



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:09 am BST

PDB ID : 5Z4U
Title : Crystal Structure of T2R-TTL complex with 7a3
Authors : Lai, Q.; Wang, Y.; Yang, J.; Yao, Y.
Deposited on : 2018-01-14
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

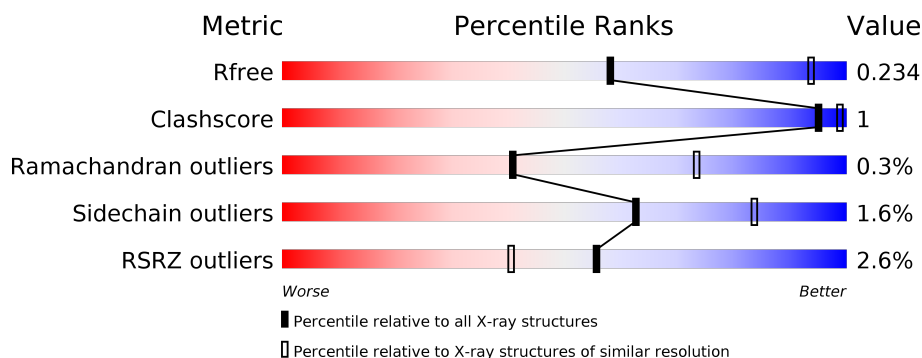
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	450	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 92% 5% • </div> </div>
1	C	450	<div> <div style="width: 96%; height: 10px; background-color: green;"></div> <div style="width: 3%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 96% • • </div> </div>
2	B	445	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 90% 5% 5% </div> </div>
2	D	445	<div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 90% • 5% </div> </div>
3	E	143	<div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% • 16% </div> </div>
4	F	384	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 10% 77% • 20% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ACP	F	401	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 17352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	170	VAL	MET	conflict	UNP Q6B856
B	296	ALA	SER	conflict	UNP Q6B856
B	316	VAL	ILE	conflict	UNP Q6B856
D	170	VAL	MET	conflict	UNP Q6B856
D	296	ALA	SER	conflict	UNP Q6B856
D	316	VAL	ILE	conflict	UNP Q6B856

- Molecule 3 is a protein called Stathmin-4.

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

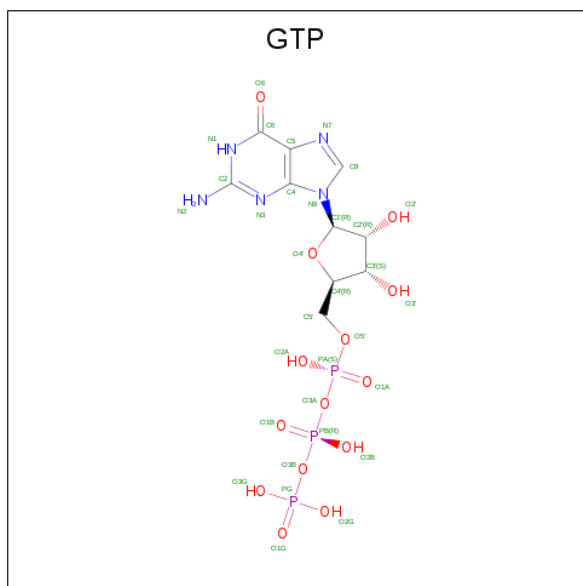
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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

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: $C_{10}H_{16}N_5O_{14}P_3$).



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

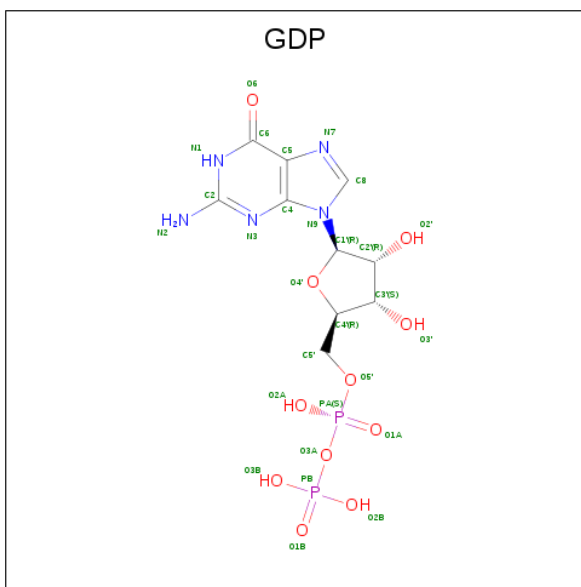
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

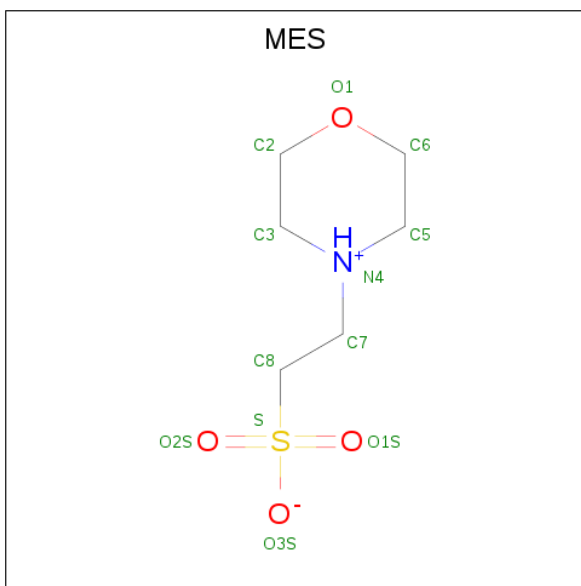
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

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



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

-
- ORTEP diagram of compound 96C. The structure shows a central pyrazole ring (N10, N12) connected to a phenyl ring (C06-C13) and a 4-(2,4,6-trimethoxyphenyl)phenyl group (C04-C13, O03-O24). The thermal ellipsoids are drawn at the 50% probability level.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total 27	C 21	N 2	O 4	0	0
10	D	1	Total 27	C 21	N 2	O 4	0	0

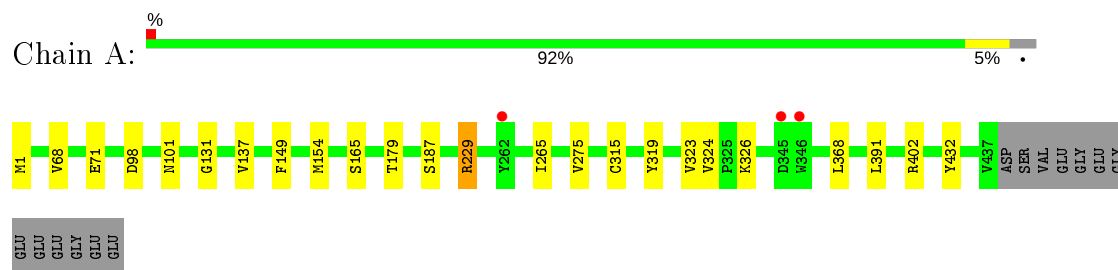
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- The chemical structure of Adenosine-5'-triphosphate (ATP) is shown. It consists of an adenine base (a purine ring system with an amino group at position 6) attached to a ribose sugar. The ribose sugar is linked to a triphosphate group at the 5' position. The triphosphate group is composed of three phosphate groups linked in series. The structure is labeled with atom names and numbers, indicating the specific atoms involved in the reaction.

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

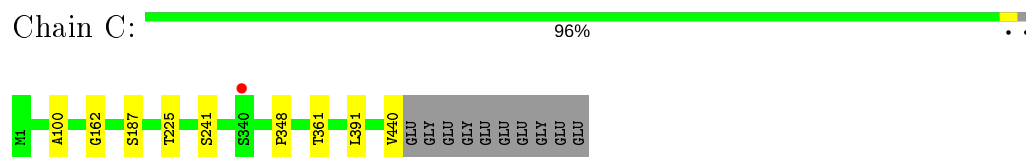
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

