



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:29 am BST

PDB ID : 5EZY  
Title : Crystal structure of T2R-TTL-taccalonolide AJ complex  
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.  
Deposited on : 2015-11-27  
Resolution : 2.05 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](mailto: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.

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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

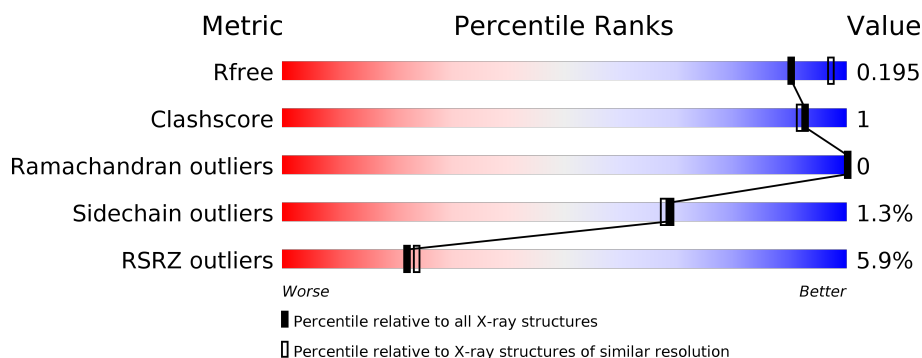
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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>2%</div> <div>95%</div> <div>• •</div> </div>
1	C	450	<div> <div>%</div> <div>94%</div> <div>• •</div> </div>
2	B	445	<div> <div>4%</div> <div>93%</div> <div>• •</div> </div>
2	D	445	<div> <div>5%</div> <div>93%</div> <div>• •</div> </div>
3	E	143	<div> <div>6%</div> <div>84%</div> <div>• 15%</div> </div>
4	F	384	<div> <div>17%</div> <div>85%</div> <div>5% • 10%</div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 36311 atoms, of which 16959 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	3	0
			6756	2169	3328	583	652	24			
1	C	440	Total	C	H	N	O	S	0	9	0
			6836	2192	3368	589	662	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	0	0
			6588	2110	3227	576	649	26			
2	D	431	Total	C	H	N	O	S	0	0	0
			6645	2126	3256	580	656	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	4	0
			2046	627	1028	186	200	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	cloning artifact	UNP P63043
E	4	ALA	-	cloning artifact	UNP P63043

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	347	Total	C	H	N	O	S	0	1	0
			5546	1832	2686	494	520	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 (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	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		

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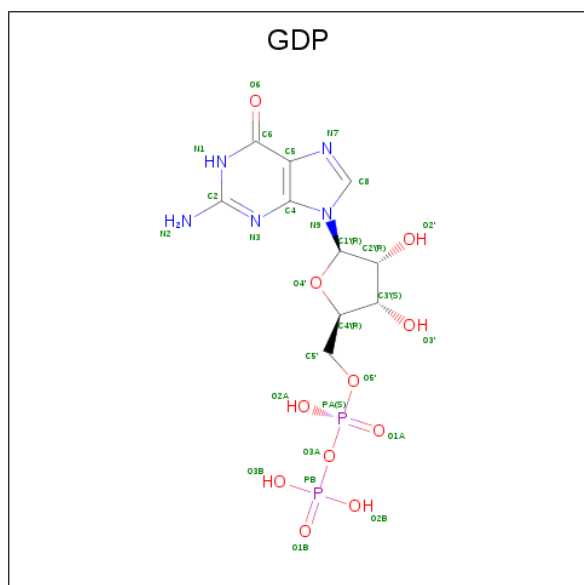
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

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

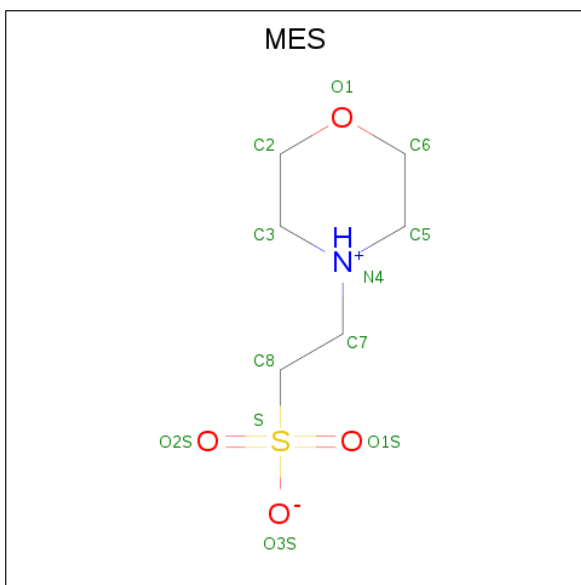
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



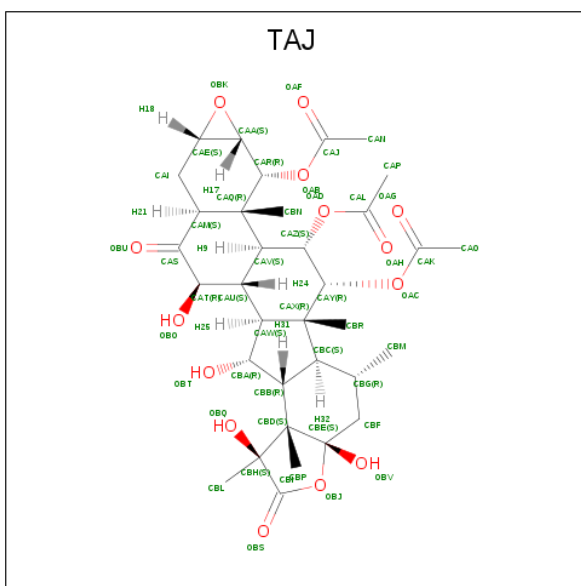
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



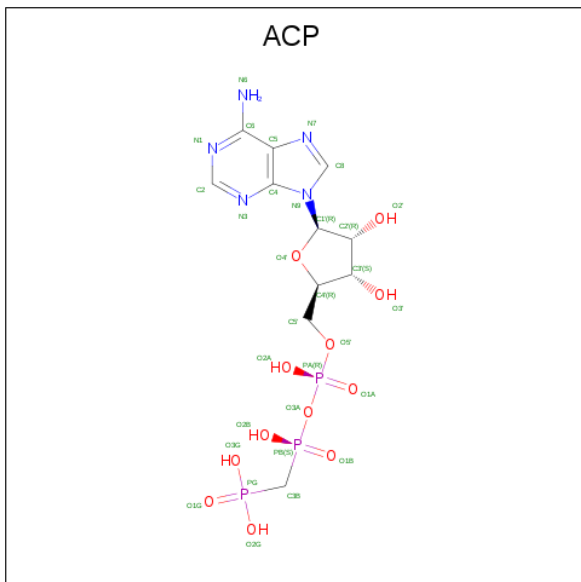
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
9	B	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0

- Molecule 10 is taccalonolide AJ (three-letter code: TAJ) (formula:  $C_{34}H_{46}O_{14}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total 48	C 34	O 14	0	0
10	D	1	Total 48	C 34	O 14	0	0

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



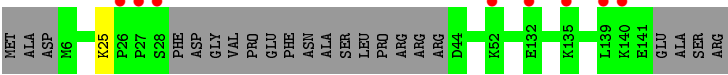
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

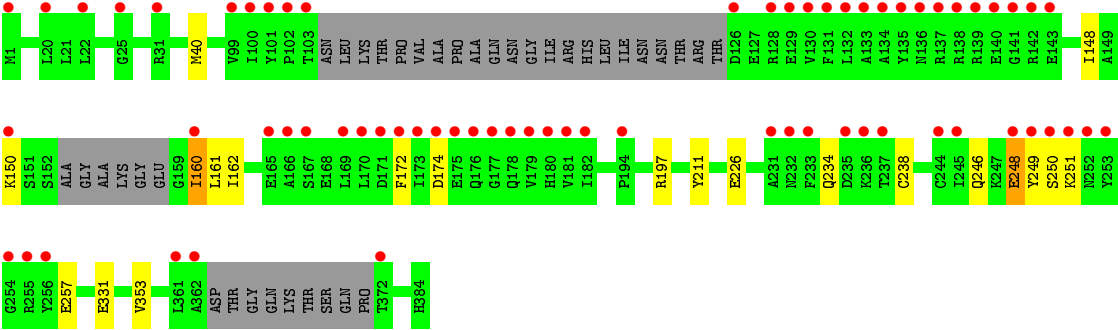
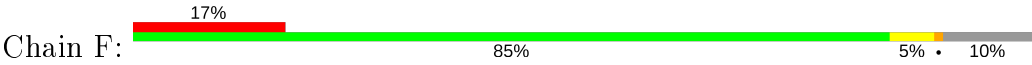
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	331	Total	O	0	0
			331	331		
12	B	275	Total	O	0	0
			275	275		
12	C	454	Total	O	0	0
			454	454		
12	D	218	Total	O	0	0
			218	218		
12	E	91	Total	O	0	0
			91	91		
12	F	178	Total	O	0	0
			178	178		







