



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:20 AM UTC

PDB ID : 5J2U / pdb_00005j2u
Title : Tubulin-MMAF complex
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Deposited on : 2016-03-30
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

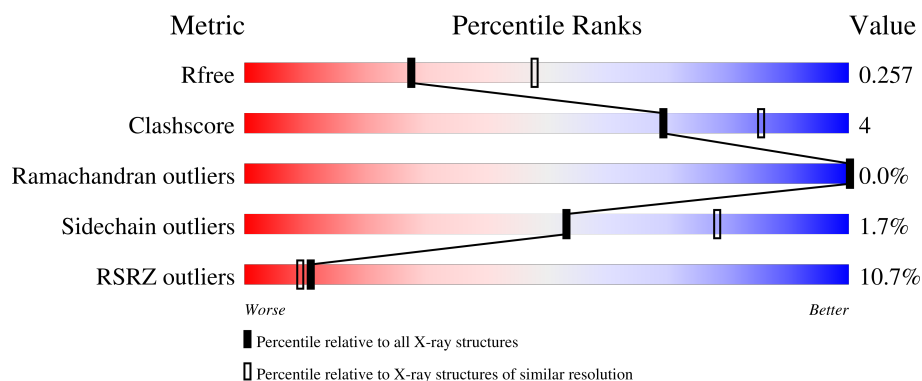
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	451	13% 90% 8% .
1	C	451	5% 89% 9% .
2	B	445	4% 88% 9% .
2	D	445	11% 87% 8% 5%
3	E	143	13% 76% 10% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	17% 74% 14% • 10%
5	G	5	20% 60% 20%
5	H	5	20% 20% 60%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 35235 atoms, of which 17304 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	439	Total	C	H	N	O	S	0	6	0
			6834	2194	3377	584	657	22			
1	C	440	Total	C	H	N	O	S	0	12	0
			6894	2212	3407	585	666	24			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	428	Total	C	H	N	O	S	4	8	0
			6685	2137	3285	580	656	27			
2	D	422	Total	C	H	N	O	S	0	4	0
			6532	2093	3204	563	645	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	6	0
			2106	644	1064	186	206	6			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	344	Total	C	H	N	O	S	0	2	0
			5605	1808	2787	479	517	14			

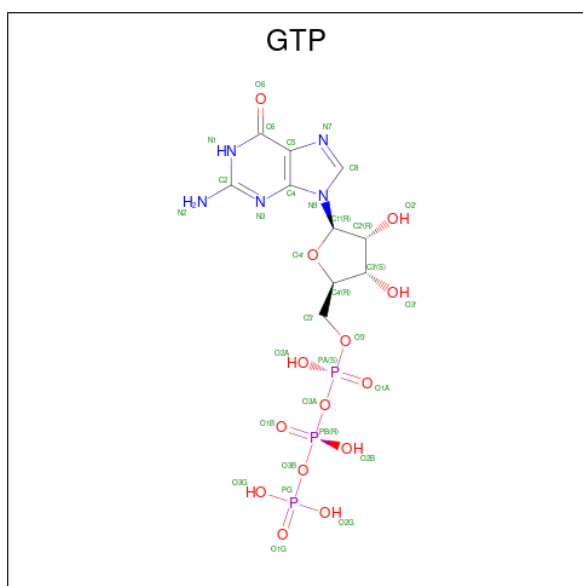
There are 6 discrepancies between the modelled and reference sequences:

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 a protein called Monomethyl auristatin F (MMAF).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	5	Total 116	C 39	H 64	N 5	O 8	0	0	0
5	H	5	Total 116	C 39	H 64	N 5	O 8	0	0	0

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		
6	C	1	Total	C	H	N	O	P	0	0
			41	10	9	5	14	3		

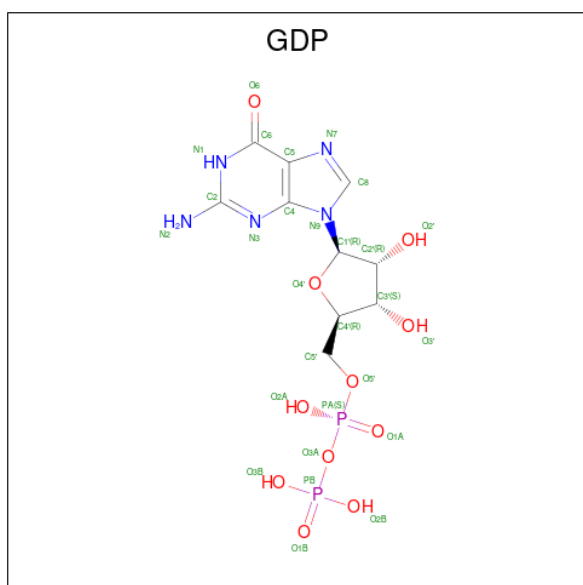
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

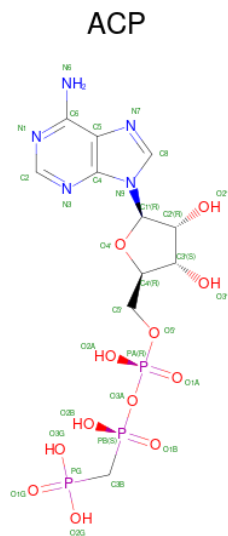
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	2	Total	Mg	0	0
			2	2		
7	C	2	Total	Mg	0	0
			2	2		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

