



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 11:55 PM UTC

PDB ID : 9U6D / pdb_00009u6d
Title : Crystal structure of tubulin-RB3-TTL in complex with X8
Authors : Yan, W.; Yang, J.H.
Deposited on : 2025-03-23
Resolution : 2.54 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

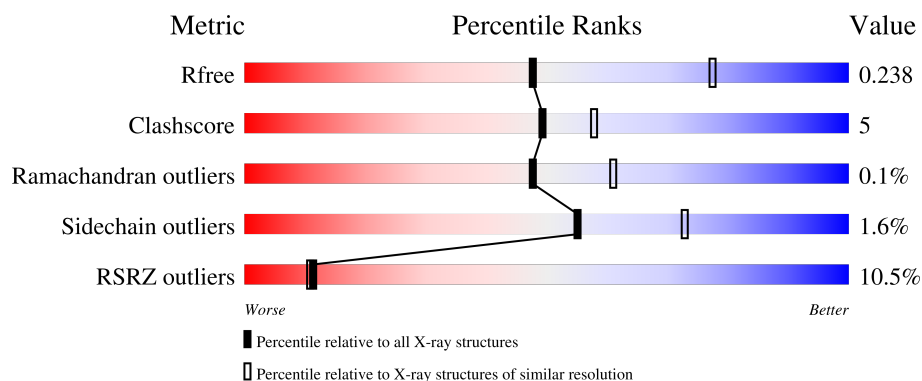
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	<div> <div>3%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	C	451	<div> <div>5%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
2	B	431	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
2	D	431	<div> <div>13%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
3	E	189	<div> <div>14%</div> <div>60%</div> <div>5%</div> <div>35%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>23%</div><div>71%</div><div>10%</div><div>•</div><div>18%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34334 atoms, of which 16655 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	438	Total	C	H	N	O	S	0	0	0
			6758	2167	3334	582	653	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6785	2175	3348	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	424	Total	C	H	N	O	S	0	0	0
			6525	2096	3192	569	643	25			
2	D	425	Total	C	H	N	O	S	0	0	0
			6472	2083	3157	565	644	23			

- 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	1	0
			2060	631	1036	186	202	5			

- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	313	Total	C	H	N	O	S	0	0	0
			4968	1609	2471	421	455	12			

There are 39 discrepancies between the modelled and reference sequences:

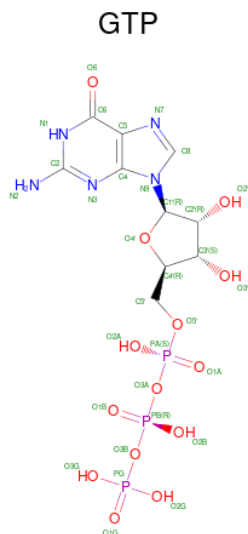
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

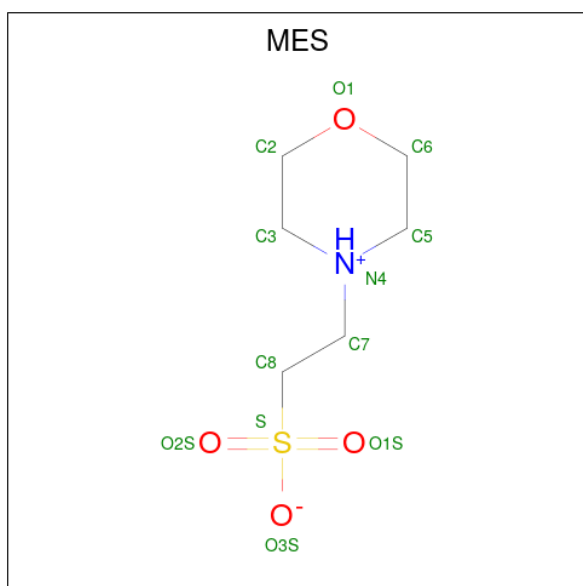
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	2	Total Ca 2 2	0	0

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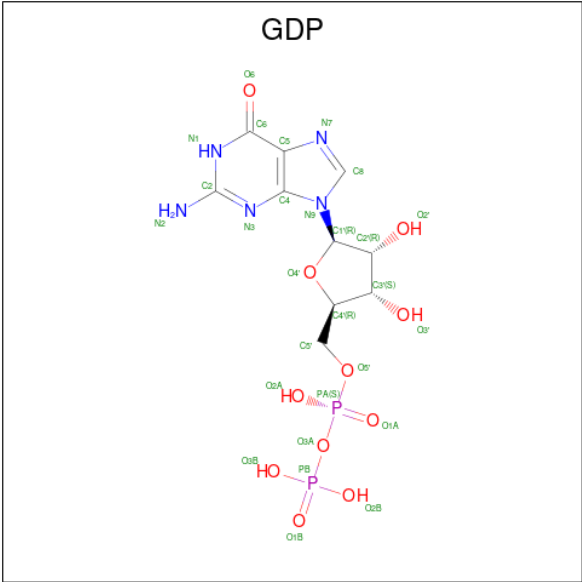
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	D	1	Total	C	F	H	N	O	0	0
			72	31	2	33	3	3		

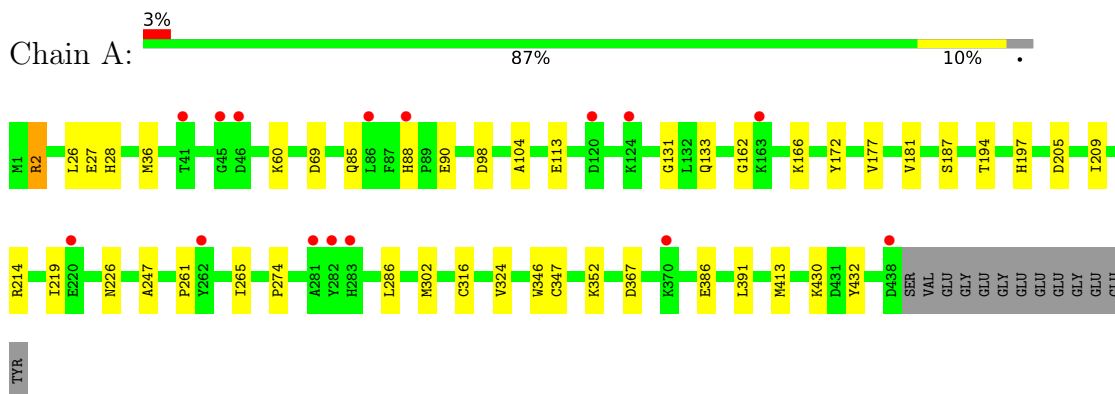
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	91	Total	O	0	0
			91	91		
11	B	93	Total	O	0	0
			93	93		
11	C	137	Total	O	0	0
			137	137		
11	D	38	Total	O	0	0
			38	38		
11	E	18	Total	O	0	0
			18	18		
11	F	51	Total	O	0	0
			51	51		