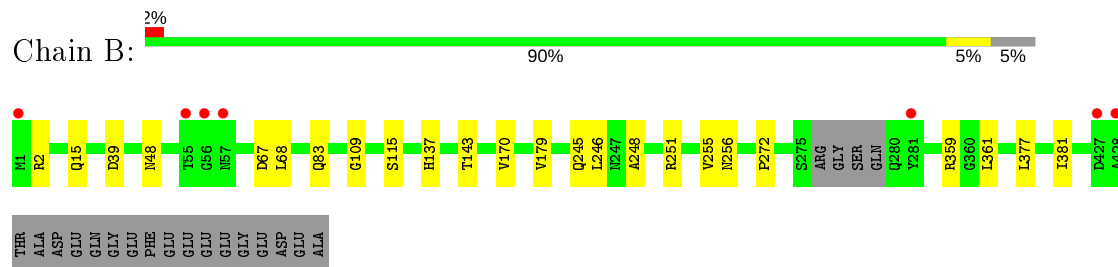
- Molecule 1: Tubulin alpha-1B chain



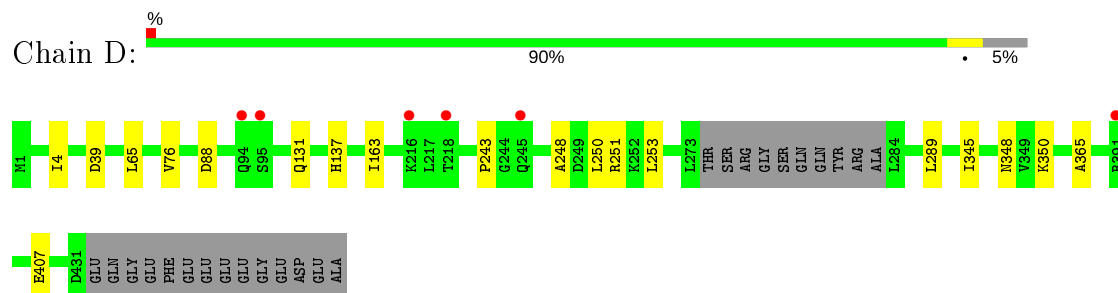
- Molecule 1: Tubulin alpha-1B chain



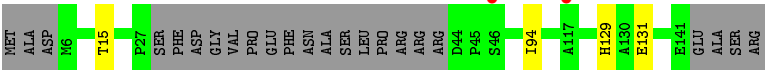
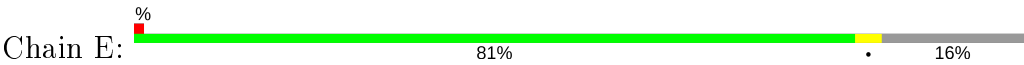
- Molecule 2: Tubulin beta-2B chain



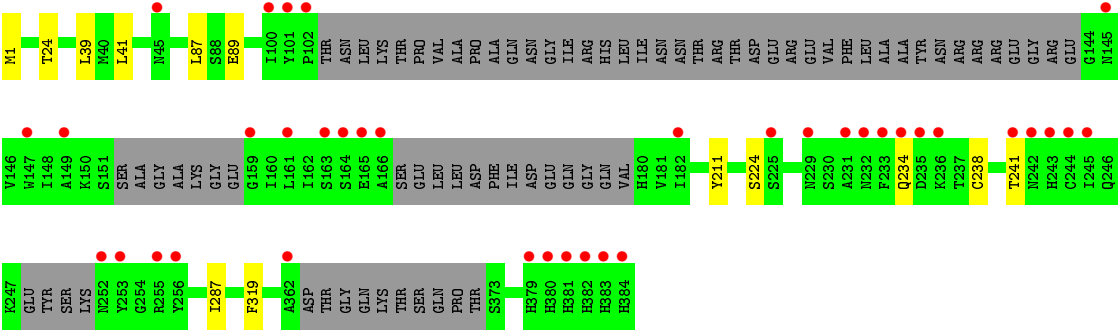
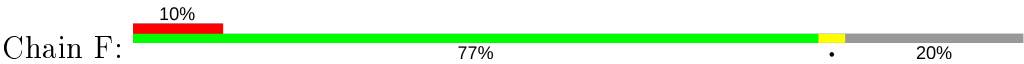
- Molecule 2: Tubulin beta-2B chain



- 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	105.49Å 158.23Å 182.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.44 – 3.18 29.81 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.9 (119.44-3.18) 92.1 (29.81-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.188 , 0.235 0.190 , 0.234	Depositor DCC
R_{free} test set	2416 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17352	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CA, GTP, ACP, MES, 96C

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	0.39	0/3525	0.60	0/4784
1	C	0.38	0/3556	0.62	0/4828
2	B	0.38	0/3425	0.59	0/4639
2	D	0.39	0/3377	0.58	0/4576
3	E	0.38	0/1002	0.54	0/1329
4	F	0.40	0/2618	0.58	0/3537
All	All	0.39	0/17503	0.59	0/23693

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3441	0	3362	17	0
1	C	3469	0	3377	4	0
2	B	3351	0	3229	11	0
2	D	3304	0	3182	9	0
3	E	994	0	1013	2	0
4	F	2553	0	2519	3	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	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	1	0
10	D	27	0	0	2	0
11	F	31	0	14	0	0
All	All	17352	0	16770	41	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 (41) 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:HH11	1:A:229[A]:ARG:CG	1.74	0.99
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.29	0.96
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	2.01	0.71
1:A:368[B]:LEU:H	1:A:368[B]:LEU:HD12	1.56	0.70
1:A:229[A]:ARG:HG3	1:A:229[A]:ARG:HH11	1.66	0.60
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.86	0.56
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.89	0.55
1:A:229[A]:ARG:NH1	1:A:229[A]:ARG:CG	2.47	0.53
2:B:170:VAL:HG13	2:B:381:ILE:HD11	1.89	0.53
1:A:368[B]:LEU:N	1:A:368[B]:LEU:HD12	2.24	0.51
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.93	0.51
1:A:187:SER:CB	1:A:391:LEU:HD21	2.41	0.50
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.95	0.49
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.93	0.48
2:D:248:ALA:HA	10:D:503:96C:N12	2.29	0.47
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.95	0.47
1:A:275:VAL:HG13	1:A:368[B]:LEU:HD21	1.97	0.47
1:C:100:ALA:CB	2:D:251:ARG:HG2	2.47	0.45
2:B:248:ALA:HB1	10:B:506:96C:C15	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:HG21	1:A:154:MET:SD	2.57	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.45
2:B:170:VAL:HG11	2:B:377:LEU:HD21	1.99	0.45
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.98	0.45
2:B:251:ARG:O	2:B:255:VAL:HG23	2.18	0.44
2:D:289:LEU:HD22	2:D:365:ALA:CB	2.48	0.44
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.53	0.44
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.52	0.43
4:F:224:SER:HB2	4:F:241:THR:HG22	1.98	0.43
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.00	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.54	0.43
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.01	0.43
2:D:4:ILE:HG13	2:D:131:GLN:HE21	1.84	0.43
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.48	0.43
2:B:68:LEU:HD21	2:B:109:GLY:HA2	2.01	0.42
2:D:407:GLU:OE1	3:E:129:HIS:NE2	2.52	0.42
2:B:251:ARG:NH1	9:B:503:MES:O2S	2.52	0.42
2:B:67:ASP:HA	2:B:143:THR:HG21	2.02	0.42
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.02	0.42
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.67	0.41
2:B:170:VAL:CG1	2:B:381:ILE:HD11	2.50	0.40
2:D:350:LYS:HG3	10:D:503:96C:C27	2.51	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%)	425 (97%)	13 (3%)	1 (0%)	47	78
1	C	444/450 (99%)	433 (98%)	11 (2%)	0	100	100
2	B	422/445 (95%)	404 (96%)	15 (4%)	3 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	417/445 (94%)	400 (96%)	15 (4%)	2 (0%)	29	66
3	E	116/143 (81%)	111 (96%)	5 (4%)	0	100	100
4	F	300/384 (78%)	280 (93%)	19 (6%)	1 (0%)	41	73
All	All	2138/2317 (92%)	2053 (96%)	78 (4%)	7 (0%)	41	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	245	GLN
2	D	39	ASP
2	D	243	PRO
2	B	39	ASP
4	F	24	THR
2	B	246	LEU
1	A	131	GLY

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	74
1	C	377/378 (100%)	373 (99%)	4 (1%)	73	88
2	B	367/382 (96%)	360 (98%)	7 (2%)	57	80
2	D	362/382 (95%)	359 (99%)	3 (1%)	81	92
3	E	108/127 (85%)	106 (98%)	2 (2%)	57	80
4	F	281/342 (82%)	275 (98%)	6 (2%)	53	79
All	All	1867/1989 (94%)	1835 (98%)	32 (2%)	62	82

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	165	SER
1	A	179	THR
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	315[A]	CYS
1	A	315[B]	CYS
1	A	324	VAL
1	A	326	LYS
1	A	402	ARG
2	B	2	ARG
2	B	15	GLN
2	B	48	ASN
2	B	83	GLN
2	B	115	SER
2	B	137	HIS
2	B	359	ARG
1	C	225	THR
1	C	241	SER
1	C	361	THR
1	C	440	VAL
2	D	88	ASP
2	D	137	HIS
2	D	253	LEU
3	E	15	THR
3	E	131	GLU
4	F	1	MET
4	F	87	LEU
4	F	89	GLU
4	F	211	TYR
4	F	234	GLN
4	F	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
2	B	83	GLN
1	C	101	ASN
1	C	249	ASN
2	D	195	ASN
2	D	292	GLN
3	E	12	ASN