● Molecule 4: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.30Å 158.50Å 180.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.20 – 2.05 45.20 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.20-2.05) 99.5 (45.20-2.05)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.187 , 0.208 0.189 , 0.195	Depositor DCC
$R_{free}$ test set	9227 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	36311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, TAJ

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	0.23	0/3514	0.42	0/4770
1	C	0.23	0/3577	0.42	0/4857
2	B	0.23	0/3436	0.41	0/4654
2	D	0.23	0/3464	0.40	0/4692
3	E	0.22	0/1044	0.33	0/1385
4	F	0.22	0/2931	0.40	0/3958
All	All	0.23	0/17966	0.40	0/24316

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	3428	3328	3329	5	0
1	C	3468	3368	3349	7	0
2	B	3361	3227	3238	6	0
2	D	3389	3256	3266	8	0
3	E	1018	1028	1007	0	0
4	F	2860	2686	2816	21	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	26	26	0	0
10	B	48	0	0	3	0
10	D	48	0	0	3	0
11	F	31	0	14	5	0
12	A	331	0	0	2	0
12	B	275	0	0	2	0
12	C	454	0	0	2	0
12	D	218	0	0	1	0
12	E	91	0	0	0	0
12	F	178	0	0	1	0
All	All	19352	16959	17093	51	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 (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:150:LYS:HE3	4:F:160:ILE:HD13	1.48	0.94
4:F:148:ILE:HD11	4:F:150:LYS:HE3	1.54	0.88
2:B:424:ASN:ND2	12:B:601:HOH:O	2.21	0.74
4:F:40:MET:SD	12:F:662:HOH:O	2.45	0.73
1:C:128:GLN:NE2	12:C:601:HOH:O	2.23	0.71
4:F:248:GLU:HB2	4:F:249:TYR:HD1	1.58	0.69
2:D:280:SER:OG	2:D:281:GLN:N	2.30	0.62
4:F:248:GLU:HB2	4:F:249:TYR:CD1	2.38	0.59
2:B:147:SER:HG	2:B:190:SER:HG	1.51	0.58
4:F:160:ILE:HD12	4:F:161:LEU:N	2.18	0.58
4:F:148:ILE:HD11	4:F:150:LYS:CE	2.31	0.57
4:F:226:GLU:OE2	4:F:250:SER:OG	2.22	0.56
1:C:234:ILE:HD13	1:C:302:MET:SD	2.45	0.56
1:C:356:ASN:ND2	12:C:607:HOH:O	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:503:TAJ:OBT	10:D:503:TAJ:OBQ	2.25	0.54
4:F:150:LYS:NZ	11:F:401:ACP:O5'	2.38	0.54
10:B:505:TAJ:CBC	10:B:505:TAJ:CBL	2.86	0.53
4:F:150:LYS:HZ2	11:F:401:ACP:C8	2.24	0.51
4:F:160:ILE:HD11	4:F:162:ILE:HG13	1.93	0.51
1:A:358:GLN:NE2	12:A:609:HOH:O	2.41	0.51
4:F:331:GLU:OE2	11:F:401:ACP:O1G	2.28	0.50
4:F:148:ILE:HD11	4:F:160:ILE:HD13	1.93	0.49
4:F:246:GLN:O	4:F:250:SER:HB3	2.12	0.49
2:B:192:HIS:O	12:B:601:HOH:O	2.19	0.49
10:D:503:TAJ:CBL	10:D:503:TAJ:CBC	2.91	0.49
4:F:161:LEU:HD22	4:F:172:PHE:CB	2.45	0.47
2:D:109:THR:OG1	2:D:110:GLU:N	2.47	0.47
10:B:505:TAJ:OBQ	10:B:505:TAJ:OBT	2.33	0.46
4:F:148:ILE:HG13	4:F:160:ILE:CD1	2.45	0.46
10:B:505:TAJ:CAY	10:B:505:TAJ:CAP	2.94	0.46
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.97	0.46
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.57	0.45
2:D:226:ASP:OD1	10:D:503:TAJ:CBL	2.65	0.45
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.48	0.45
2:B:400:ARG:NH1	1:C:439:SER:OG	2.50	0.44
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.99	0.44
2:B:303:ALA:O	2:B:305:CYS:N	2.49	0.44
1:C:209:ILE:HD11	1:C:302:MET:SD	2.58	0.44
2:D:79:ARG:NH1	12:D:611:HOH:O	2.48	0.44
4:F:161:LEU:HD22	4:F:172:PHE:HB2	1.98	0.44
4:F:150:LYS:NZ	11:F:401:ACP:H8	2.33	0.44
2:D:292:THR:HG22	2:D:335:VAL:HG21	2.01	0.43
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.00	0.43
1:A:394:LYS:NZ	12:A:608:HOH:O	2.38	0.42
1:C:320:ARG:HA	1:C:356:ASN:O	2.19	0.42
2:D:283:TYR:HD1	2:D:286:LEU:HB3	1.84	0.42
2:B:136:GLN:HA	2:B:167:ASN:O	2.21	0.41
4:F:150:LYS:HZ2	11:F:401:ACP:H8	1.83	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.41
1:A:209:ILE:HD11	1:A:302:MET:SD	2.60	0.41
4:F:251:LYS:O	4:F:251:LYS:HG2	2.21	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	438/450 (97%)	430 (98%)	8 (2%)	0	100	100
1	C	447/450 (99%)	437 (98%)	10 (2%)	0	100	100
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	429/445 (96%)	421 (98%)	8 (2%)	0	100	100
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100
4	F	340/384 (88%)	327 (96%)	13 (4%)	0	100	100
All	All	2200/2317 (95%)	2153 (98%)	47 (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	371/378 (98%)	370 (100%)	1 (0%)	92	93
1	C	380/378 (100%)	373 (98%)	7 (2%)	59	55
2	B	369/383 (96%)	363 (98%)	6 (2%)	62	59
2	D	372/383 (97%)	369 (99%)	3 (1%)	81	82
3	E	113/127 (89%)	112 (99%)	1 (1%)	78	79
4	F	314/342 (92%)	307 (98%)	7 (2%)	52	46
All	All	1919/1991 (96%)	1894 (99%)	25 (1%)	69	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	437	VAL
2	B	50	ASN
2	B	139	HIS
2	B	278	ARG
2	B	286	LEU
2	B	318	ILE
2	B	390	ARG
1	C	2	ARG
1	C	71	GLU
1	C	245	ASP
1	C	251	ASP
1	C	293	ASN
1	C	347[A]	CYS
1	C	347[B]	CYS
2	D	19	LYS
2	D	139	HIS
2	D	220	THR
3	E	25	LYS
4	F	160	ILE
4	F	174	ASP
4	F	211	TYR
4	F	234	GLN
4	F	238	CYS
4	F	248	GLU
4	F	353	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	TAJ	D	503	2	51,54,54	2.32	9 (17%)	60,94,94	2.23	18 (30%)
8	GDP	B	501	6	24,30,30	1.07	2 (8%)	31,47,47	1.90	7 (22%)
5	GTP	C	501	6	26,34,34	0.94	1 (3%)	33,54,54	1.68	6 (18%)
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.69	6 (18%)
10	TAJ	B	505	2	51,54,54	2.49	10 (19%)	60,94,94	2.13	16 (26%)
11	ACP	F	401	-	27,33,33	2.27	11 (40%)	32,52,52	1.52	4 (12%)
9	MES	B	503	-	12,12,12	2.14	1 (8%)	14,16,16	1.88	4 (28%)
5	GTP	D	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.76	6 (18%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.47	2 (14%)

