7	-2.44	106.80	110.67
10	B	504	89U	C03-C04-C07	-2.44	117.86	122.68
10	D	502	89U	C03-C04-C07	-2.43	117.87	122.68
5	D	501	GTP	C5-C6-N1	2.42	119.41	113.25
5	A	501	GTP	C5-C6-N1	2.40	119.36	113.25
5	C	501	GTP	C5-C6-N1	2.39	119.34	113.25
10	D	502	89U	O24-C20-C19	-2.34	120.36	124.30
5	A	501	GTP	O6-C6-C5	-2.33	120.37	126.53
9	B	505	MES	O2S-S-C8	2.33	110.25	106.73
11	F	401	ACP	O3G-PG-O2G	-2.29	101.43	107.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	O6-C6-C5	-2.29	120.50	126.53
5	C	501	GTP	O6-C6-C5	-2.26	120.56	126.53
11	F	401	ACP	O2B-PB-O1B	2.19	117.09	109.95
11	F	401	ACP	N3-C4-N9	2.15	130.83	127.17
9	B	503	MES	O2S-S-C8	2.13	109.95	106.73
10	B	504	89U	O24-C20-C19	-2.10	120.77	124.30
11	F	401	ACP	C4-C5-N7	-2.04	108.25	110.58
8	B	501	GDP	O2B-PB-O3A	2.02	111.42	104.64
9	B	503	MES	C7-N4-C3	2.01	116.59	111.24

There are no chirality outliers.

All (48) 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-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	505	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O3S
10	B	504	89U	C04-C07-C16-C17
10	B	504	89U	C08-C07-C16-C17
10	D	502	89U	C04-C07-C16-C17
10	D	502	89U	C08-C07-C16-C17
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	C4'-C5'-O5'-PA
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
9	B	505	MES	C8-C7-N4-C5
9	B	505	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3A-PA-O1A
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PG-C3B-PB-O3A
9	B	505	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3A-PA-O1A
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	O4'-C4'-C5'-O5'

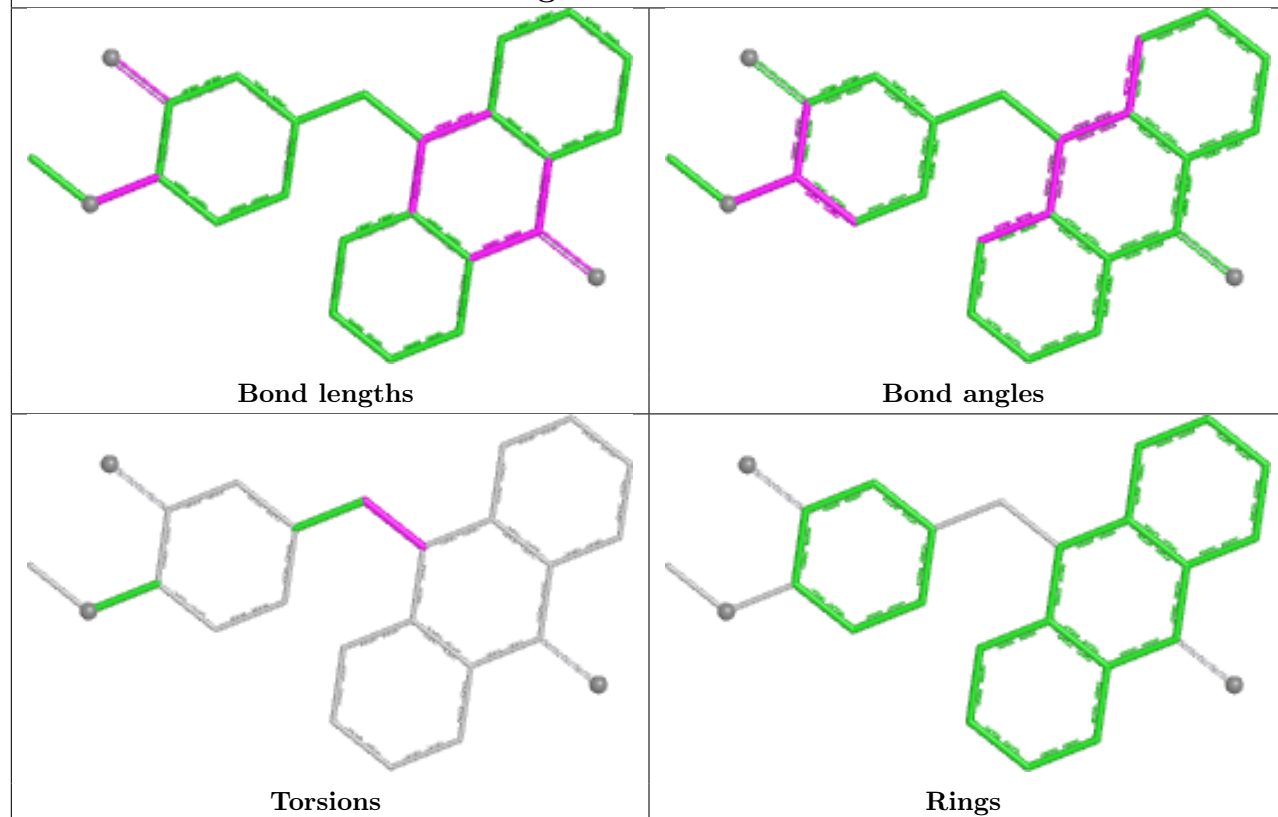
There are no ring outliers.

1 monomer is involved in 1 short contact:

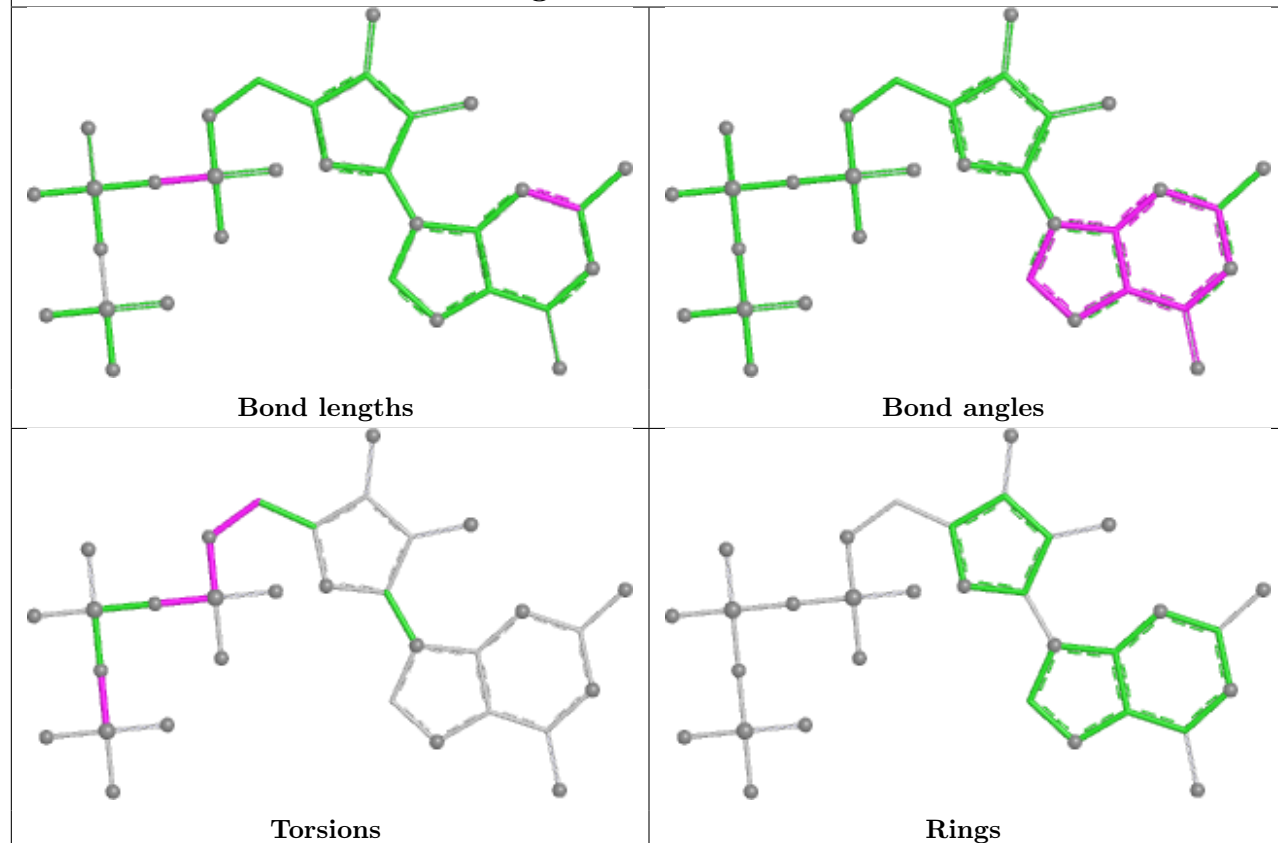
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	1	0

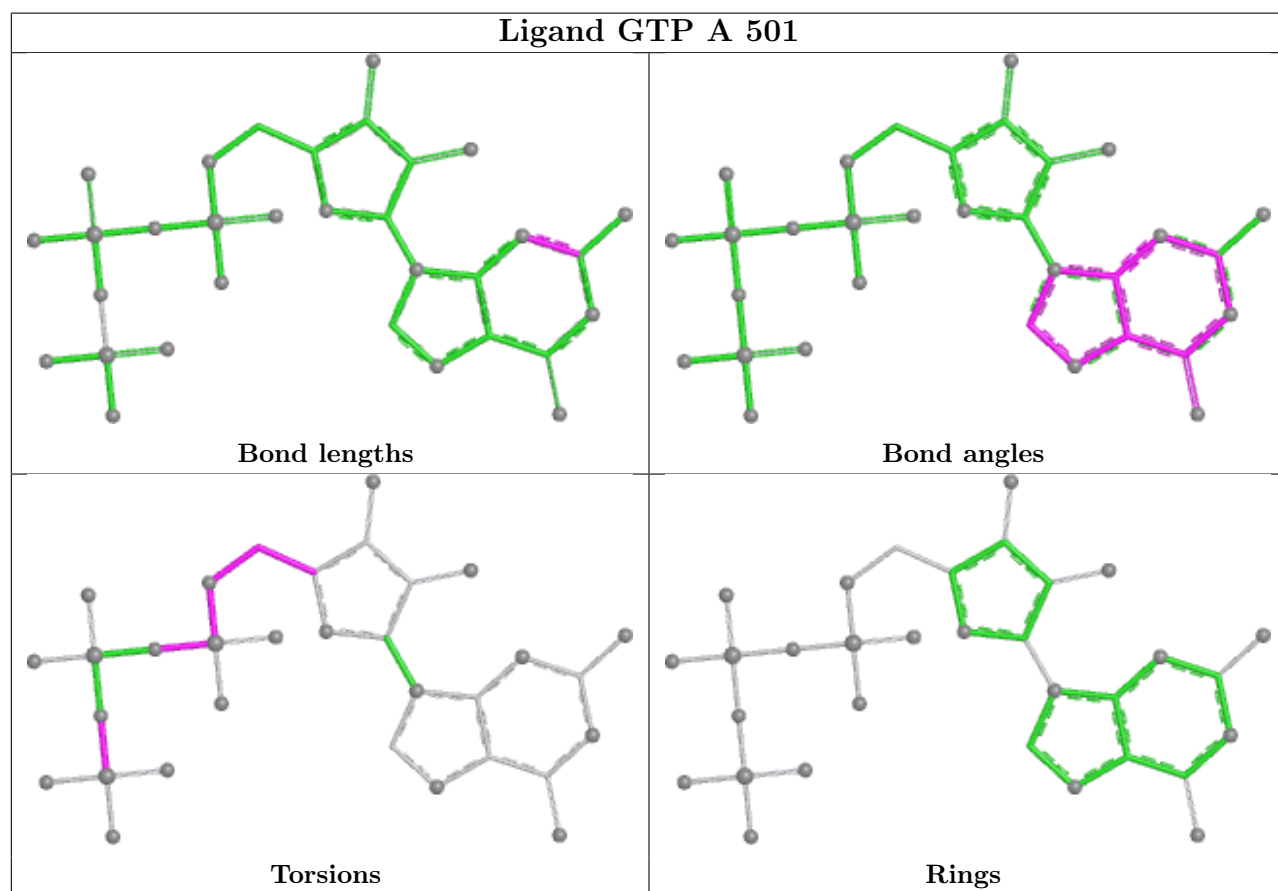
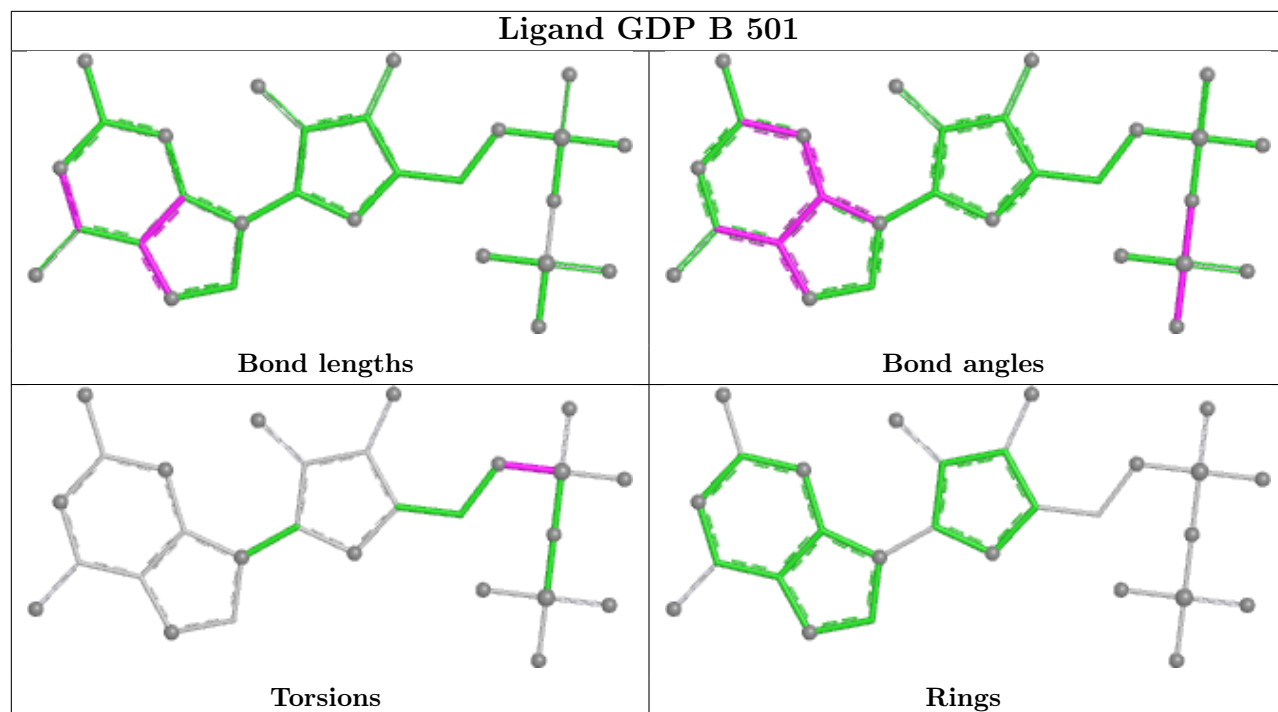
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 89U B 504