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Mol	Chain	Res	Type
3	E	136	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 carbohydrates 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$
11	ACP	F	401	-	27,33,33	1.46	6 (22%)	32,52,52	1.35	3 (9%)
10	96C	D	503	-	26,29,29	2.49	6 (23%)	33,40,40	1.39	3 (9%)
9	MES	B	503	-	12,12,12	2.17	1 (8%)	14,16,16	6.99	8 (57%)
9	MES	B	505	-	12,12,12	2.00	1 (8%)	14,16,16	6.30	8 (57%)
5	GTP	C	501	6	26,34,34	1.14	2 (7%)	33,54,54	1.87	8 (24%)
8	GDP	B	501	6	24,30,30	1.29	2 (8%)	31,47,47	2.06	6 (19%)
5	GTP	A	501	6	26,34,34	1.18	2 (7%)	33,54,54	1.96	9 (27%)
5	GTP	D	501	6	26,34,34	1.19	2 (7%)	33,54,54	2.01	8 (24%)
10	96C	B	506	-	26,29,29	2.28	5 (19%)	33,40,40	1.12	3 (9%)

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
11	ACP	F	401	-	-	5/15/38/38	0/3/3/3
10	96C	D	503	-	-	4/17/17/17	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
9	MES	B	505	-	-	3/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
5	GTP	D	501	6	-	7/18/38/38	0/3/3/3
10	96C	B	506	-	-	6/17/17/17	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	96C	C14-C13	-9.16	1.38	1.49
10	B	506	96C	C14-C13	-7.92	1.40	1.49
9	B	503	MES	C8-S	-6.91	1.67	1.77
9	B	505	MES	C8-S	-6.33	1.68	1.77
10	B	506	96C	C08-C07	-5.36	1.39	1.49
8	B	501	GDP	C6-C5	4.81	1.49	1.41
10	D	503	96C	C08-C07	-4.63	1.41	1.49
10	D	503	96C	C13-N12	-4.46	1.31	1.35
5	D	501	GTP	C6-C5	4.33	1.48	1.41
5	A	501	GTP	C6-C5	4.12	1.48	1.41
10	B	506	96C	C13-N12	-3.95	1.32	1.35
5	C	501	GTP	C6-C5	3.87	1.48	1.41
10	D	503	96C	C09-N10	-3.70	1.31	1.35
11	F	401	ACP	PB-O3A	3.56	1.62	1.58
10	B	506	96C	C09-N10	-2.86	1.32	1.35
11	F	401	ACP	PG-O2G	2.85	1.61	1.54
11	F	401	ACP	PG-O3G	2.77	1.61	1.54
5	C	501	GTP	C5-C4	2.63	1.47	1.40
11	F	401	ACP	C5-C4	2.58	1.47	1.40
10	B	506	96C	O17-C16	2.57	1.41	1.37
5	D	501	GTP	C5-C4	2.48	1.47	1.40
5	A	501	GTP	C5-C4	2.47	1.47	1.40
8	B	501	GDP	C5-C4	2.40	1.47	1.40
10	D	503	96C	O23-C22	2.38	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	96C	O17-C16	2.36	1.40	1.37
11	F	401	ACP	PB-O2B	2.04	1.61	1.56
11	F	401	ACP	C2-N3	2.00	1.35	1.32

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O3S-S-C8	-13.62	83.73	105.77
9	B	505	MES	O3S-S-O1S	-12.40	80.97	111.27
9	B	503	MES	O3S-S-O1S	-10.87	84.71	111.27
9	B	503	MES	O3S-S-O2S	-10.86	84.75	111.27
9	B	505	MES	O3S-S-O2S	-10.81	84.87	111.27
9	B	503	MES	O1S-S-C8	10.66	119.75	106.92
9	B	503	MES	O2S-S-C8	10.16	119.15	106.92
9	B	505	MES	O1S-S-C8	9.91	118.85	106.92
9	B	505	MES	O3S-S-C8	-9.42	90.53	105.77
9	B	505	MES	O2S-S-C8	8.83	117.55	106.92
8	B	501	GDP	C2-N3-C4	5.40	121.53	115.36
10	D	503	96C	C11-N10-N12	5.19	126.60	120.50
5	D	501	GTP	C6-C5-C4	-4.78	116.23	120.80
9	B	503	MES	C2-C3-N4	4.75	117.30	110.10
5	D	501	GTP	C2-N3-C4	4.73	120.76	115.36
5	A	501	GTP	C6-C5-C4	-4.71	116.30	120.80
8	B	501	GDP	C6-C5-C4	-4.64	116.36	120.80
8	B	501	GDP	C6-N1-C2	4.54	123.14	115.93
5	C	501	GTP	C6-N1-C2	4.46	123.02	115.93
5	A	501	GTP	C6-N1-C2	4.38	122.89	115.93
5	C	501	GTP	C5-C6-N1	-4.33	117.51	123.43
5	A	501	GTP	C2-N3-C4	4.30	120.27	115.36
5	D	501	GTP	C6-N1-C2	4.24	122.67	115.93
5	C	501	GTP	C6-C5-C4	-4.03	116.95	120.80
5	A	501	GTP	C5-C6-N1	-4.01	117.94	123.43
8	B	501	GDP	C5-C6-N1	-3.94	118.04	123.43
8	B	501	GDP	N3-C2-N1	-3.94	121.97	127.22
5	C	501	GTP	C2-N3-C4	3.91	119.82	115.36
5	D	501	GTP	N3-C2-N1	-3.79	122.17	127.22
5	D	501	GTP	C5-C6-N1	-3.62	118.48	123.43
11	F	401	ACP	N3-C2-N1	-3.59	123.07	128.68
5	A	501	GTP	N3-C2-N1	-3.49	122.56	127.22
8	B	501	GDP	C4-C5-N7	-3.29	105.97	109.40
5	C	501	GTP	N3-C2-N1	-3.17	122.99	127.22
11	F	401	ACP	C3'-C2'-C1'	3.10	105.65	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	506	96C	O23-C22-C19	3.09	120.59	115.16
10	B	506	96C	C11-N10-N12	2.99	124.02	120.50
9	B	503	MES	C5-N4-C3	2.93	115.41	108.83
10	D	503	96C	C02-O03-C04	2.91	125.44	117.99
9	B	503	MES	C6-C5-N4	2.86	114.44	110.10
11	F	401	ACP	C4-C5-N7	-2.78	106.50	109.40
5	A	501	GTP	C4-C5-N7	-2.76	106.53	109.40
10	B	506	96C	O23-C22-C25	-2.66	119.53	124.12
5	D	501	GTP	PB-O3B-PG	-2.48	124.31	132.83
5	D	501	GTP	PA-O3A-PB	-2.42	124.53	132.83
5	C	501	GTP	PB-O3B-PG	-2.41	124.54	132.83
5	D	501	GTP	C4-C5-N7	-2.35	106.95	109.40
9	B	505	MES	O2S-S-O1S	2.23	121.67	113.95
5	C	501	GTP	C4-C5-N7	-2.19	107.12	109.40
5	C	501	GTP	PA-O3A-PB	-2.10	125.62	132.83
5	A	501	GTP	PA-O3A-PB	-2.09	125.64	132.83
5	A	501	GTP	C1'-N9-C4	-2.08	123.00	126.64
9	B	505	MES	C7-N4-C5	-2.07	105.93	111.23
5	A	501	GTP	O3G-PG-O2G	2.06	115.51	107.64
10	D	503	96C	O17-C16-C19	2.05	118.77	115.16
9	B	505	MES	C2-C3-N4	2.01	113.15	110.10

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O3G
9	B	503	MES	N4-C7-C8-S
9	B	503	MES	C7-C8-S-O1S
9	B	505	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O1A
10	D	503	96C	C19-C16-O17-C18
10	B	506	96C	C25-C22-O23-C24
10	D	503	96C	C15-C16-O17-C18
10	B	506	96C	C19-C22-O23-C24
10	D	503	96C	N12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
10	D	503	96C	N12-C13-C14-C25
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
10	B	506	96C	C19-C16-O17-C18
10	B	506	96C	C15-C16-O17-C18
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	503	MES	C7-C8-S-O2S
9	B	505	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O2G
5	D	501	GTP	C4'-C5'-O5'-PA
10	B	506	96C	N12-C13-C14-C25
5	C	501	GTP	C4'-C5'-O5'-PA
8	B	501	GDP	PB-O3A-PA-O2A
10	B	506	96C	N12-C13-C14-C15
5	D	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O1A
9	B	505	MES	N4-C7-C8-S