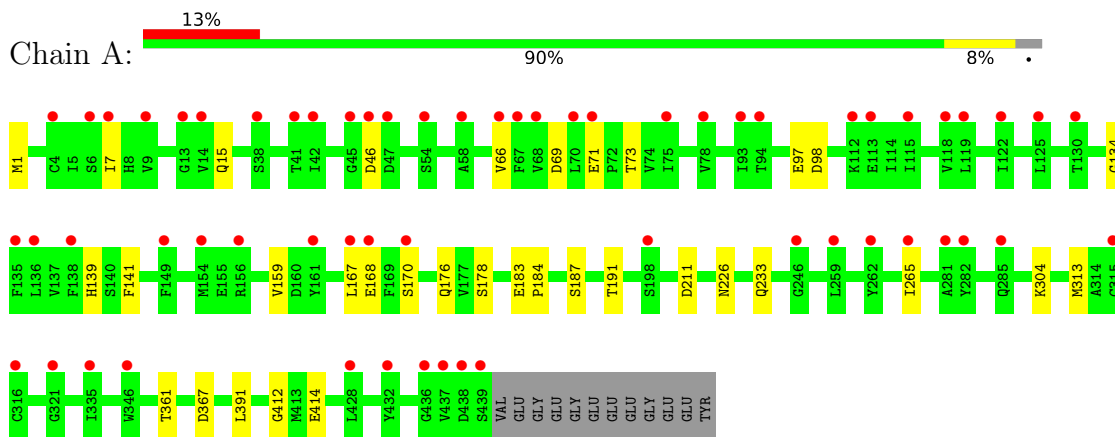
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	12	Total O 12 12	0	0
11	B	52	Total O 52 52	0	0
11	C	47	Total O 47 47	0	0
11	D	9	Total O 9 9	0	0
11	E	9	Total O 9 9	0	0
11	F	9	Total O 9 9	0	0

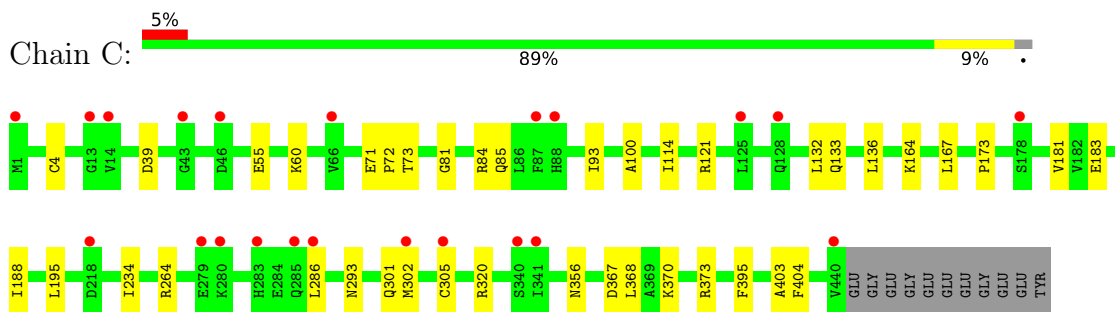
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

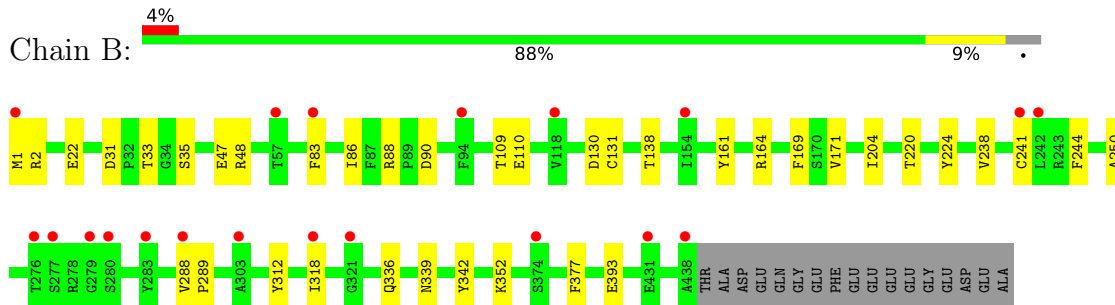
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain



- Molecule 2: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.57Å 155.39Å 182.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.65 – 2.50 56.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (56.65-2.50) 86.4 (56.65-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.216 , 0.250 0.226 , 0.257	Depositor DCC
R_{free} test set	2000 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35235	wwPDB-VP
Average B, all atoms (Å ²)	78.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3WT, MVA, ACP, GTP, MG, 3WU, CA, GDP

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	0.40	0/3554	0.73	1/4826 (0.0%)
1	C	0.46	1/3601 (0.0%)	0.73	0/4892
2	B	0.36	0/3503	0.67	0/4743
2	D	0.34	0/3413	0.76	4/4624 (0.1%)
3	E	0.32	0/1068	0.70	0/1418
4	F	0.37	0/2886	0.75	3/3899 (0.1%)
5	G	2.56	1/18 (5.6%)	1.51	0/20
5	H	2.54	2/18 (11.1%)	1.07	0/20
All	All	0.40	4/18061 (0.0%)	0.73	8/24442 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	1
5	G	0	2
5	H	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	5	PHE	CG-CD2	6.96	1.53	1.38
5	G	5	PHE	CG-CD2	6.87	1.53	1.38
1	C	133	GLN	C-O	-5.17	1.18	1.24
5	H	5	PHE	CE2-CZ	5.05	1.53	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	109	THR	N-CA-C	16.41	131.43	111.40
2	D	110	GLU	N-CA-C	-12.38	98.66	113.88
4	F	238	CYS	N-CA-C	-10.07	100.13	114.12
2	D	109	THR	CB-CA-C	-8.15	97.11	110.79
2	D	110	GLU	N-CA-CB	7.32	120.32	110.59

