Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 12:25 PM JST

PDB ID	:	5ZXH
Title	:	The structure of MT189-tubulin complex
Authors	:	Li, Z.P.; Wang, Y.X.; Meng, T.; Yang, J.L.; Chen, Q.
Deposited on	:	2018-05-21
Resolution	:	2.80 Å(reported)

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

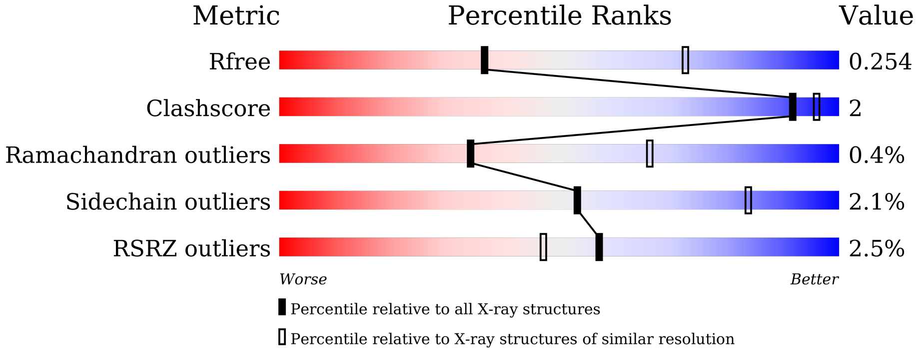
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

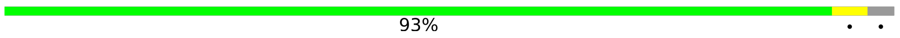
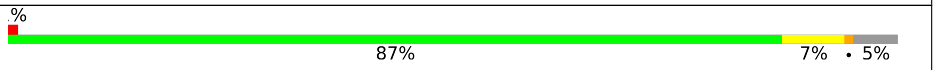
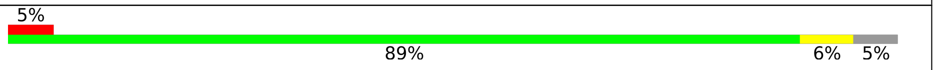
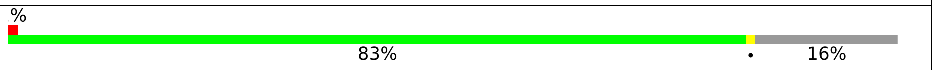
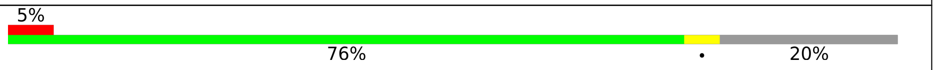
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	
1	C	450	
2	B	445	
2	D	445	
3	E	143	
4	F	384	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17367 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total 3441	C 2179	N 586	O 652	S 24	0	4	0
1	C	440	Total 3469	C 2193	N 588	O 663	S 25	0	7	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total 3351	C 2106	N 574	O 645	S 26	0	2	0
2	D	421	Total 3304	C 2078	N 562	O 638	S 26	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	170	VAL	MET	engineered mutation	UNP Q6B856
B	316	VAL	ILE	engineered mutation	UNP Q6B856
D	170	VAL	MET	engineered mutation	UNP Q6B856
D	316	VAL	ILE	engineered mutation	UNP Q6B856

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total 994	C 614	N 180	O 195	S 5	0	0	0

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

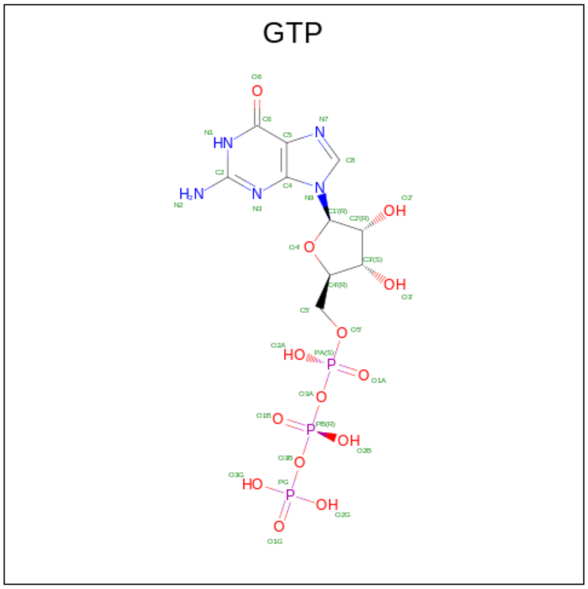
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	309	2553	1645	438	455	15	0	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
5	C	1	32	10	5	14	3	0	0
5	D	1	32	10	5	14	3	0	0

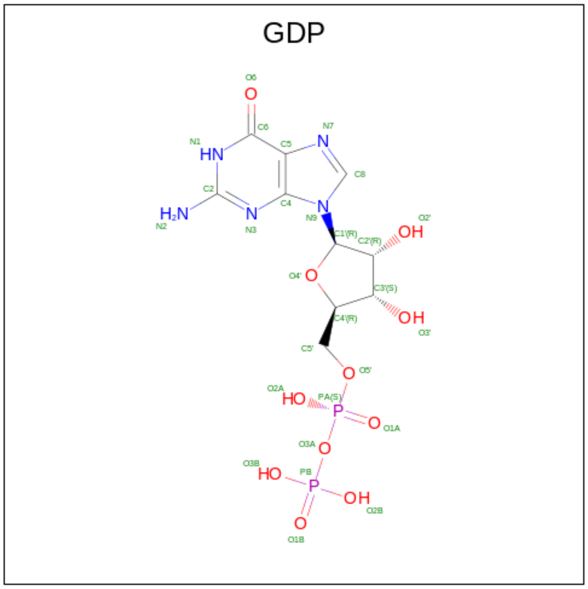
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

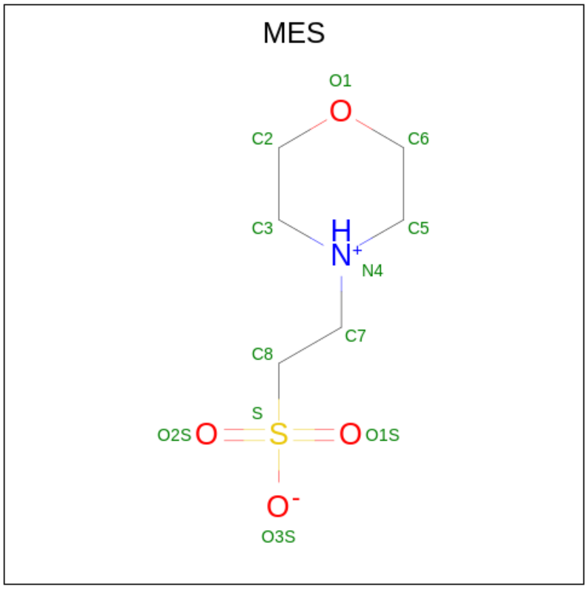
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



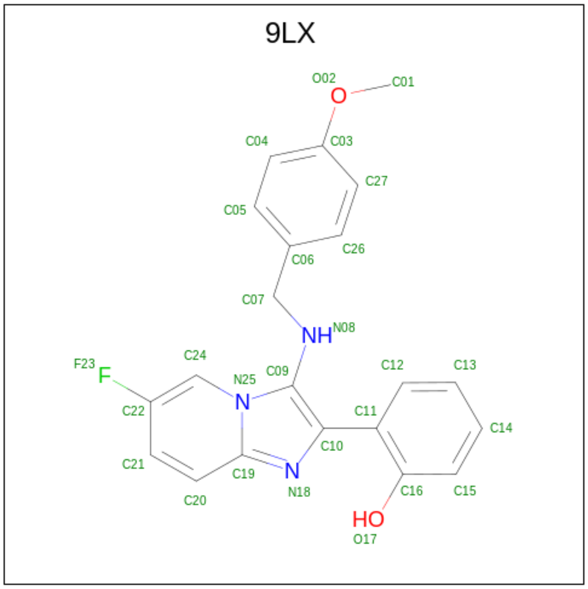
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



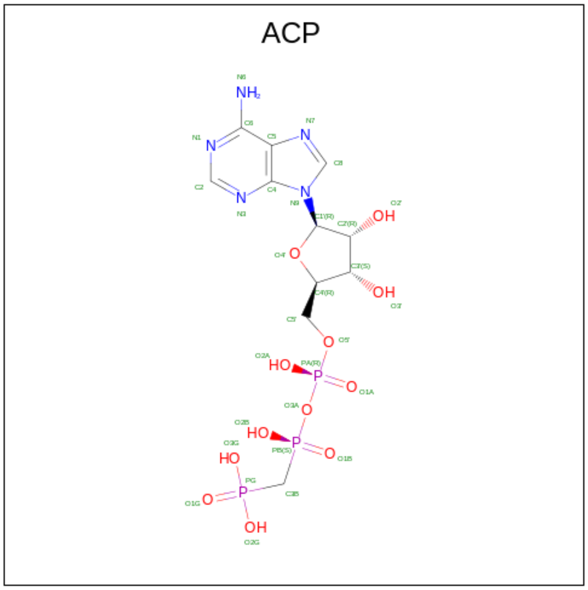
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is 2-(6-fluoro-3-{[(4-methoxyphenyl)methyl]amino}imidazo[1,2-a]pyridin-2-yl)phenol (three-letter code: 9LX) (formula: $C_{21}H_{18}FN_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
10	B	1	27	21	1	3	2	0	0
10	D	1	27	21	1	3	2	0	0

