



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:20 AM UTC

PDB ID : 4O2A / pdb_00004o2a
Title : Tubulin-BAL27862 complex
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Deposited on : 2013-12-17
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

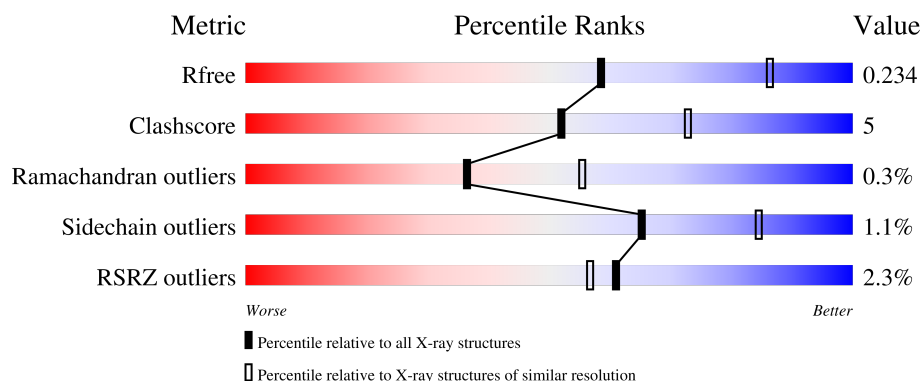
1 Overall quality at a glance

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	86% 11% .
1	C	451	% 88% 9% ..
2	B	445	% 82% 12% 6%
2	D	445	3% 80% 13% . 5%
3	E	143	6% 83% . 13%

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Mol	Chain	Length	Quality of chain
4	F	384	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	2RR	D	604	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	12	0
			3487	2214	587	662	24			
1	C	440	Total	C	N	O	S	0	15	0
			3504	2224	587	667	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	16	0
			3371	2127	566	650	28			
2	D	421	Total	C	N	O	S	0	4	0
			3324	2091	562	643	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	5	0
			1045	646	188	205	6			

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 TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	4	0
			2740	1766	465	495	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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	2	Total	Mg	0	0
			2	2		
6	D	2	Total	Mg	0	0
			2	2		

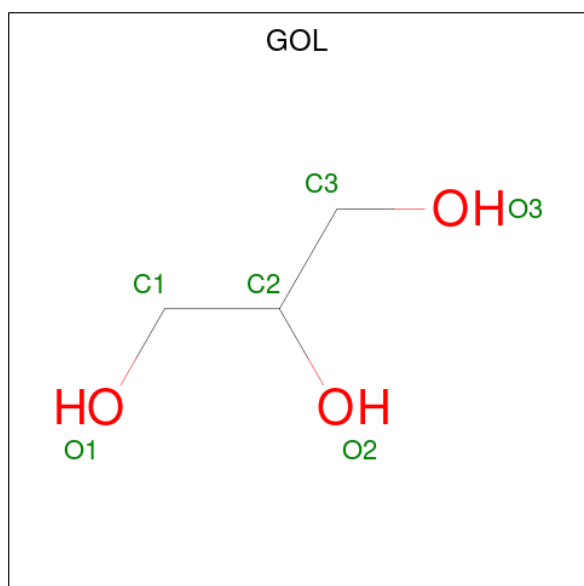
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

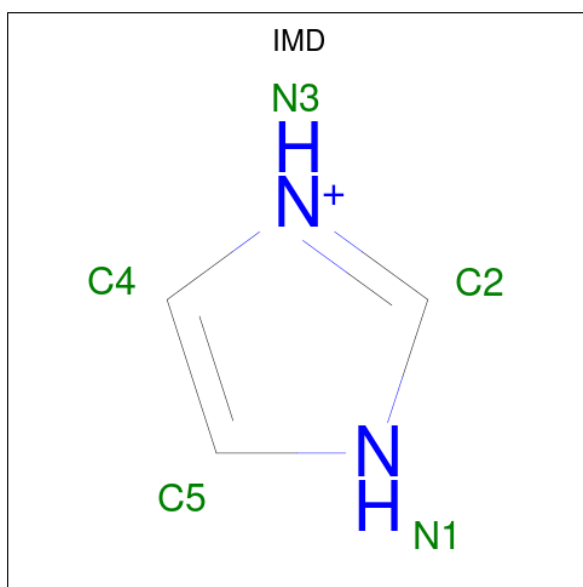
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



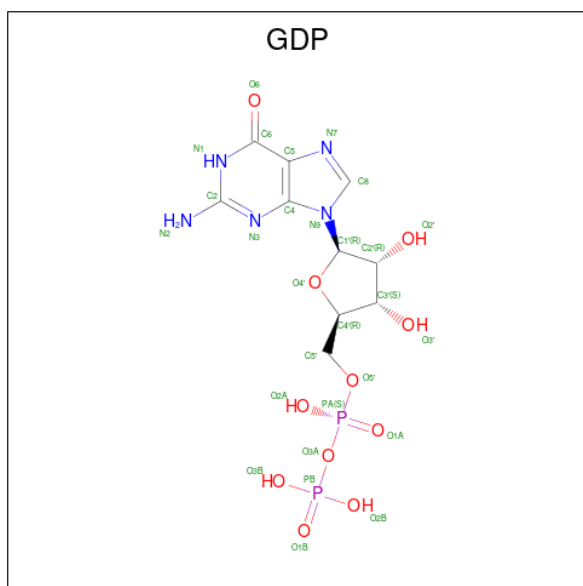
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0

- Molecule 10 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	N	0	0
			5	3	2		

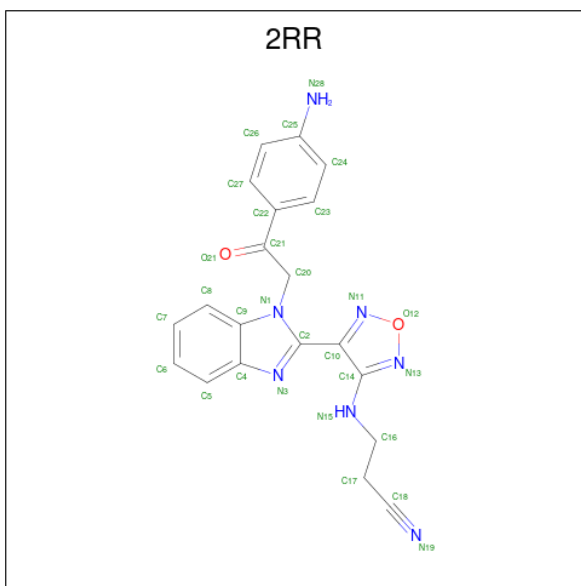
- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

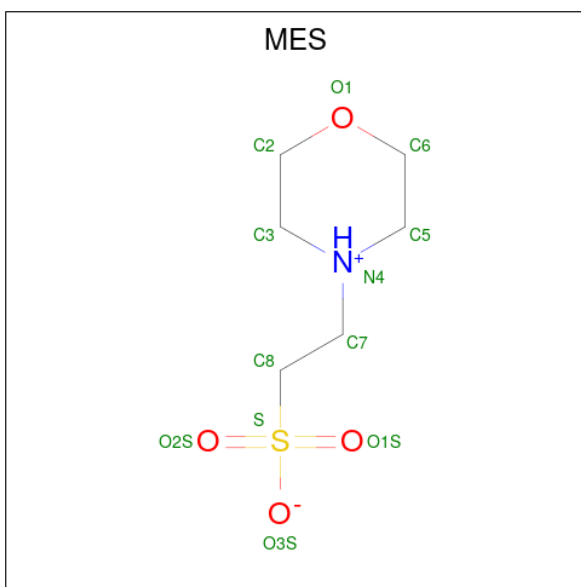
- Molecule 12 is 3-[(4-{1-[2-(4-aminophenyl)-2-oxoethyl]-1H-benzimidazol-2-yl})-1,2,5-oxadiaz

ol-3-yl)amino]propanenitrile (CCD ID: 2RR) (formula: $C_{20}H_{17}N_7O_2$).