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	149	ALA	Peptide
5	G	4	3WU	Peptide,Mainchain
5	H	4	3WU	Peptide,Mainchain

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	3457	3377	3390	22	0
1	C	3487	3407	3424	23	0
2	B	3400	3285	3287	24	0
2	D	3328	3204	3215	21	1
3	E	1042	1064	1070	12	0
4	F	2818	2787	2796	31	1
5	G	52	64	43	0	0
5	H	52	64	43	2	0
6	A	32	9	12	1	0
6	C	32	9	12	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
8	A	1	0	0	0	0
9	B	28	10	12	0	0
9	D	28	10	12	1	0
10	F	31	14	14	0	0
11	A	12	0	0	0	0
11	B	52	0	0	3	0
11	C	47	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	9	0	0	1	0
11	E	9	0	0	1	0
11	F	9	0	0	1	0
All	All	17931	17304	17330	124	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 124 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)
3:E:46:SER:OG	3:E:49:GLU:HB2	1.29	1.29
4:F:82:LYS:NZ	4:F:127:GLU:OE2	1.92	1.02
3:E:46:SER:HG	3:E:49:GLU:HB2	1.26	0.98
3:E:46:SER:OG	3:E:49:GLU:CB	2.17	0.92
1:C:60:LYS:NZ	1:C:85:GLN:O	2.09	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:338:LYS:NZ	4:F:88:SER:OG[3_545]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	443/451 (98%)	421 (95%)	22 (5%)	0	100	100
1	C	450/451 (100%)	431 (96%)	19 (4%)	0	100	100
2	B	433/445 (97%)	418 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	422/445 (95%)	400 (95%)	22 (5%)	0	100	100
3	E	125/143 (87%)	123 (98%)	2 (2%)	0	100	100
4	F	338/384 (88%)	316 (94%)	21 (6%)	1 (0%)	36	55
5	G	1/5 (20%)	1 (100%)	0	0	100	100
5	H	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2213/2329 (95%)	2111 (95%)	101 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	237	THR

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	376/379 (99%)	373 (99%)	3 (1%)	73	88
1	C	383/379 (101%)	378 (99%)	5 (1%)	61	82
2	B	377/383 (98%)	373 (99%)	4 (1%)	65	84
2	D	369/383 (96%)	365 (99%)	4 (1%)	65	84
3	E	116/127 (91%)	113 (97%)	3 (3%)	40	68
4	F	310/342 (91%)	295 (95%)	15 (5%)	23	46
5	G	2/2 (100%)	2 (100%)	0	100	100
5	H	2/2 (100%)	2 (100%)	0	100	100
All	All	1935/1997 (97%)	1901 (98%)	34 (2%)	53	77

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	226	GLU
4	F	236	LYS

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Mol	Chain	Res	Type
4	F	272	MET
2	D	77	SER
1	C	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	104	ASN
4	F	243	HIS
4	F	268	ASN
4	F	246	GLN
4	F	183	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
5	3WU	G	4	5	12,12,13	1.25	1 (8%)	9,15,17	1.39	1 (11%)
5	3WT	H	3	5	11,12,13	1.02	1 (9%)	9,14,16	1.89	1 (11%)
5	3WT	G	3	5	11,12,13	1.09	1 (9%)	9,14,16	2.12	2 (22%)
5	MVA	H	1	5	6,7,8	1.35	1 (16%)	6,8,10	1.18	0
5	3WU	H	4	5	12,12,13	1.30	1 (8%)	9,15,17	1.62	3 (33%)
5	MVA	G	1	5	6,7,8	1.33	1 (16%)	6,8,10	1.05	0

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
5	3WU	G	4	5	-	0/12/19/21	0/1/1/1
5	3WT	H	3	5	-	4/17/17/18	-
5	3WT	G	3	5	-	6/17/17/18	-
5	MVA	H	1	5	-	3/6/8/10	-
5	3WU	H	4	5	-	0/12/19/21	0/1/1/1
5	MVA	G	1	5	-	0/6/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	4	3WU	C3-CA	-2.54	1.49	1.53
5	H	4	3WU	C3-CA	-2.52	1.49	1.53
5	G	3	3WT	C26-C	2.52	1.56	1.50
5	H	3	3WT	C26-C	2.36	1.56	1.50
5	H	1	MVA	CA-N	-2.18	1.43	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	3WT	C25-N-CA	5.73	121.62	114.23
5	H	3	3WT	C25-N-CA	5.13	120.85	114.23
5	H	4	3WU	C3-CA-N	3.56	109.69	103.19
5	G	4	3WU	C3-CA-N	3.21	109.04	103.19
5	G	3	3WT	O-C-C26	-2.15	119.13	125.38

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1	MVA	C-CA-CB-CG2
5	H	1	MVA	O-C-CA-CB
5	G	3	3WT	C20-CA-N-C25
5	G	3	3WT	O5-C20-C26-C
5	H	3	3WT	C20-CA-N-C25

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	3	3WT	1	0
5	H	1	MVA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	GDP	D	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.69	5 (11%)
6	GTP	A	501	7	33,34,34	1.06	4 (12%)	50,54,54	1.59	8 (16%)
10	ACP	F	401	-	31,33,33	2.15	11 (35%)	47,52,52	1.91	13 (27%)
9	GDP	B	501	-	29,30,30	1.21	3 (10%)	45,47,47	1.62	5 (11%)
6	GTP	C	501	7	33,34,34	0.96	2 (6%)	50,54,54	1.55	8 (16%)