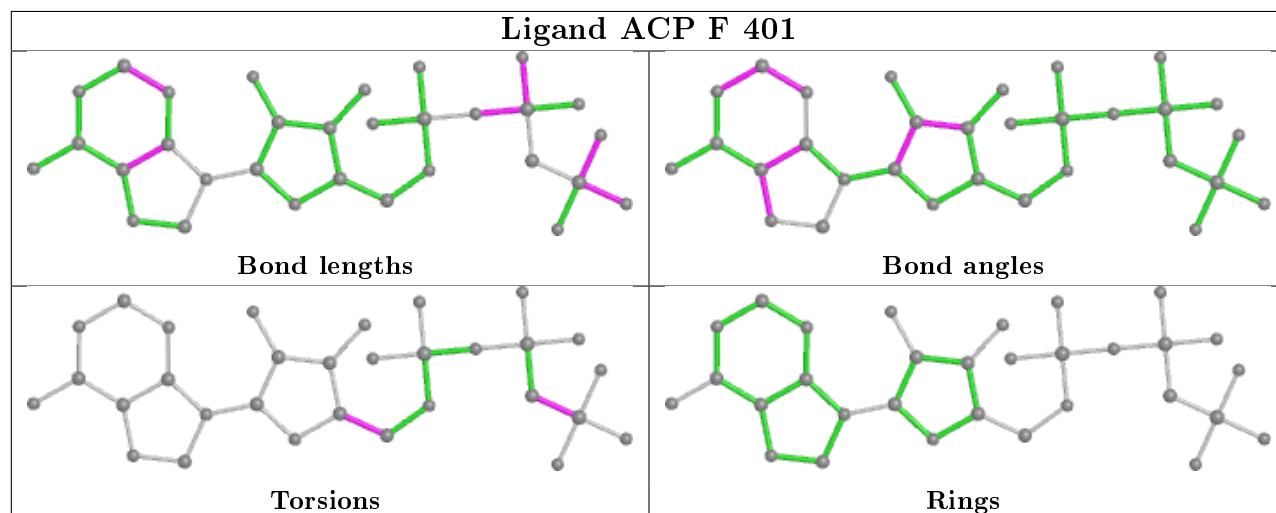
There are no ring outliers.

3 monomers are involved in 4 short contacts:

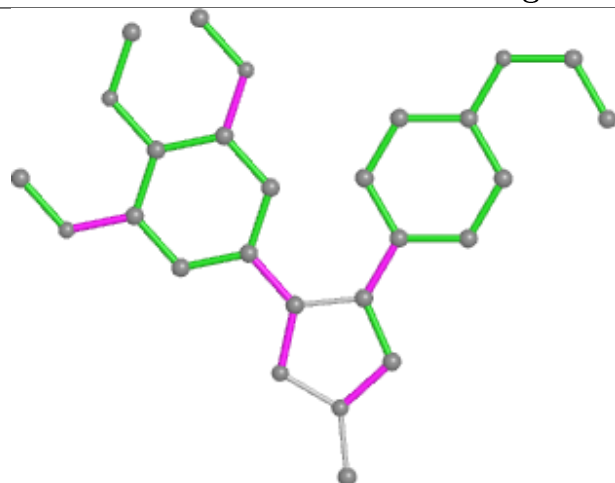
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	96C	2	0
9	B	503	MES	1	0
10	B	506	96C	1	0

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

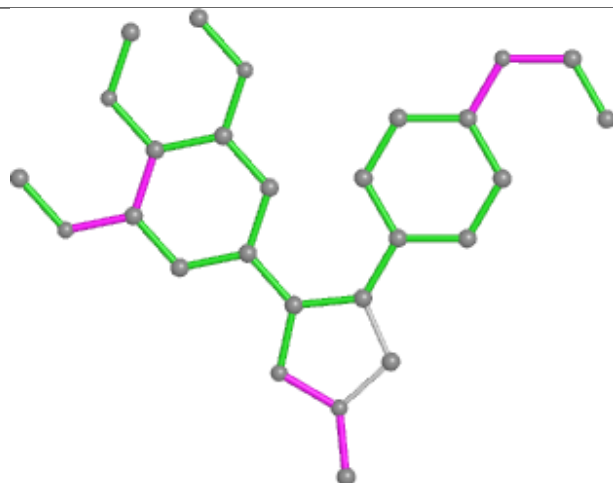
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