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	TAJ	D	503	2	-	4/12/145/145	-
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
10	TAJ	B	505	2	-	7/12/145/145	-
11	ACP	F	401	-	-	3/15/38/38	0/3/3/3
9	MES	B	503	-	-	5/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	TAJ	CAT-CAS	-11.66	1.38	1.52
10	D	503	TAJ	CAT-CAS	-9.98	1.40	1.52
10	D	503	TAJ	CAM-CAS	-7.81	1.38	1.51
10	B	505	TAJ	CAM-CAS	-7.76	1.38	1.51
9	B	504	MES	C8-S	-7.51	1.66	1.77
9	B	503	MES	C8-S	-7.19	1.67	1.77
11	F	401	ACP	PG-O2G	-5.45	1.42	1.54
11	F	401	ACP	PG-O1G	4.47	1.59	1.50
11	F	401	ACP	C2'-C1'	-4.43	1.47	1.53
10	D	503	TAJ	CBF-CBE	4.31	1.55	1.51
10	B	505	TAJ	CBF-CBE	4.30	1.55	1.51
10	B	505	TAJ	CBH-CBD	-3.89	1.51	1.57
10	D	503	TAJ	CBH-CBD	-3.78	1.51	1.57
10	B	505	TAJ	CAX-CAW	-3.70	1.50	1.56
11	F	401	ACP	PB-O1B	-3.70	1.42	1.51
10	B	505	TAJ	CAQ-CAM	-3.62	1.49	1.56
10	B	505	TAJ	CAA-CAE	3.59	1.51	1.46
10	D	503	TAJ	CAQ-CAM	-3.57	1.49	1.56
8	B	501	GDP	C6-C5	3.49	1.47	1.41
10	D	503	TAJ	CAX-CAW	-3.46	1.50	1.56
10	D	503	TAJ	CAA-CAE	3.15	1.51	1.46
5	A	501	GTP	C6-N1	3.13	1.38	1.33
5	D	501	GTP	C6-N1	3.09	1.38	1.33
5	C	501	GTP	C6-N1	2.86	1.38	1.33
11	F	401	ACP	C4-N3	-2.83	1.31	1.35
11	F	401	ACP	O4'-C4'	-2.75	1.38	1.45
10	B	505	TAJ	OBV-CBE	2.55	1.44	1.40
11	F	401	ACP	C5-N7	-2.47	1.30	1.39
10	D	503	TAJ	OBV-CBE	2.41	1.43	1.40
11	F	401	ACP	PA-O2A	-2.34	1.44	1.55
11	F	401	ACP	C2'-C3'	-2.31	1.47	1.53
8	B	501	GDP	C5-C4	2.25	1.46	1.40
10	B	505	TAJ	CBB-CBA	2.25	1.57	1.53
11	F	401	ACP	PA-O1A	-2.24	1.42	1.50
10	B	505	TAJ	CAX-CBC	-2.10	1.52	1.56
11	F	401	ACP	O3'-C3'	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	TAJ	CBB-CBA	2.02	1.57	1.53

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	TAJ	OBS-CBI-CBH	-7.37	120.87	128.28
10	D	503	TAJ	OBS-CBI-CBH	-7.24	121.01	128.28
10	D	503	TAJ	CAI-CAM-CAS	-6.31	105.03	113.18
5	D	501	GTP	N3-C2-N1	-5.48	119.91	127.22
5	A	501	GTP	N3-C2-N1	-5.33	120.11	127.22
5	C	501	GTP	N3-C2-N1	-5.27	120.19	127.22
10	B	505	TAJ	CAR-OAB-CAJ	-4.97	110.55	117.81
10	B	505	TAJ	OBJ-CBI-CBH	4.91	115.11	110.11
8	B	501	GDP	C6-N1-C2	4.85	123.63	115.93
10	D	503	TAJ	OBJ-CBI-CBH	4.69	114.88	110.11
10	D	503	TAJ	CAR-OAB-CAJ	-4.60	111.09	117.81
8	B	501	GDP	C6-C5-C4	-4.49	116.51	120.80
10	B	505	TAJ	CAX-CBC-CBB	-4.32	98.19	107.51
10	D	503	TAJ	CAX-CBC-CBB	-4.12	98.61	107.51
5	D	501	GTP	C2-N3-C4	4.12	120.06	115.36
8	B	501	GDP	C5-C6-N1	-4.10	117.82	123.43
5	A	501	GTP	C2-N3-C4	4.00	119.93	115.36
10	D	503	TAJ	CAZ-OAD-CAL	-3.94	111.62	117.72
8	B	501	GDP	C2-N3-C4	3.84	119.74	115.36
10	B	505	TAJ	CAA-OBK-CAE	3.77	63.00	60.59
5	C	501	GTP	C2-N3-C4	3.66	119.54	115.36
8	B	501	GDP	N3-C2-N1	-3.61	122.41	127.22
9	B	503	MES	C5-N4-C3	3.54	116.80	108.83
9	B	503	MES	O3S-S-C8	3.45	111.35	105.77
10	D	503	TAJ	CAI-CAM-CAQ	-3.45	106.93	111.73
10	D	503	TAJ	CAA-OBK-CAE	3.39	62.76	60.59
11	F	401	ACP	C4-C5-N7	-3.34	105.92	109.40
5	C	501	GTP	C5-C6-N1	-3.28	118.95	123.43
9	B	504	MES	C5-N4-C3	3.24	116.12	108.83
10	B	505	TAJ	CAI-CAM-CAQ	-3.22	107.25	111.73
5	D	501	GTP	PB-O3B-PG	-3.20	121.83	132.83
10	B	505	TAJ	OBK-CAA-CAR	-3.18	109.53	116.05
10	B	505	TAJ	OBV-CBE-OBJ	3.11	114.72	109.03
5	A	501	GTP	C5-C6-N1	-3.07	119.23	123.43
10	B	505	TAJ	CAI-CAM-CAS	-3.06	109.23	113.18
5	D	501	GTP	C5-C6-N1	-2.99	119.34	123.43
5	C	501	GTP	C6-N1-C2	2.99	120.67	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	O2'-C2'-C3'	-2.98	102.18	111.82
5	D	501	GTP	PA-O3A-PB	-2.95	122.72	132.83
5	C	501	GTP	PB-O3B-PG	-2.93	122.76	132.83
10	D	503	TAJ	OBV-CBE-OBJ	2.93	114.39	109.03
5	C	501	GTP	PA-O3A-PB	-2.87	122.99	132.83
10	D	503	TAJ	OBK-CAA-CAR	-2.85	110.21	116.05
11	F	401	ACP	O2B-PB-C3B	2.84	118.22	106.58
9	B	504	MES	O3S-S-C8	2.82	110.33	105.77
10	D	503	TAJ	OBU-CAS-CAM	-2.79	118.31	122.75
10	B	505	TAJ	OAD-CAL-CAP	2.78	116.21	111.09
5	A	501	GTP	C6-N1-C2	2.77	120.33	115.93
5	D	501	GTP	C6-N1-C2	2.76	120.31	115.93
5	A	501	GTP	PA-O3A-PB	-2.74	123.44	132.83
5	A	501	GTP	PB-O3B-PG	-2.72	123.50	132.83
10	D	503	TAJ	OAC-CAK-CAO	2.71	116.08	111.09
10	B	505	TAJ	CBE-OBJ-CBI	-2.65	105.90	110.38
8	B	501	GDP	PA-O3A-PB	-2.64	123.75	132.83
10	D	503	TAJ	CBE-OBJ-CBI	-2.63	105.94	110.38
10	B	505	TAJ	OAC-CAK-CAO	2.60	115.87	111.09
11	F	401	ACP	N3-C2-N1	-2.53	124.72	128.68
10	B	505	TAJ	CAY-OAC-CAK	-2.52	114.13	117.81
10	D	503	TAJ	CAY-OAC-CAK	-2.45	114.23	117.81
10	B	505	TAJ	OBV-CBE-CBD	-2.42	107.51	114.38
9	B	503	MES	O1S-S-C8	2.30	109.69	106.92
10	D	503	TAJ	OAD-CAL-CAP	2.30	115.32	111.09
10	B	505	TAJ	CAV-CAZ-CAY	-2.29	109.30	113.90
10	B	505	TAJ	OBK-CAA-CAE	-2.24	57.24	59.89
10	D	503	TAJ	OBV-CBE-CBD	-2.22	108.08	114.38
10	D	503	TAJ	OBK-CAA-CAE	-2.17	57.32	59.89
9	B	503	MES	C6-O1-C2	2.16	117.10	109.89
8	B	501	GDP	C4-C5-N7	-2.12	107.19	109.40
10	D	503	TAJ	CAQ-CAV-CAZ	-2.09	113.27	115.64