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



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

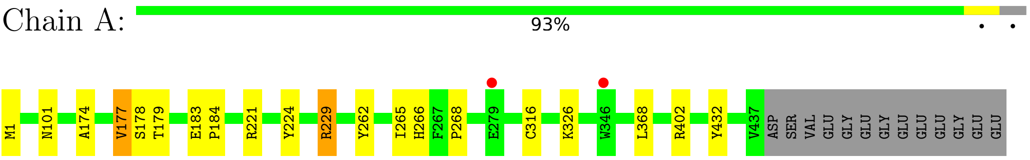
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	7	7	7	0	0
12	B	4	4	4	0	0
12	C	4	4	4	0	0

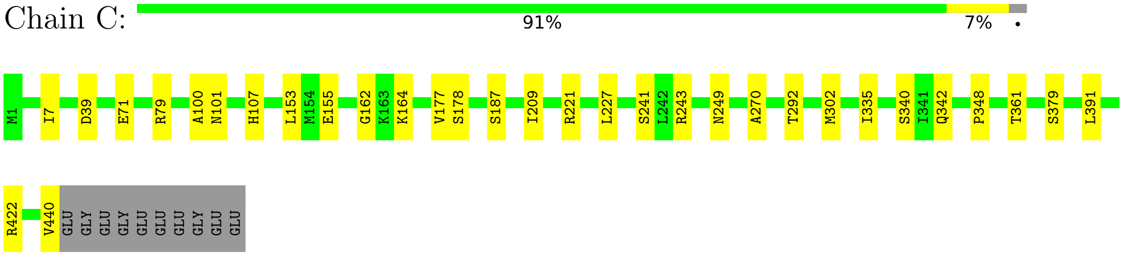
3 Residue-property plots

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.

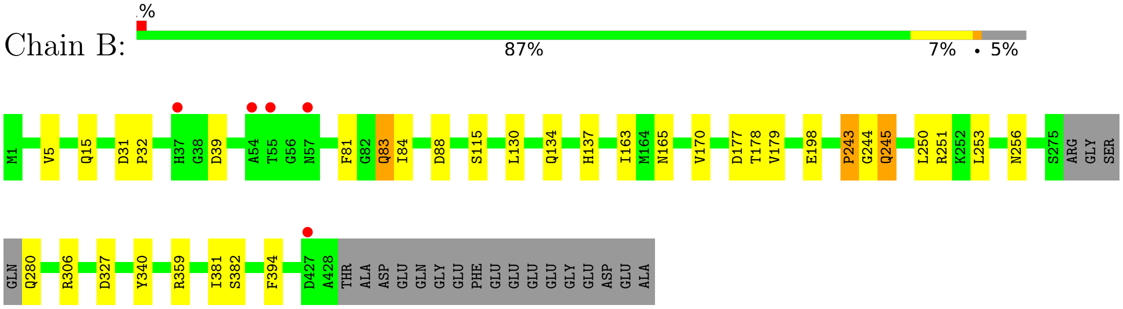
- Molecule 1: Tubulin alpha-1B chain



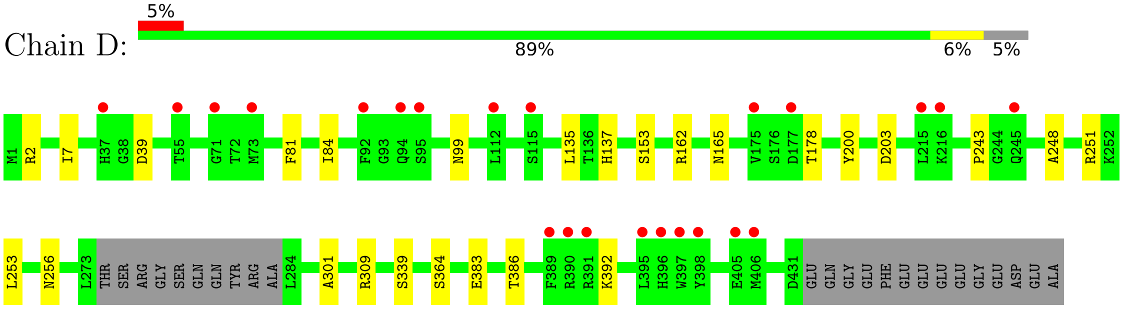
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain

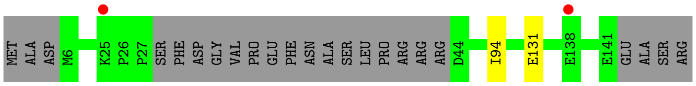


- Molecule 2: Tubulin beta-2B chain



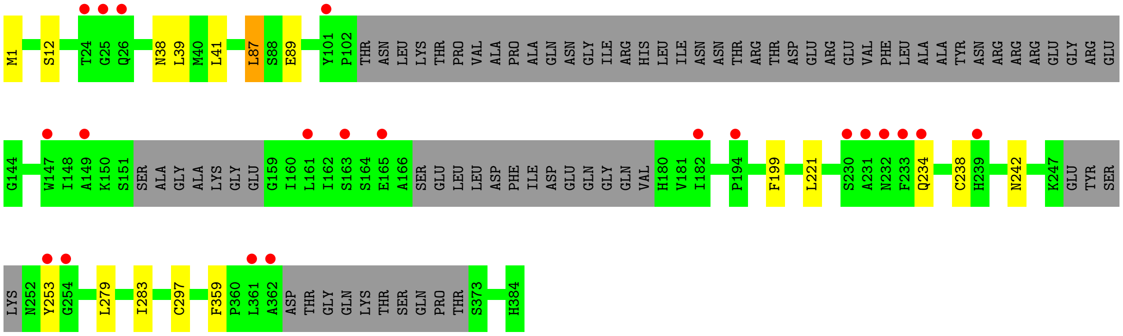
- Molecule 3: Stathmin-4

Chain E:



- Molecule 4: Tubulin tyrosine ligase

Chain F:



4 Data and refinement statistics

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.91Å 157.06Å 182.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 46.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.80) 99.5 (46.84-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.259 0.210 , 0.254	Depositor DCC
R_{free} test set	3753 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17367	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, MES, 9LX, CA, GDP, GTP, ACP

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	0.52	0/3525	0.73	0/4784
1	C	0.55	0/3556	0.74	4/4828 (0.1%)
2	B	0.53	0/3425	0.72	0/4639
2	D	0.49	0/3377	0.68	0/4576
3	E	0.52	0/1002	0.68	0/1329
4	F	0.49	0/2618	0.65	0/3537
All	All	0.52	0/17503	0.71	4/23693 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	243	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	79	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	422	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	3441	0	3362	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3469	0	3377	13	0
2	B	3351	0	3226	17	0
2	D	3304	0	3179	10	0
3	E	994	0	1013	1	0
4	F	2553	0	2519	6	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	1	0
10	B	27	0	0	0	0
10	D	27	0	0	0	0
11	F	31	0	14	1	0
12	A	7	0	0	0	0
12	B	4	0	0	0	0
12	C	4	0	0	0	0
All	All	17367	0	16764	56	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 2.

All (56) 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)
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:HH11	1.83	0.90
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:HG2	1.52	0.74
1:A:174:ALA:O	1:A:178:SER:HB2	1.96	0.66
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:HG3	1.60	0.66
2:B:251:ARG:NH1	9:B:503:MES:O2S	2.27	0.65
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	2.10	0.62
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:H	1.64	0.62
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.50	0.60
4:F:87:LEU:HD21	4:F:297:CYS:HB2	1.87	0.56
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:N	2.21	0.55
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.90	0.53
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.90	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.45	0.52
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.73	0.52
1:A:177:VAL:HG22	1:A:177:VAL:O	2.10	0.51
2:D:7:ILE:O	2:D:135:LEU:HD12	2.10	0.51
1:C:101:ASN:HD22	2:D:256:ASN:HD21	1.57	0.51
2:D:81:PHE:O	2:D:84:ILE:HG22	2.11	0.50
2:D:203:ASP:HB3	2:D:301:ALA:HA	1.93	0.50
2:B:306:ARG:NH1	2:B:340:TYR:OH	2.45	0.50
1:C:270:ALA:HB3	1:C:302:MET:CE	2.43	0.49
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.96	0.48
2:B:177:ASP:O	2:B:178:THR:HG23	2.13	0.48
2:B:198:GLU:OE2	2:B:253:LEU:HD23	2.14	0.47
1:A:177:VAL:HG21	1:A:224:TYR:CE1	2.50	0.47
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.97	0.47
1:C:100:ALA:CB	2:D:251:ARG:HG2	2.45	0.46
1:A:221:ARG:NE	2:B:327:ASP:OD2	2.49	0.46
2:B:170:VAL:HG13	2:B:381:ILE:HD11	1.97	0.46
2:B:83:GLN:HE21	2:B:83:GLN:HA	1.80	0.46
2:B:5:VAL:HG23	2:B:130:LEU:CD1	2.45	0.46
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.97	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.45
2:B:243:PRO:CB	2:B:244:GLY:CA	2.94	0.45
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.47	0.45
2:B:5:VAL:HG23	2:B:130:LEU:HD11	1.99	0.45
2:D:309:ARG:NH1	2:D:339:SER:O	2.46	0.45
2:D:165:ASN:HD21	2:D:200:TYR:HE2	1.63	0.45
2:B:81:PHE:O	2:B:84:ILE:HG22	2.17	0.44
2:D:383:GLU:HA	2:D:386:THR:HG22	1.99	0.44
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.99	0.44
1:C:107:HIS:HE1	1:C:155:GLU:OE1	2.01	0.44
1:A:266:HIS:O	1:A:268:PRO:HD3	2.17	0.43
4:F:242:ASN:HD21	11:F:401:ACP:H5'2	1.83	0.43
2:B:179:VAL:HG21	2:B:394:PHE:CZ	2.54	0.43
1:C:270:ALA:HB3	1:C:302:MET:HE3	2.01	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.42
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.01	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.50	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.55	0.41
1:C:241:SER:HA	1:C:249:ASN:HD21	1.85	0.41
2:D:203:ASP:OD1	2:D:203:ASP:C	2.58	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.22	0.40
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.56	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	439/450 (98%)	429 (98%)	10 (2%)	0	100	100
1	C	444/450 (99%)	434 (98%)	9 (2%)	1 (0%)	47	78
2	B	422/445 (95%)	404 (96%)	15 (4%)	3 (1%)	22	53
2	D	417/445 (94%)	393 (94%)	20 (5%)	4 (1%)	15	44
3	E	116/143 (81%)	109 (94%)	7 (6%)	0	100	100
4	F	300/384 (78%)	289 (96%)	10 (3%)	1 (0%)	41	72
All	All	2138/2317 (92%)	2058 (96%)	71 (3%)	9 (0%)	34	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	D	39	ASP
2	D	248	ALA
2	D	392	LYS
2	B	245	GLN
4	F	253	TYR
2	B	39	ASP