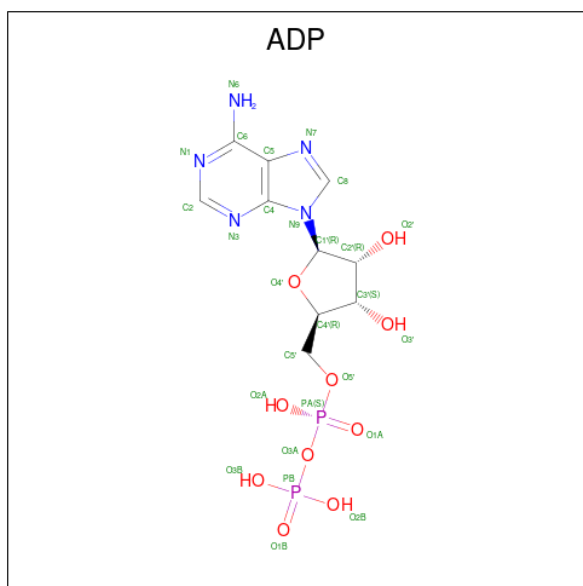
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			29	20	7	2		
12	D	1	Total	C	N	O	0	0
			29	20	7	2		

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



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

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

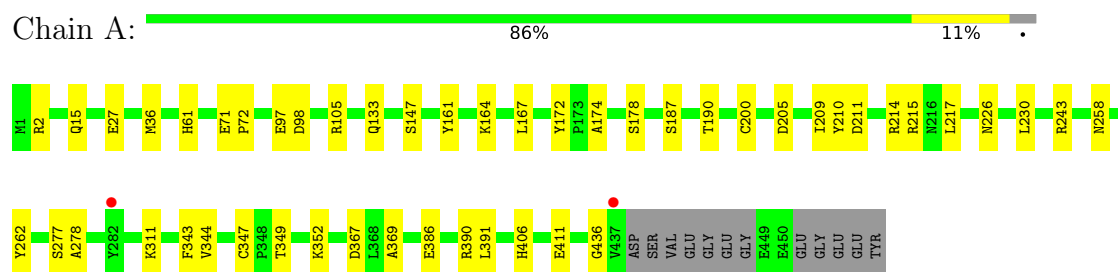
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	63	Total	O	0	0
			63	63		
15	B	70	Total	O	0	0
			70	70		
15	C	144	Total	O	0	0
			144	144		
15	D	26	Total	O	0	0
			26	26		
15	E	13	Total	O	0	0
			13	13		
15	F	18	Total	O	0	0
			18	18		

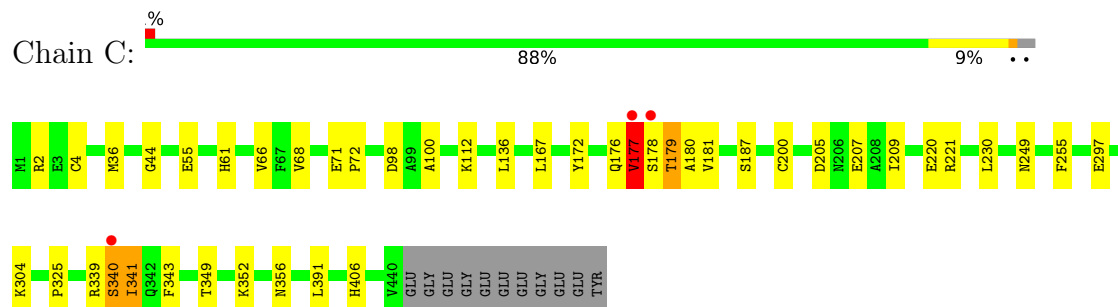
3 Residue-property plots [i](#)

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.