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	GDP	D	501	-	-	3/16/32/32	0/3/3/3
6	GTP	A	501	7	-	7/22/38/38	0/3/3/3
10	ACP	F	401	-	-	7/19/38/38	0/3/3/3
9	GDP	B	501	-	-	4/16/32/32	0/3/3/3
6	GTP	C	501	7	-	7/22/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	ACP	PG-O1G	5.20	1.60	1.50
10	F	401	ACP	C5-C4	4.72	1.47	1.39
10	F	401	ACP	PB-O1B	4.14	1.61	1.51
10	F	401	ACP	PB-O2B	-3.73	1.47	1.56
10	F	401	ACP	PG-O3G	-3.35	1.47	1.55

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	401	ACP	C5-C4-N3	-5.78	118.76	126.72
9	D	501	GDP	C5-C4-N3	-5.53	119.59	128.39
10	F	401	ACP	N3-C4-N9	5.24	136.07	127.17
6	C	501	GTP	C5-C4-N3	-5.15	120.19	128.39
9	B	501	GDP	C5-C4-N3	-5.08	120.31	128.39

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	GTP	PB-O3B-PG-O2G
6	A	501	GTP	PB-O3B-PG-O3G
6	A	501	GTP	C5'-O5'-PA-O3A
6	A	501	GTP	C5'-O5'-PA-O1A
6	A	501	GTP	C5'-O5'-PA-O2A

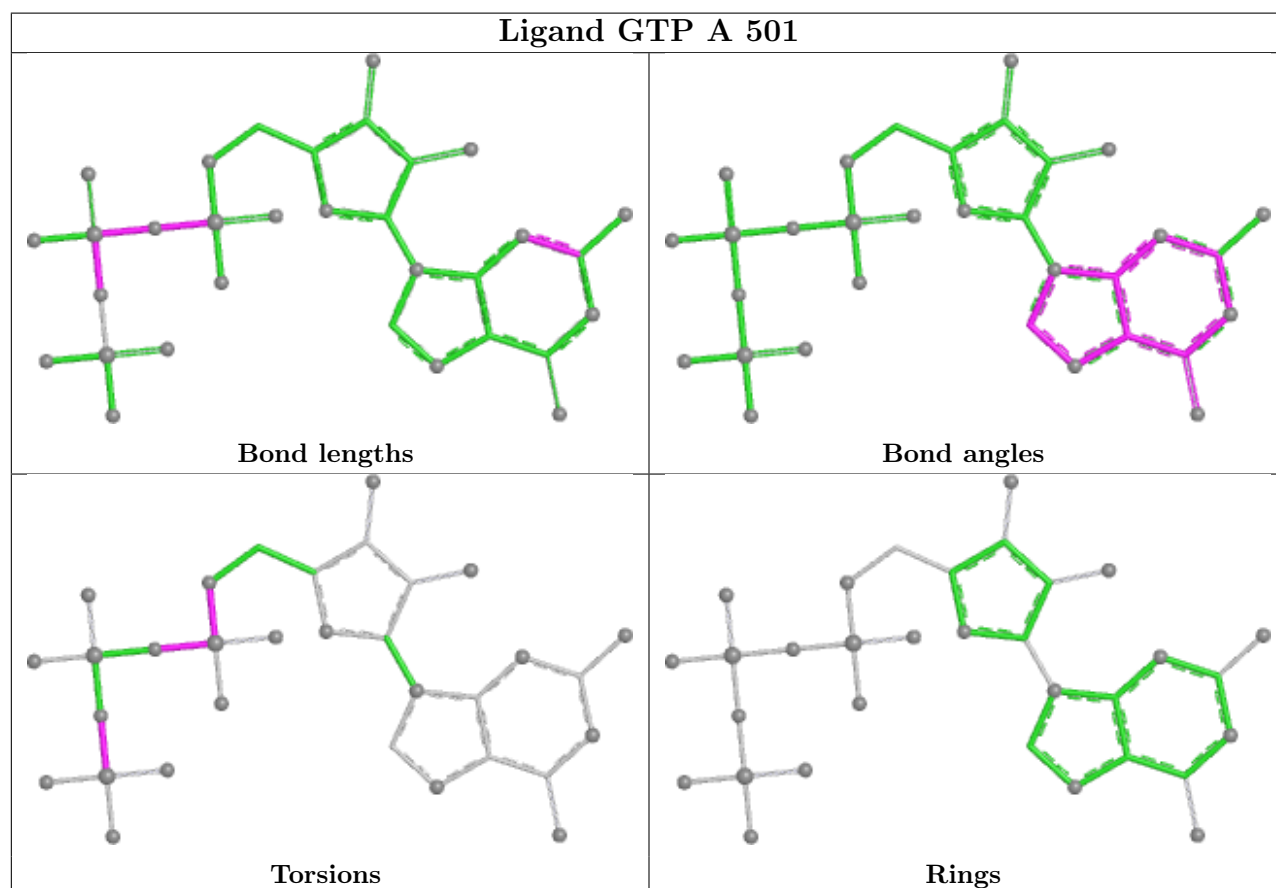
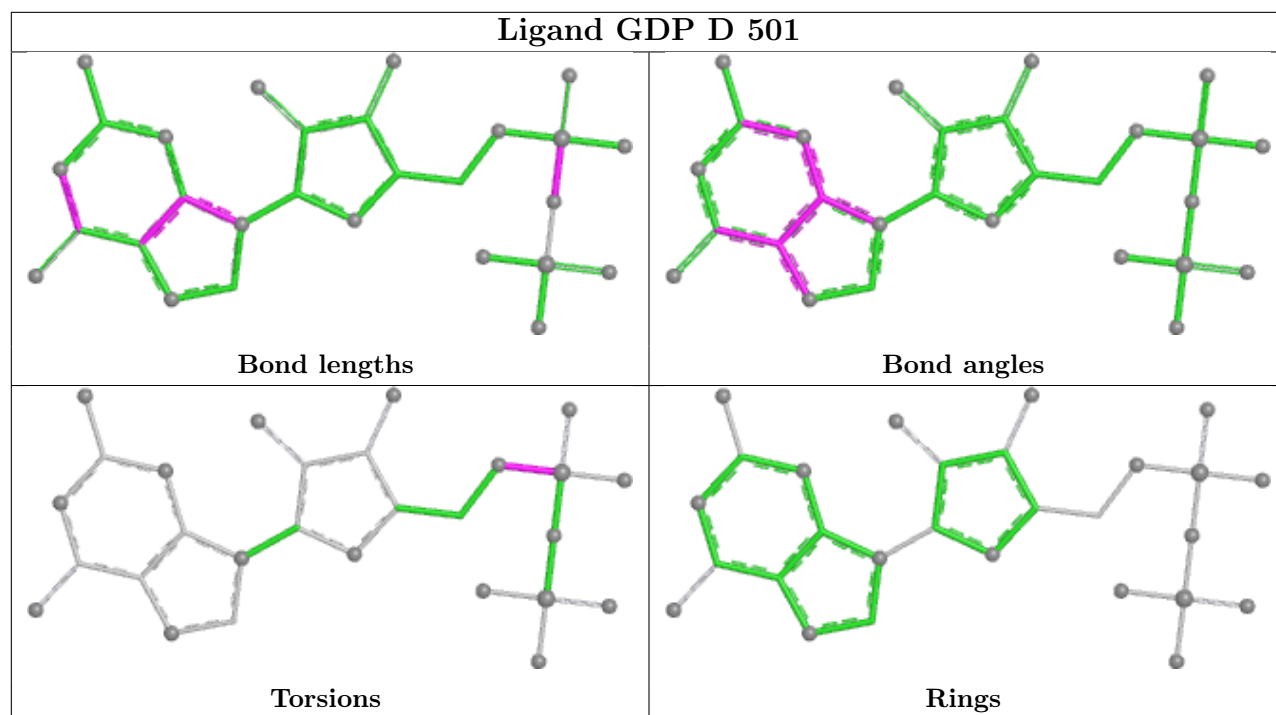
There are no ring outliers.