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Mol	Chain	Res	Type
1	C	164	LYS
2	D	243	PRO

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	372/378 (98%)	362 (97%)	10 (3%)	44	78
1	C	377/378 (100%)	368 (98%)	9 (2%)	49	81
2	B	367/383 (96%)	358 (98%)	9 (2%)	47	80
2	D	362/383 (94%)	356 (98%)	6 (2%)	60	87
3	E	108/127 (85%)	107 (99%)	1 (1%)	78	94
4	F	281/342 (82%)	275 (98%)	6 (2%)	53	84
All	All	1867/1991 (94%)	1826 (98%)	41 (2%)	53	83

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	177	VAL
1	A	179	THR
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	262	TYR
1	A	316[A]	CYS
1	A	316[B]	CYS
1	A	326	LYS
1	A	402	ARG
2	B	15	GLN
2	B	83	GLN
2	B	88	ASP
2	B	115	SER
2	B	137	HIS
2	B	245	GLN

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Mol	Chain	Res	Type
2	B	280	GLN
2	B	359	ARG
2	B	382	SER
1	C	71	GLU
1	C	177	VAL
1	C	178	SER
1	C	221	ARG
1	C	340	SER
1	C	342	GLN
1	C	361	THR
1	C	379	SER
1	C	440	VAL
2	D	2	ARG
2	D	137	HIS
2	D	153	SER
2	D	162	ARG
2	D	253	LEU
2	D	364	SER
3	E	131	GLU
4	F	1	MET
4	F	12	SER
4	F	87	LEU
4	F	89	GLU
4	F	234	GLN
4	F	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
2	B	11	GLN
2	B	52	ASN
2	B	83	GLN
2	B	190	HIS
1	C	101	ASN
1	C	128	GLN
1	C	133	GLN
1	C	249	ASN
1	C	372	GLN
2	D	99	ASN
4	F	252	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
9	MES	B	505	-	12,12,12	2.10	1 (8%)	14,16,16	6.37	9 (64%)
10	9LX	D	503	-	26,30,30	2.07	2 (7%)	27,42,42	1.26	1 (3%)
5	GTP	D	501	6	26,34,34	0.88	1 (3%)	32,54,54	1.47	9 (28%)
10	9LX	B	506	-	26,30,30	2.53	4 (15%)	27,42,42	1.15	2 (7%)
11	ACP	F	401	-	27,33,33	1.78	6 (22%)	32,52,52	1.34	3 (9%)
8	GDP	B	501	6	24,30,30	1.00	1 (4%)	30,47,47	1.04	3 (10%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	32,54,54	1.45	4 (12%)
9	MES	B	503	-	12,12,12	2.21	1 (8%)	14,16,16	6.68	9 (64%)
5	GTP	C	501	6	26,34,34	0.94	1 (3%)	32,54,54	1.26	2 (6%)

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
9	MES	B	505	-	-	2/6/14/14	0/1/1/1
10	9LX	D	503	-	-	4/8/11/11	0/4/4/4
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3
10	9LX	B	506	-	-	5/8/11/11	0/4/4/4
11	ACP	F	401	-	-	6/15/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	506	9LX	C11-C10	-11.01	1.38	1.49
10	D	503	9LX	C11-C10	-8.92	1.40	1.49
9	B	503	MES	C8-S	-7.07	1.67	1.77
9	B	505	MES	C8-S	-6.76	1.67	1.77
11	F	401	ACP	PG-O1G	5.53	1.61	1.50
10	B	506	9LX	C19-N18	4.27	1.37	1.33
11	F	401	ACP	PB-O3A	3.35	1.62	1.58
10	D	503	9LX	C19-N18	3.14	1.36	1.33
11	F	401	ACP	PG-O3G	3.03	1.61	1.54
10	B	506	9LX	C10-N18	-2.66	1.32	1.37
11	F	401	ACP	PG-O2G	-2.58	1.49	1.54
8	B	501	GDP	C2'-C1'	-2.50	1.50	1.53
11	F	401	ACP	C5-C4	2.48	1.47	1.40
5	A	501	GTP	C6-N1	-2.38	1.34	1.37
5	C	501	GTP	C6-N1	-2.34	1.34	1.37
11	F	401	ACP	PB-O2B	2.10	1.61	1.56
10	B	506	9LX	O17-C16	2.09	1.40	1.36
5	D	501	GTP	C6-N1	-2.04	1.34	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	505	MES	O3S-S-O1S	-12.92	79.72	111.27
9	B	503	MES	O3S-S-C8	-12.09	86.22	105.77
9	B	503	MES	O3S-S-O2S	-11.40	83.42	111.27
9	B	503	MES	O3S-S-O1S	-11.13	84.07	111.27
9	B	505	MES	O3S-S-O2S	-11.12	84.11	111.27
9	B	505	MES	O1S-S-C8	10.22	119.22	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O2S-S-C8	9.73	118.63	106.92
9	B	503	MES	O1S-S-C8	9.26	118.06	106.92
9	B	505	MES	O3S-S-C8	-8.70	91.70	105.77
9	B	505	MES	O2S-S-C8	8.17	116.75	106.92
9	B	503	MES	C2-C3-N4	4.34	116.69	110.10
11	F	401	ACP	N3-C2-N1	-3.70	122.89	128.68
10	D	503	9LX	C01-O02-C03	3.69	125.52	117.51
5	D	501	GTP	O3G-PG-O3B	-3.44	93.09	104.64
5	A	501	GTP	PA-O3A-PB	-3.27	121.60	132.83
5	A	501	GTP	O3G-PG-O2G	3.15	119.66	107.64
9	B	505	MES	C2-C3-N4	2.99	114.63	110.10
11	F	401	ACP	C4-C5-N7	-2.88	106.40	109.40
11	F	401	ACP	C3’-C2’-C1’	2.79	105.18	100.98
9	B	503	MES	C6-C5-N4	2.74	114.25	110.10
9	B	503	MES	C5-N4-C3	2.70	114.90	108.83
5	D	501	GTP	PA-O3A-PB	-2.57	124.02	132.83
5	A	501	GTP	C8-N7-C5	2.55	107.86	102.99
5	C	501	GTP	C8-N7-C5	2.49	107.74	102.99
5	D	501	GTP	O3G-PG-O1G	2.47	120.35	110.68
8	B	501	GDP	O3B-PB-O2B	2.47	117.06	107.64
9	B	505	MES	C7-N4-C5	-2.41	105.07	111.23
5	D	501	GTP	C8-N7-C5	2.39	107.55	102.99
5	D	501	GTP	O3G-PG-O2G	2.39	116.78	107.64
9	B	505	MES	C6-C5-N4	2.33	113.64	110.10
5	A	501	GTP	O6-C6-C5	-2.31	119.86	124.37
9	B	505	MES	O2S-S-O1S	2.27	121.82	113.95
5	C	501	GTP	PB-O3B-PG	-2.27	125.03	132.83
10	B	506	9LX	C24-C22-C21	-2.21	117.71	122.01
5	D	501	GTP	C5-C6-N1	2.18	117.81	113.95
8	B	501	GDP	O6-C6-C5	-2.17	120.13	124.37
10	B	506	9LX	F23-C22-C21	2.17	122.23	118.54
9	B	503	MES	O1-C6-C5	-2.15	107.06	111.80
5	D	501	GTP	PB-O3B-PG	-2.14	125.49	132.83
8	B	501	GDP	C8-N7-C5	2.11	107.02	102.99
5	D	501	GTP	O4’-C1’-C2’	-2.03	103.97	106.93
5	D	501	GTP	O6-C6-C5	-2.01	120.44	124.37

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
9	B	503	MES	N4-C7-C8-S
9	B	503	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O1S
10	B	506	9LX	C09-C10-C11-C12
10	B	506	9LX	C09-C10-C11-C16
10	B	506	9LX	C06-C07-N08-C09
10	D	503	9LX	C09-C10-C11-C12
10	D	503	9LX	C09-C10-C11-C16
10	D	503	9LX	C06-C07-N08-C09
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
5	D	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	O4'-C4'-C5'-O5'
5	D	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	505	MES	C7-C8-S-O2S
11	F	401	ACP	C3'-C4'-C5'-O5'
10	B	506	9LX	C27-C03-O02-C01
10	B	506	9LX	C04-C03-O02-C01
10	D	503	9LX	C27-C03-O02-C01
5	A	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	503	MES	C7-C8-S-O2S
5	C	501	GTP	C4'-C5'-O5'-PA