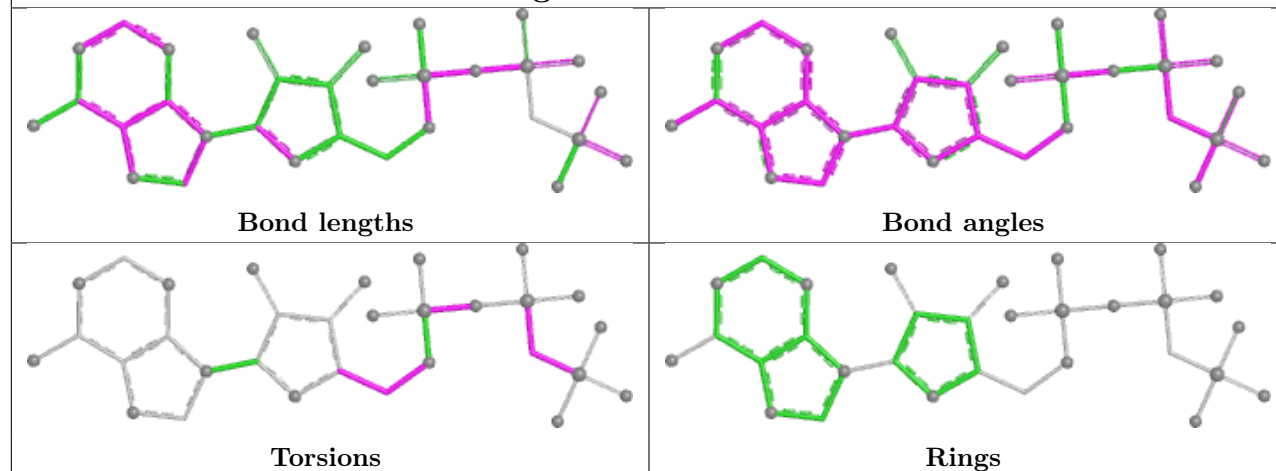


Ligand GTP C 501

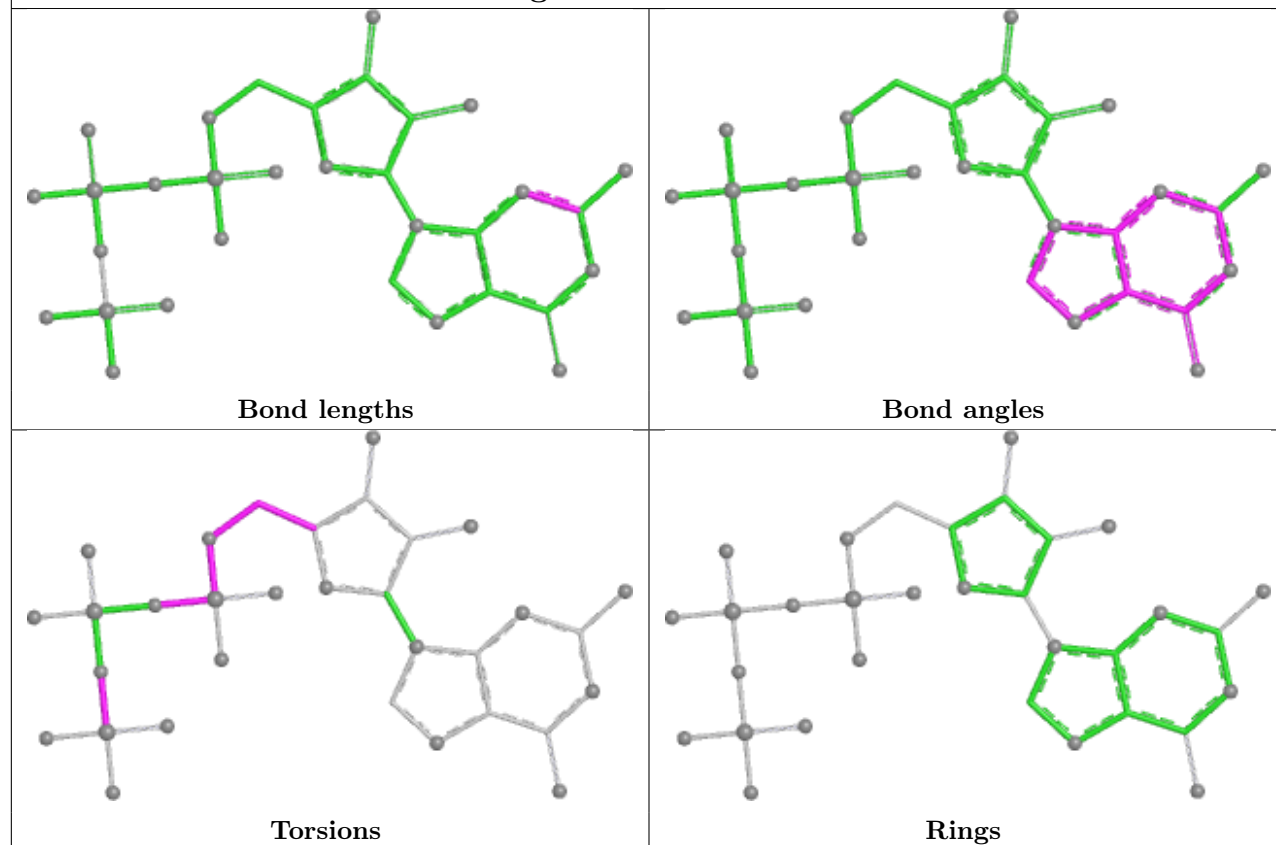


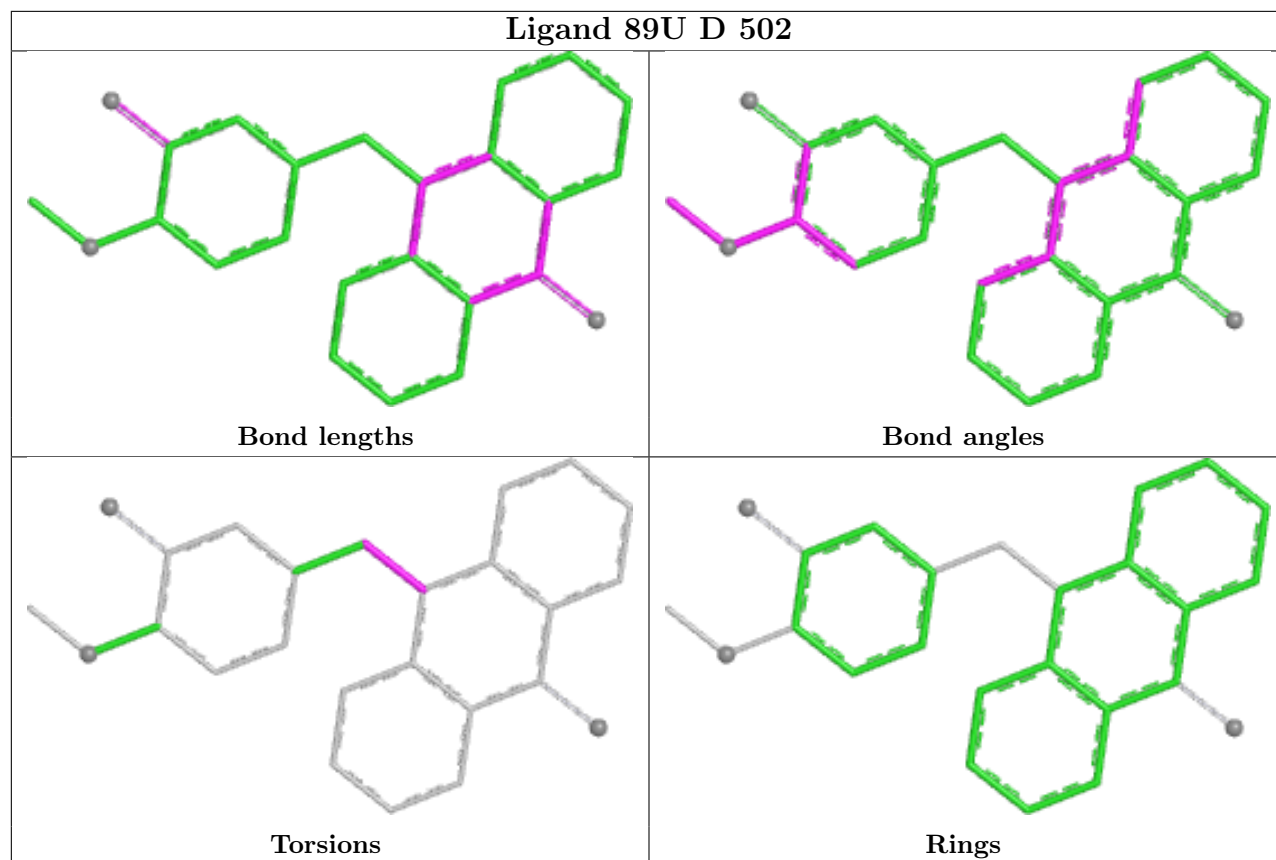


Ligand ACP F 401



Ligand GTP D 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	437/450 (97%)	0.68	28 (6%)	25 27	19, 41, 72, 100	4 (0%)
1	C	440/450 (97%)	0.08	11 (2%)	58 60	14, 28, 57, 79	3 (0%)
2	B	427/445 (95%)	0.69	52 (12%)	8 9	18, 39, 80, 141	2 (0%)
2	D	421/445 (94%)	1.54	128 (30%)	1 1	25, 55, 95, 129	1 (0%)
3	E	121/143 (84%)	1.37	30 (24%)	2 2	25, 54, 95, 110	1 (0%)
4	F	334/384 (86%)	2.00	152 (45%)	0 0	20, 69, 145, 159	1 (0%)
All	All	2180/2317 (94%)	0.97	401 (18%)	3 4	14, 45, 103, 159	12 (0%)