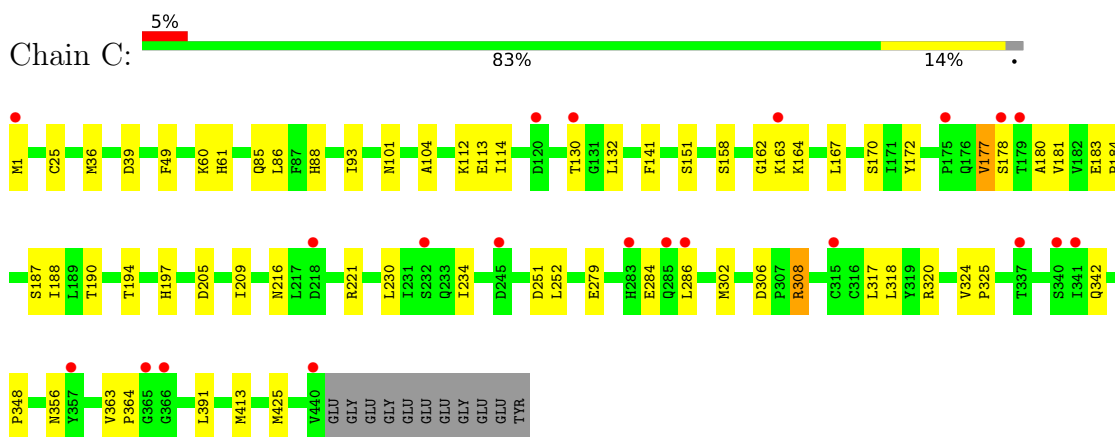
3 Residue-property plots [i](#)

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.

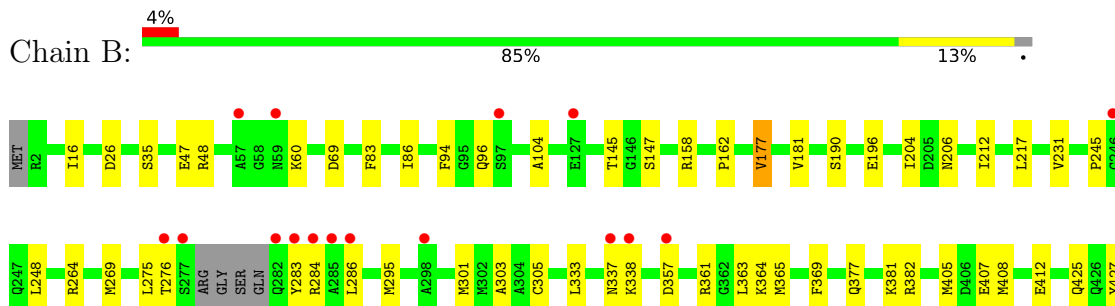
- Molecule 1: Tubulin alpha-1B chain

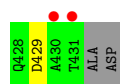


- Molecule 1: Tubulin alpha-1B chain

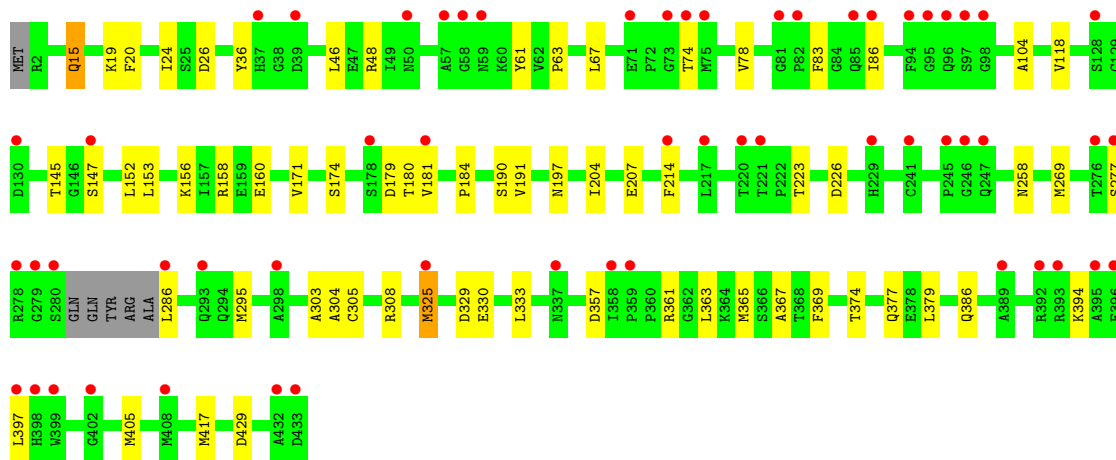
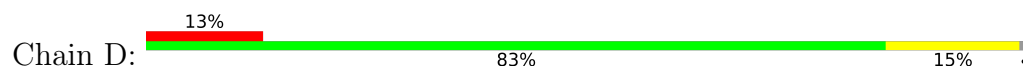