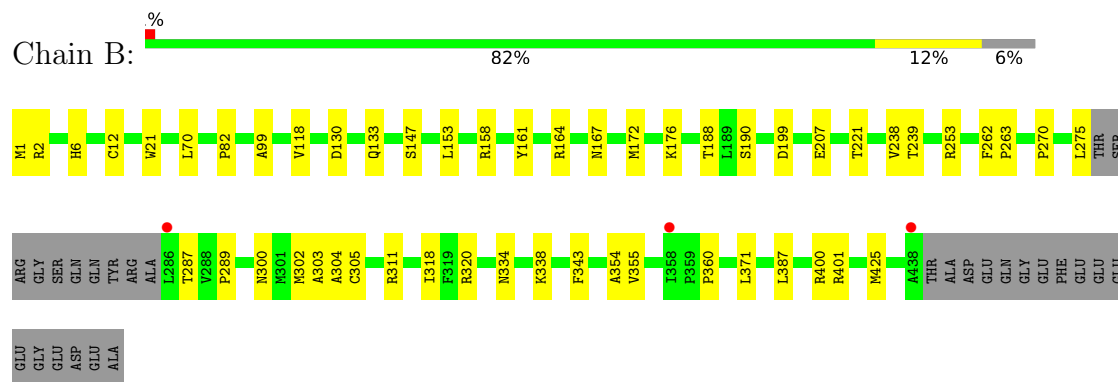
- Molecule 1: Tubulin alpha-1B chain



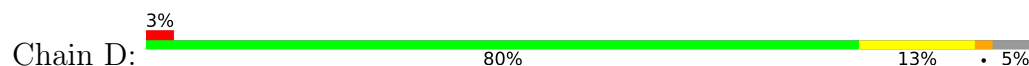
- Molecule 1: Tubulin alpha-1B chain

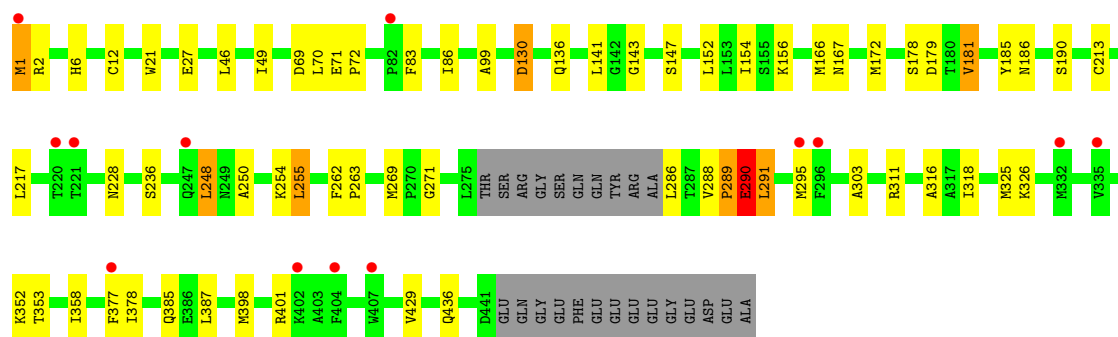


- Molecule 2: Tubulin beta-2B chain

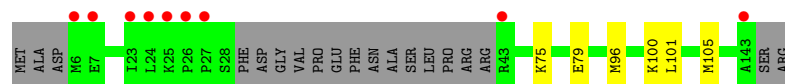
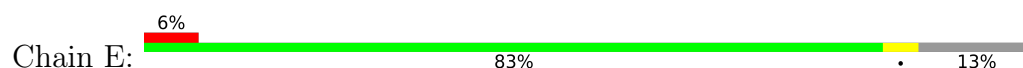


- Molecule 2: Tubulin beta-2B chain

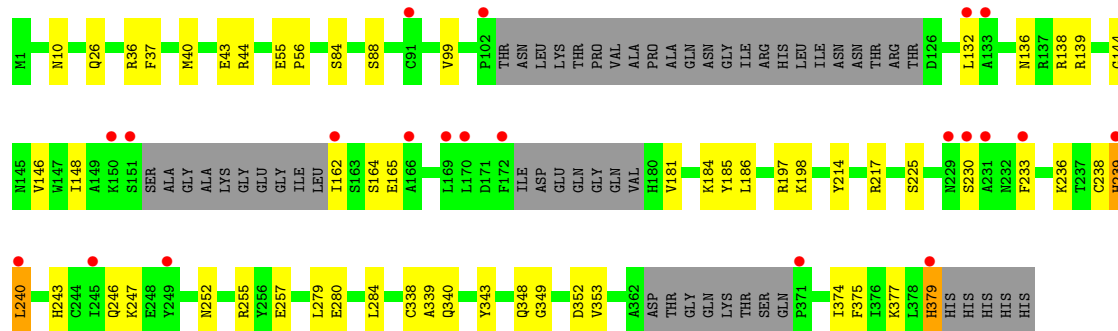




● Molecule 3: Stathmin-4



● 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	104.53Å 158.12Å 179.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.36 – 2.50 59.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.36-2.50) 99.7 (59.36-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.194 , 0.232 0.198 , 0.234	Depositor DCC
R_{free} test set	5155 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18043	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, GOL, CA, GTP, 2RR, CL, MES, IMD, ADP

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	0.27	0/3600	0.72	4/4886 (0.1%)
1	C	0.29	0/3628	0.72	0/4926
2	B	0.28	0/3489	0.69	2/4724 (0.0%)
2	D	0.29	0/3409	0.74	7/4619 (0.2%)
3	E	0.25	0/1069	0.63	0/1419
4	F	0.27	0/2815	0.67	0/3801
All	All	0.28	0/18010	0.71	13/24375 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	289	PRO	CA-C-N	7.39	135.00	121.70
2	D	289	PRO	C-N-CA	7.39	135.00	121.70
1	A	262	TYR	CA-C-N	6.32	125.82	119.24
1	A	262	TYR	C-N-CA	6.32	125.82	119.24
2	B	262	PHE	CA-C-N	5.27	125.33	119.32

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	3487	0	3433	25	0
1	C	3504	0	3447	33	0
2	B	3371	0	3289	31	0
2	D	3324	0	3215	48	0
3	E	1045	0	1066	4	0
4	F	2740	0	2729	38	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	6	0	8	0	0
10	A	5	0	5	0	0
11	B	28	0	12	2	0
11	D	28	0	12	2	0
12	B	29	0	17	2	0
12	D	29	0	17	17	0
13	B	12	0	12	2	0
14	F	27	0	12	3	0
15	A	63	0	0	0	0
15	B	70	0	0	1	0
15	C	144	0	0	1	0
15	D	26	0	0	1	0
15	E	13	0	0	0	0
15	F	18	0	0	2	0
All	All	18043	0	17298	177	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 5.

The worst 5 of 177 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:238:CYS:SG	4:F:239:HIS:CE1	2.03	1.50
4:F:238:CYS:SG	4:F:239:HIS:ND1	2.11	1.22
1:C:180:ALA:N	12:D:604:2RR:H16	1.87	0.89
4:F:238:CYS:SG	4:F:239:HIS:HE1	1.67	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:C	12:D:604:2RR:H16	2.06	0.80

There are no symmetry-related clashes.

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	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	43	63
1	C	453/451 (100%)	443 (98%)	9 (2%)	1 (0%)	43	63
2	B	430/445 (97%)	417 (97%)	11 (3%)	2 (0%)	24	43
2	D	421/445 (95%)	402 (96%)	17 (4%)	2 (0%)	24	43
3	E	125/143 (87%)	124 (99%)	1 (1%)	0	100	100
4	F	325/384 (85%)	313 (96%)	12 (4%)	0	100	100
All	All	2201/2319 (95%)	2130 (97%)	65 (3%)	6 (0%)	36	55

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	290	GLU
2	D	181	VAL
1	C	177	VAL
1	A	178	SER
2	B	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	382/379 (101%)	382 (100%)	0	100	100
1	C	386/379 (102%)	380 (98%)	6 (2%)	55	79
2	B	378/383 (99%)	375 (99%)	3 (1%)	73	88
2	D	368/383 (96%)	359 (98%)	9 (2%)	43	70
3	E	115/127 (91%)	115 (100%)	0	100	100
4	F	303/342 (89%)	299 (99%)	4 (1%)	61	82
All	All	1932/1993 (97%)	1910 (99%)	22 (1%)	65	84

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	286	LEU
2	D	401	ARG
2	D	291	LEU
4	F	236	LYS
1	C	179	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	183	GLN
4	F	306	HIS
2	B	193	GLN
2	B	249	ASN
1	C	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	IMD	A	506	-	5,5,5	0.64	0	5,5,5	0.44	0
11	GDP	B	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.74	6 (13%)
14	ADP	F	401	-	28,29,29	1.40	5 (17%)	43,45,45	1.81	11 (25%)
5	GTP	A	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.54	8 (16%)
12	2RR	B	504	-	32,32,32	1.10	2 (6%)	38,44,44	1.48	6 (15%)
12	2RR	D	604	-	32,32,32	1.15	4 (12%)	38,44,44	1.68	9 (23%)
13	MES	B	505	-	12,12,12	2.34	1 (8%)	15,16,16	2.35	5 (33%)
9	GOL	A	505	-	5,5,5	0.39	0	5,5,5	0.29	0
11	GDP	D	602	6	29,30,30	1.17	3 (10%)	45,47,47	1.73	5 (11%)
5	GTP	C	501	6	33,34,34	1.01	3 (9%)	50,54,54	1.54	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
10	IMD	A	506	-	-	-	0/1/1/1
11	GDP	B	501	-	-	4/16/32/32	0/3/3/3
14	ADP	F	401	-	-	2/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
12	2RR	B	504	-	-	1/17/17/17	0/4/4/4
12	2RR	D	604	-	-	5/17/17/17	0/4/4/4
13	MES	B	505	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	A	505	-	-	2/4/4/4	-
11	GDP	D	602	6	-	5/16/32/32	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	505	MES	C8-S	-7.85	1.66	1.77
14	F	401	ADP	C5-C4	4.67	1.47	1.39
11	D	602	GDP	C5-C4	3.16	1.47	1.38
11	B	501	GDP	C5-C4	3.08	1.47	1.38
12	D	604	2RR	C14-N15	3.06	1.41	1.35