All (401) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	8.2
4	F	240	LEU	7.6
2	D	397	TRP	7.5
4	F	161	LEU	7.5
2	B	248	ALA	6.8
4	F	233	PHE	6.5
2	D	394	PHE	6.3
4	F	169	LEU	6.3
4	F	166	ALA	6.2
4	F	182	ILE	6.2
2	D	247	ASN	6.1
4	F	181	VAL	5.9
4	F	103	THR	5.9
4	F	231	ALA	5.6
4	F	245	ILE	5.5
2	D	217	LEU	5.4
4	F	239	HIS	5.4
2	D	1	MET	5.4
2	D	92	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	57	ASN	5.3
4	F	243	HIS	5.3
2	D	248	ALA	5.3
2	B	247	ASN	5.3
4	F	173	ILE	5.2
2	B	55	THR	5.1
4	F	162	ILE	5.1
1	C	440	VAL	5.0
4	F	186	LEU	5.0
2	D	81	PHE	4.9
4	F	241	THR	4.8
2	B	56	GLY	4.8
4	F	320	MET	4.8
2	D	219	THR	4.7
2	D	30	ILE	4.7
1	A	437	VAL	4.6
2	D	179	VAL	4.6
4	F	131	PHE	4.6
4	F	172	PHE	4.6
4	F	362	ALA	4.6
2	D	72	THR	4.5
2	B	279	GLN	4.5
4	F	180	HIS	4.5
4	F	228	TYR	4.5
4	F	237	THR	4.4
2	D	362	LYS	4.4
3	E	6	MET	4.4
2	D	393	ALA	4.3
4	F	191	LEU	4.3
2	D	360	GLY	4.3
2	D	284	LEU	4.3
2	B	54	ALA	4.3
4	F	100	ILE	4.3
2	D	390	ARG	4.2
2	B	428	ALA	4.2
2	D	246	LEU	4.2
2	D	69	GLU	4.2
4	F	244	CYS	4.2
4	F	230	SER	4.1
2	B	280	GLN	4.1
1	A	282	TYR	4.1
1	A	279[A]	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	98	TYR	4.1
2	D	245	GLN	4.1
1	C	340	SER	4.0
4	F	148	ILE	4.0
4	F	379	HIS	4.0
4	F	227	PRO	4.0
4	F	179	VAL	4.0
4	F	133	ALA	4.0
4	F	170	LEU	4.0
4	F	177	GLY	4.0
2	D	80	PRO	3.9
2	D	55	THR	3.9
4	F	99	VAL	3.9
4	F	130	VAL	3.9
2	B	245	GLN	3.9
4	F	147	TRP	3.9
2	D	42	LEU	3.9
4	F	238	CYS	3.9
2	B	48	ASN	3.9
4	F	194	PRO	3.9
2	D	388	MET	3.9
2	B	2	ARG	3.9
2	D	210	ILE	3.8
3	E	115[A]	HIS	3.8
1	C	357	TYR	3.8
2	D	37	HIS	3.8
2	D	180	VAL	3.8
4	F	101	TYR	3.7
2	D	176	SER	3.7
2	D	48	ASN	3.7
2	D	73	MET	3.7
4	F	330	ILE	3.7
3	E	139	LEU	3.7
4	F	144	GLY	3.7
4	F	192	LEU	3.7
3	E	141	GLU	3.7
4	F	195	GLY	3.6
4	F	372	THR	3.6
4	F	256	TYR	3.6
2	B	278	SER	3.6
2	D	95	SER	3.6
4	F	236	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	178	GLN	3.6
3	E	28	SER	3.6
4	F	252	ASN	3.6
1	C	337	THR	3.6
2	D	76	VAL	3.6
4	F	335	ALA	3.6
4	F	253	TYR	3.6
4	F	132	LEU	3.5
4	F	260	ASN	3.5
2	D	97	ALA	3.5
2	D	34	GLY	3.5
2	B	282	ARG	3.5
4	F	146	VAL	3.5
4	F	199	PHE	3.5
4	F	361	LEU	3.5
2	D	70	PRO	3.5
1	A	262	TYR	3.5
2	D	211	CYS	3.4
2	D	56	GLY	3.4
4	F	263	PHE	3.4
4	F	91	CYS	3.4
1	A	88	HIS	3.4
2	D	356	ILE	3.4
2	B	190	HIS	3.4
4	F	141	GLY	3.4
2	B	58	LYS	3.4
3	E	44	ASP	3.4
4	F	22	LEU	3.4
4	F	185	TYR	3.4
2	D	126	SER	3.4
4	F	225	SER	3.4
2	B	277	GLY	3.4
2	D	93	GLY	3.4
2	D	84	ILE	3.3
4	F	20	LEU	3.3
1	A	436	GLY	3.3
2	D	273	LEU	3.3
4	F	234	GLN	3.3
2	D	293	MET	3.3
4	F	247	LYS	3.3
4	F	17	VAL	3.3
4	F	232	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	102	PRO	3.3
2	B	336	LYS	3.3
4	F	167	SER	3.3
4	F	226	GLU	3.2
2	D	177	ASP	3.2
2	B	42	LEU	3.2
2	B	246	LEU	3.2
4	F	380	HIS	3.2
2	D	35	SER	3.2
2	B	283	ALA	3.2
2	D	82	GLY	3.2
2	D	215	LEU	3.2
4	F	336	PRO	3.2
2	B	323	MET	3.2
4	F	200	ASP	3.2
1	A	281	ALA	3.1
2	D	391	ARG	3.1
2	D	406	MET	3.1
4	F	138	ARG	3.1
4	F	24	THR	3.1
4	F	145	ASN	3.1
2	D	85	PHE	3.1
2	D	431	ASP	3.1
3	E	25	LYS	3.1
4	F	257	GLU	3.1
1	A	283	HIS	3.1
4	F	25	GLY	3.1
4	F	142	ARG	3.1
2	D	286	VAL	3.0
2	D	214	THR	3.0
4	F	90	SER	3.0
4	F	196	HIS	3.0
4	F	223	THR	3.0
2	D	83	GLN	3.0
4	F	88	SER	3.0
2	D	57	ASN	3.0
4	F	254	GLY	3.0
2	B	333	VAL	3.0
2	B	427	ASP	3.0
2	D	71	GLY	3.0
1	C	1	MET	3.0
2	B	281	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	33	ASP	2.9
2	D	395	LEU	2.9
2	D	396	HIS	2.9
1	A	163	LYS	2.9
4	F	139	ARG	2.9
2	D	33	THR	2.9
4	F	163	SER	2.9
2	D	96	GLY	2.9
3	E	45	PRO	2.9
2	D	212	PHE	2.9
4	F	283	ILE	2.9
1	C	284	GLU	2.9
2	D	285	THR	2.9