2 monomers are involved in 2 short contacts:

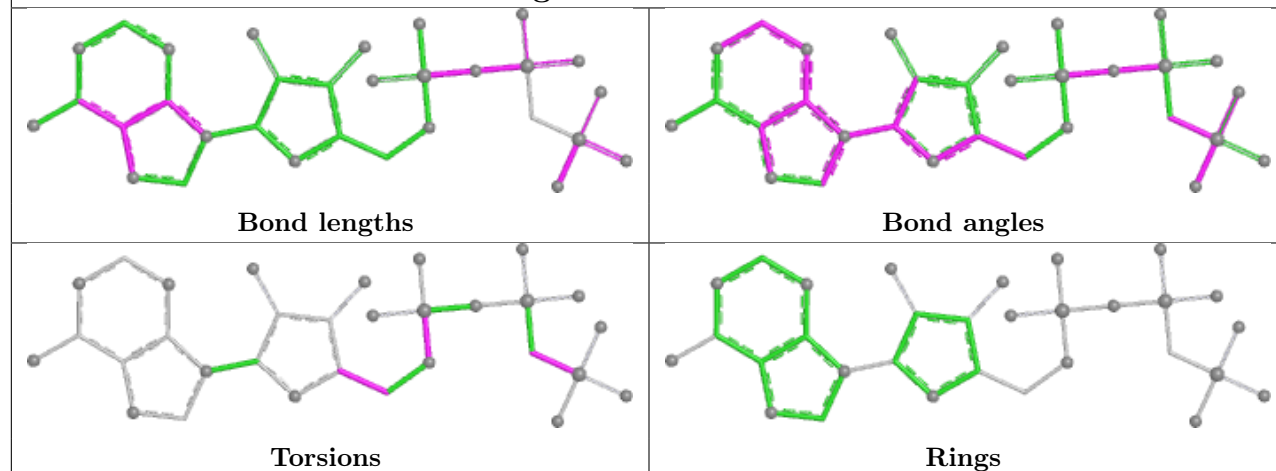
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
6	A	501	GTP	1	0