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	501	GDP	C5-C4-N3	-5.94	118.94	128.39
11	D	602	GDP	C5-C4-N3	-5.87	119.05	128.39
13	B	505	MES	C5-N4-C3	5.54	120.77	108.84
14	F	401	ADP	C5-C4-N3	-5.34	119.37	126.72
11	B	501	GDP	C2-N3-C4	5.02	120.95	112.30

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

7 monomers are involved in 29 short contacts:

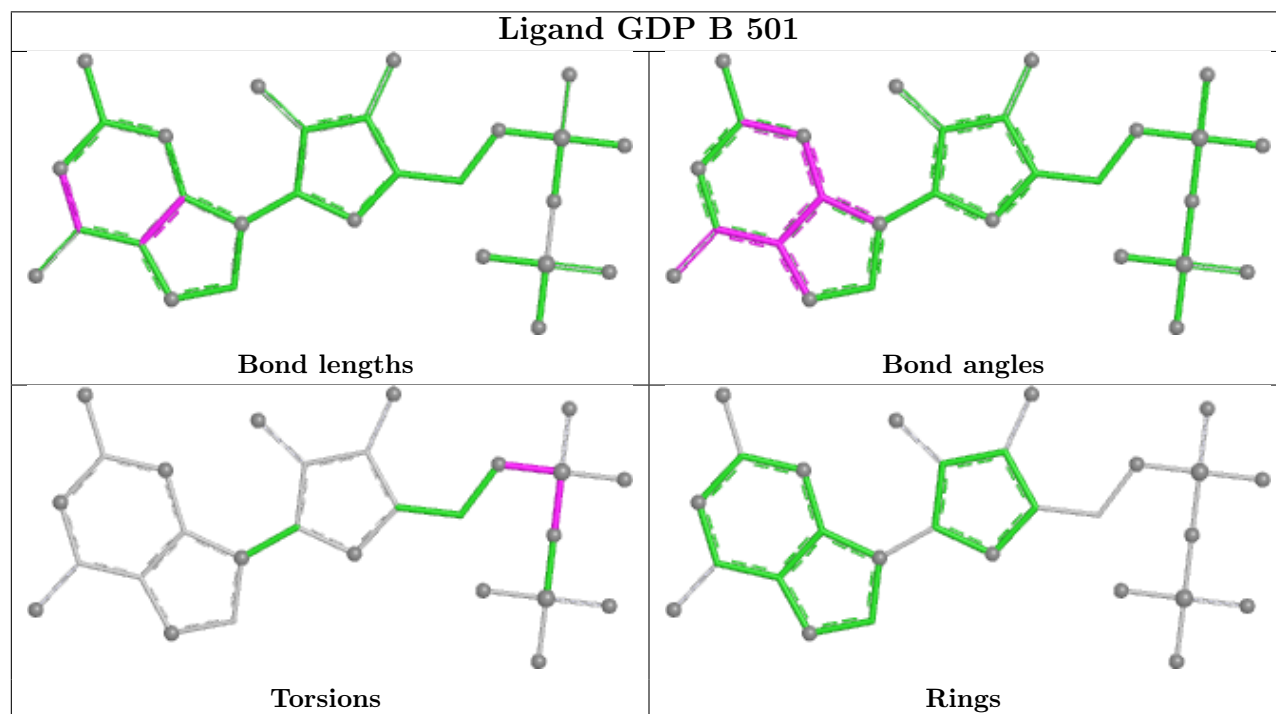
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	501	GDP	2	0
14	F	401	ADP	3	0
5	A	501	GTP	1	0
12	B	504	2RR	2	0