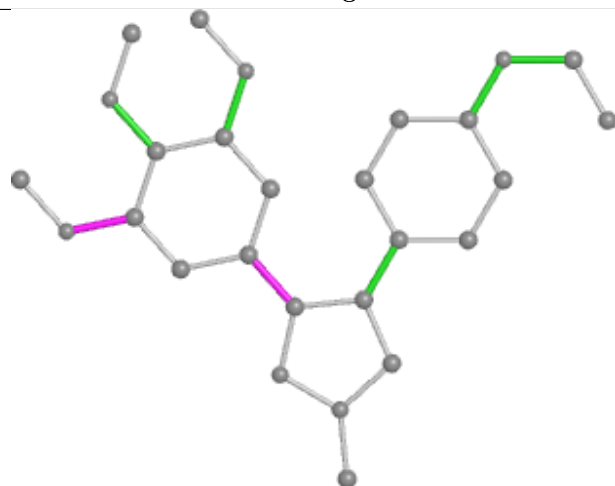
Ligand 96C D 503



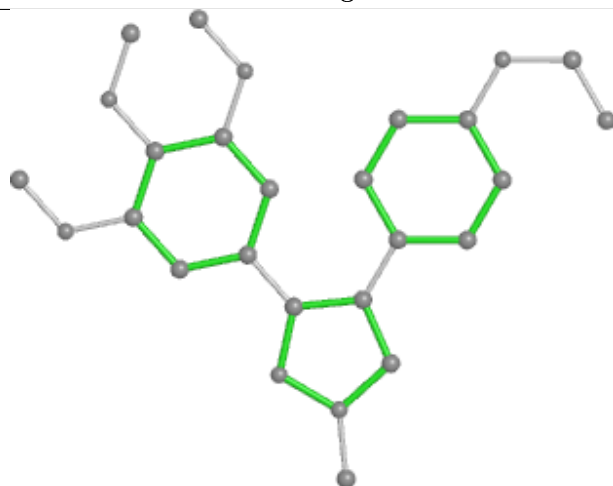
Bond lengths



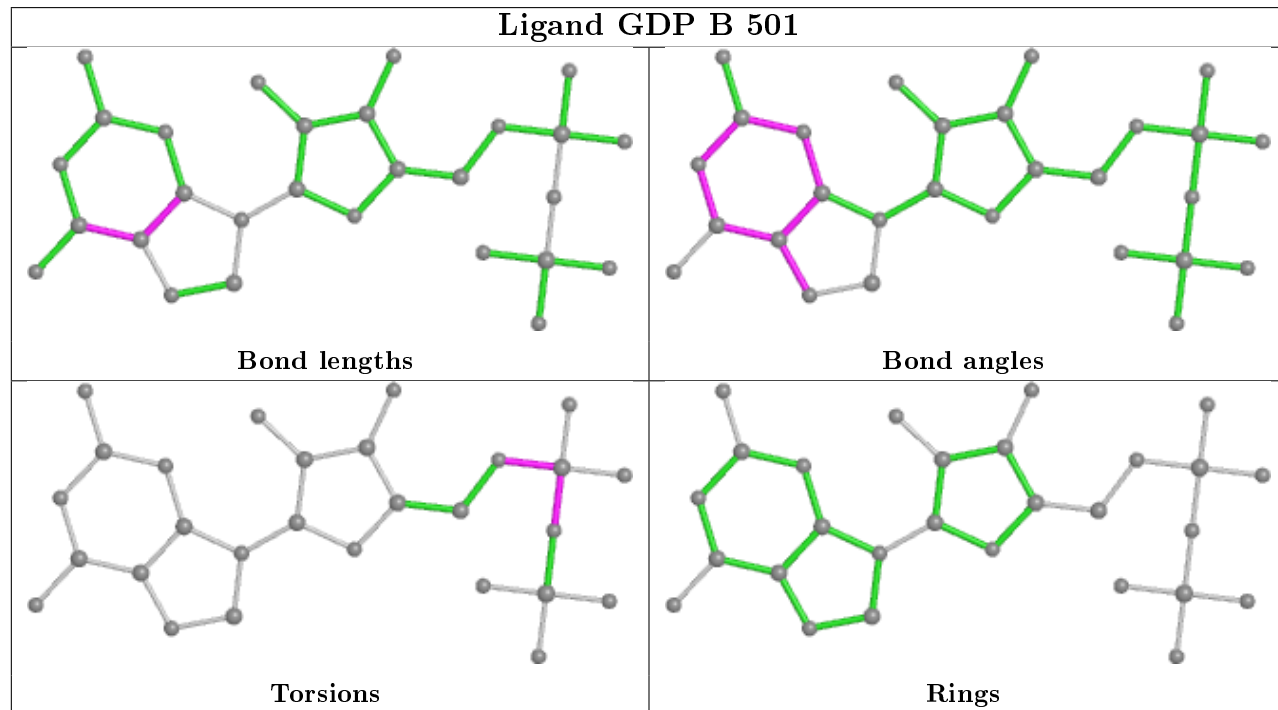
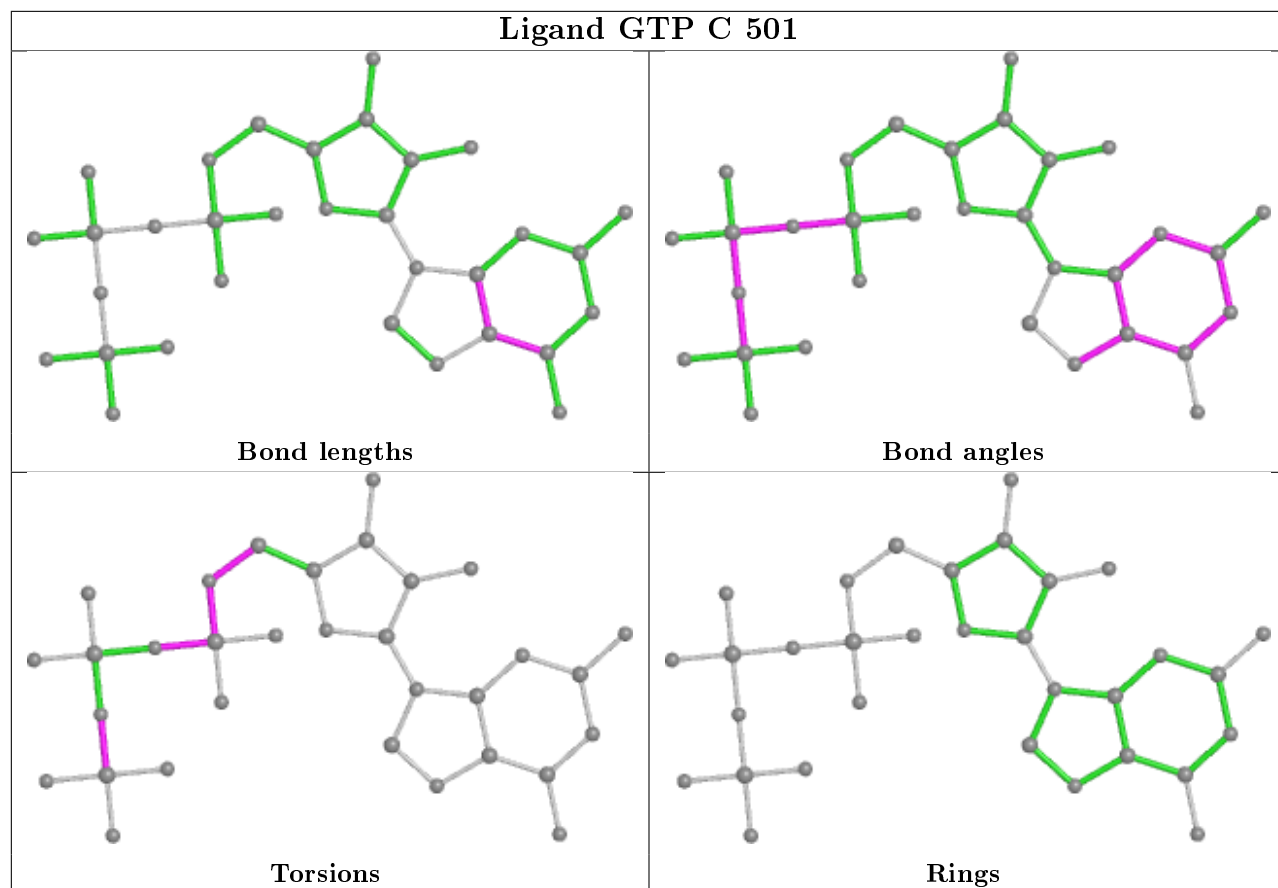
Bond angles

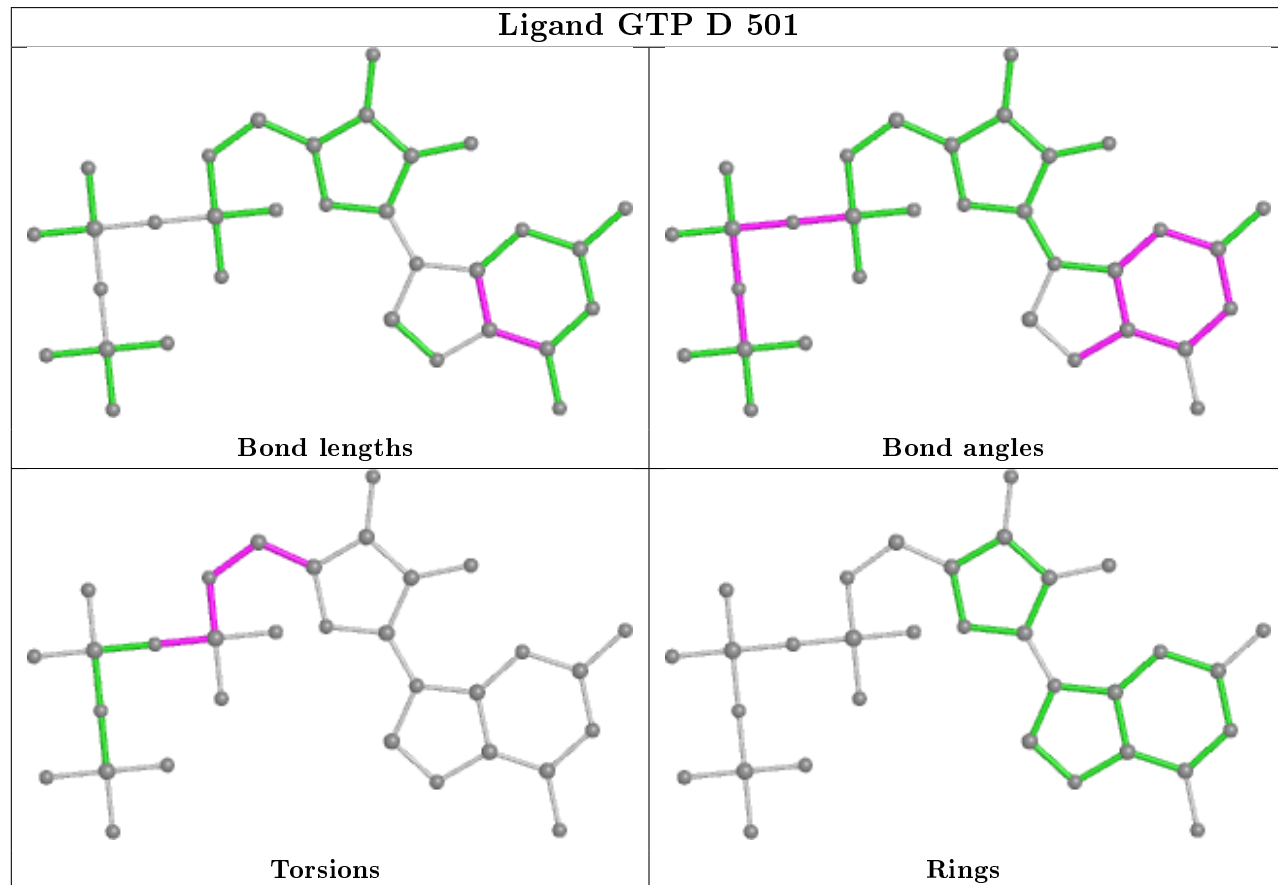
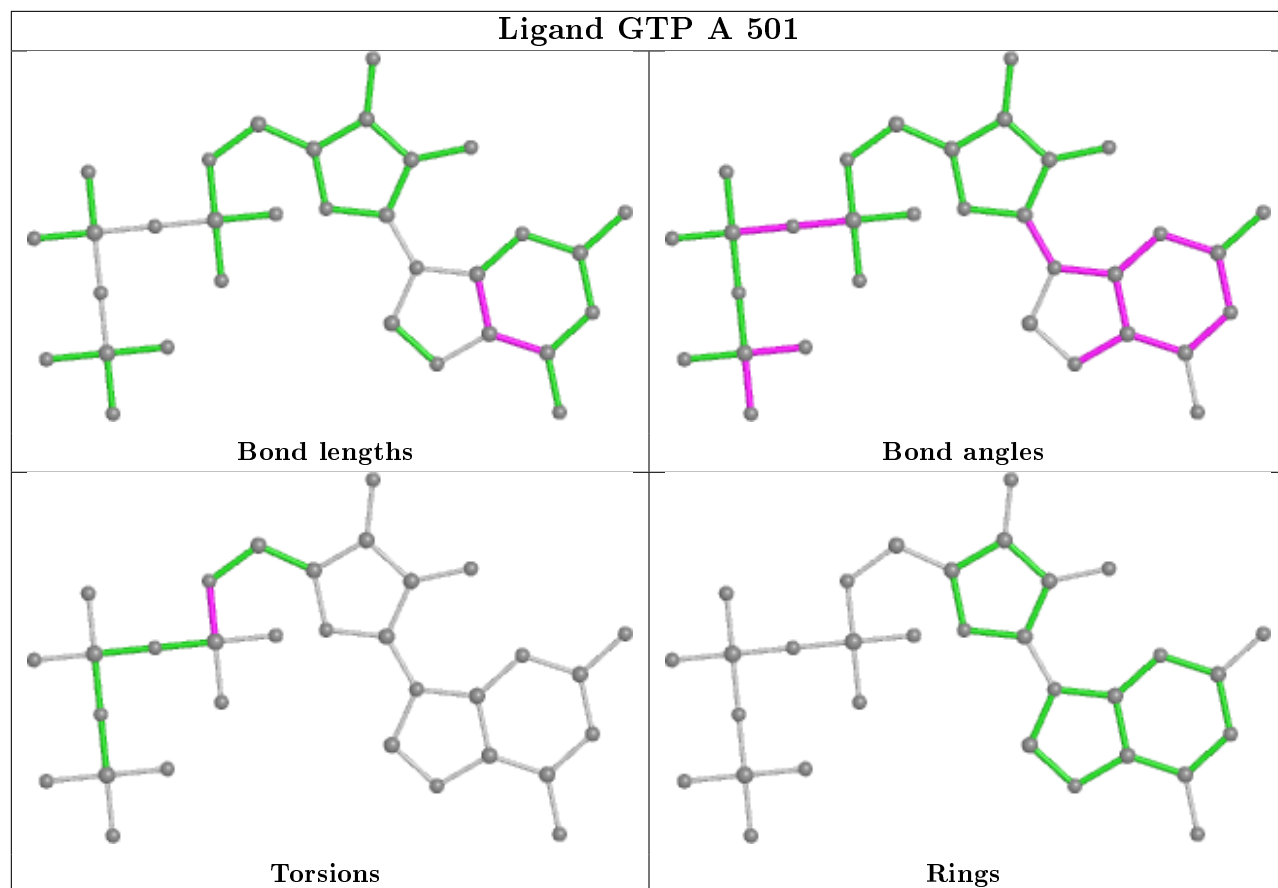