1	A	176[A]	GLN	2.9
2	B	194[A]	GLU	2.9
2	D	244	GLY	2.8
4	F	224	SER	2.8
2	D	222	TYR	2.8
4	F	135	TYR	2.8
2	D	387	ALA	2.8
4	F	18	SER	2.8
3	E	59	GLU	2.8
4	F	92	THR	2.8
3	E	52	LYS	2.8
2	D	77	ARG	2.8
4	F	333	ASN	2.8
2	B	212	PHE	2.8
2	D	358	PRO	2.7
3	E	26	PRO	2.7
2	D	90	PHE	2.7
2	D	178	THR	2.7
4	F	259	GLY	2.7
3	E	46	SER	2.7
4	F	164	SER	2.7
3	E	27	PRO	2.7
1	C	346	TRP	2.7
2	D	68	LEU	2.7
2	D	361	LEU	2.7
4	F	136	ASN	2.7
2	D	32	PRO	2.7
4	F	198	LYS	2.7
2	D	170	MET	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	137	ARG	2.7
3	E	24	LEU	2.7
4	F	342	LEU	2.7
2	B	59	TYR	2.7
4	F	183	GLN	2.7
2	D	45	GLU	2.7
2	D	216	LYS	2.7
4	F	242	ASN	2.7
4	F	140	GLU	2.7
2	D	400	GLY	2.7
4	F	337	ALA	2.6
2	B	41	ASP	2.6
4	F	235	ASP	2.6
2	D	146	GLY	2.6
3	E	23	ILE	2.6
3	E	12	ASN	2.6
4	F	171	ASP	2.6
1	A	159	VAL	2.6
2	B	38	GLY	2.6
2	D	221	THR	2.6
3	E	22	VAL	2.6
2	D	220	PRO	2.6
2	D	54	ALA	2.6
4	F	27	TRP	2.6
2	B	33	THR	2.6
2	D	323	MET	2.6
3	E	133	VAL	2.6
2	D	108	GLU	2.6
4	F	129	GLU	2.6
2	D	41	ASP	2.6
2	D	128	ASP	2.6
2	B	219	THR	2.6
2	D	175	VAL	2.6
2	B	37	HIS	2.6
2	D	58	LYS	2.6
4	F	193	GLU	2.5
2	D	10	GLY	2.5
2	D	94	GLN	2.5
4	F	89	GLU	2.5
4	F	331	GLU	2.5
2	D	46	ARG	2.5
1	A	178	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	53	LYS	2.5
4	F	75	ALA	2.5
2	D	116	VAL	2.5
2	D	320	ARG	2.5
3	E	7	GLU	2.5
4	F	351	VAL	2.5
2	D	398	TYR	2.5
4	F	189	PRO	2.5
4	F	31	ARG	2.4
2	D	59	TYR	2.4
4	F	21	LEU	2.4
1	C	283	HIS	2.4
2	D	227	HIS	2.4
4	F	197	ARG	2.4
4	F	222	ARG	2.4
4	F	344	ALA	2.4
2	D	140	GLY	2.4
4	F	258	GLU	2.4
2	B	338	SER	2.4
4	F	12	SER	2.4
1	A	250	VAL	2.4
2	D	165	ASN	2.4
2	D	38	GLY	2.4
2	D	218	THR	2.4
2	B	275	SER	2.4
2	B	84	ILE	2.4
1	C	248	LEU	2.4
4	F	221	LEU	2.4
4	F	176	GLN	2.4
4	F	246	GLN	2.4
2	D	39	ASP	2.4
2	D	87	PRO	2.4
1	A	365	GLY	2.4
4	F	261	GLU	2.4
1	C	245	ASP	2.3
2	B	39	ASP	2.3
2	D	31	ASP	2.3
2	B	350	LYS	2.3
2	D	392	LYS	2.3
4	F	321	VAL	2.3
2	D	359	ARG	2.3
1	A	92	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	196	GLU	2.3
2	D	416	ASN	2.3
1	A	179	THR	2.3
2	B	214	THR	2.3
2	D	86	ARG	2.3
2	D	291	GLN	2.3
4	F	340	GLN	2.3
2	D	112	LEU	2.3
2	D	172	SER	2.3
3	E	122	ARG	2.3
4	F	168	GLU	2.3
3	E	50	ILE	2.3
2	D	228	LEU	2.3
4	F	28	LYS	2.3
4	F	229	ASN	2.3
2	D	385	PHE	2.2
4	F	13	VAL	2.3
4	F	126	ASP	2.2
2	B	80	PRO	2.2
1	A	350	GLY	2.2
2	B	276	ARG	2.2
4	F	1	MET	2.2
4	F	73	ARG	2.2
2	D	405	GLU	2.2
4	F	165	GLU	2.2
2	D	113	VAL	2.2
2	D	119	VAL	2.2
2	D	389	PHE	2.2
1	A	57	GLY	2.2
2	B	274	THR	2.2
4	F	174	ASP	2.2
1	A	134	GLY	2.2
3	E	103	GLN	2.2
4	F	306	HIS	2.2
2	D	399	THR	2.2
4	F	15	ALA	2.2
2	B	126	SER	2.2
2	B	36	TYR	2.2
3	E	9	ILE	2.2
2	B	165	ASN	2.2
2	B	327	ASP	2.2
3	E	127	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	175	GLU	2.2
4	F	134	ALA	2.2
4	F	14	TYR	2.1
1	A	86	LEU	2.1
1	A	346	TRP	2.1
2	B	363	MET	2.1
2	D	363	MET	2.1
2	D	169	VAL	2.1
4	F	10	ASN	2.1
1	A	124	LYS	2.1
1	A	372	GLN	2.1
2	D	402	GLY	2.1
4	F	23	ALA	2.1
2	D	2	ARG	2.1
2	D	208	TYR	2.1
2	D	44	LEU	2.1
3	E	62	LYS	2.1
3	E	140	LYS	2.1
4	F	376	ILE	2.1
1	A	90	GLU	2.1
1	A	232	SER	2.1
2	B	215	LEU	2.1
3	E	48	GLU	2.1
4	F	270	TYR	2.1
1	A	128	GLN	2.1
1	C	128	GLN	2.1
2	B	40	SER	2.1
2	D	40	SER	2.1
2	D	78	SER	2.1
2	D	145	SER	2.1
2	D	153	SER	2.1
4	F	143	GLU	2.1
2	B	30	ILE	2.1
2	B	337	ASN	2.1
4	F	316	GLY	2.1
4	F	255	ARG	2.1
1	A	82	THR	2.0
4	F	273	ASP	2.0
2	D	106	TYR	2.0
3	E	135	LYS	2.0
4	F	32	LYS	2.0
2	D	53	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	274	ALA	2.0
2	D	129	CYS	2.0
3	E	136	ASN	2.0
2	B	320	ARG	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