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

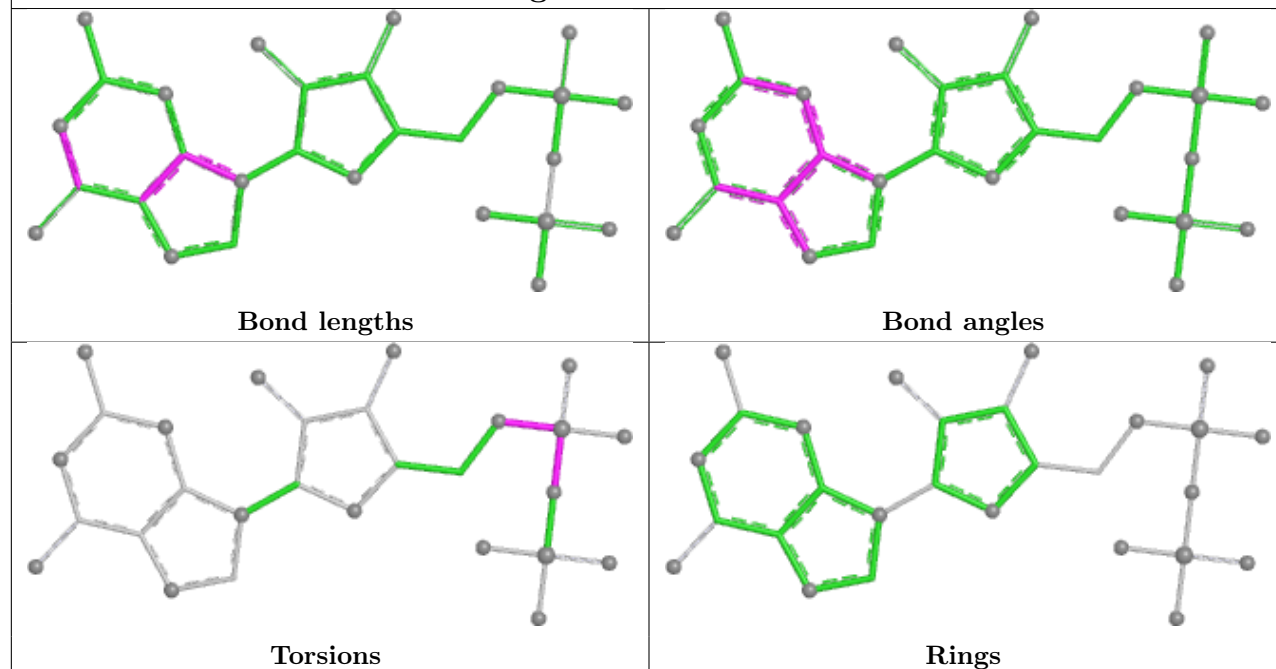
equivalents in the CSD to analyse the geometry.