- Molecule 2: Tubulin beta chain

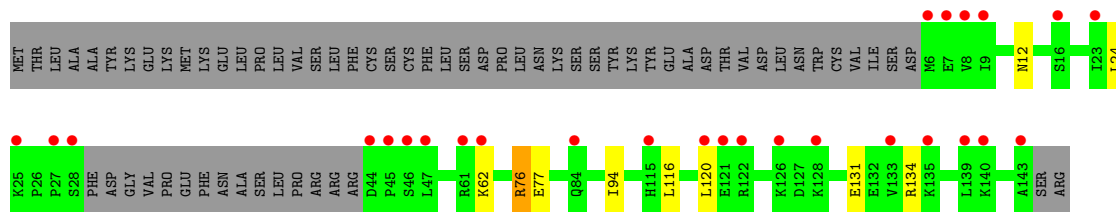




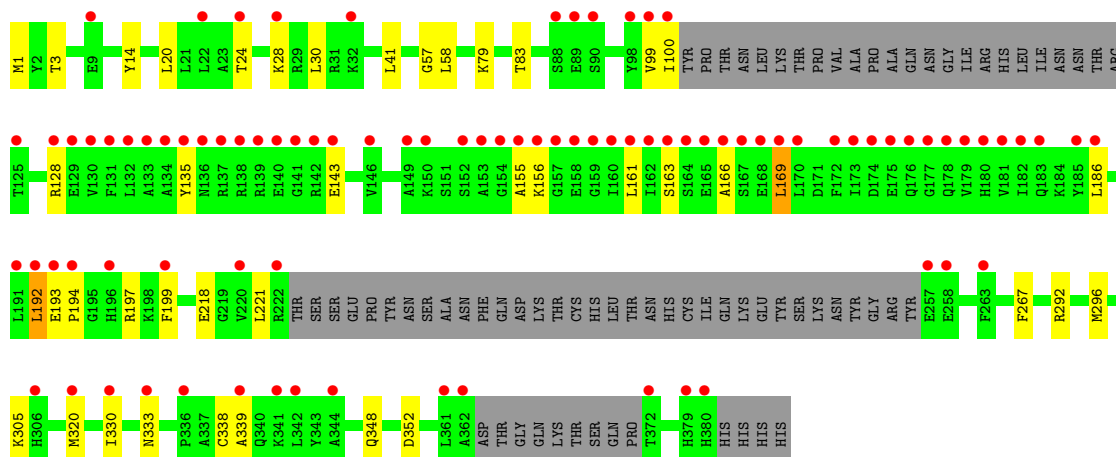
• Molecule 2: Tubulin beta chain



• 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	104.85Å 157.58Å 181.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.99 – 2.54 62.99 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (62.99-2.54) 99.7 (62.99-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.209 , 0.238 0.209 , 0.238	Depositor DCC
R_{free} test set	5107 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34334	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: GTP, CA, A1L8Z, MG, MES, 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	0.19	0/3502	0.43	0/4754
1	C	0.21	0/3515	0.45	0/4772
2	B	0.20	0/3407	0.45	0/4617
2	D	0.24	0/3388	0.46	0/4594
3	E	0.15	0/1033	0.35	0/1371
4	F	0.14	0/2549	0.36	0/3446
All	All	0.20	0/17394	0.43	0/23554

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	3424	3334	3334	32	0
1	C	3437	3348	3348	47	0
2	B	3333	3192	3211	40	1
2	D	3315	3157	3177	38	1
3	E	1024	1036	1035	6	0
4	F	2497	2471	2470	31	0
5	A	32	9	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	9	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
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	B	12	13	13	0	0
9	B	28	10	12	1	0
9	D	28	10	12	1	0
10	B	39	33	0	0	0
10	D	39	33	0	0	0
11	A	91	0	0	6	0
11	B	93	0	0	5	0
11	C	137	0	0	4	0
11	D	38	0	0	5	0
11	E	18	0	0	0	0
11	F	51	0	0	2	0
All	All	17679	16655	16636	183	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 5.

The worst 5 of 183 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:C:36:MET:HE3	1:C:39:ASP:HB2	1.58	0.86
1:A:2:ARG:HG3	1:A:131:GLY:O	1.87	0.73
2:D:329:ASP:O	2:D:333:LEU:HD13	1.89	0.72
2:B:407:GLU:OE2	11:B:601:HOH:O	2.10	0.70
2:B:276:THR:HG21	2:B:363:LEU:HD21	1.73	0.69

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:B:284:ARG:HH21	2:D:160:GLU:OE1[4_455]	1.52	0.08

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	436/451 (97%)	427 (98%)	8 (2%)	1 (0%)	43	56
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	420/431 (97%)	407 (97%)	13 (3%)	0	100	100
2	D	421/431 (98%)	410 (97%)	10 (2%)	1 (0%)	43	56
3	E	120/189 (64%)	117 (98%)	3 (2%)	0	100	100
4	F	305/384 (79%)	282 (92%)	22 (7%)	1 (0%)	36	45
All	All	2140/2337 (92%)	2072 (97%)	65 (3%)	3 (0%)	48	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
4	F	192	LEU
2	D	304	ALA

5.3.2 Protein sidechains [i](#)

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	369/379 (97%)	366 (99%)	3 (1%)	73	84
1	C	371/379 (98%)	365 (98%)	6 (2%)	55	73
2	B	365/370 (99%)	360 (99%)	5 (1%)	59	75
2	D	361/370 (98%)	353 (98%)	8 (2%)	45	64
3	E	111/171 (65%)	108 (97%)	3 (3%)	39	58
4	F	267/342 (78%)	262 (98%)	5 (2%)	50	69
All	All	1844/2011 (92%)	1814 (98%)	30 (2%)	55	73

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	15	GLN
4	F	169	LEU
2	D	74	THR
4	F	305	LYS
3	E	77	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	107	HIS
1	C	406	HIS
3	E	124	GLN
2	D	349	ASN
2	D	398	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 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	A1L8Z	B	506	-	42,43,43	3.31	22 (52%)	52,59,59	2.46	19 (36%)
10	A1L8Z	D	504	-	42,43,43	3.03	22 (52%)	52,59,59	2.90	20 (38%)
9	GDP	D	503	6	29,30,30	1.18	2 (6%)	45,47,47	1.80	9 (20%)
5	GTP	A	501	6	33,34,34	0.92	1 (3%)	50,54,54	1.63	10 (20%)
8	MES	B	502	-	12,12,12	2.23	1 (8%)	15,16,16	1.59	3 (20%)
5	GTP	C	501	6	33,34,34	2.25	5 (15%)	50,54,54	1.95	12 (24%)
9	GDP	B	505	6	29,30,30	1.15	2 (6%)	45,47,47	1.82	10 (22%)