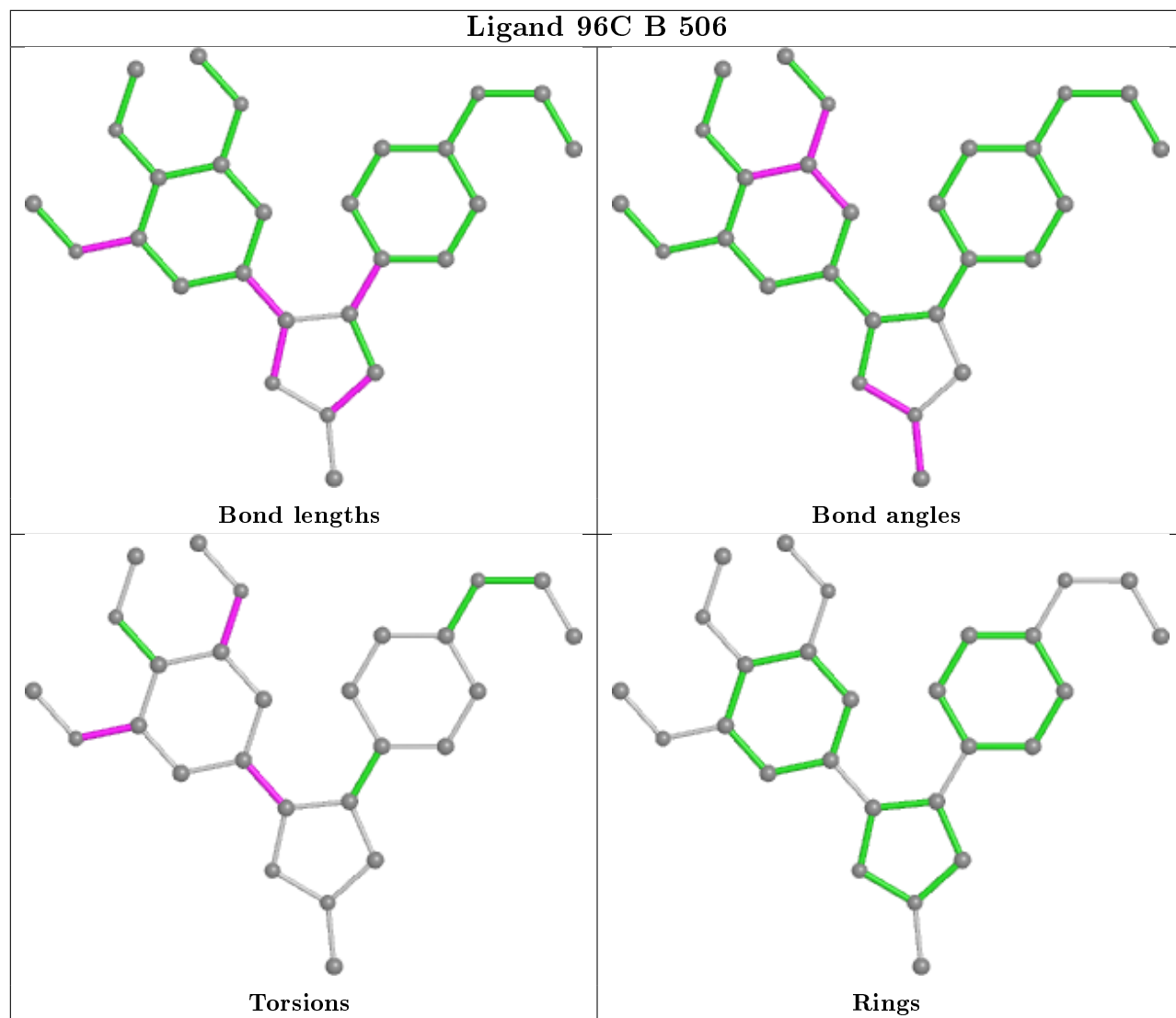
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	-0.33	3 (0%)	87 81	33, 54, 82, 106	0
1	C	440/450 (97%)	-0.57	1 (0%)	95 94	23, 40, 70, 83	1 (0%)
2	B	424/445 (95%)	-0.38	7 (1%)	70 57	29, 50, 80, 110	1 (0%)
2	D	421/445 (94%)	-0.11	6 (1%)	75 63	36, 68, 104, 118	4 (0%)
3	E	120/143 (83%)	0.18	2 (1%)	70 57	42, 71, 102, 112	0
4	F	309/384 (80%)	0.22	38 (12%)	4 2	41, 77, 146, 209	0
All	All	2151/2317 (92%)	-0.24	57 (2%)	56 40	23, 57, 102, 209	6 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	232	ASN	6.4
4	F	244	CYS	5.9
4	F	234	GLN	3.9
2	B	1	MET	3.8
4	F	253	TYR	3.6
4	F	233	PHE	3.6
4	F	231	ALA	3.6
4	F	384	HIS	3.5
2	D	216	LYS	3.4
4	F	163	SER	3.3
4	F	102	PRO	3.2
4	F	161	LEU	3.2
4	F	362	ALA	3.2
4	F	379	HIS	3.1
2	D	245	GLN	3.1
4	F	383	HIS	3.1
1	A	345	ASP	3.0
4	F	165	GLU	3.0
4	F	241	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	55	THR	3.0
2	B	57	ASN	2.9
4	F	100	ILE	2.9
4	F	245	ILE	2.9
4	F	256	TYR	2.9
4	F	159	GLY	2.8
4	F	381	HIS	2.8
4	F	101	TYR	2.8
4	F	182	ILE	2.7
2	D	94	GLN	2.7
4	F	252	ASN	2.6
1	A	346	TRP	2.6
4	F	225	SER	2.6
4	F	164	SER	2.6
4	F	145	ASN	2.6
4	F	229	ASN	2.6
4	F	235	ASP	2.6
2	B	56	GLY	2.5
4	F	45	ASN	2.5
4	F	242	ASN	2.5
2	D	95	SER	2.5
2	D	218	THR	2.5
4	F	149	ALA	2.5
2	D	391	ARG	2.4
3	E	117	ALA	2.3
4	F	255	ARG	2.2
4	F	382	HIS	2.2
4	F	243	HIS	2.1
4	F	147	TRP	2.1
4	F	166	ALA	2.1
4	F	236	LYS	2.1
4	F	380	HIS	2.1
3	E	46	SER	2.1
2	B	427	ASP	2.1
1	A	262	TYR	2.1
2	B	428	ALA	2.1
2	B	281	TYR	2.0
1	C	340	SER	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 carbohydrates in this entry.