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A

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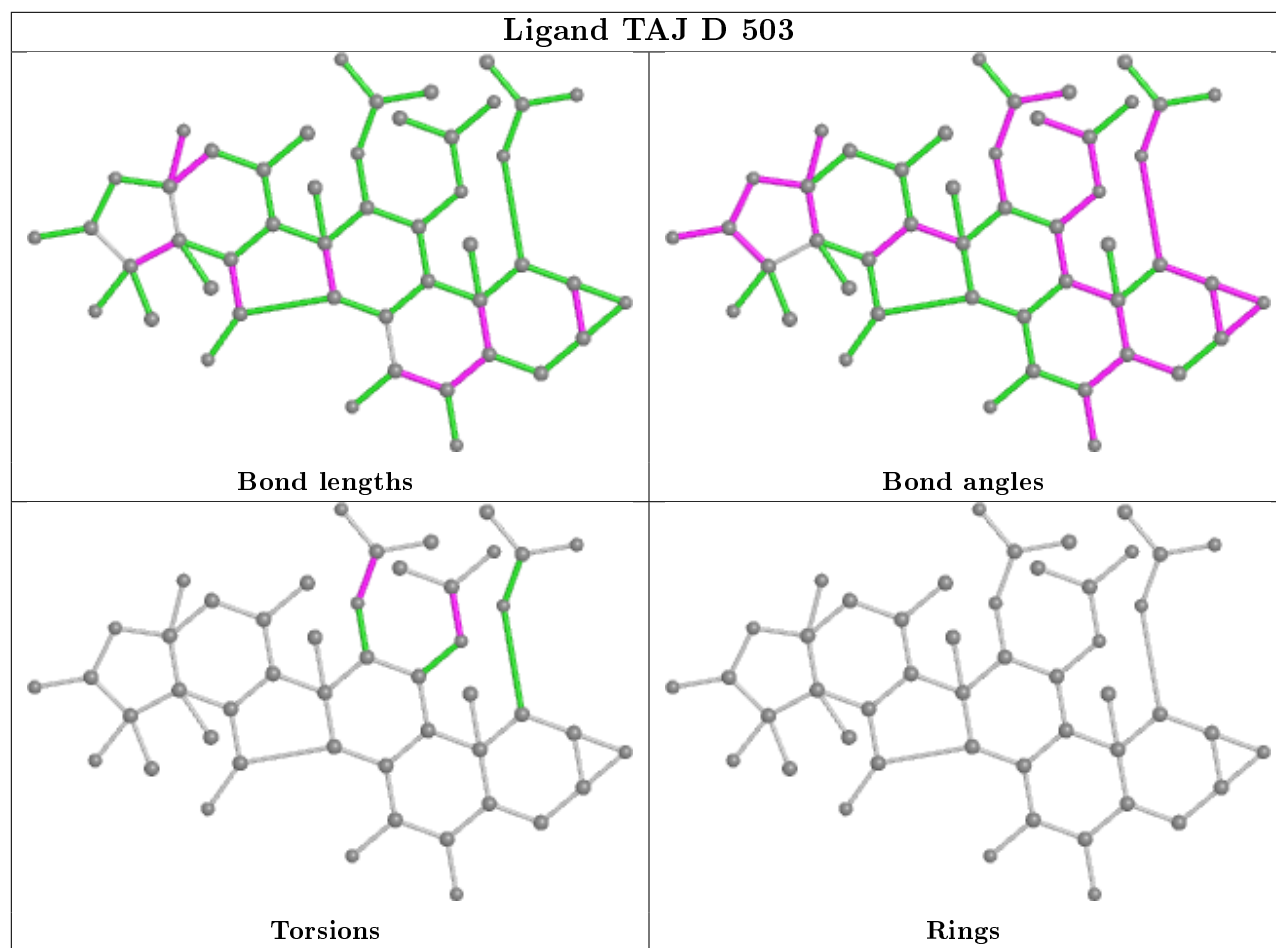
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
10	D	503	TAJ	OAH-CAL-OAD-CAZ
10	D	503	TAJ	CAP-CAL-OAD-CAZ
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	504	MES	C7-C8-S-O1S
10	B	505	TAJ	OAH-CAL-OAD-CAZ
10	B	505	TAJ	CAN-CAJ-OAB-CAR
10	B	505	TAJ	CAP-CAL-OAD-CAZ
10	B	505	TAJ	OAF-CAJ-OAB-CAR
10	B	505	TAJ	CAO-CAK-OAC-CAY
10	D	503	TAJ	CAO-CAK-OAC-CAY
10	B	505	TAJ	OAG-CAK-OAC-CAY
10	D	503	TAJ	OAG-CAK-OAC-CAY
9	B	503	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O3S
9	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	504	MES	C8-C7-N4-C5
8	B	501	GDP	PB-O3A-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	505	TAJ	CAA-CAR-OAB-CAJ
5	A	501	GTP	PB-O3A-PA-O1A

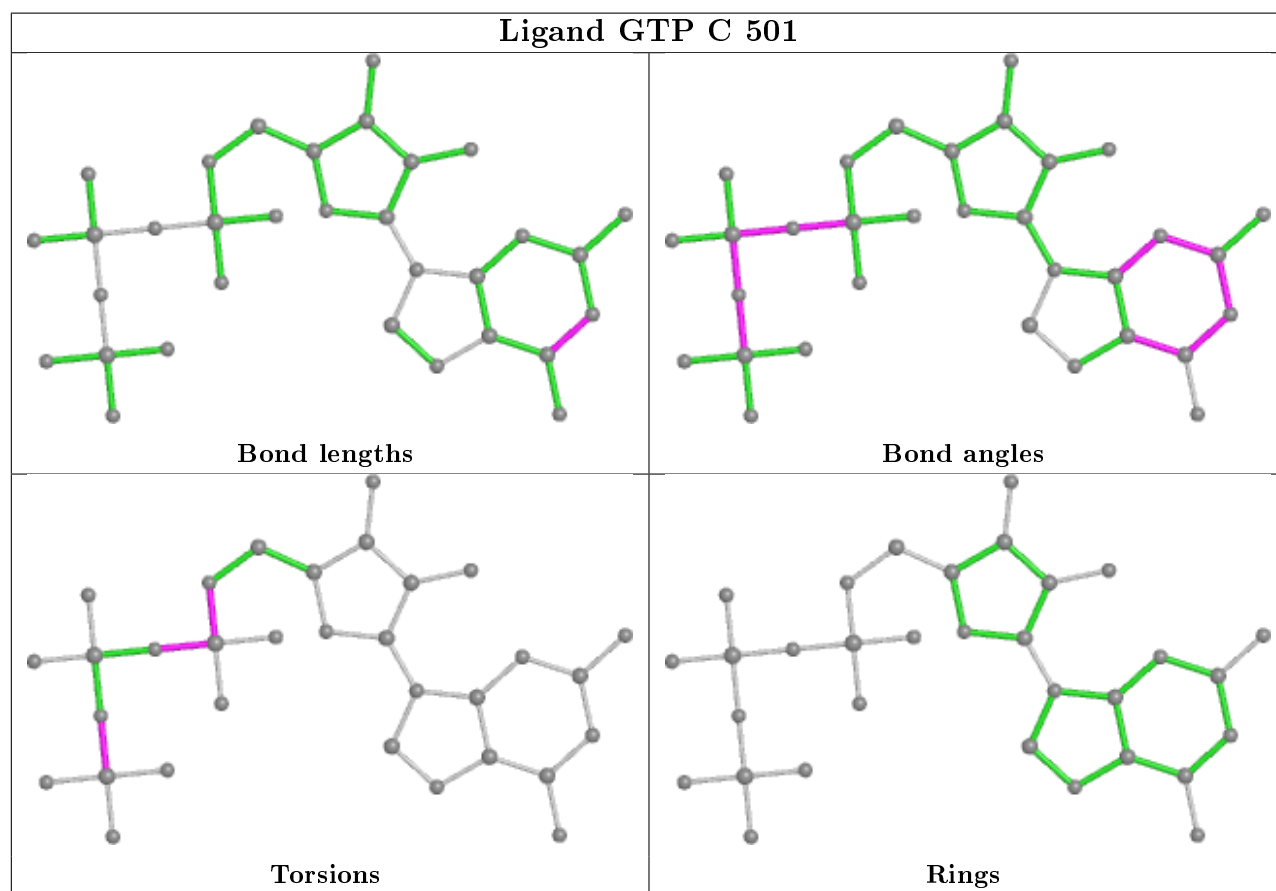
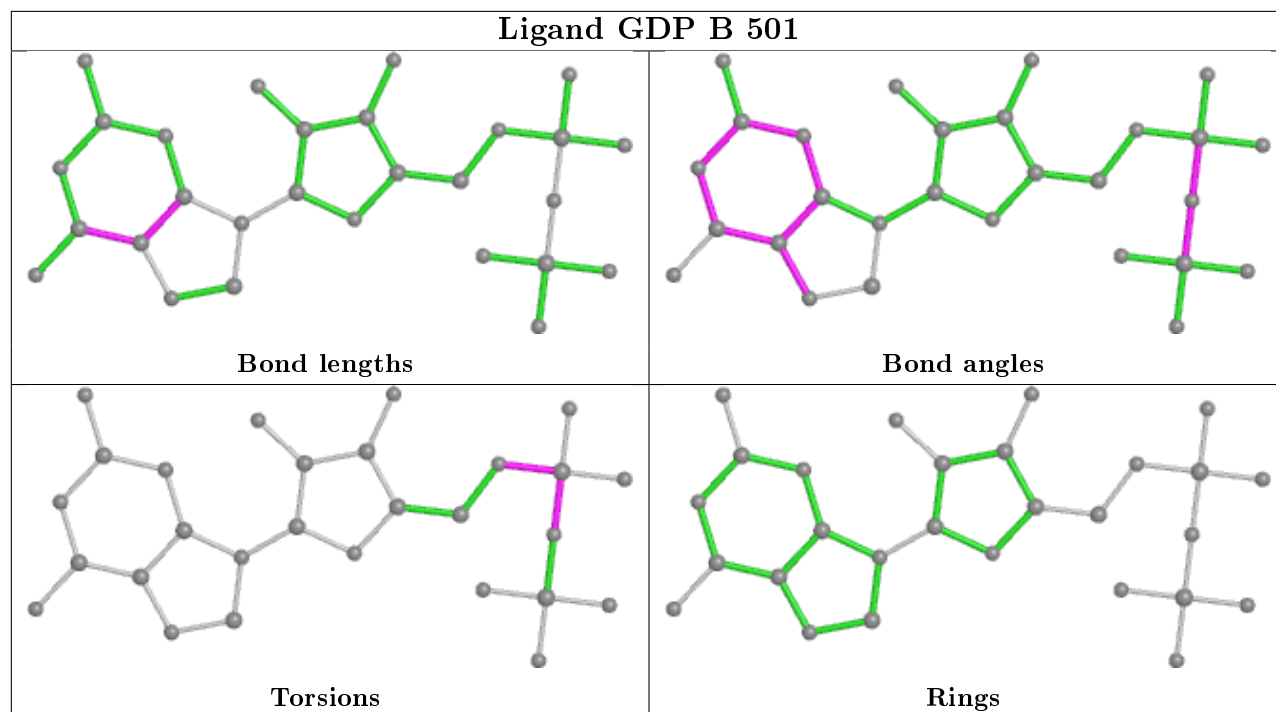
There are no ring outliers.