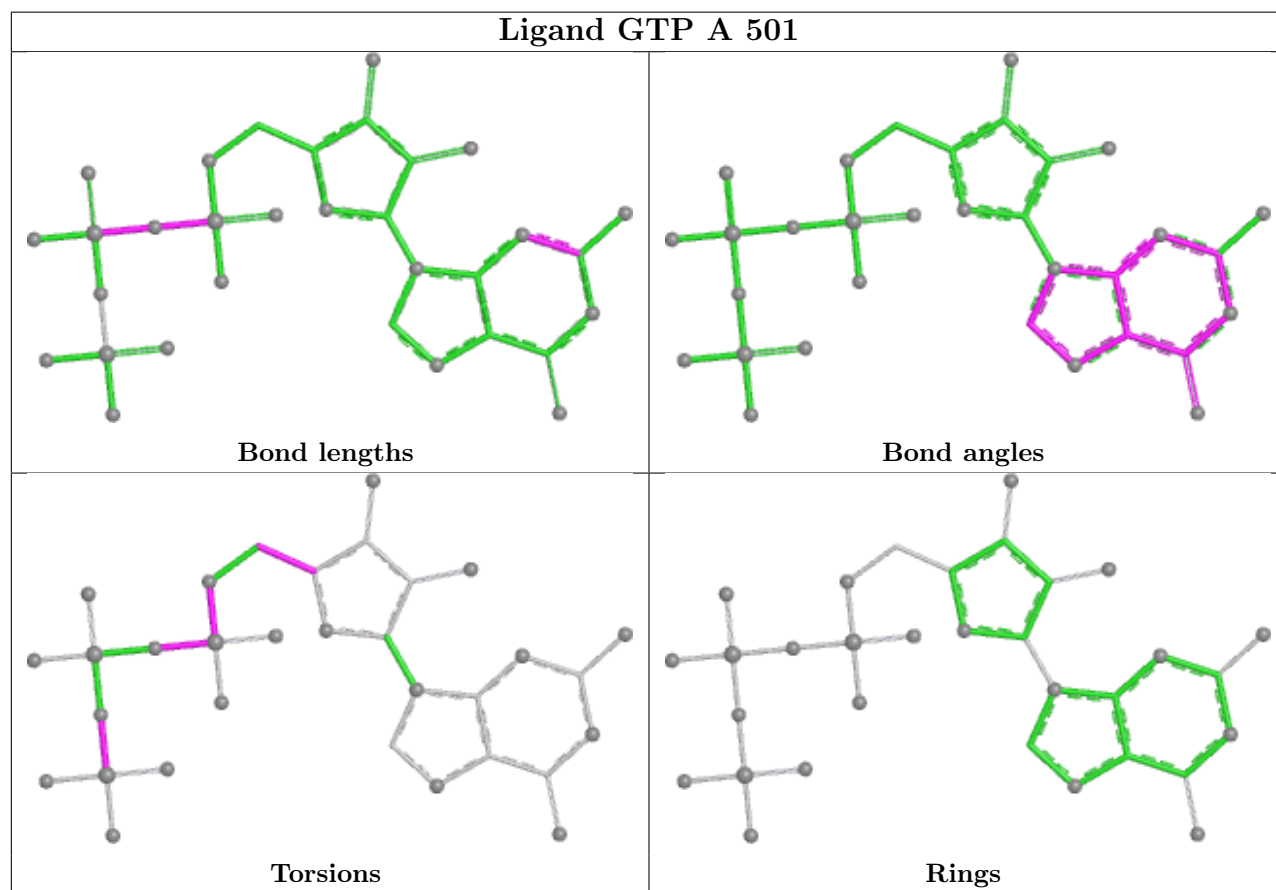
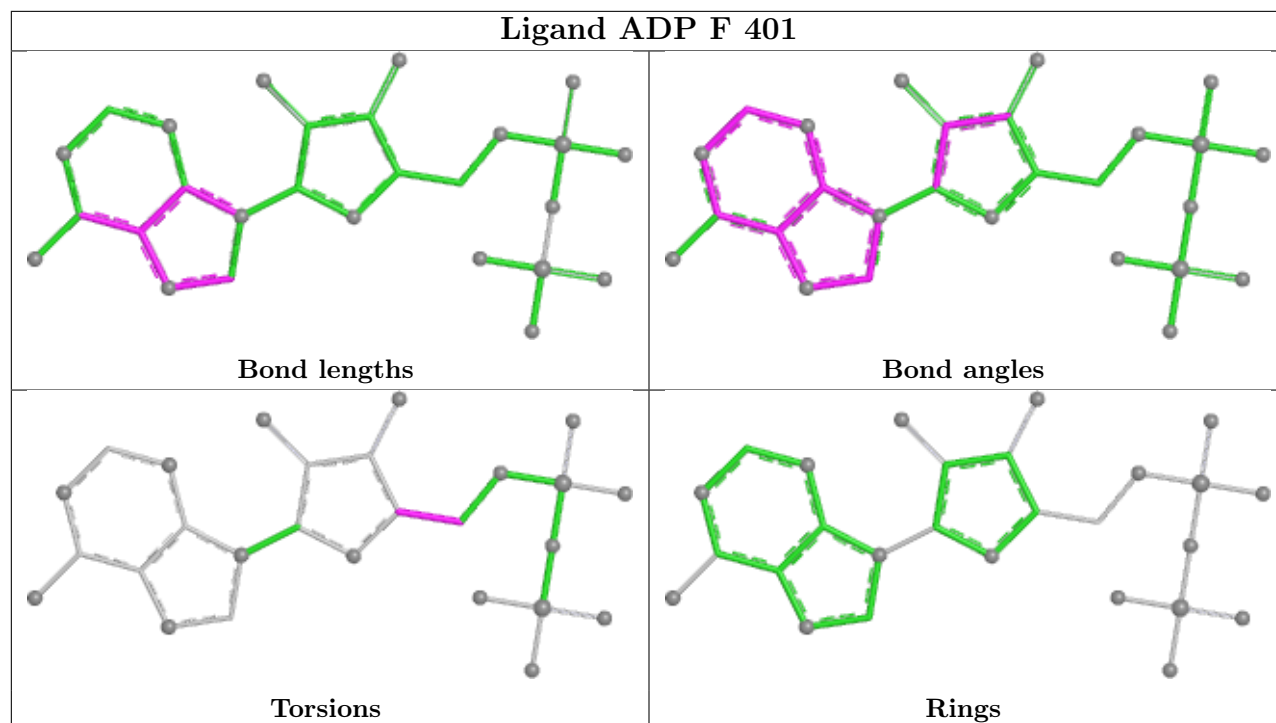
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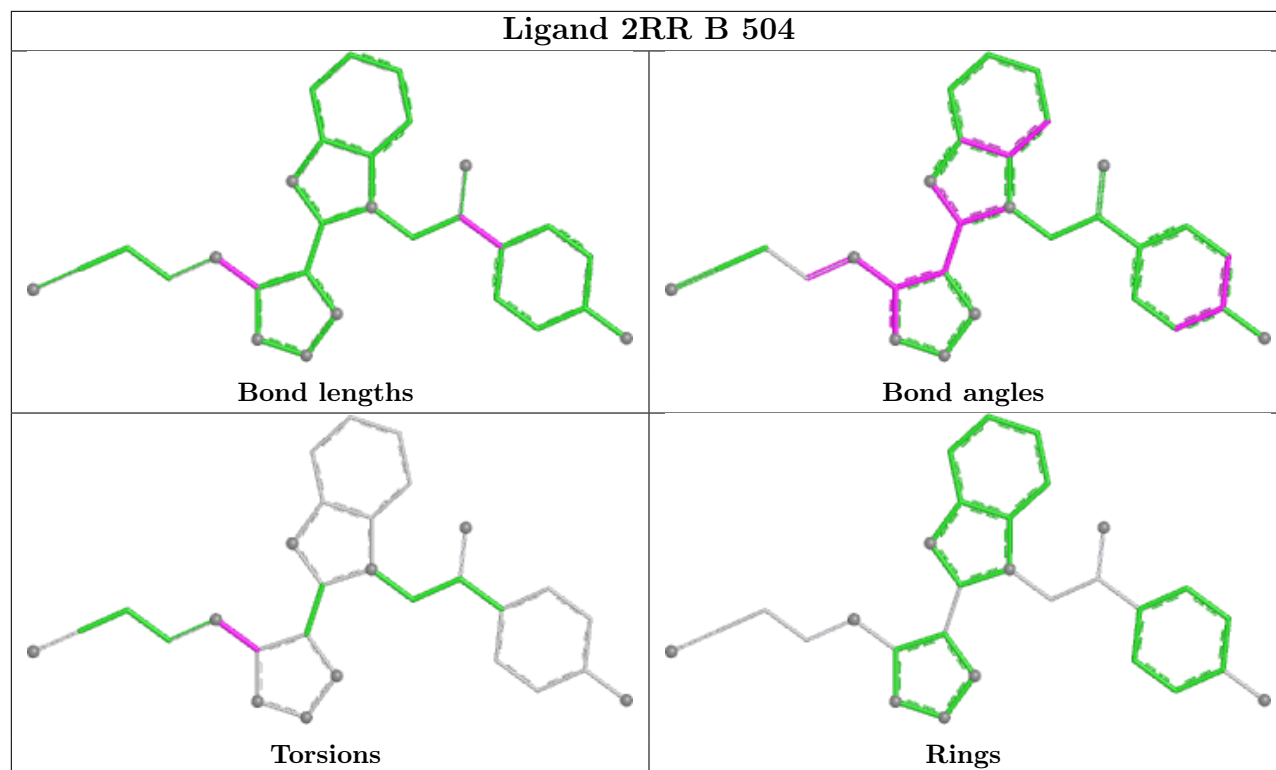
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	604	2RR	17	0
13	B	505	MES	2	0
11	D	602	GDP	2	0

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.