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	A1L8Z	B	506	-	-	10/27/42/42	0/5/5/5
10	A1L8Z	D	504	-	-	6/27/42/42	1/5/5/5
9	GDP	D	503	6	-	1/16/32/32	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
8	MES	B	502	-	-	1/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
9	GDP	B	505	6	-	1/16/32/32	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	506	A1L8Z	C28-N3	8.68	1.47	1.35
5	C	501	GTP	PB-O3A	7.59	1.67	1.59
8	B	502	MES	C8-S	-7.42	1.67	1.77
5	C	501	GTP	PB-O3B	7.38	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	504	A1L8Z	C7-C8	6.15	1.64	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	504	A1L8Z	C7-C8-N1	9.05	128.62	116.06
10	B	506	A1L8Z	C7-C8-N1	7.74	126.79	116.06
10	D	504	A1L8Z	C6-C7-C8	-7.42	99.16	113.56
10	D	504	A1L8Z	C31-C29-C28	7.17	128.94	117.25
9	D	503	GDP	C5-C4-N3	-6.11	118.66	128.39

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

All (1) ring outliers are listed below:

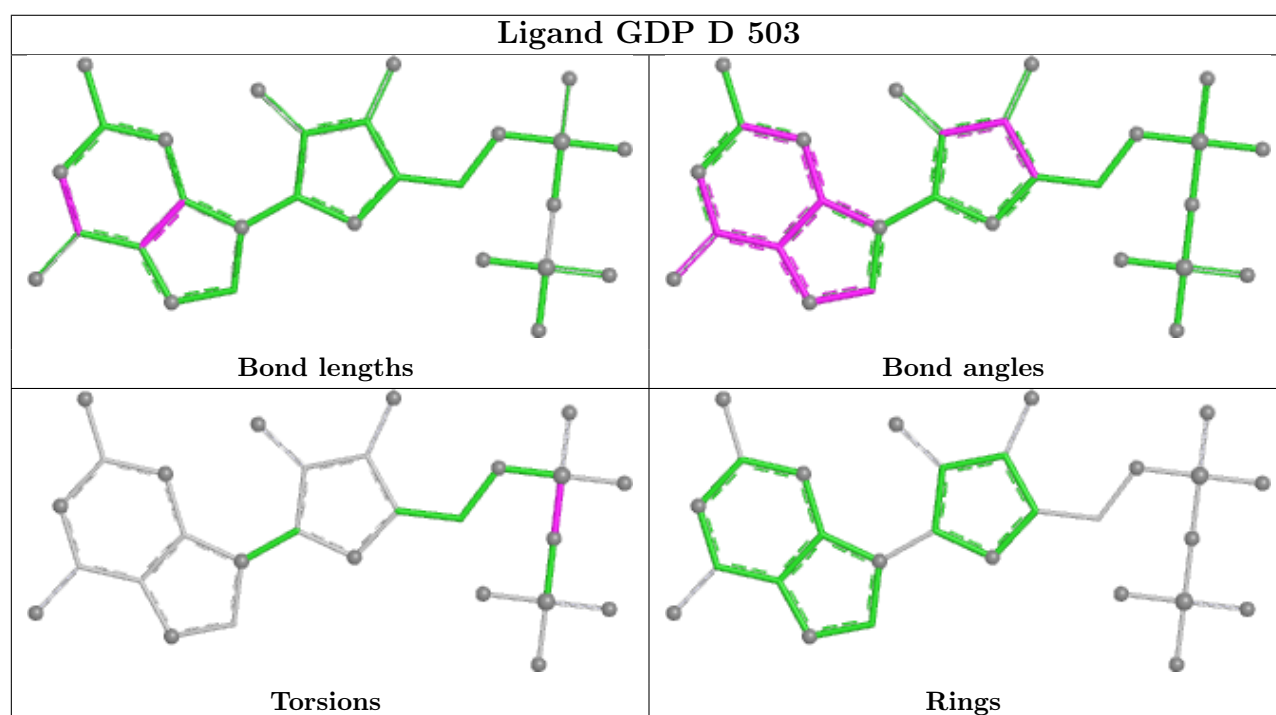
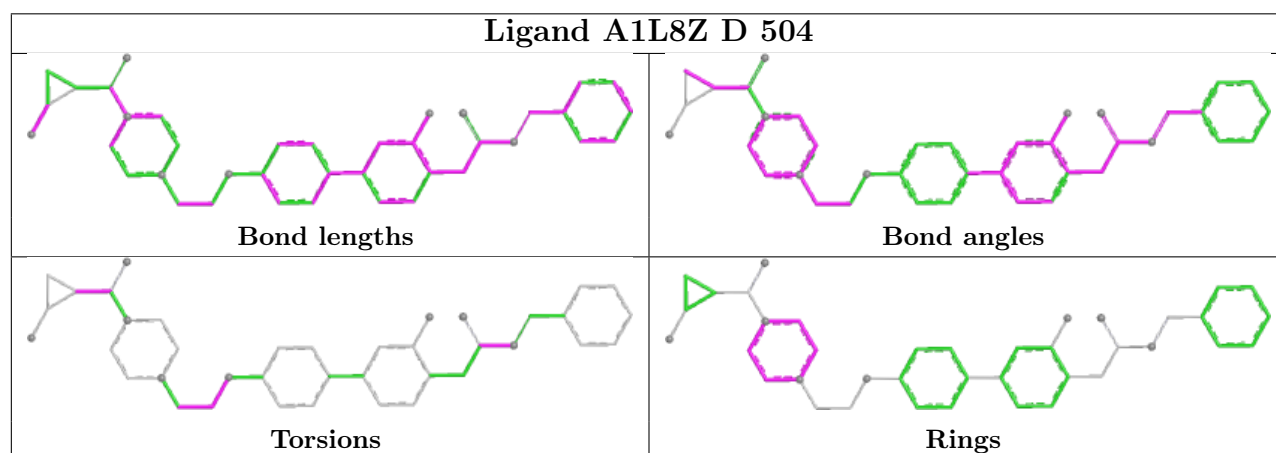
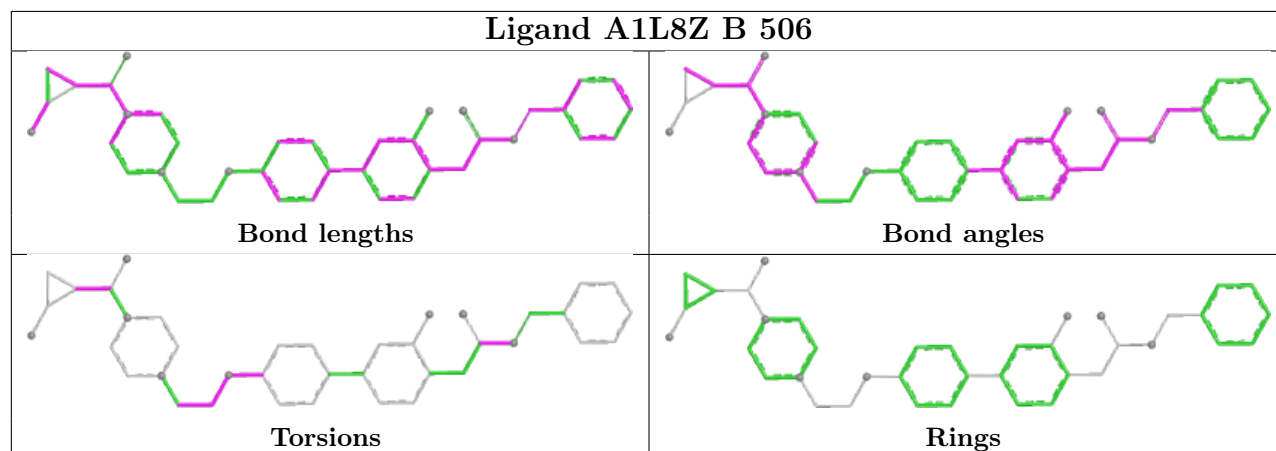
Mol	Chain	Res	Type	Atoms
10	D	504	A1L8Z	C24-C25-C26-C27-N2-N3