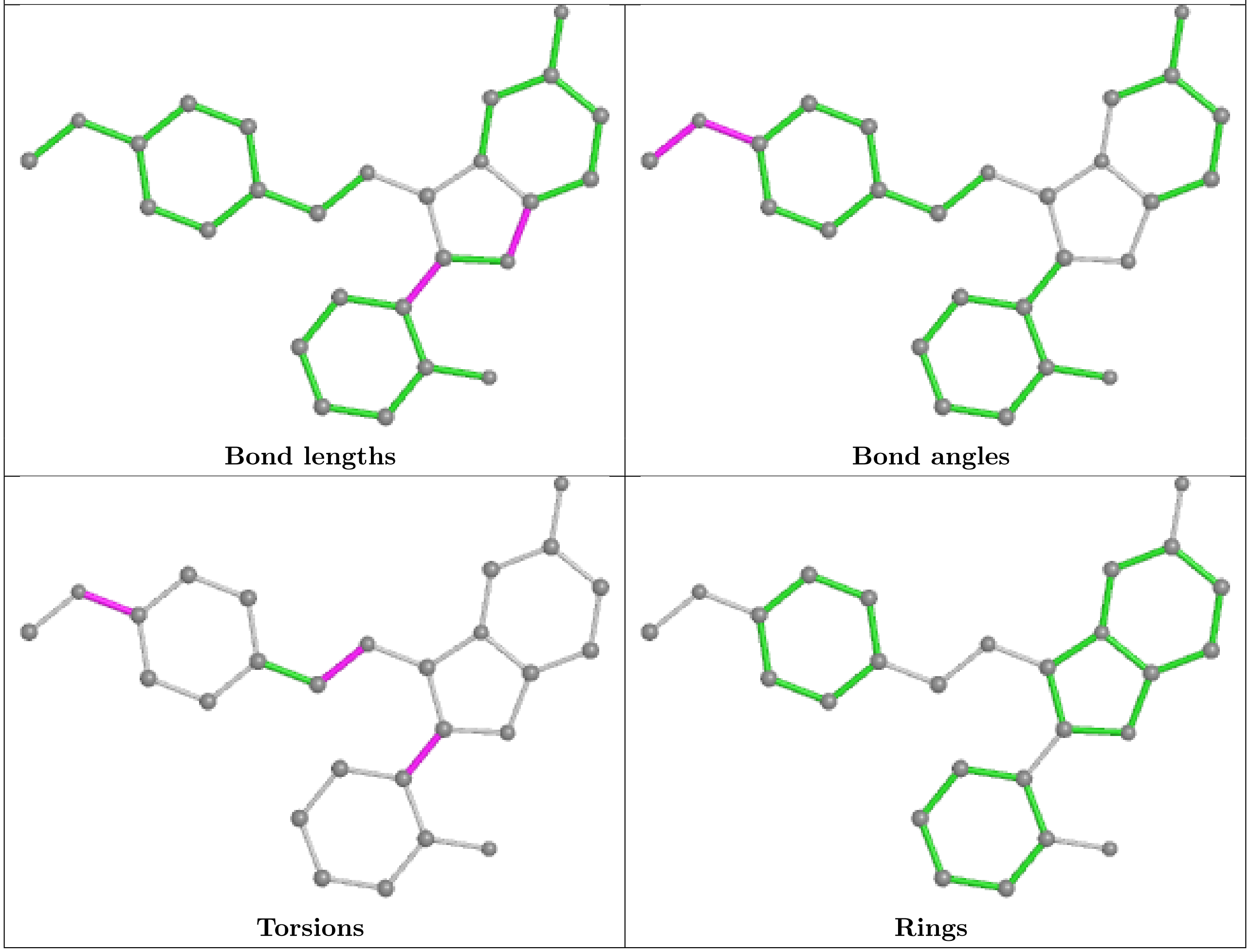
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	1	0
9	B	503	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 9LX D 503



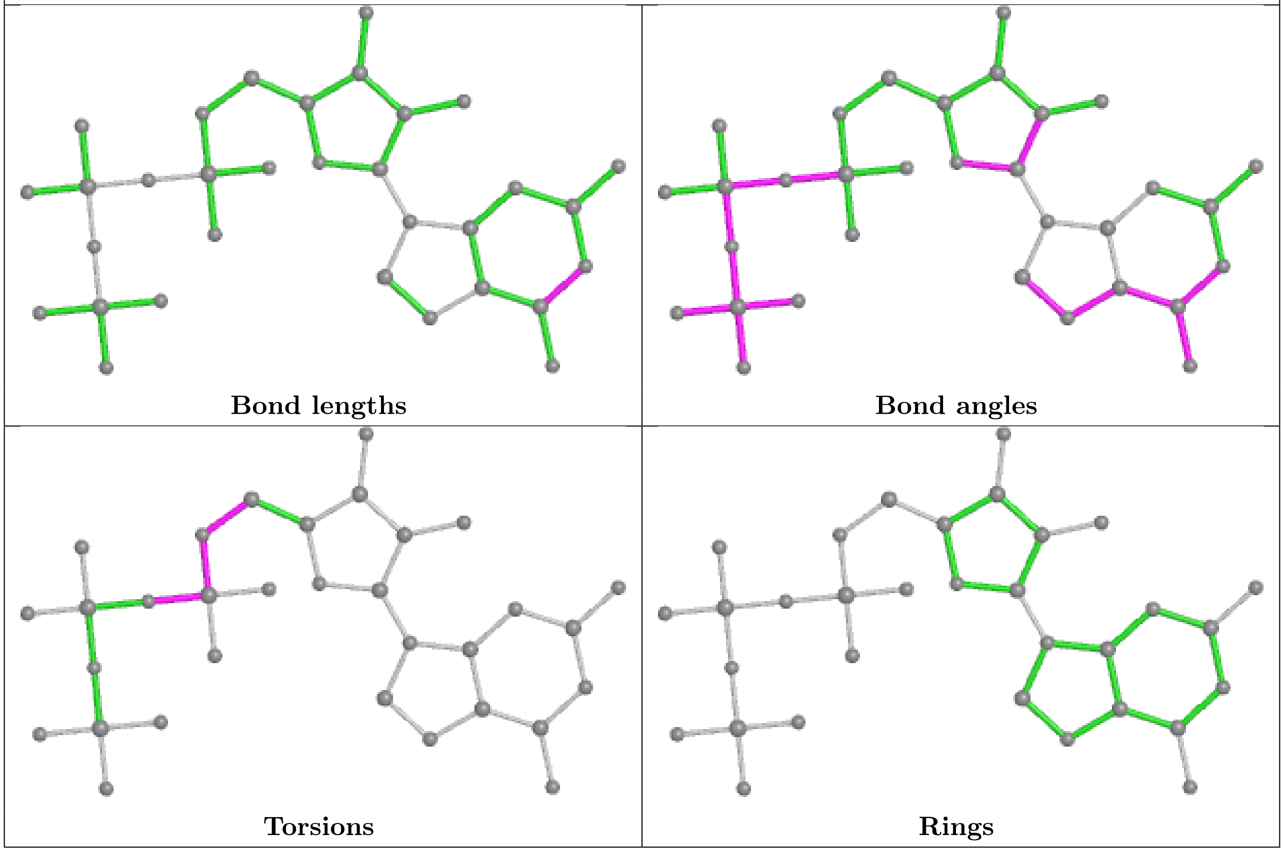
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP D 501