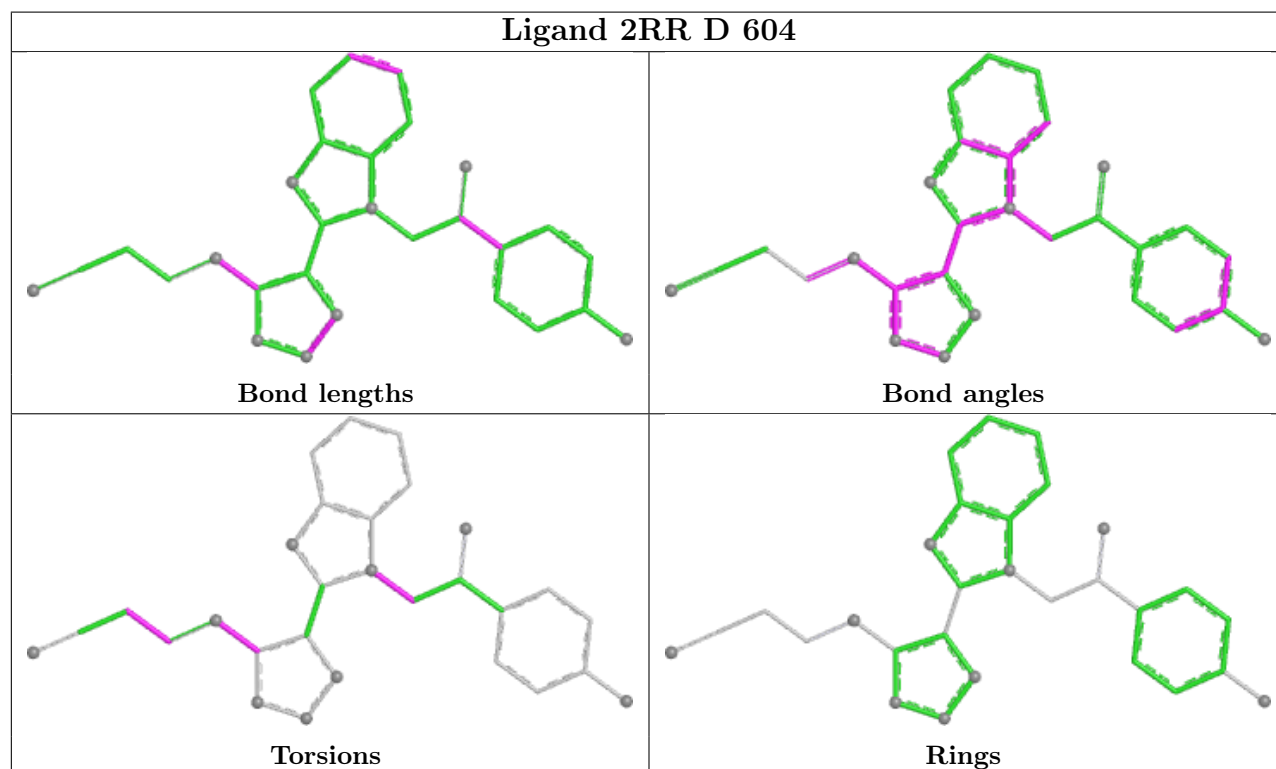


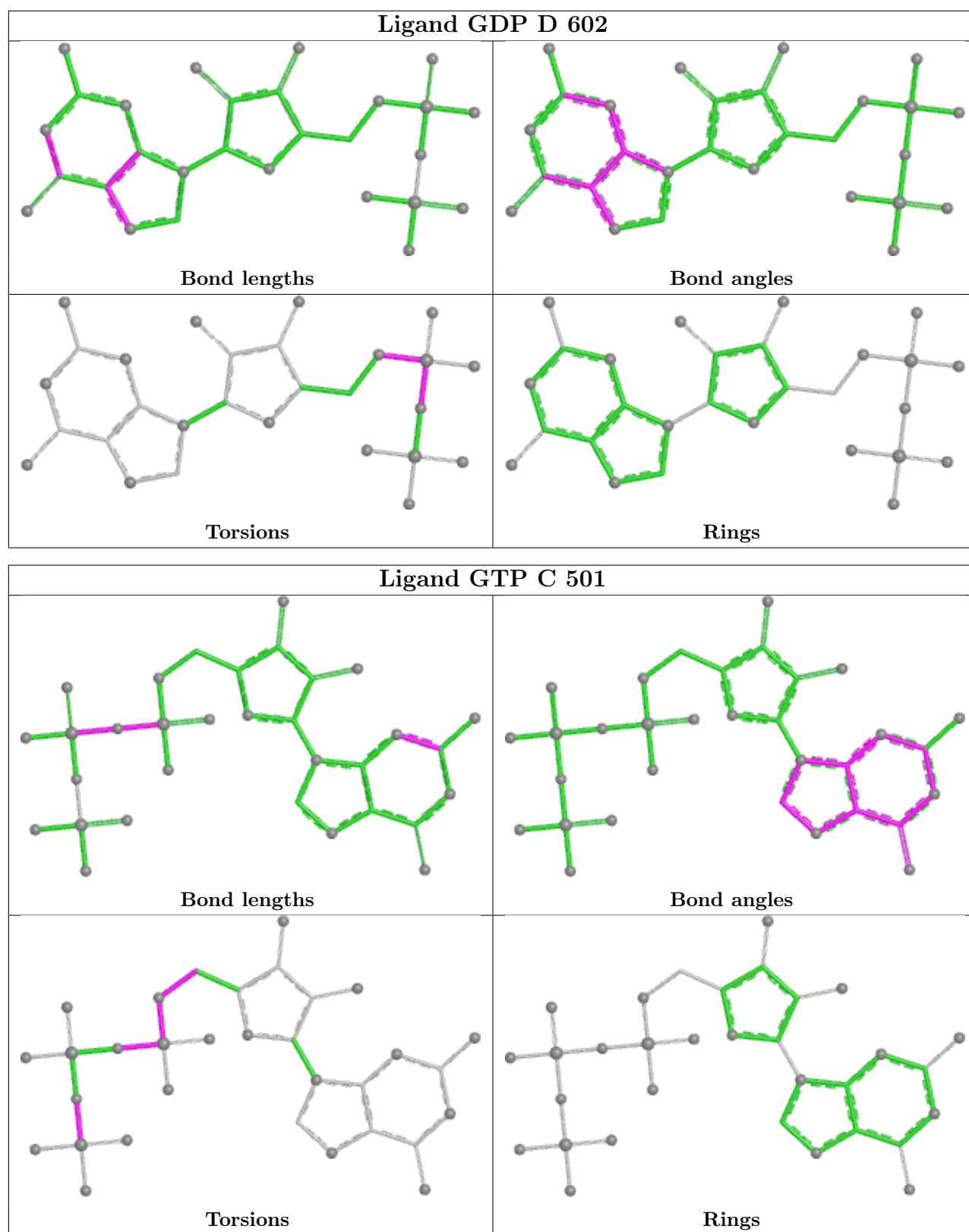


Ligand 2RR B 504



Ligand 2RR D 604





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	439/451 (97%)	-0.31	2 (0%) 87 85	18, 43, 76, 114	12 (2%)
1	C	440/451 (97%)	-0.54	3 (0%) 84 81	15, 31, 65, 98	15 (3%)
2	B	418/445 (93%)	-0.27	3 (0%) 84 81	15, 41, 77, 112	18 (4%)
2	D	421/445 (94%)	0.15	13 (3%) 51 47	24, 57, 93, 116	10 (2%)
3	E	124/143 (86%)	0.14	9 (7%) 21 19	24, 58, 102, 130	5 (4%)
4	F	331/384 (86%)	0.27	21 (6%) 26 23	23, 65, 143, 162	4 (1%)
All	All	2173/2319 (93%)	-0.15	51 (2%) 61 57	15, 46, 98, 162	64 (2%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	VAL	4.9
4	F	371	PRO	4.6
4	F	379	HIS	4.5
3	E	143	ALA	4.5
2	B	438	ALA	4.3

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 ⓘ

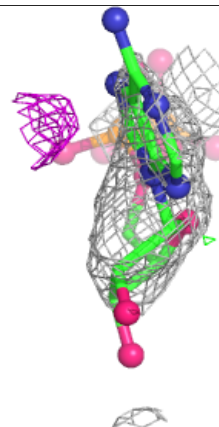
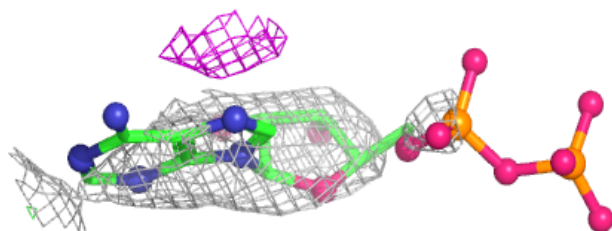
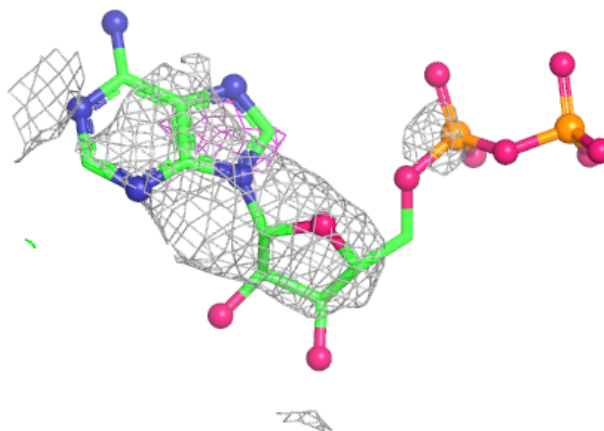
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ADP	F	401	27/27	0.68	0.17	165,168,234,394	0