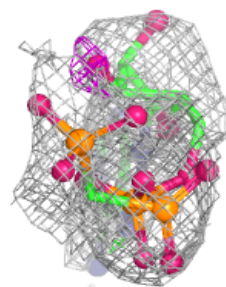
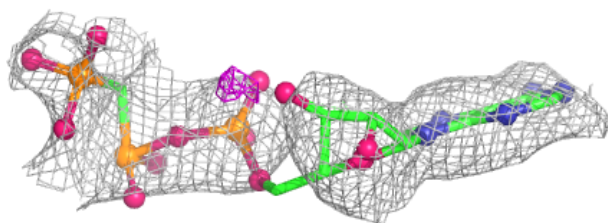
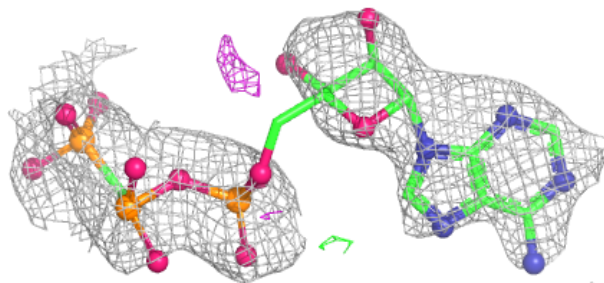
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	D	503	1/1	0.63	0.19	69,69,69,69	0
11	ACP	F	401	31/31	0.71	0.18	78,90,123,137	0
9	MES	B	505	12/12	0.79	0.17	60,82,95,119	0
10	89U	D	502	25/25	0.84	0.18	31,46,60,73	0
10	89U	B	504	25/25	0.86	0.18	30,43,52,53	0
5	GTP	D	501	32/32	0.88	0.16	45,56,78,138	0
9	MES	B	503	12/12	0.90	0.11	31,40,49,51	0
7	CA	A	503	1/1	0.91	0.08	62,62,62,62	0
8	GDP	B	501	28/28	0.95	0.09	13,24,31,34	0
5	GTP	A	501	32/32	0.96	0.08	14,24,33,35	0
5	GTP	C	501	32/32	0.97	0.07	9,18,24,27	0
6	MG	B	502	1/1	0.98	0.06	16,16,16,16	0
7	CA	C	503	1/1	0.98	0.03	40,40,40,40	0
6	MG	C	502	1/1	0.98	0.06	19,19,19,19	0
6	MG	A	502	1/1	0.98	0.04	24,24,24,24	0