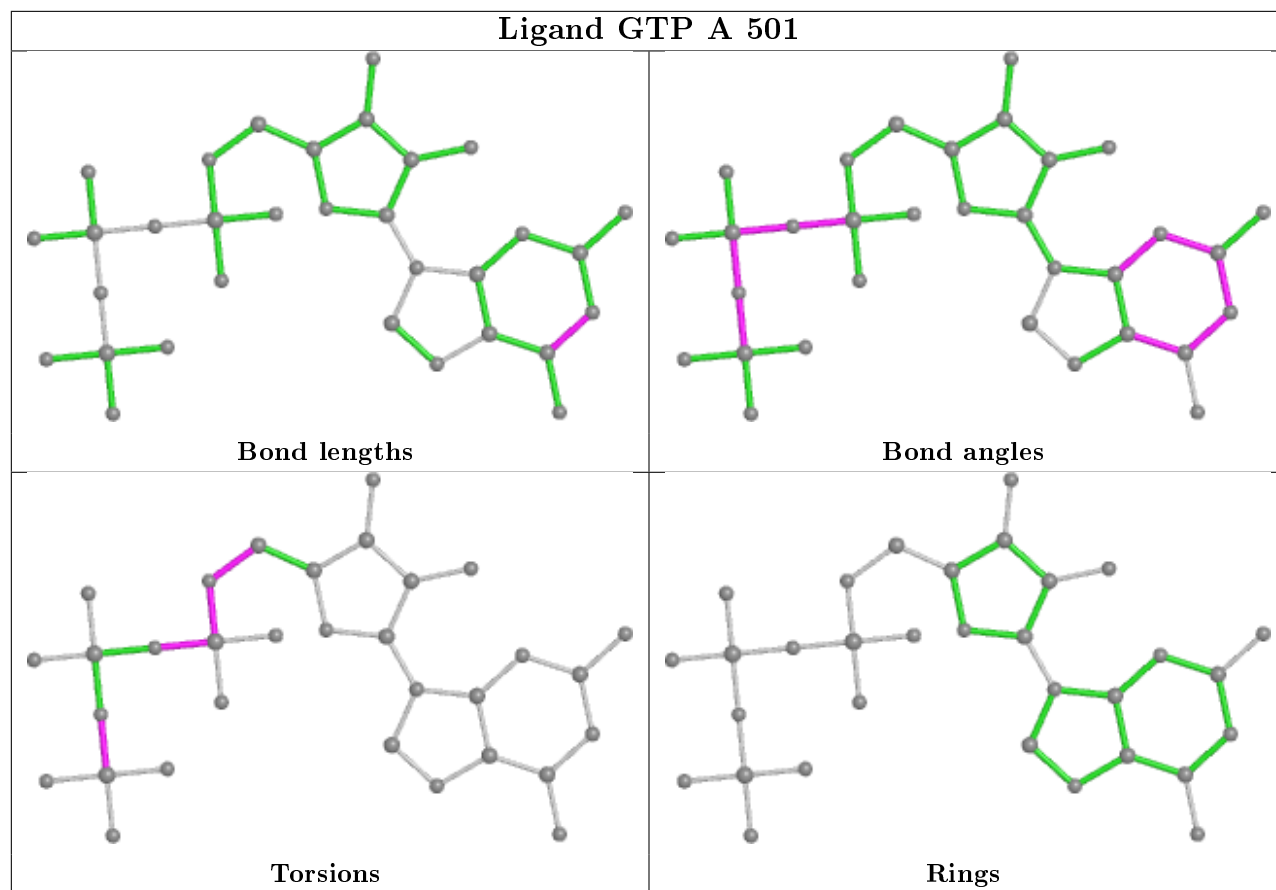
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	TAJ	3	0
10	B	505	TAJ	3	0
11	F	401	ACP	5	0

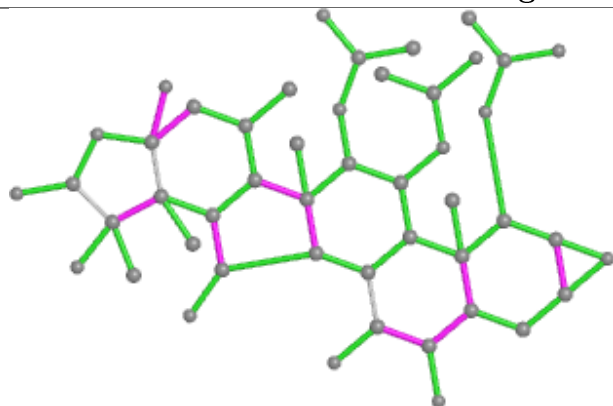
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