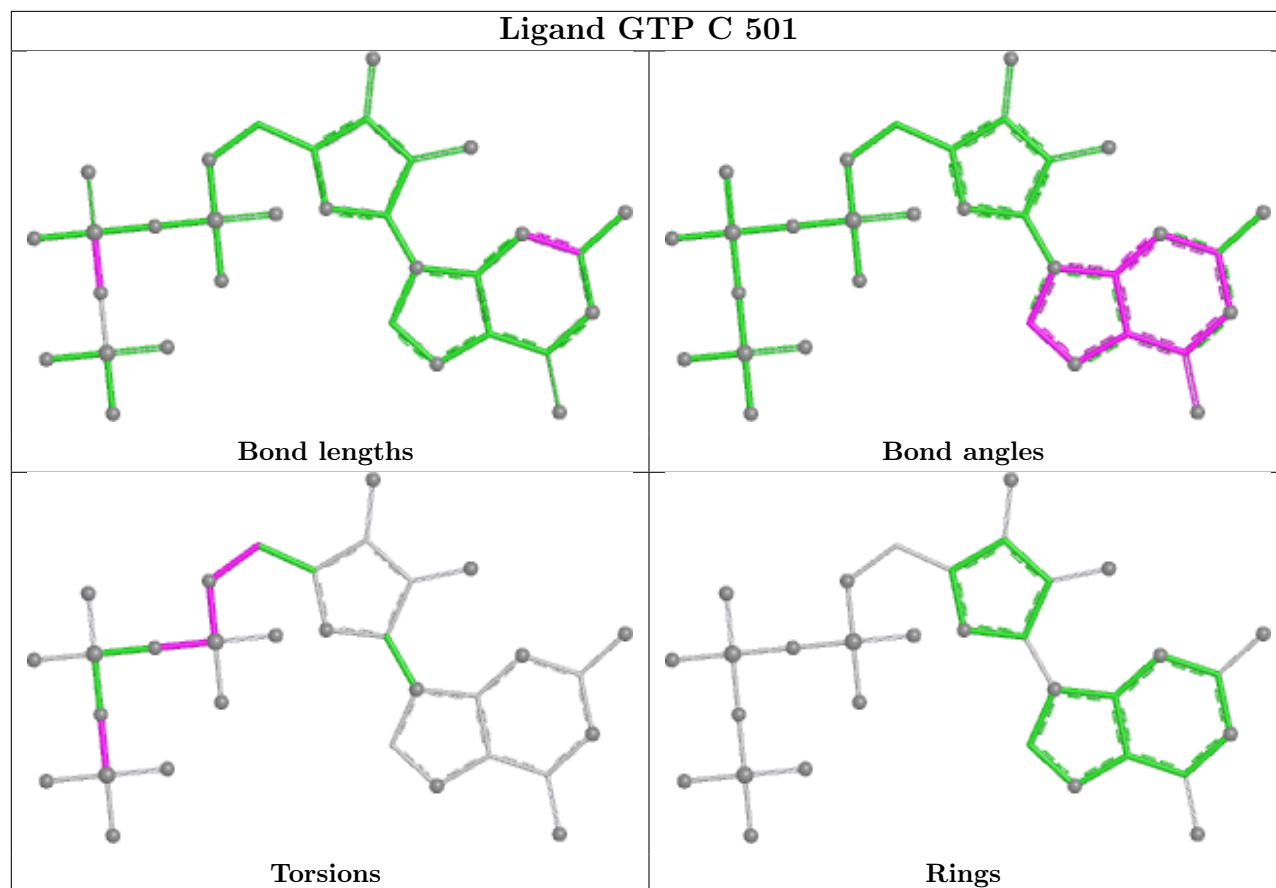


Ligand ACP F 401



Ligand GDP B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	1.11	60 (13%) 6 5	37, 74, 113, 166	6 (1%)
1	C	440/451 (97%)	0.50	22 (5%) 34 30	27, 54, 81, 121	12 (2%)
2	B	428/445 (96%)	0.69	20 (4%) 36 32	30, 61, 91, 143	7 (1%)
2	D	422/445 (94%)	1.08	50 (11%) 9 7	35, 78, 110, 141	6 (1%)
3	E	123/143 (86%)	1.08	18 (14%) 6 4	29, 79, 124, 149	6 (4%)
4	F	344/384 (89%)	1.45	65 (18%) 3 2	56, 106, 179, 302	2 (0%)
5	G	2/5 (40%)	0.79	0 100 100	49, 49, 49, 53	0
5	H	2/5 (40%)	2.00	1 (50%) 0 0	95, 95, 95, 127	0
All	All	2200/2329 (94%)	0.95	236 (10%) 11 9	27, 72, 139, 302	39 (1%)

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	6.6
4	F	150	LYS	6.0
2	D	195	VAL	6.0
1	A	149	PHE	5.2
1	C	305	CYS	5.1

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

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
5	MVA	H	1	8/9	0.79	0.18	99,119,139,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	3WU	H	4	12/13	0.79	0.16	77,93,111,111	0
5	3WT	H	3	13/14	0.84	0.18	84,106,123,128	0
5	3WU	G	4	12/13	0.92	0.10	36,47,58,60	0
5	3WT	G	3	13/14	0.92	0.13	36,49,55,61	0
5	MVA	G	1	8/9	0.94	0.09	33,44,51,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

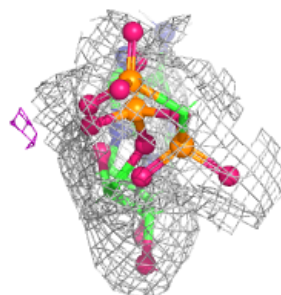
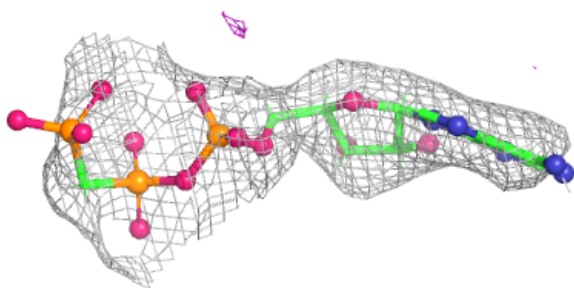
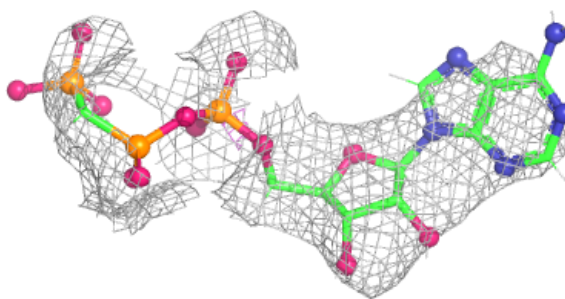
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	ACP	F	401	31/31	0.80	0.15	121,145,169,178	0
7	MG	B	502	1/1	0.83	0.26	74,74,74,74	0
7	MG	A	502	1/1	0.85	0.26	55,55,55,55	0
9	GDP	D	501	28/28	0.89	0.14	63,75,96,109	0
8	CA	A	503	1/1	0.89	0.10	123,123,123,123	0
7	MG	C	503	1/1	0.90	0.14	87,87,87,87	0
7	MG	B	503	1/1	0.90	0.10	52,52,52,52	0
6	GTP	A	501	32/32	0.93	0.11	49,57,69,79	0
6	GTP	C	501	32/32	0.96	0.10	37,46,57,72	0
9	GDP	B	501	28/28	0.96	0.09	33,40,55,57	0
7	MG	C	502	1/1	0.99	0.05	39,39,39,39	0

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

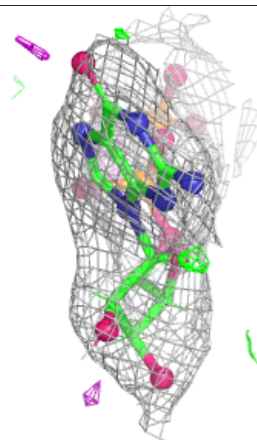
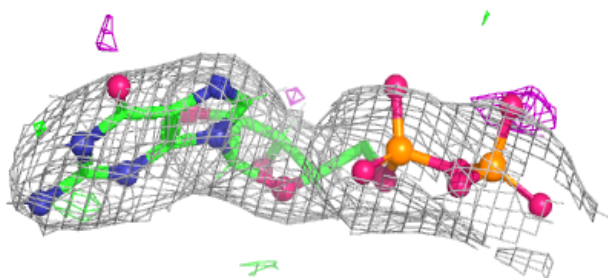
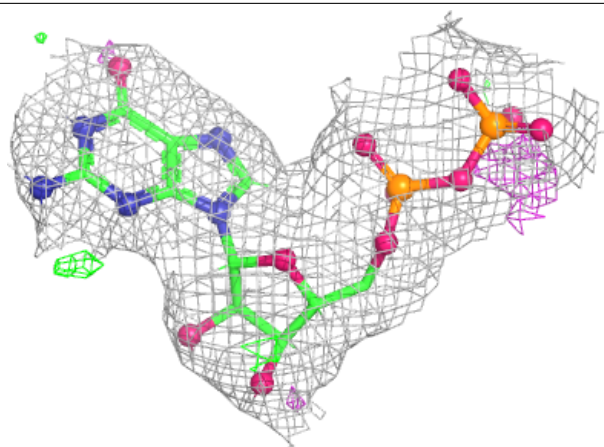
Electron density around ACP F 401:

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

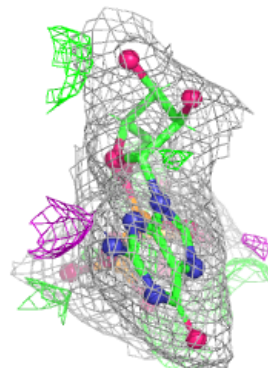
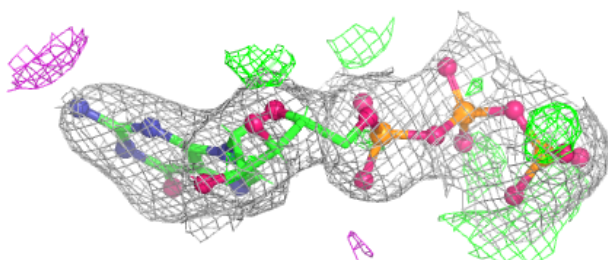
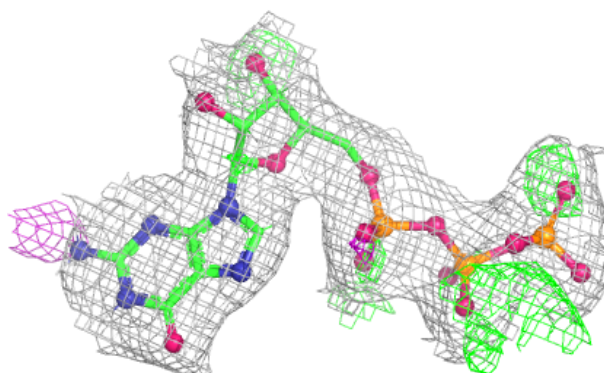


Electron density around GDP D 501:

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

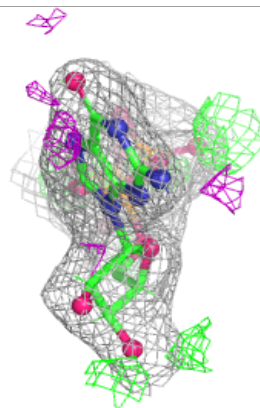
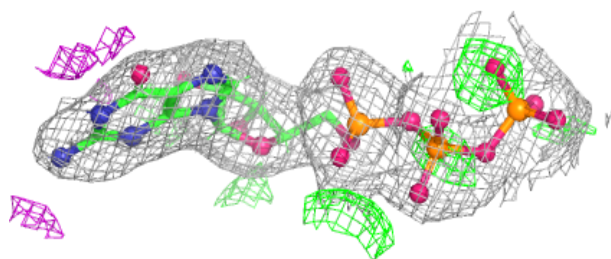
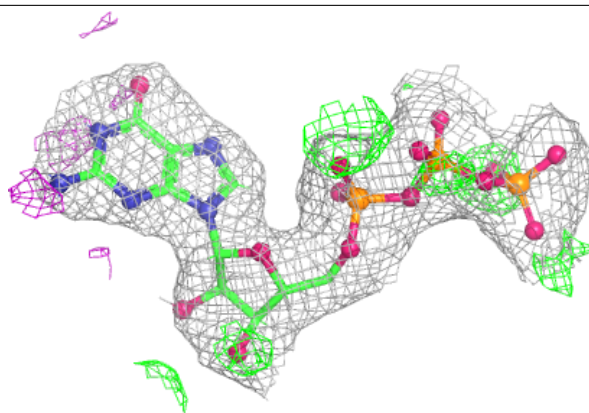
**Electron density around GTP A 501:**

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

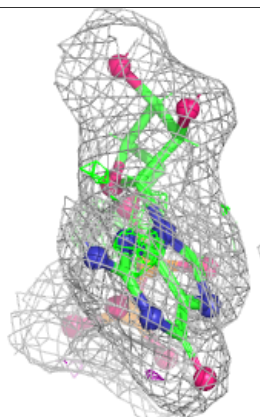
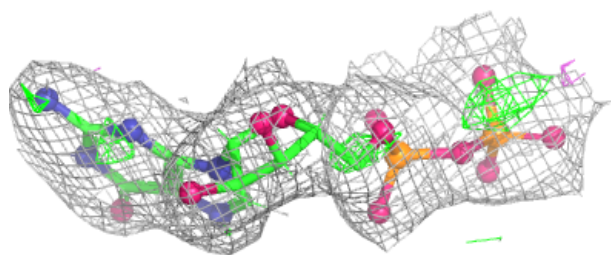
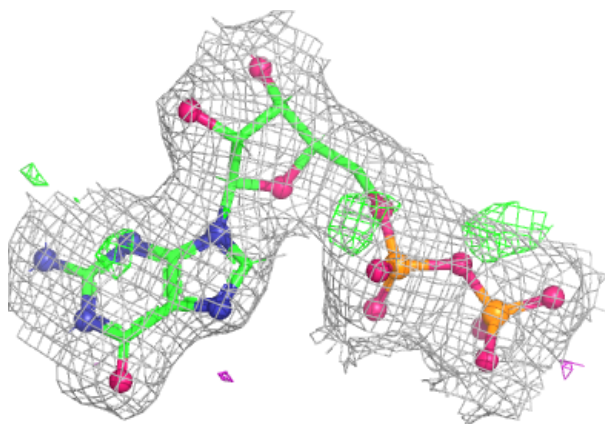


Electron density around GTP C 501:

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

There are no such residues in this entry.