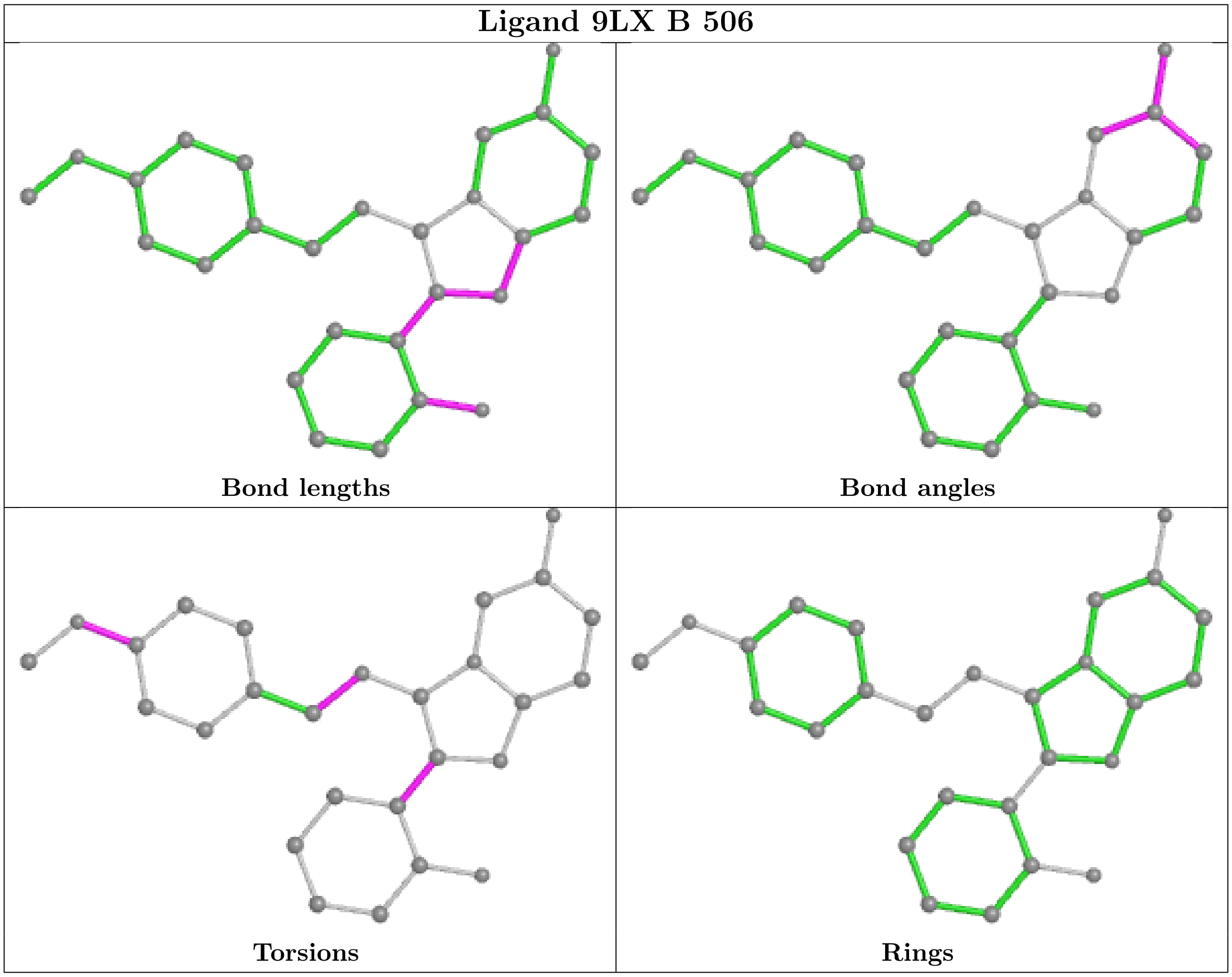
Bond lengths

Bond angles

Torsions

Rings

Ligand 9LX B 506



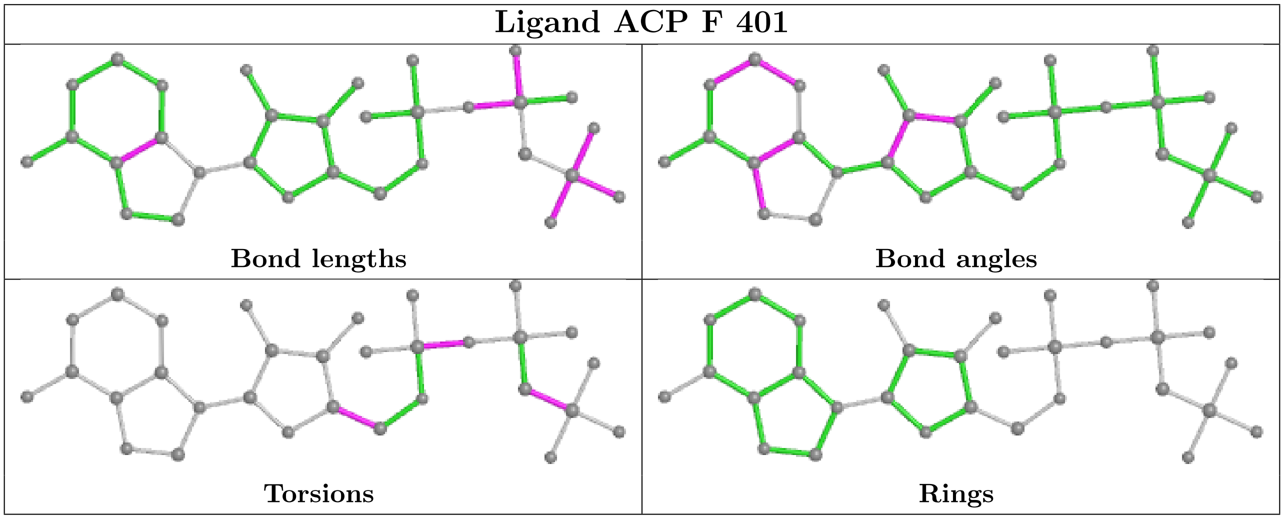
Bond lengths

Bond angles

Torsions

Rings

Ligand ACP F 401



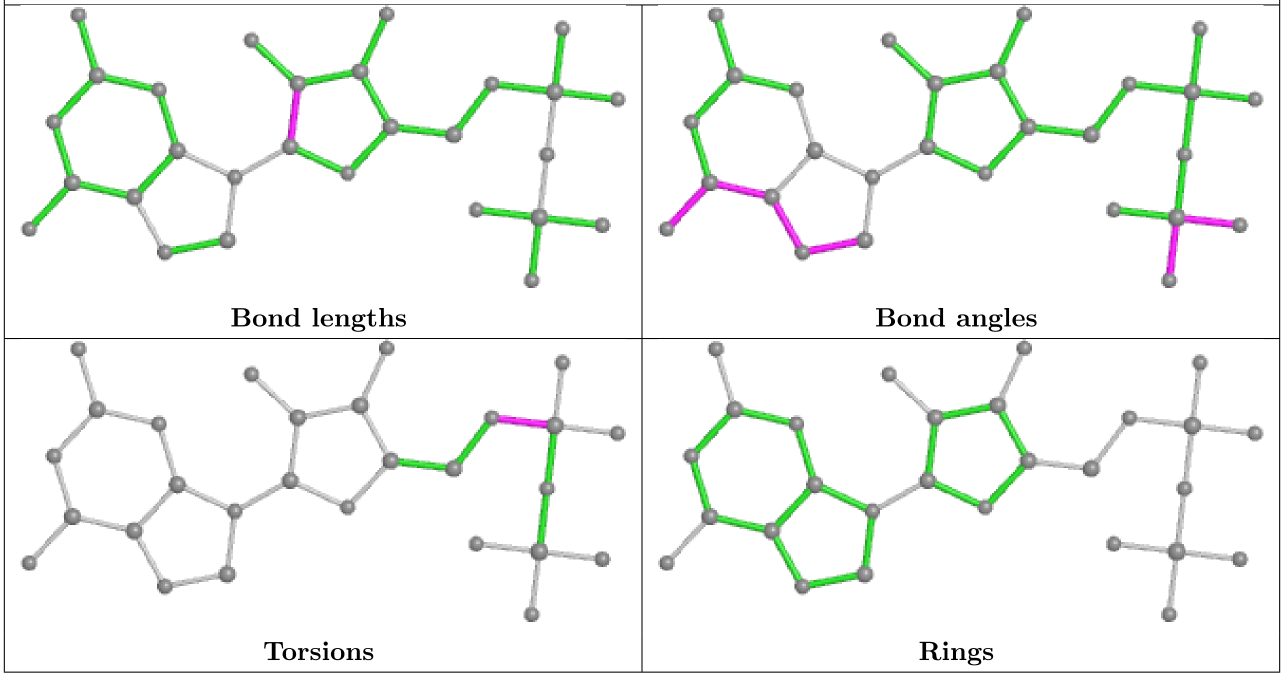
Bond lengths

Bond angles

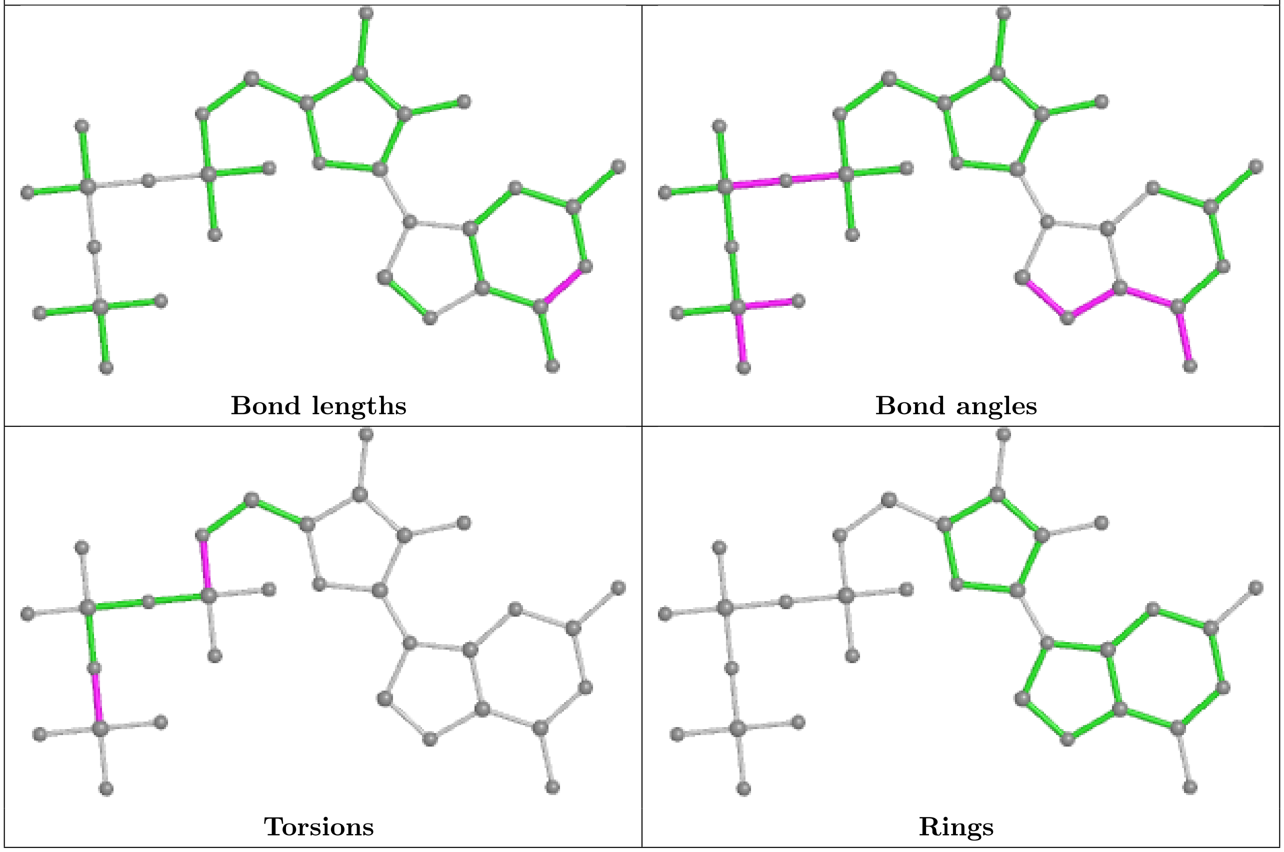
Torsions

Rings

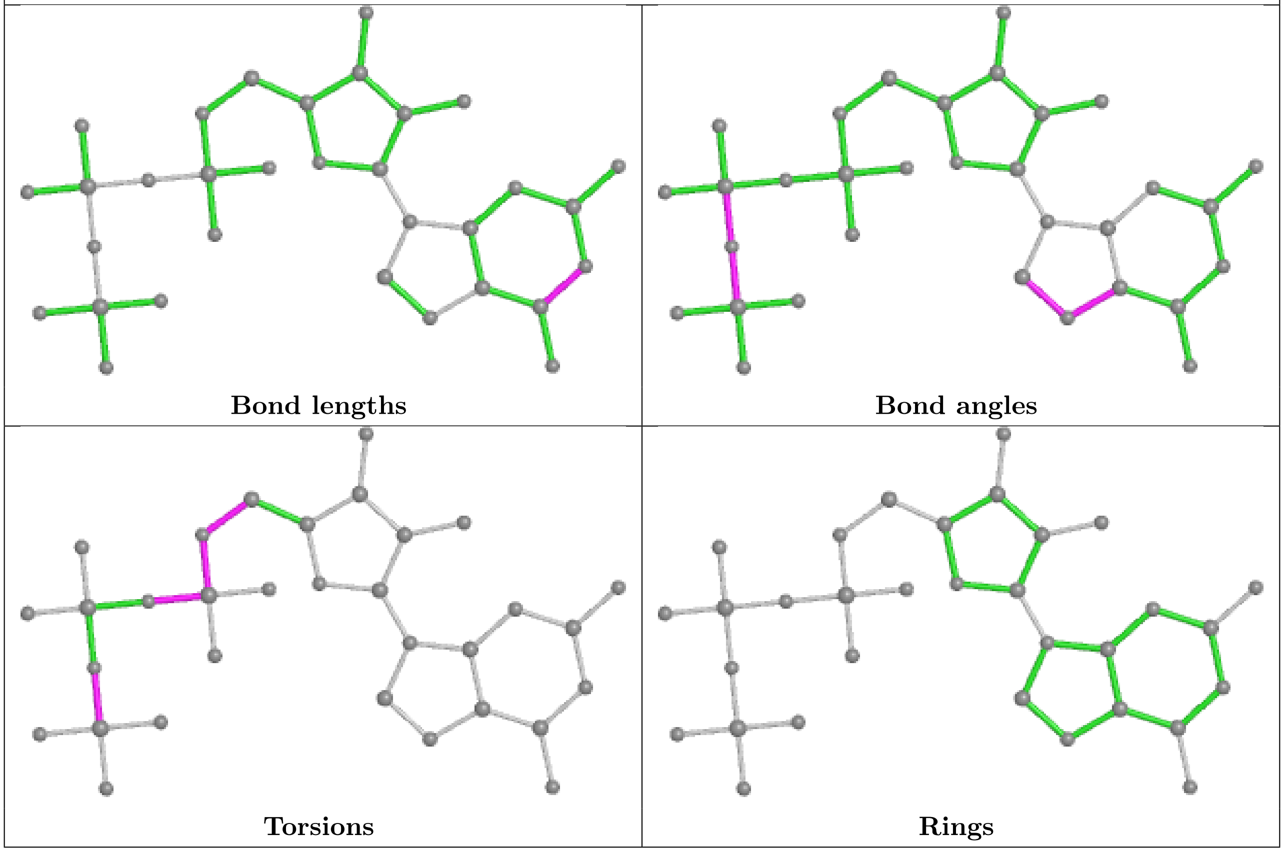
Ligand GDP B 501


Bond lengths
Bond angles
Torsions
Rings

Ligand GTP A 501


Bond lengths
Bond angles
Torsions
Rings

Ligand GTP C 501



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.21	2 (0%)	91	88	19, 39, 66, 81	0
1	C	440/450 (97%)	-0.35	0	100	100	13, 29, 55, 73	1 (0%)
2	B	424/445 (95%)	-0.24	5 (1%)	79	73	17, 36, 67, 89	1 (0%)
2	D	421/445 (94%)	0.24	23 (5%)	25	16	22, 55, 89, 113	4 (0%)
3	E	120/143 (83%)	0.26	2 (1%)	70	63	26, 54, 91, 120	0
4	F	309/384 (80%)	0.24	21 (6%)	17	10	27, 59, 100, 118	0
All	All	2151/2317 (92%)	-0.07	53 (2%)	57	47	13, 42, 81, 120	6 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	5.4
2	B	55	THR	4.0
4	F	161	LEU	3.9
4	F	182	ILE	3.9
4	F	232	ASN	3.7
2	D	389	PHE	3.4
4	F	362	ALA	3.3
2	D	390	ARG	3.3
4	F	25	GLY	3.1
2	D	37	HIS	3.0
4	F	165	GLU	3.0
2	D	73	MET	2.9
2	D	112	LEU	2.9
2	D	115	SER	2.8
4	F	234	GLN	2.8
2	D	406	MET	2.7
2	B	57	ASN	2.7
4	F	361	LEU	2.6
4	F	163	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	95	SER	2.5
2	D	71	GLY	2.5
2	D	395	LEU	2.5