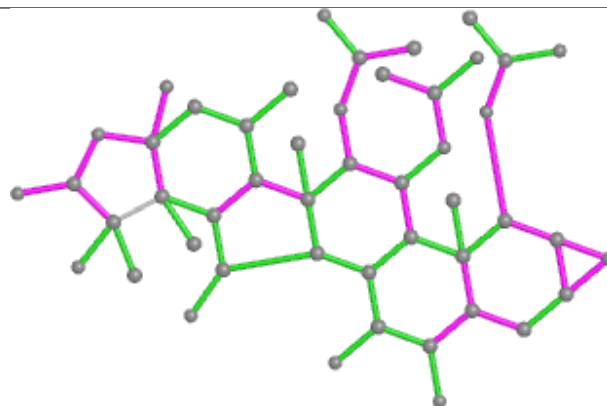




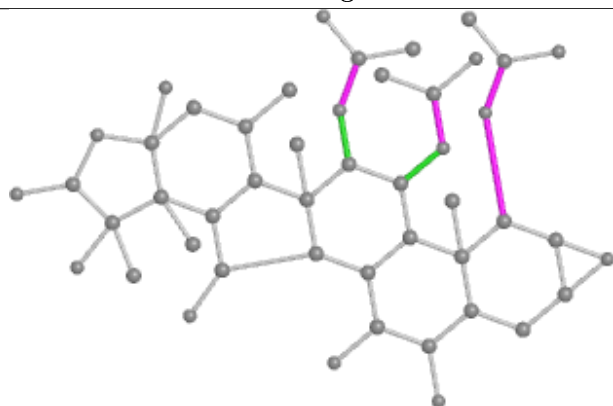
## Ligand TAJ B 505



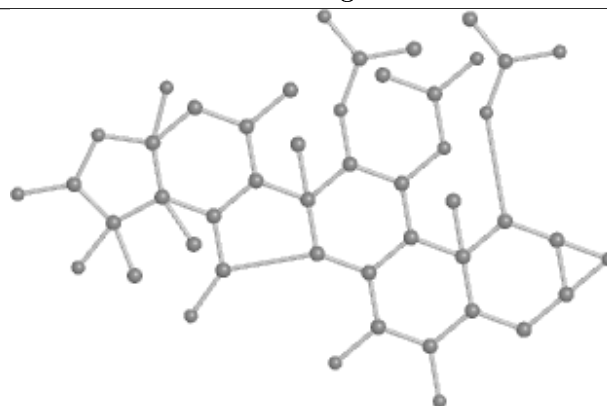
Bond lengths



Bond angles

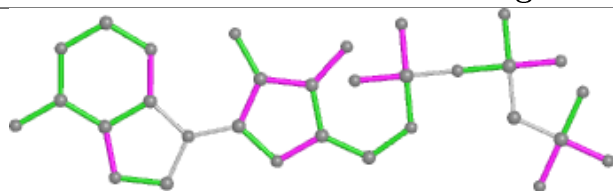


Torsions

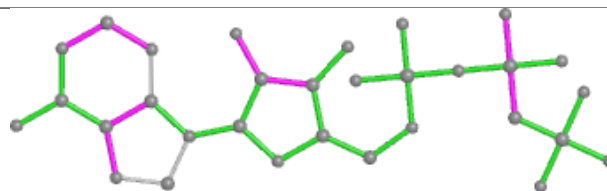


Rings

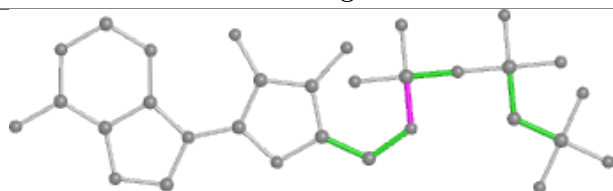
## Ligand ACP F 401



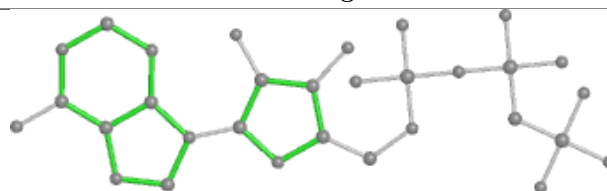
Bond lengths



Bond angles

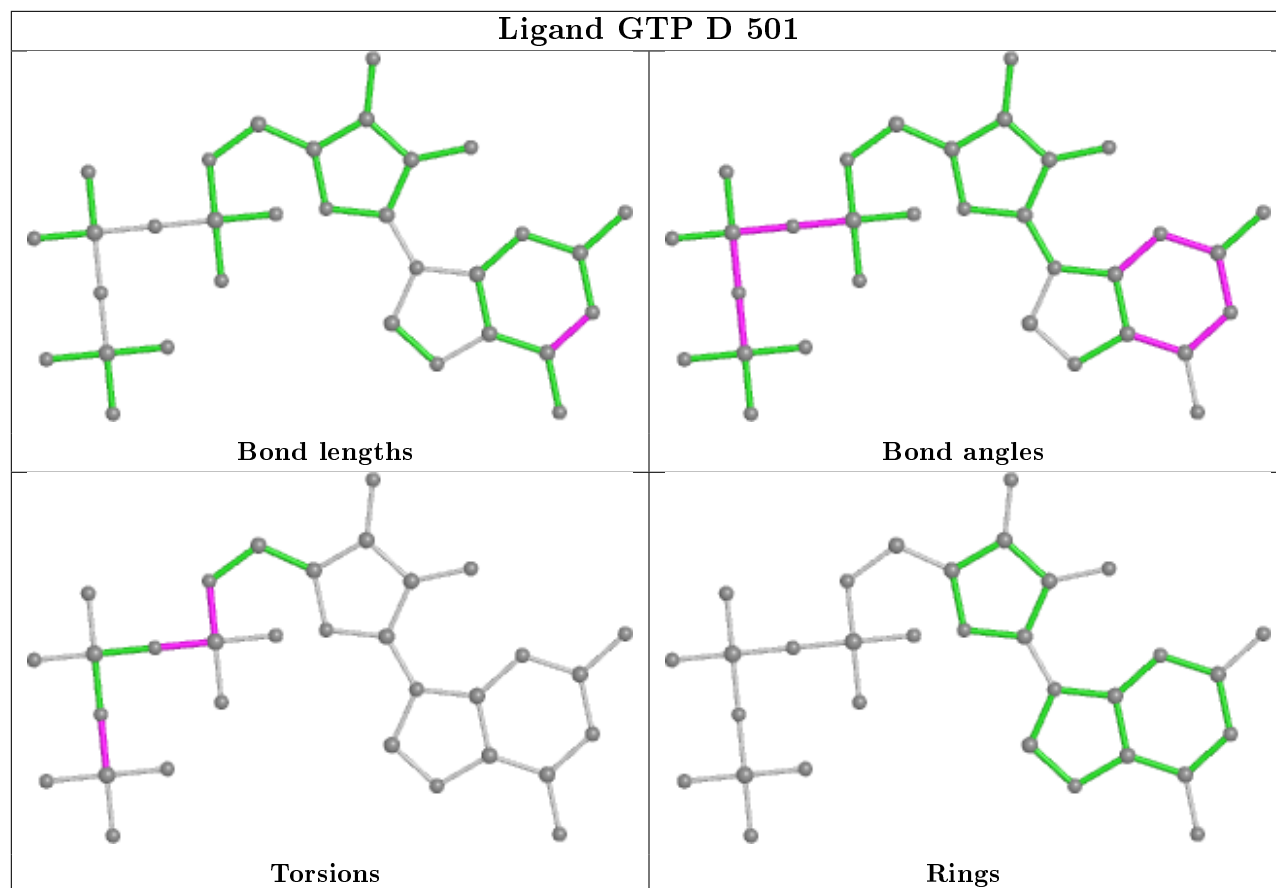


Torsions



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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/450 (97%)	-0.11	10 (2%) 60 64	14, 26, 51, 64	0
1	C	440/450 (97%)	-0.27	4 (0%) 84 86	11, 20, 45, 70	0
2	B	427/445 (95%)	0.08	16 (3%) 41 45	13, 29, 59, 90	0
2	D	431/445 (96%)	0.27	24 (5%) 24 26	14, 32, 69, 128	0
3	E	121/143 (84%)	0.28	8 (6%) 18 19	17, 39, 67, 80	0
4	F	347/384 (90%)	0.70	67 (19%) 1 0	19, 40, 90, 115	0
All	All	2203/2317 (95%)	0.12	129 (5%) 22 24	11, 30, 68, 128	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	283	TYR	9.2
2	B	57	THR	8.0
2	D	284	ARG	7.9
4	F	142	ARG	7.5
2	D	285	ALA	6.9
4	F	130	VAL	6.9
4	F	177	GLY	6.6
4	F	249	TYR	6.3
2	D	220	THR	6.2
4	F	101	TYR	6.1
4	F	372	THR	5.9
2	D	57	THR	5.8
4	F	173	ILE	5.7
4	F	182	ILE	5.6
4	F	176	GLN	5.4
4	F	103	THR	5.4
4	F	132	LEU	5.0
4	F	178	GLN	5.0
2	D	400	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
3	E	139	LEU	4.9
4	F	362	ALA	4.8
4	F	248	GLU	4.6
2	D	281	GLN	4.6
4	F	231	ALA	4.6
2	B	59	ASN	4.4
4	F	179	VAL	4.4
1	A	262	TYR	4.3
2	D	404	PHE	4.2
4	F	245	ILE	4.2
2	B	56	ALA	4.2
4	F	102	PRO	4.2
4	F	174	ASP	4.1
2	D	221	THR	4.1
1	A	282	TYR	4.1
2	B	279	GLY	4.0
4	F	133	ALA	4.0
2	D	75	MET	4.0
4	F	138	ARG	4.0
4	F	129	GLU	3.9
3	E	28	SER	3.9
4	F	251	LYS	3.9
4	F	25	GLY	3.8
2	D	282	GLN	3.8
4	F	160	ILE	3.7
4	F	137	ARG	3.7
4	F	131	PHE	3.7
4	F	236	LYS	3.6
2	D	94	PHE	3.6
4	F	233	PHE	3.6
4	F	99	VAL	3.6
2	D	58	GLY	3.5
2	B	220	THR	3.5
2	B	281	GLN	3.4
2	B	33	THR	3.4
2	B	280	SER	3.3
4	F	244	CYS	3.3
3	E	26	PRO	3.3
4	F	172	PHE	3.3
2	D	59	ASN	3.2
4	F	1	MET	3.2
4	F	169	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	170	LEU	3.2
4	F	361	LEU	3.2
2	B	58	GLY	3.1
4	F	141	GLY	3.1
2	D	286	LEU	3.1
2	B	41	ASP	3.1
3	E	140	LYS	3.1
2	D	401	ARG	3.1
2	B	60	LYS	3.1
2	B	221	THR	3.0
2	B	82	PRO	3.0
4	F	167	SER	2.9
2	D	219	LEU	2.9
4	F	128	ARG	2.9
2	B	219	LEU	2.9
4	F	136	ASN	2.9
4	F	134	ALA	2.9
4	F	100	ILE	2.8
2	D	215	ARG	2.8
1	C	340	SER	2.8
4	F	181	VAL	2.8
1	A	281	ALA	2.8
4	F	135	TYR	2.7
4	F	175	GLU	2.7
4	F	235	ASP	2.7
2	D	280	SER	2.6
4	F	180	HIS	2.6
4	F	256	TYR	2.6
1	A	180	ALA	2.6
1	A	365	GLY	2.6
4	F	171	ASP	2.5
4	F	150	LYS	2.5
1	C	1	MET	2.5
4	F	252	ASN	2.5
4	F	166	ALA	2.5
1	C	440	VAL	2.5
4	F	194	PRO	2.5
3	E	27	PRO	2.4
4	F	143	GLU	2.4
4	F	254	GLY	2.4
3	E	52	LYS	2.4
2	D	37	HIS	2.4