3 monomers are involved in 3 short contacts:

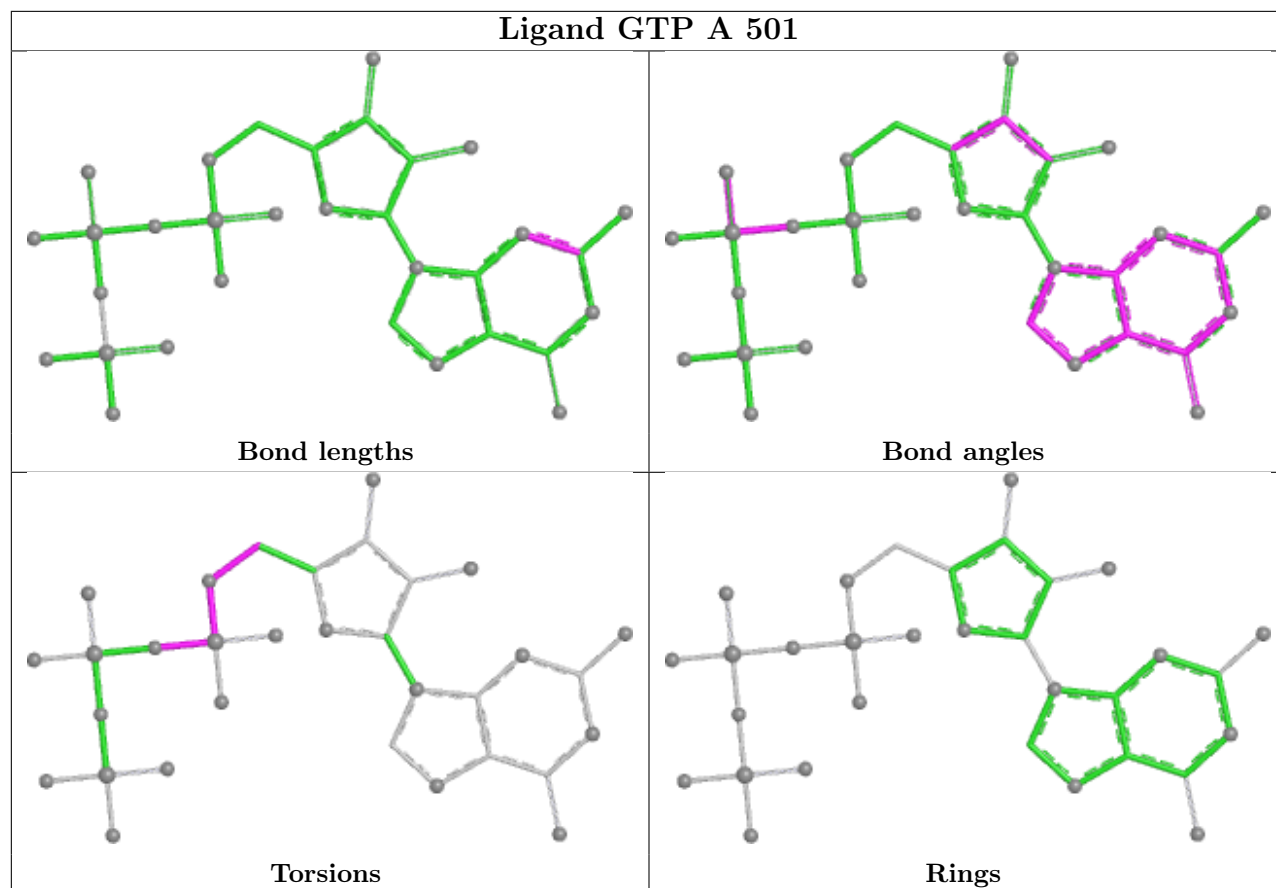
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	503	GDP	1	0
5	A	501	GTP	1	0
9	B	505	GDP	1	0