4	F	253	TYR	2.5
2	D	397	TRP	2.5
2	B	37	HIS	2.5
4	F	194	PRO	2.4
2	B	54	ALA	2.3
2	D	94	GLN	2.3
2	D	245	GLN	2.3
2	D	215	LEU	2.3
2	D	398	TYR	2.3
2	D	405	GLU	2.3
4	F	230	SER	2.2
4	F	231	ALA	2.2
4	F	26	GLN	2.2
4	F	254	GLY	2.2
4	F	24	THR	2.2
2	D	396	HIS	2.2
2	D	175	VAL	2.2
2	D	92	PHE	2.2
2	D	177	ASP	2.1
2	D	55	THR	2.1
2	D	391	ARG	2.1
4	F	101	TYR	2.1
3	E	138	GLU	2.1
4	F	147	TRP	2.1
4	F	149	ALA	2.1
3	E	25	LYS	2.1
2	B	427	ASP	2.1
4	F	239	HIS	2.0
2	D	216	LYS	2.0
1	A	279	GLU	2.0
1	A	346	TRP	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

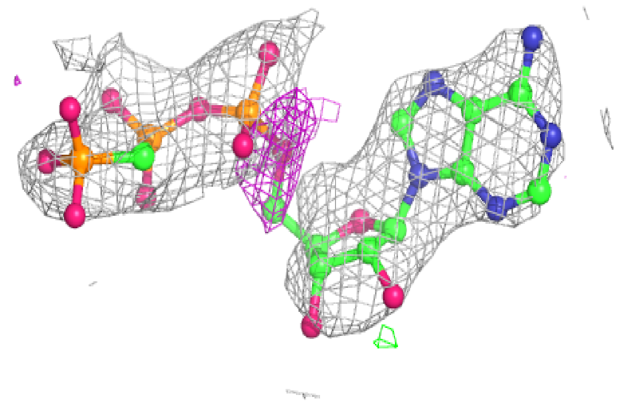
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

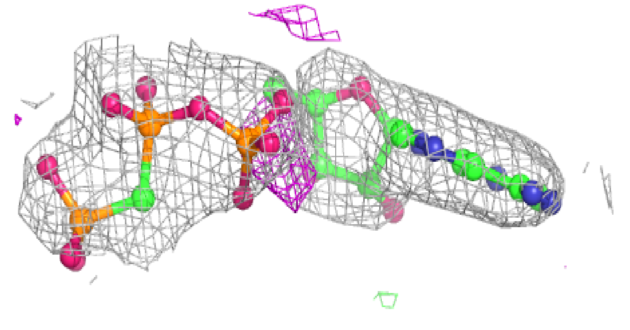
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
6	MG	B	502	1/1	0.82	0.35	37,37,37,37	0
11	ACP	F	401	31/31	0.84	0.29	76,86,136,142	0
7	CA	B	504	1/1	0.89	0.15	82,82,82,82	0
9	MES	B	505	12/12	0.92	0.25	66,72,81,81	0
9	MES	B	503	12/12	0.93	0.18	66,71,73,80	0
6	MG	D	502	1/1	0.93	0.11	42,42,42,42	0
7	CA	C	503	1/1	0.93	0.09	56,56,56,56	0
10	9LX	D	503	27/27	0.94	0.18	40,52,56,58	0
7	CA	A	503	1/1	0.94	0.05	62,62,62,62	0
5	GTP	D	501	32/32	0.95	0.13	39,45,50,58	0
10	9LX	B	506	27/27	0.96	0.17	28,29,33,34	0
8	GDP	B	501	28/28	0.97	0.15	17,22,25,28	0
6	MG	A	502	1/1	0.97	0.14	25,25,25,25	0
5	GTP	A	501	32/32	0.98	0.17	19,22,24,24	0
6	MG	C	502	1/1	0.98	0.12	17,17,17,17	0
5	GTP	C	501	32/32	0.98	0.14	18,20,23,24	0