6.4 Ligands ⓘ

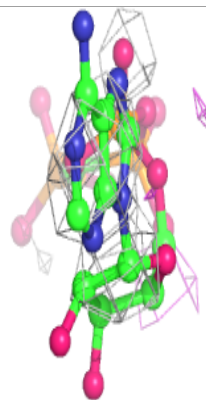
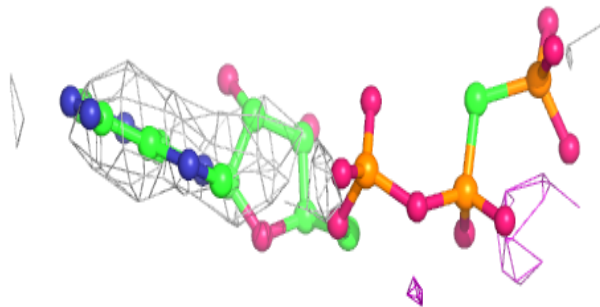
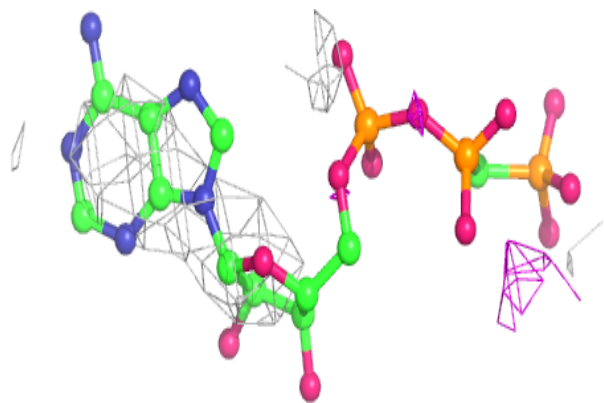
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ACP	F	401	31/31	0.60	0.56	168,201,276,282	0
9	MES	B	503	12/12	0.90	0.23	76,80,82,82	0
7	CA	A	503	1/1	0.91	0.15	94,94,94,94	0
7	CA	B	504	1/1	0.91	0.10	75,75,75,75	0
9	MES	B	505	12/12	0.92	0.31	102,105,109,111	0
10	96C	D	503	27/27	0.93	0.20	69,73,77,77	0
5	GTP	D	501	32/32	0.93	0.20	62,69,75,82	0
6	MG	B	502	1/1	0.96	0.14	17,17,17,17	0
10	96C	B	506	27/27	0.96	0.16	48,50,52,53	0
7	CA	C	503	1/1	0.97	0.07	70,70,70,70	0
5	GTP	C	501	32/32	0.97	0.17	33,39,42,43	0
8	GDP	B	501	28/28	0.97	0.14	34,37,39,40	0
5	GTP	A	501	32/32	0.97	0.13	38,41,45,48	0
6	MG	D	502	1/1	0.97	0.14	32,32,32,32	0
6	MG	C	502	1/1	0.98	0.29	22,22,22,22	0
6	MG	A	502	1/1	0.98	0.36	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.

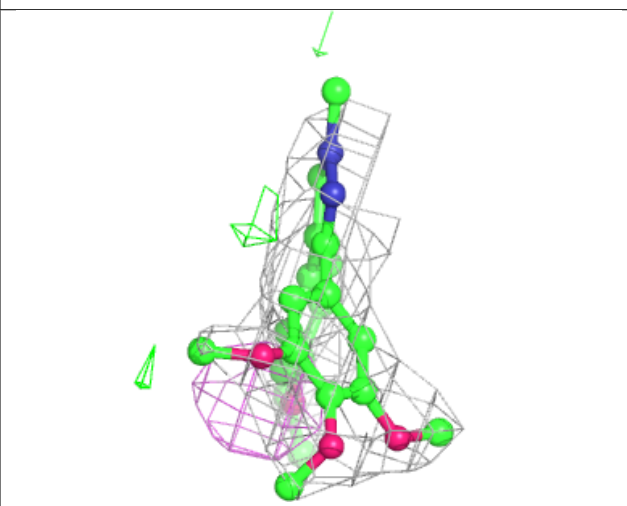
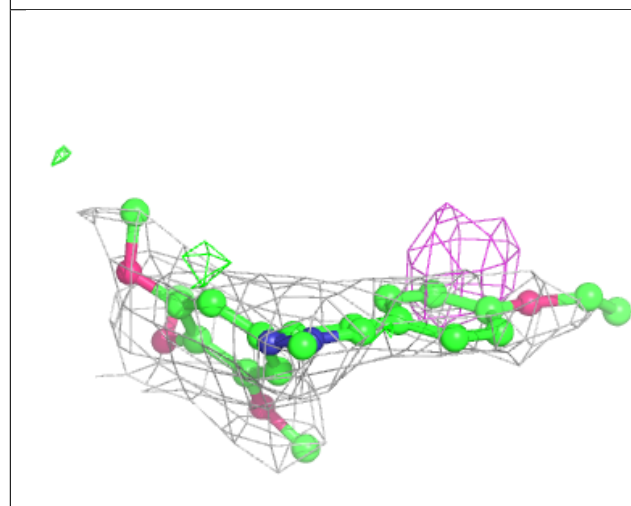
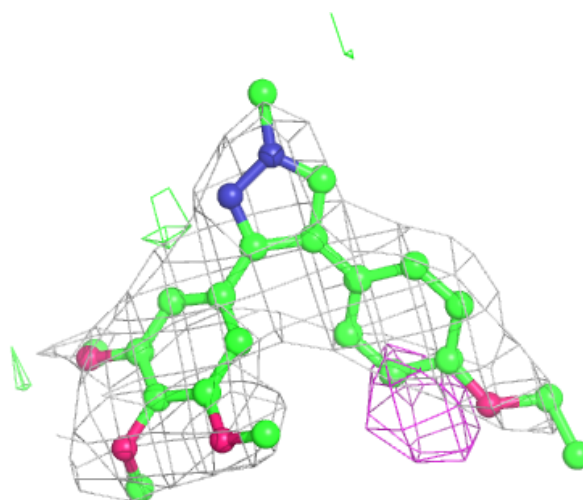
Electron density around ACP F 401:

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



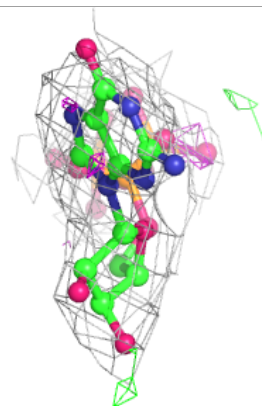
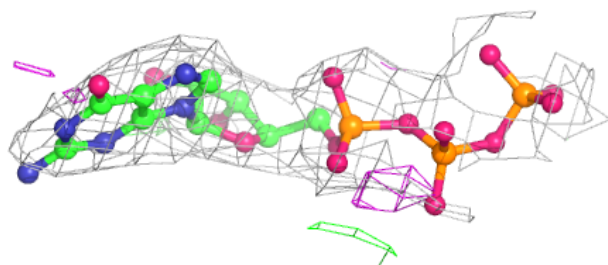
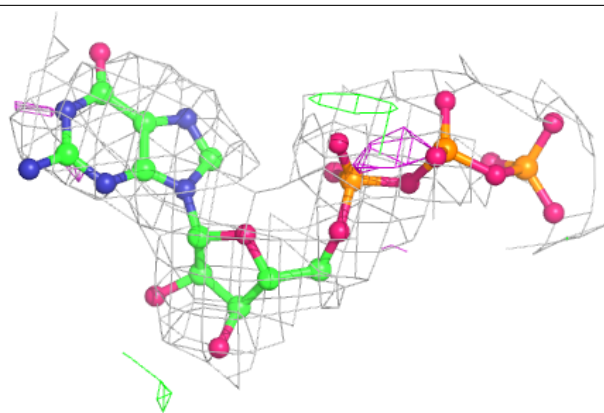
Electron density around 96C D 503:

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



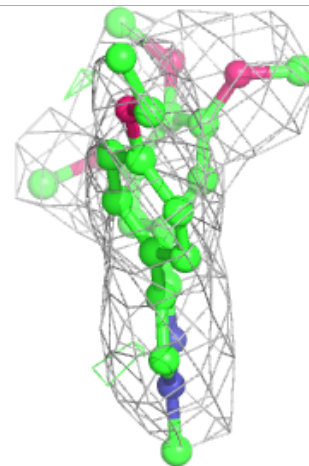
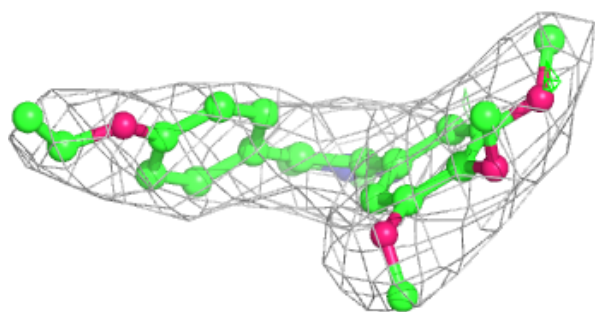
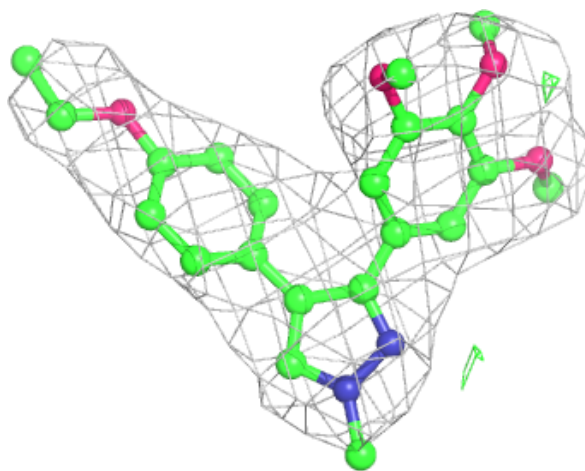
Electron density around GTP D 501:

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



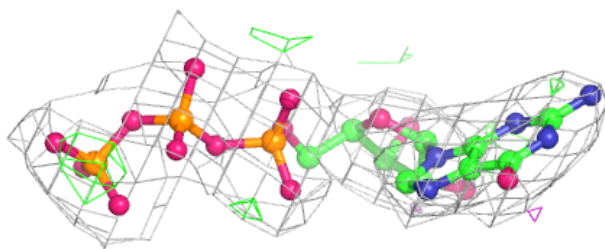
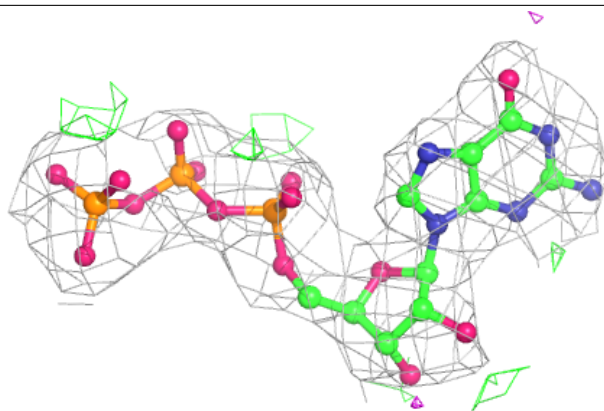
Electron density around 96C B 506:

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



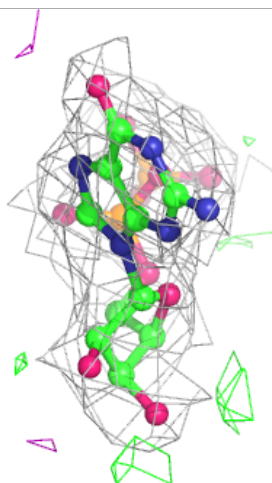
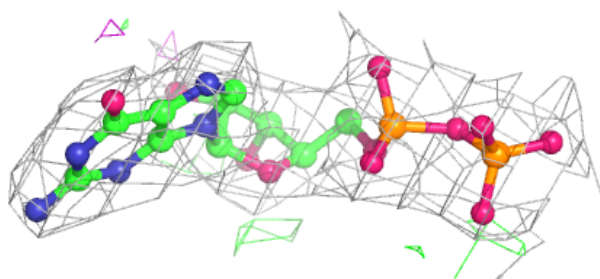
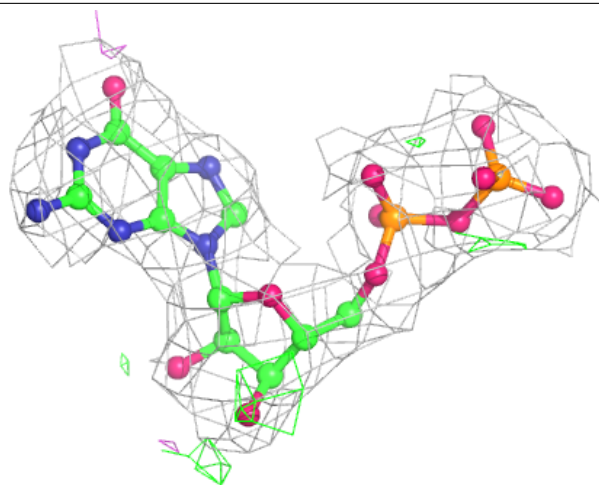
Electron density around GTP C 501:

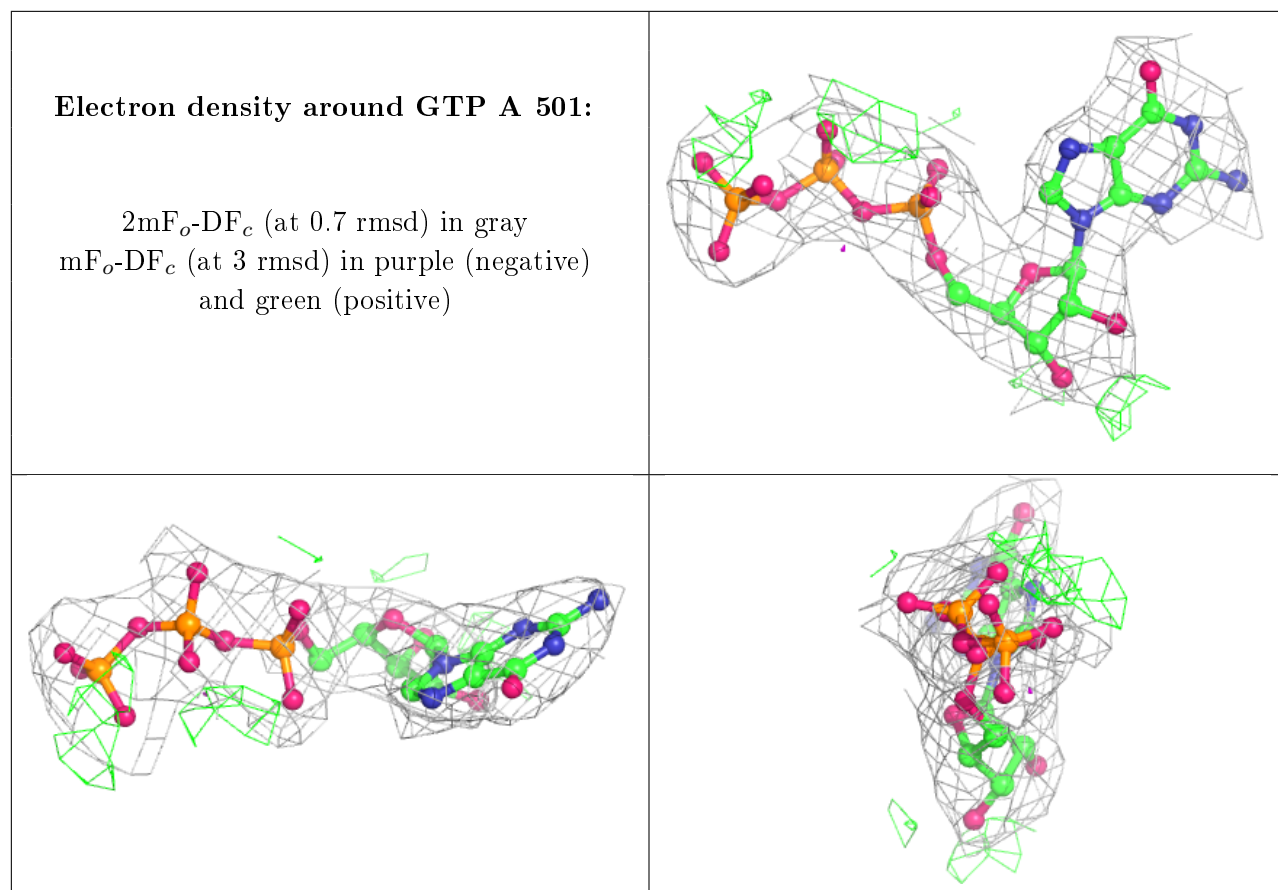
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 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.