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

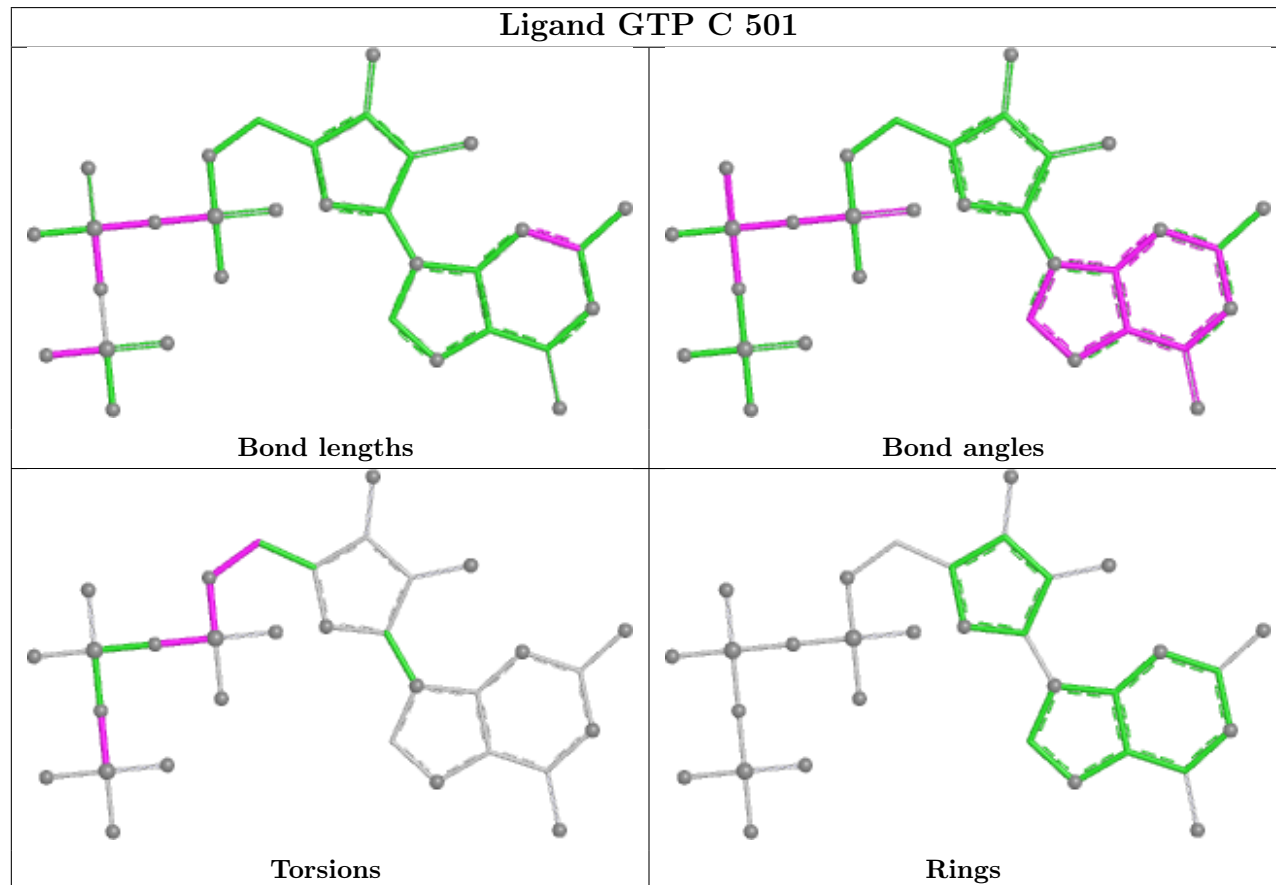
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