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	2.4
4	F	253	TYR	2.4
1	A	57	GLY	2.4
4	F	139	ARG	2.4
4	F	126	ASP	2.4
4	F	22	LEU	2.3
2	D	409	THR	2.3
4	F	232	ASN	2.3
4	F	237	THR	2.3
4	F	255	ARG	2.3
2	B	55	GLU	2.2
3	E	135	LYS	2.2
4	F	31	ARG	2.2
2	D	397	ALA	2.2
4	F	20	LEU	2.2
1	A	42	ILE	2.1
3	E	132	GLU	2.1
4	F	165	GLU	2.1
1	C	253	THR	2.1
2	B	61	TYR	2.1
2	D	402	LYS	2.1
1	A	346	TRP	2.1
4	F	140	GLU	2.0
1	A	437	VAL	2.0
2	D	33	THR	2.0
4	F	250	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [\(i\)](#)

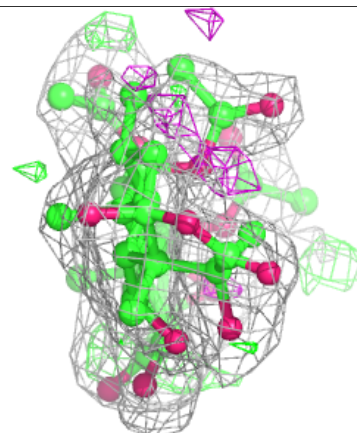
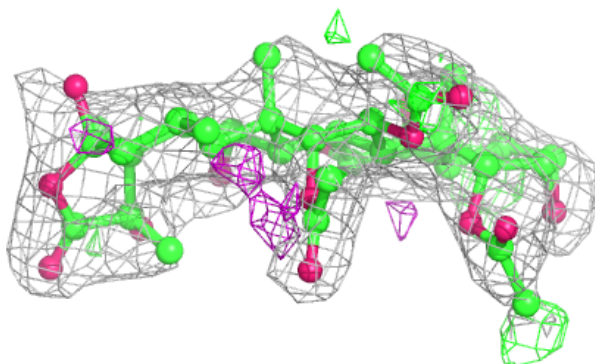
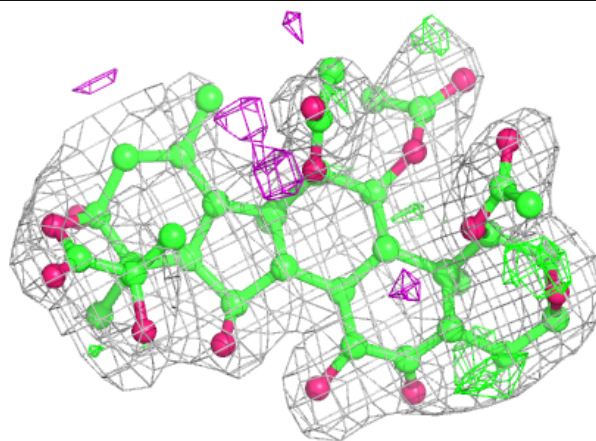
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	TAJ	B	505	48/48	0.80	0.19	53,62,71,79	0
10	TAJ	D	503	48/48	0.87	0.14	44,57,71,77	0
9	MES	B	504	12/12	0.92	0.17	35,44,52,54	0
9	MES	B	503	12/12	0.93	0.13	28,38,56,68	0
11	ACP	F	401	31/31	0.93	0.12	37,50,86,90	0
7	CA	A	503	1/1	0.95	0.05	37,37,37,37	0
6	MG	C	502	1/1	0.95	0.18	15,15,15,15	0
8	GDP	B	501	28/28	0.96	0.14	14,20,26,26	0
5	GTP	D	501	32/32	0.96	0.10	20,27,37,40	0
5	GTP	A	501	32/32	0.97	0.19	14,18,21,24	0
6	MG	D	502	1/1	0.98	0.05	33,33,33,33	0
6	MG	A	502	1/1	0.98	0.21	18,18,18,18	0
5	GTP	C	501	32/32	0.98	0.15	11,14,17,17	0
7	CA	C	503	1/1	0.99	0.04	26,26,26,26	0
6	MG	B	502	1/1	0.99	0.15	11,11,11,11	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.

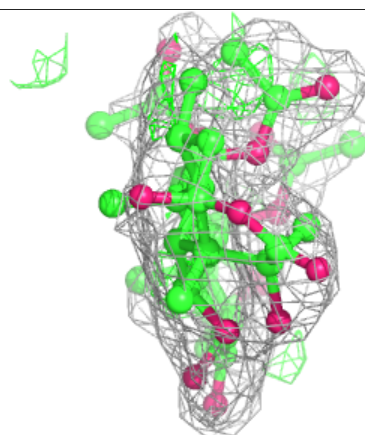
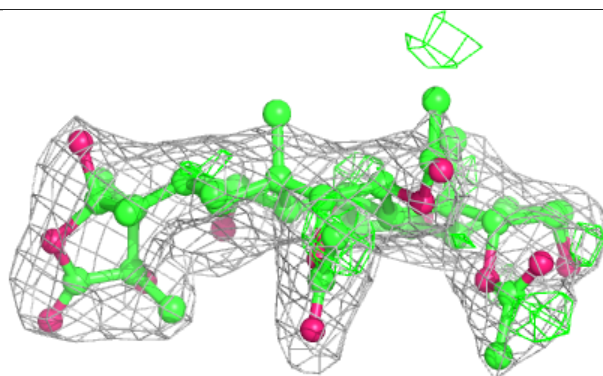
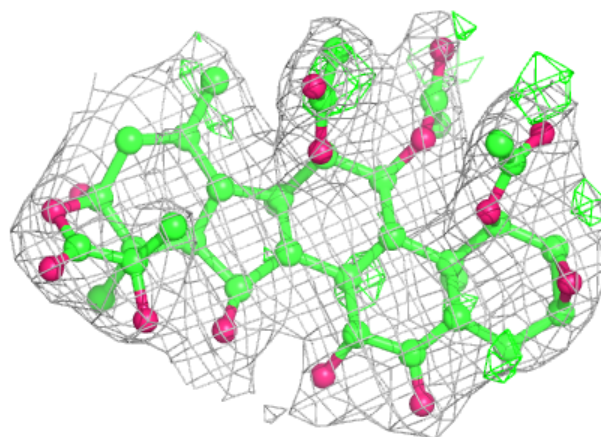
#### Electron density around TAJ B 505:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)