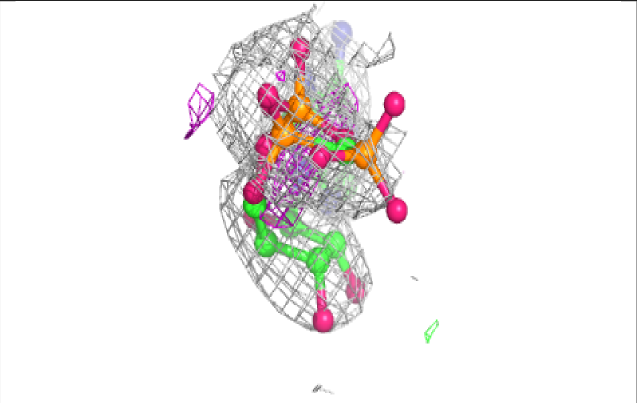
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

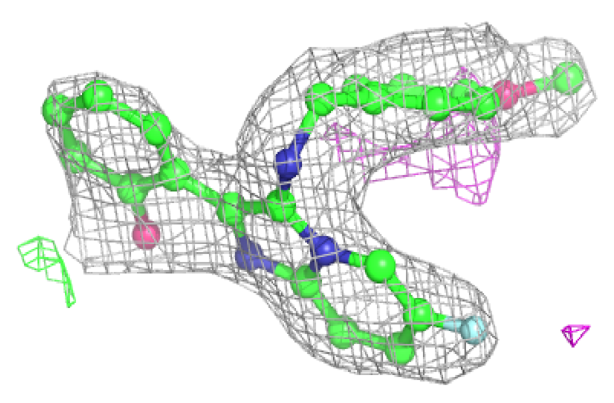


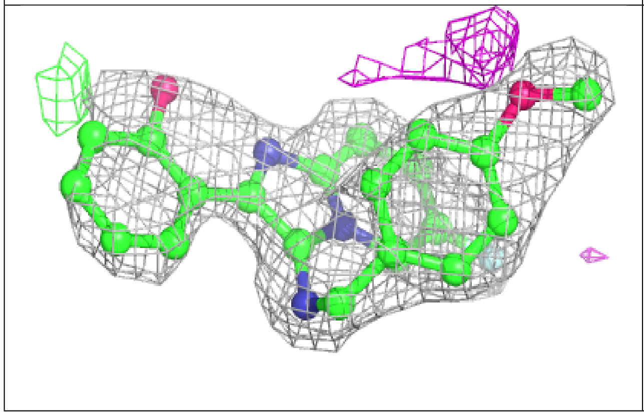


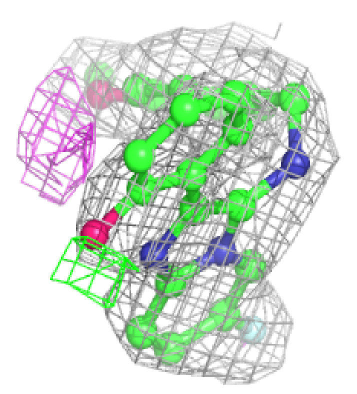


Electron density around 9LX D 503:

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

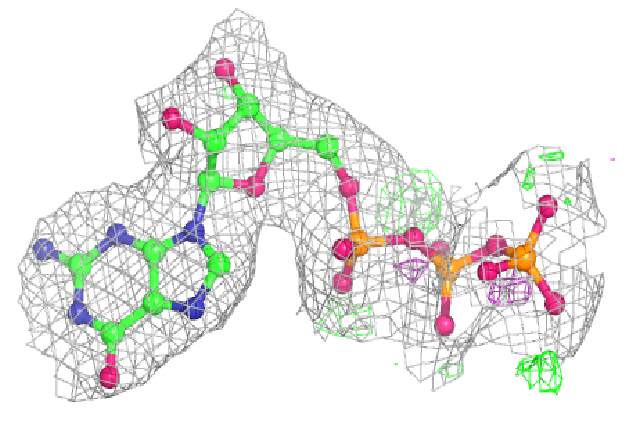


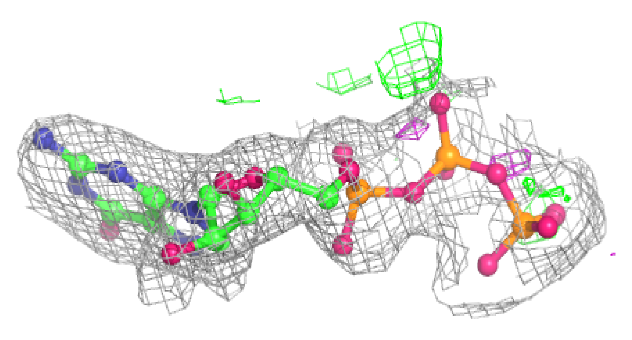


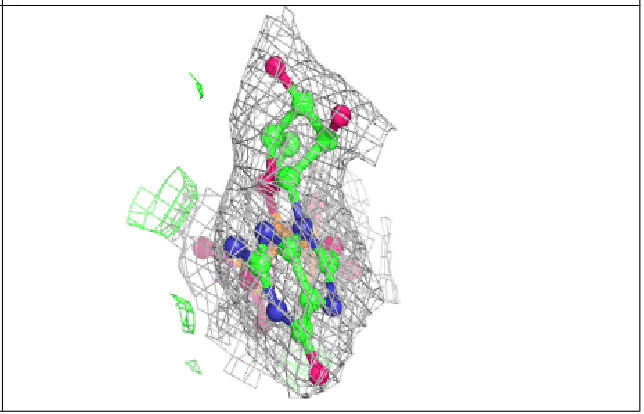


Electron density around GTP D 501:

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

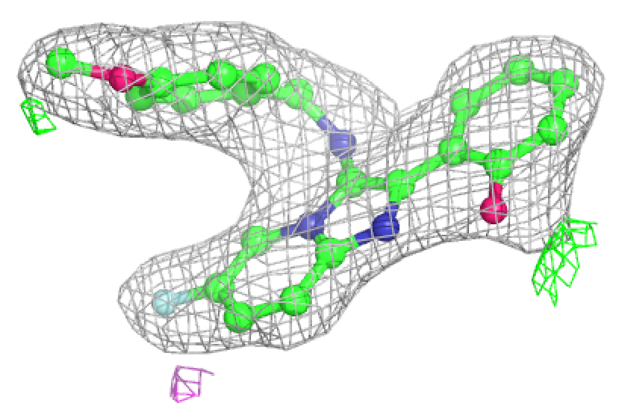


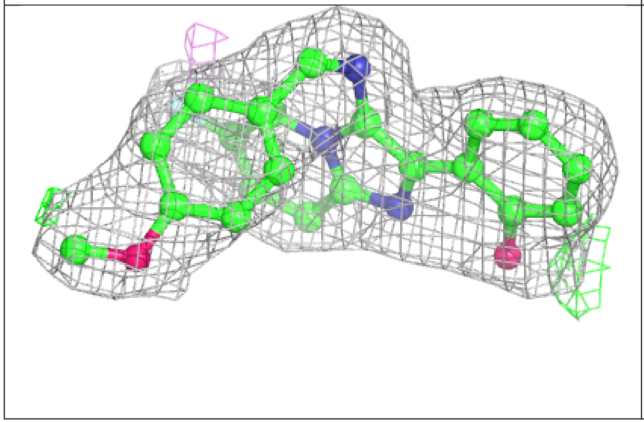


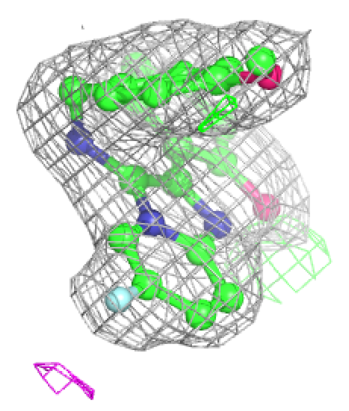


Electron density around 9LX B 506:

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

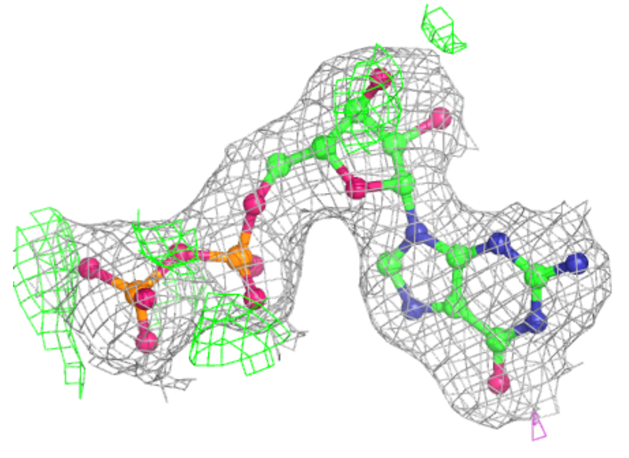


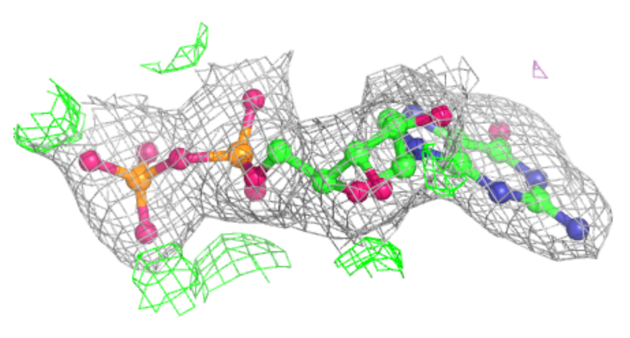


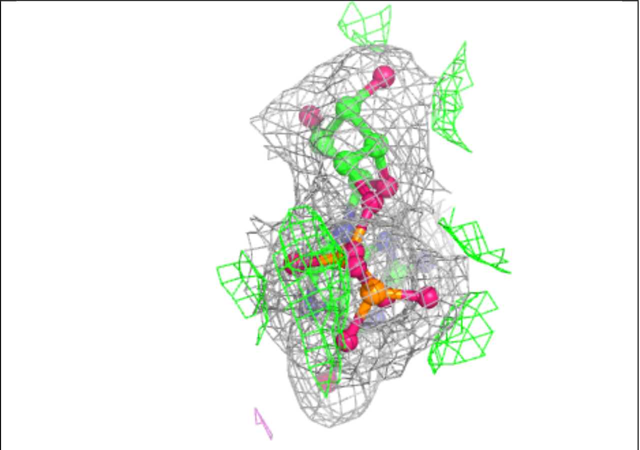


Electron density around GDP B 501:

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

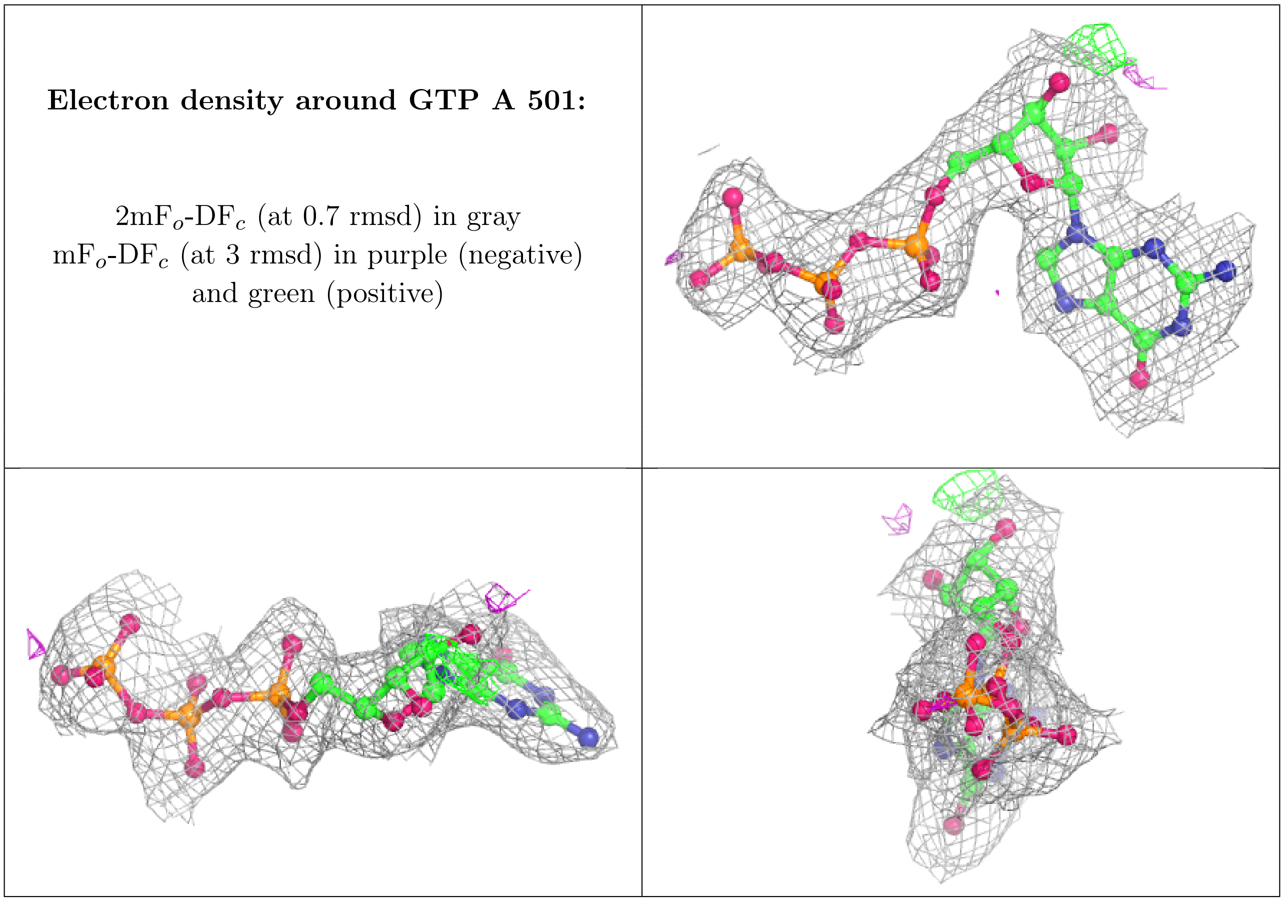


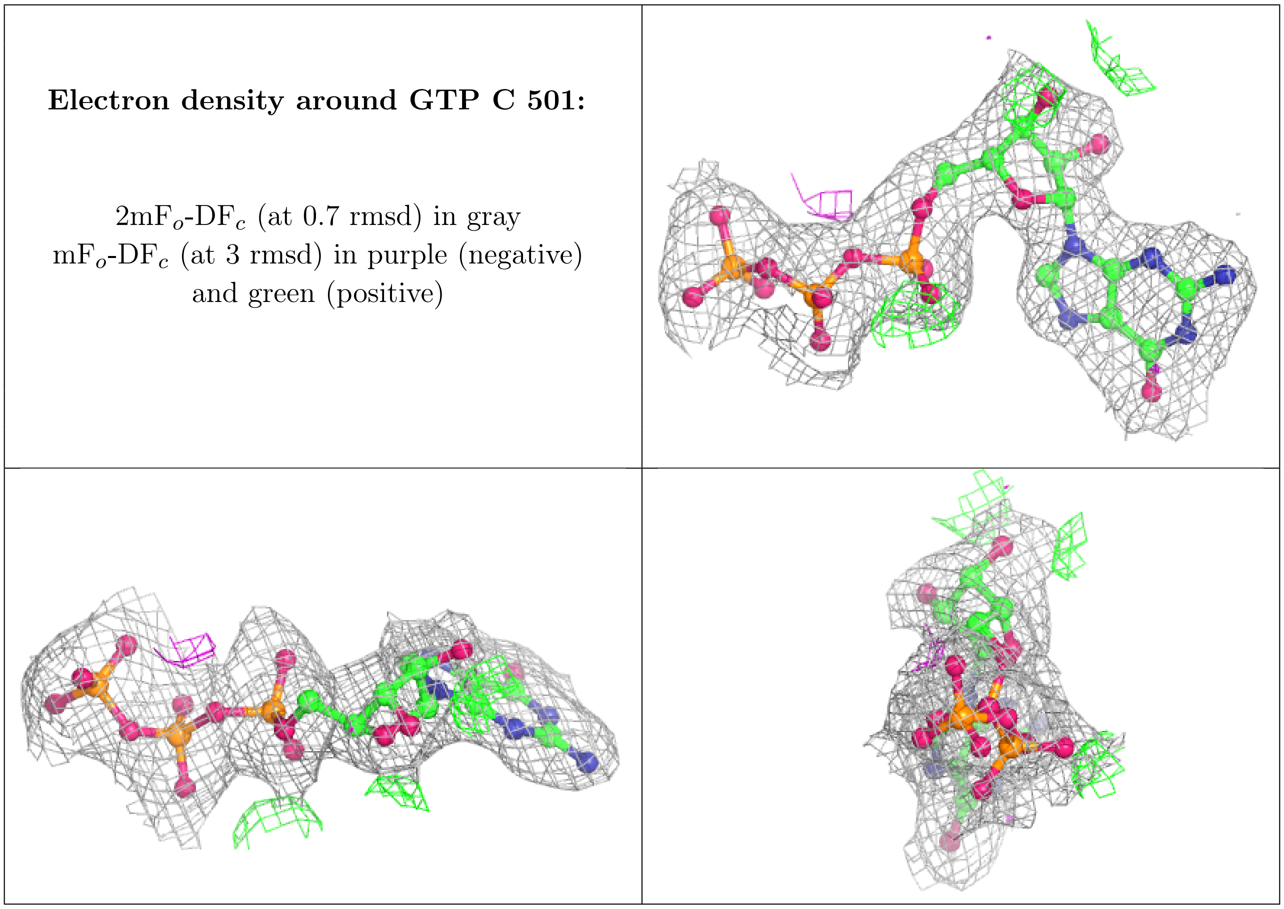




Electron density around GTP A 501:

$2mF_o$-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 ⓘ

There are no such residues in this entry.