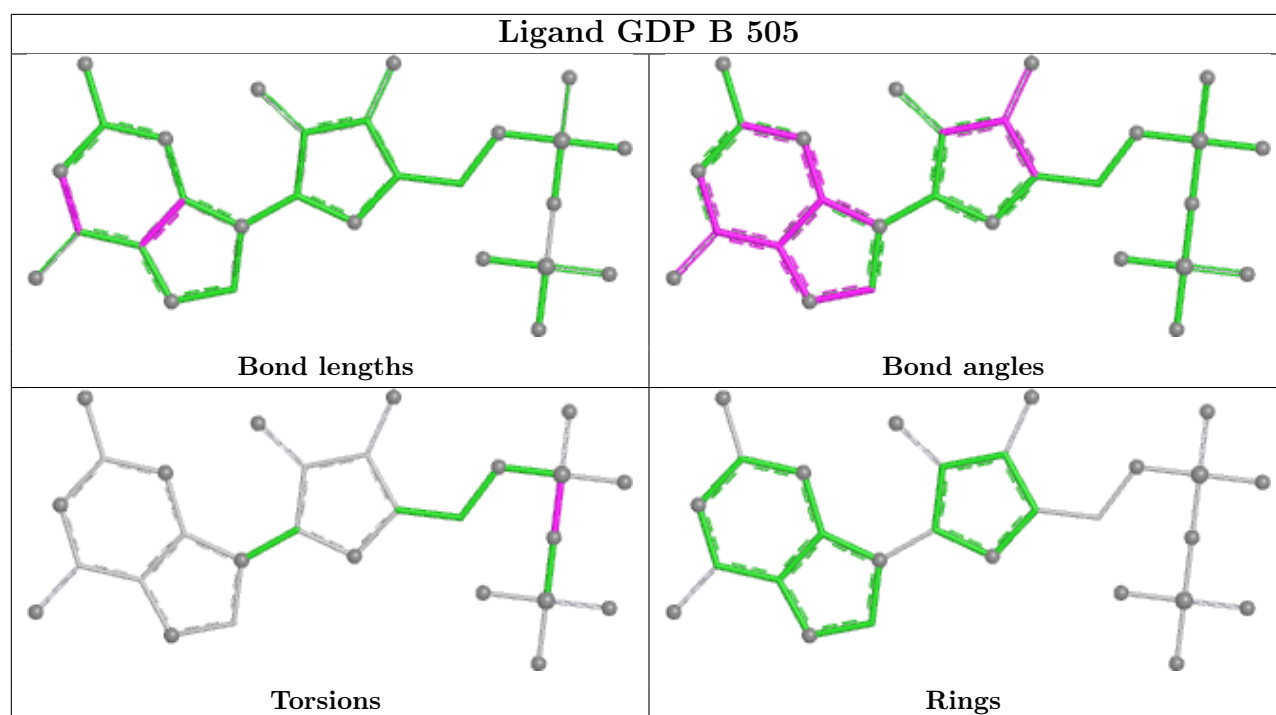


Ligand GTP A 501



Ligand GTP C 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	438/451 (97%)	0.28	15 (3%)	48	49	29, 45, 71, 97	0
1	C	440/451 (97%)	0.02	21 (4%)	35	35	23, 37, 61, 78	0
2	B	424/431 (98%)	0.28	18 (4%)	40	41	26, 44, 74, 96	0
2	D	425/431 (98%)	0.88	57 (13%)	7	5	32, 59, 88, 102	0
3	E	123/189 (65%)	1.24	27 (21%)	2	2	35, 65, 95, 112	1 (0%)
4	F	313/384 (81%)	1.32	89 (28%)	1	1	34, 67, 120, 135	0
All	All	2163/2337 (92%)	0.55	227 (10%)	11	11	23, 50, 89, 135	1 (0%)

The worst 5 of 227 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	6.5
4	F	169	LEU	6.4
4	F	132	LEU	6.2
4	F	172	PHE	5.7
2	D	94	PHE	5.7

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 oligosaccharides in this entry.

6.4 Ligands

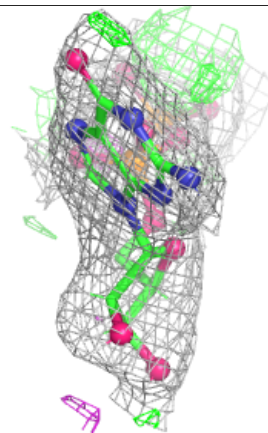
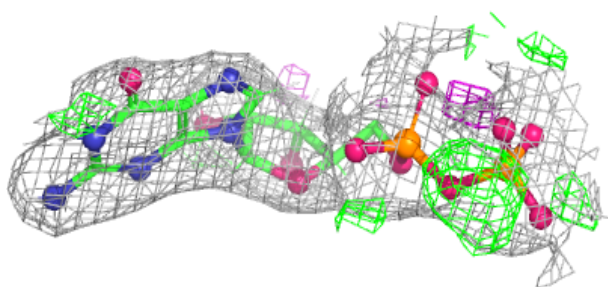
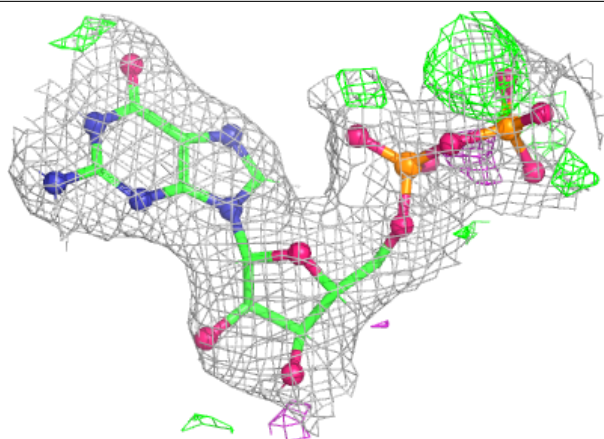
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	401	1/1	0.27	0.36	97,97,97,97	0
6	MG	D	501	1/1	0.38	0.23	72,72,72,72	0
7	CA	D	502	1/1	0.66	0.21	94,94,94,94	0
7	CA	A	503	1/1	0.68	0.22	94,94,94,94	0
7	CA	B	504	1/1	0.71	0.15	79,79,79,79	0
7	CA	B	503	1/1	0.82	0.21	88,88,88,88	0
7	CA	E	201	1/1	0.87	0.12	81,81,81,81	0
9	GDP	D	503	28/28	0.90	0.13	41,57,75,81	0
10	A1L8Z	B	506	39/39	0.91	0.14	28,44,59,64	0
10	A1L8Z	D	504	39/39	0.91	0.13	37,49,60,67	0
8	MES	B	502	12/12	0.94	0.10	36,47,56,57	0
6	MG	B	501	1/1	0.95	0.13	31,31,31,31	0
6	MG	A	502	1/1	0.95	0.14	34,34,34,34	0
7	CA	C	503	1/1	0.96	0.06	58,58,58,58	0
5	GTP	A	501	32/32	0.96	0.08	24,32,40,45	0
9	GDP	B	505	28/28	0.96	0.10	25,34,44,61	0
5	GTP	C	501	32/32	0.98	0.07	22,29,38,45	0
6	MG	C	502	1/1	0.99	0.03	29,29,29,29	0

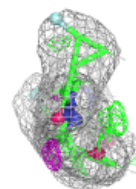
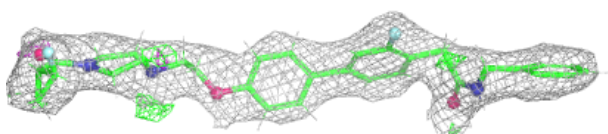
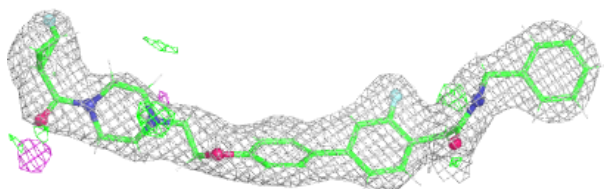
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP 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)

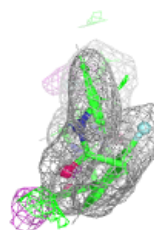
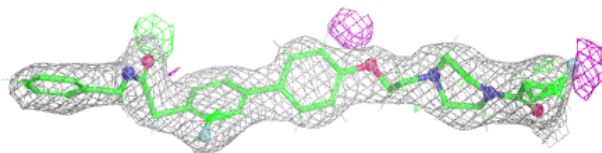
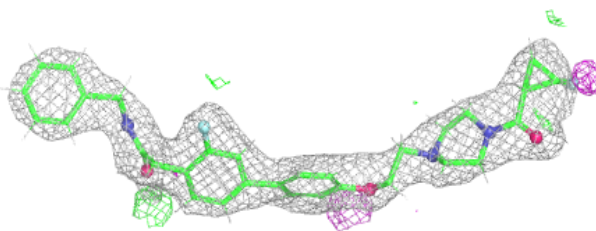
**Electron density around A1L8Z B 506:**