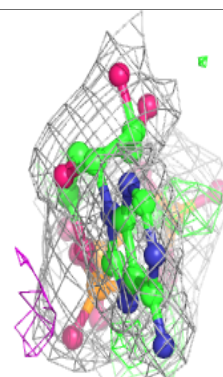
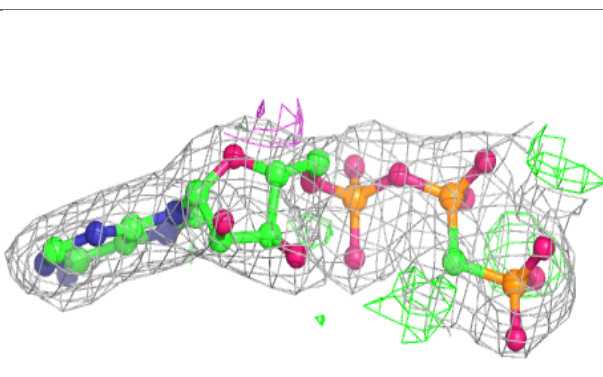
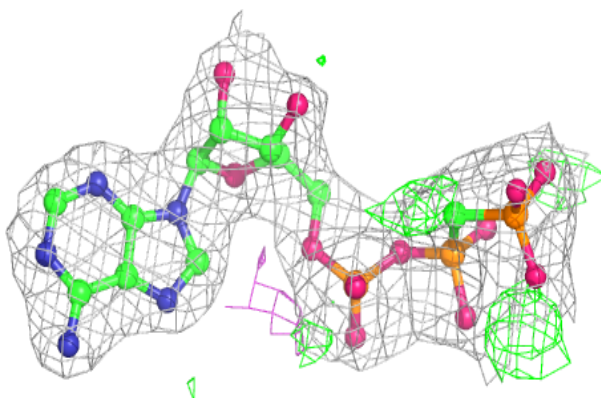


**Electron density around TAJ D 503:**

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

**Electron density around ACP F 401:**

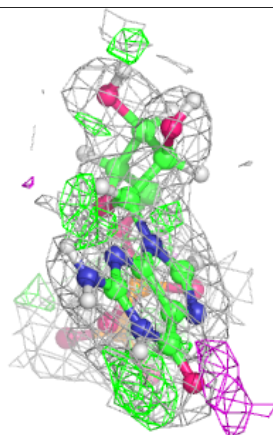
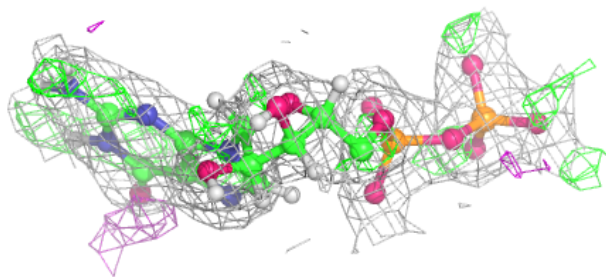
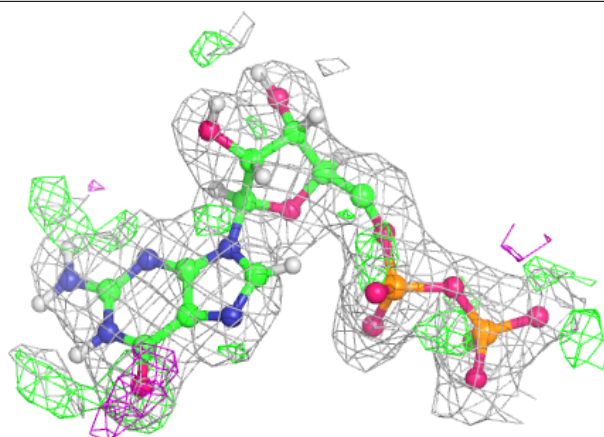
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



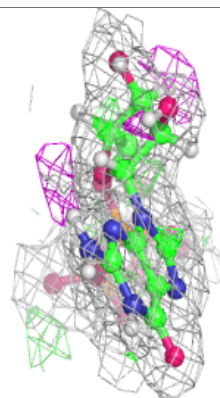
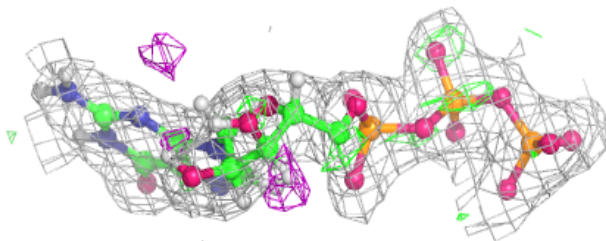
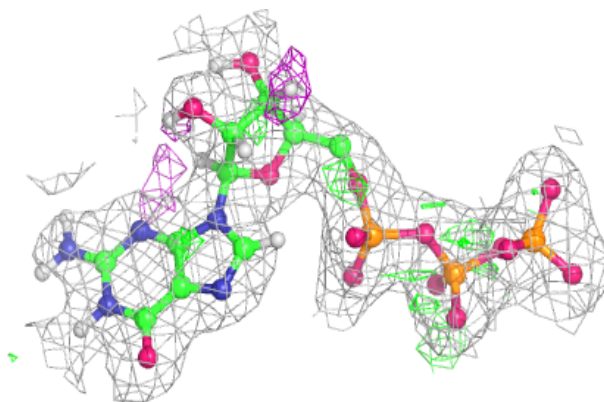


**Electron density around GDP B 501:**

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

**Electron density around GTP D 501:**

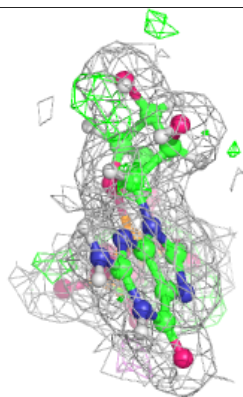
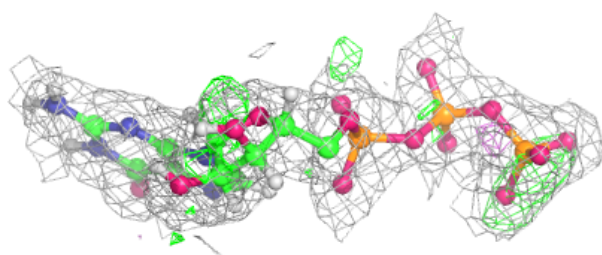
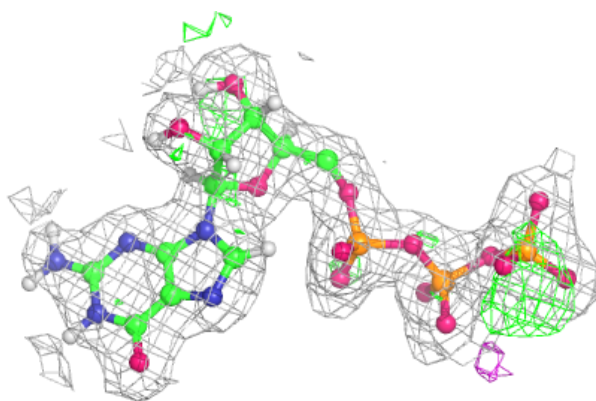
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



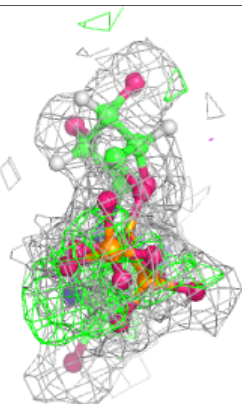
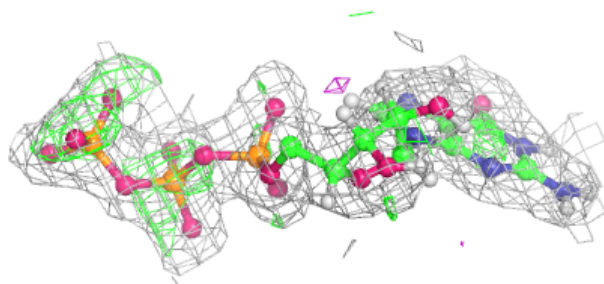
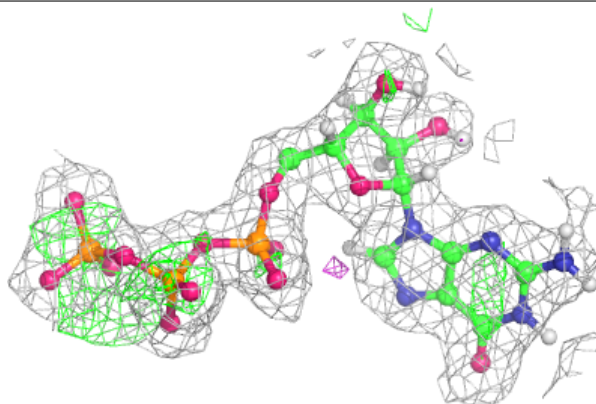


**Electron density around GTP A 501:**

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

**Electron density around 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.