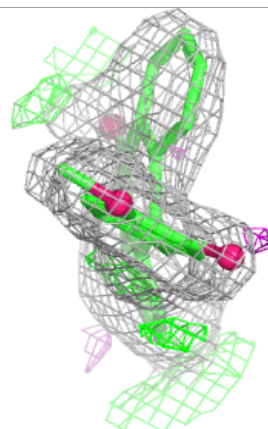
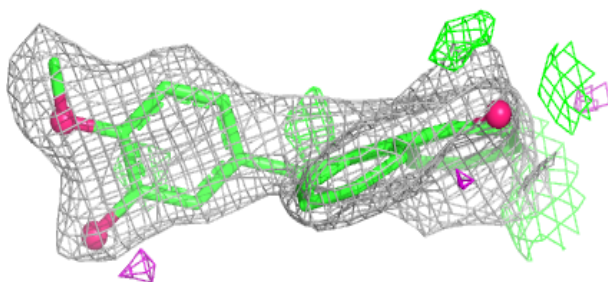
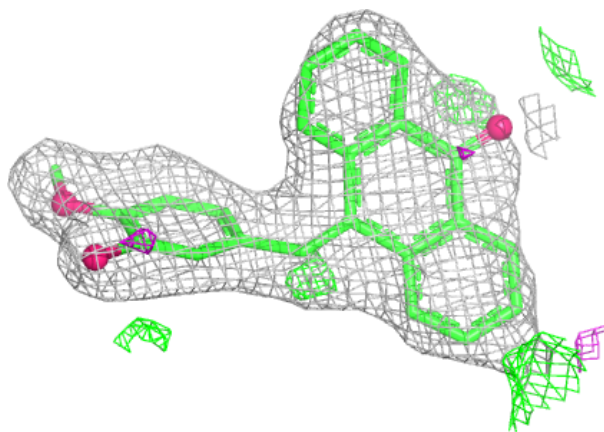
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

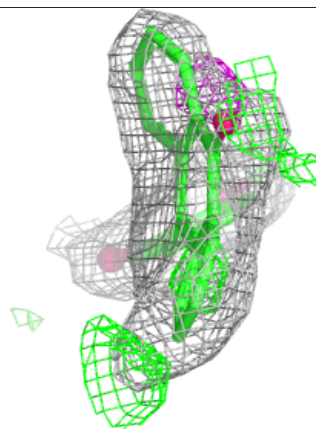
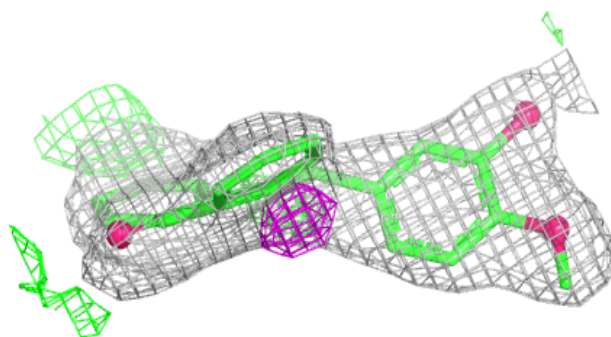
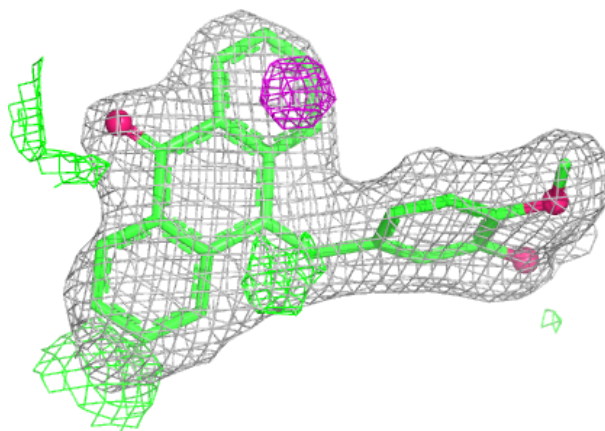
**Electron density around 89U D 502:**