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

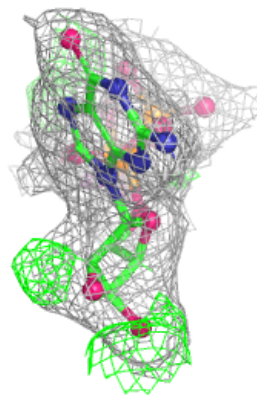
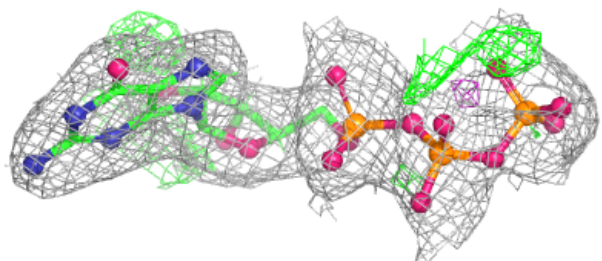
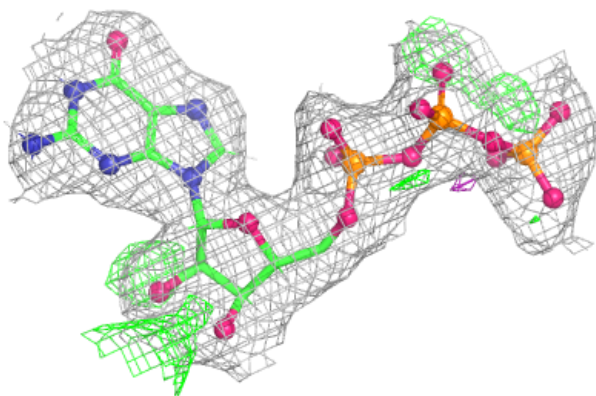


Electron density around A1L8Z D 504:

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

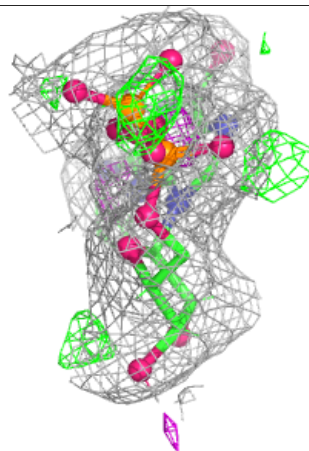
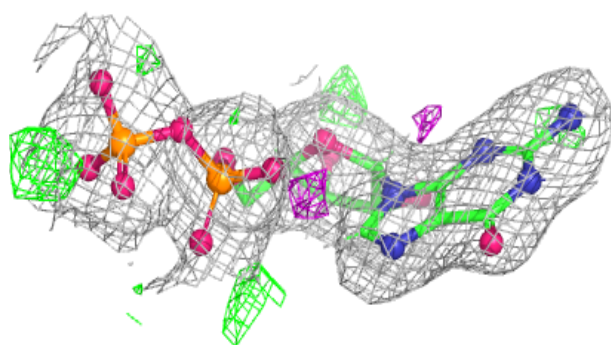
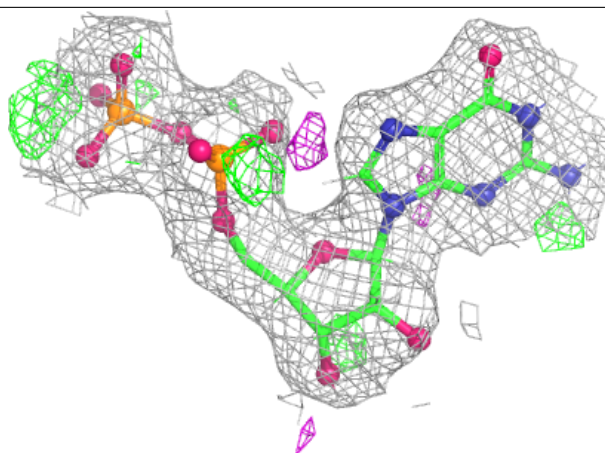
**Electron density around GTP A 501:**

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

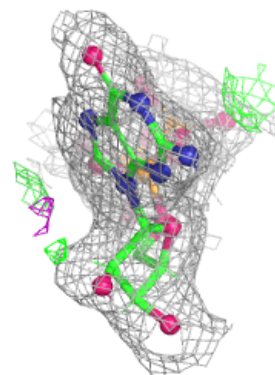
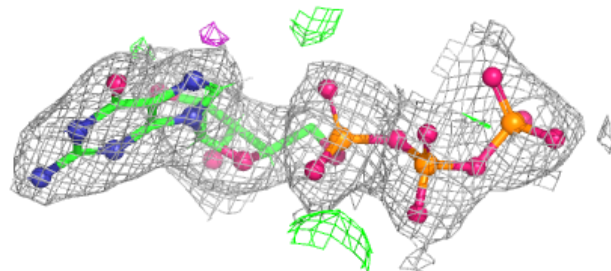
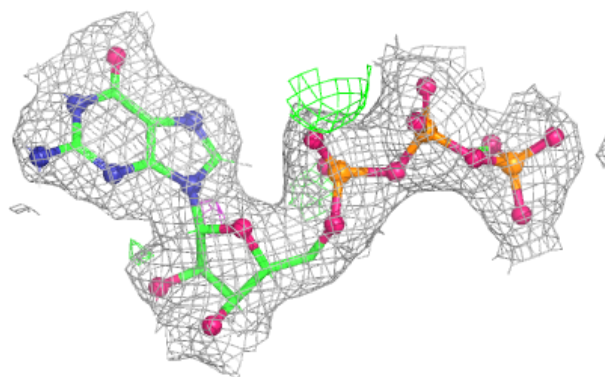


Electron density around GDP B 505:

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

**Electron density around GTP C 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.