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



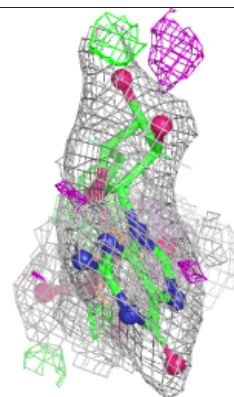
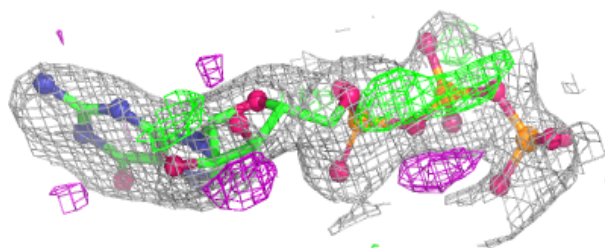
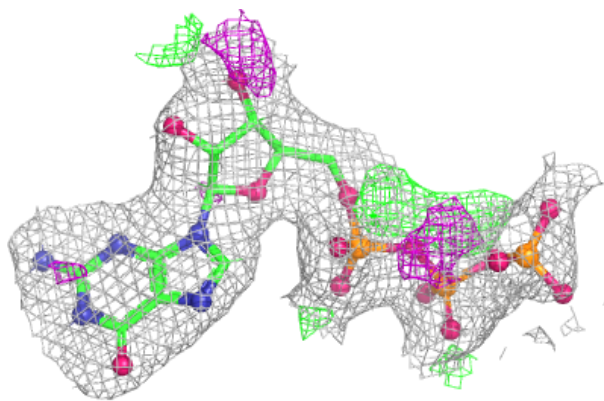
Electron density around 89U B 504:

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



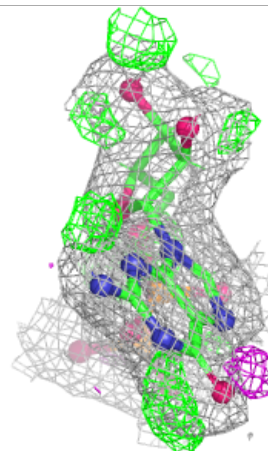
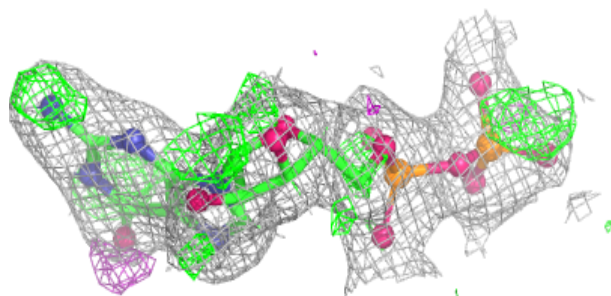
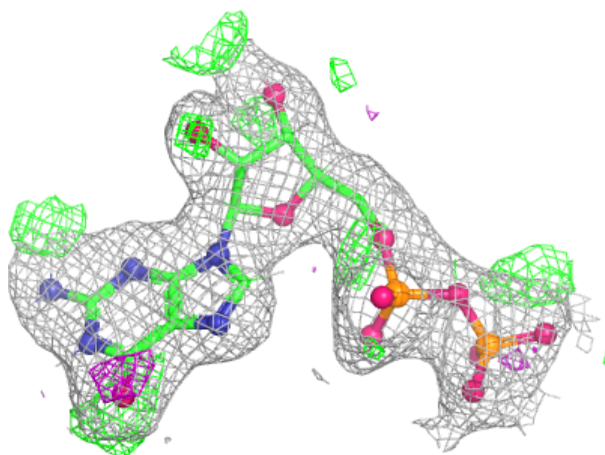
Electron density around GTP D 501:

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



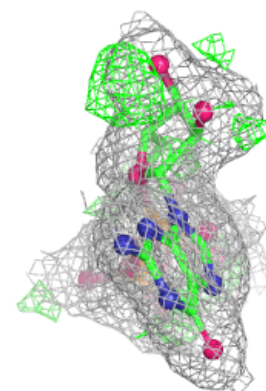
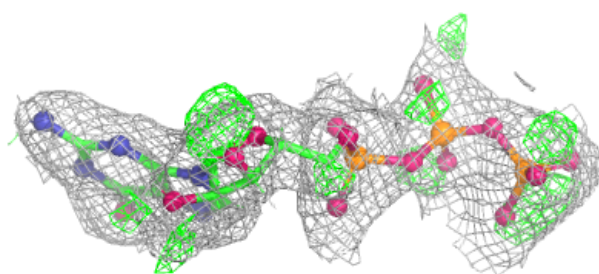
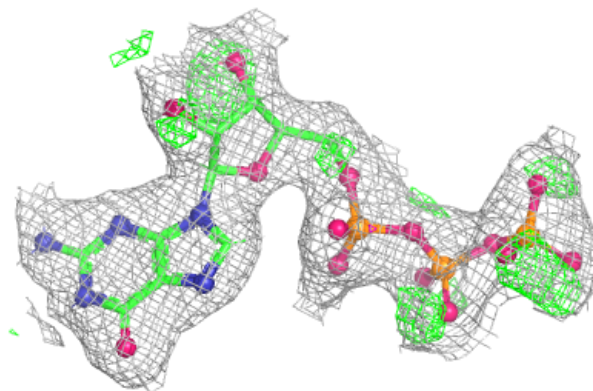
Electron density around GDP B 501:

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

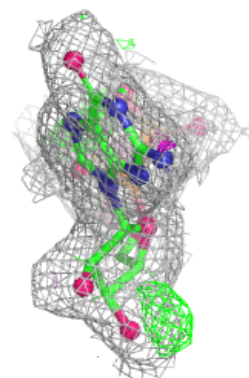
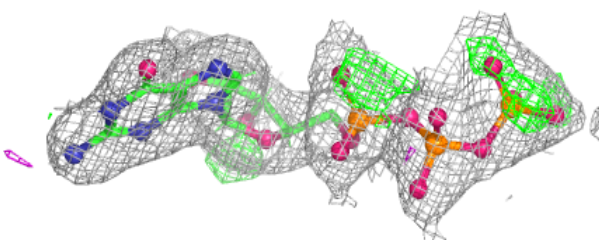
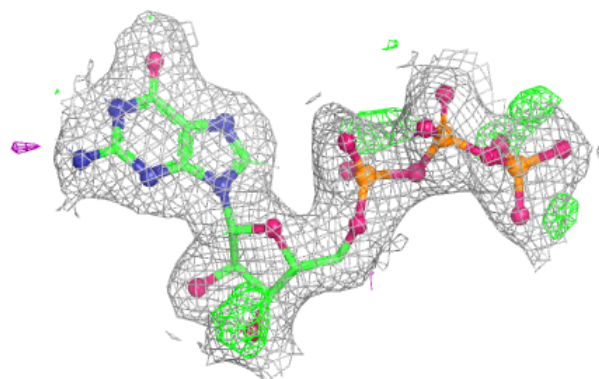


Electron density around GTP A 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.