12	2RR	D	604	29/29	0.70	0.19	60,72,78,80	0
7	CA	B	503	1/1	0.85	0.19	81,81,81,81	0
10	IMD	A	506	5/5	0.86	0.23	92,92,94,95	0
9	GOL	A	505	6/6	0.89	0.19	90,97,99,99	0
8	CL	A	504	1/1	0.89	0.10	78,78,78,78	0
6	MG	B	502	1/1	0.90	0.26	47,47,47,47	0
11	GDP	D	602	28/28	0.92	0.08	35,44,62,69	0
13	MES	B	505	12/12	0.93	0.10	41,50,67,67	0
12	2RR	B	504	29/29	0.93	0.09	34,47,54,55	0
6	MG	D	603	1/1	0.95	0.05	44,44,44,44	0
11	GDP	B	501	28/28	0.96	0.06	18,27,36,43	0
7	CA	E	700	1/1	0.96	0.13	84,84,84,84	0
6	MG	B	506	1/1	0.96	0.08	42,42,42,42	0
7	CA	A	503	1/1	0.97	0.06	62,62,62,62	0
6	MG	A	502	1/1	0.97	0.03	25,25,25,25	0
5	GTP	A	501	32/32	0.97	0.06	13,31,36,67	0
5	GTP	C	501	32/32	0.98	0.05	11,22,35,62	0
7	CA	C	502	1/1	0.98	0.03	58,58,58,58	0
6	MG	D	601	1/1	0.98	0.06	23,23,23,23	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.

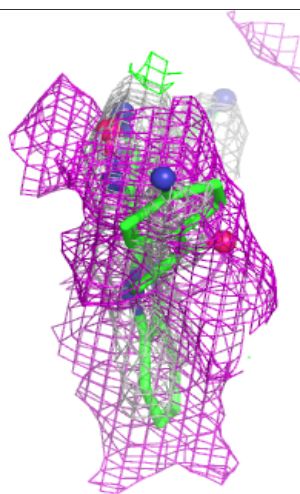
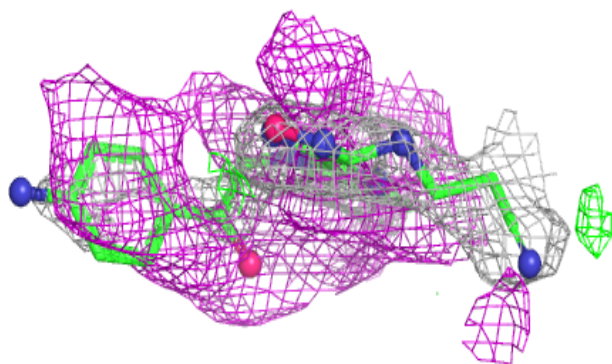
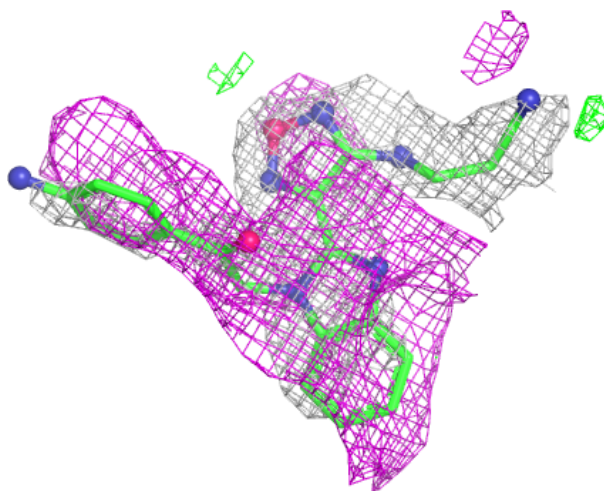
Electron density around ADP F 401:

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



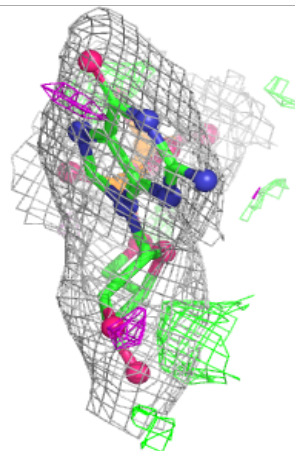
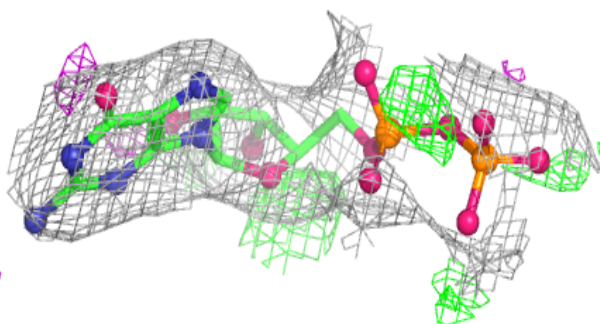
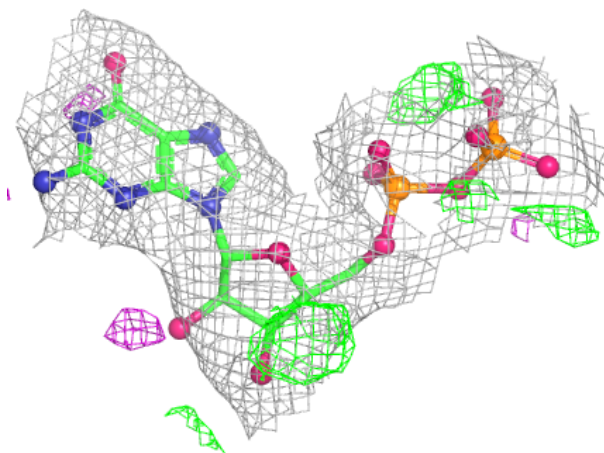
Electron density around 2RR D 604:

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



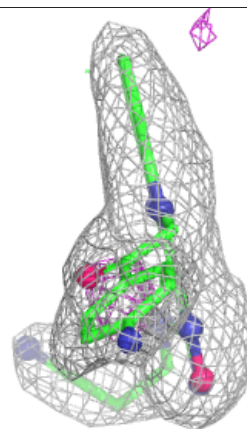
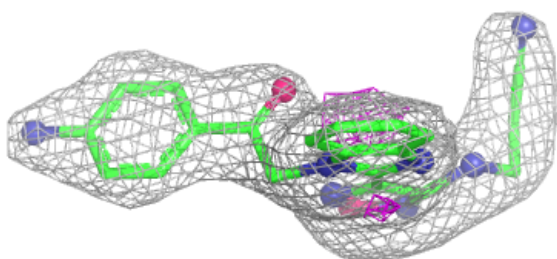
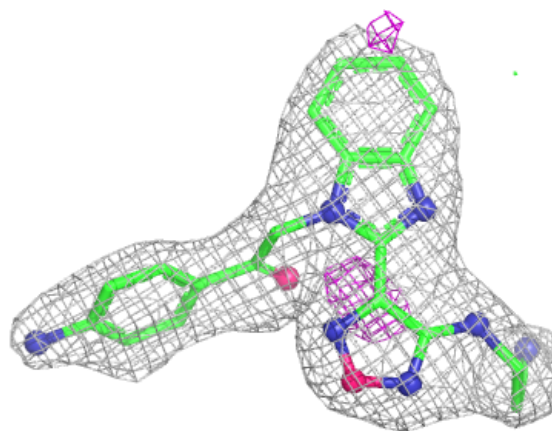
Electron density around GDP D 602:

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



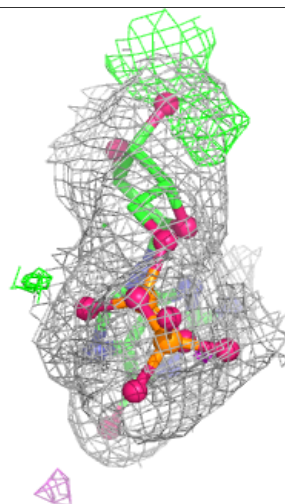
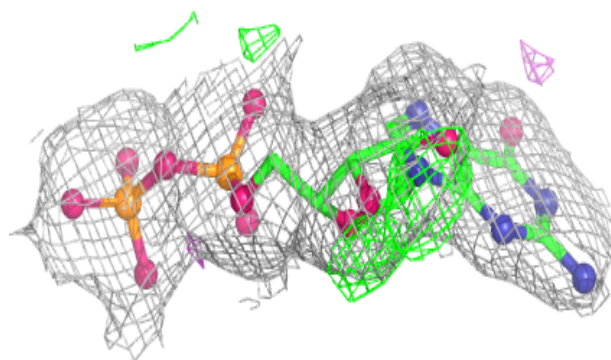
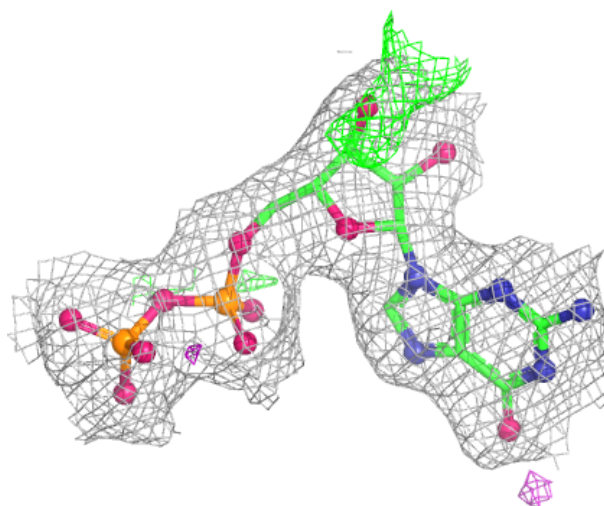
Electron density around 2RR B 504:

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



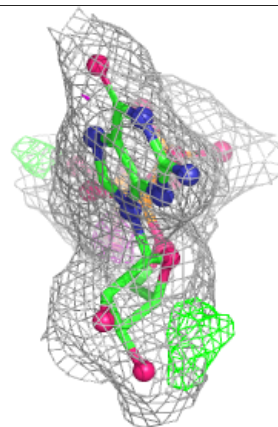
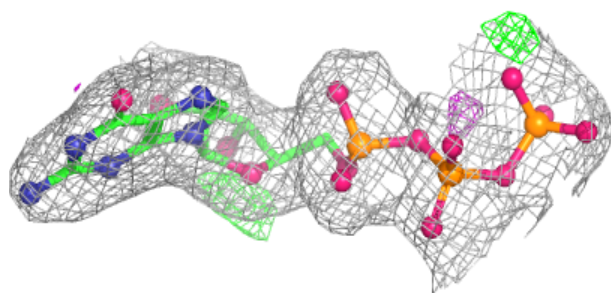
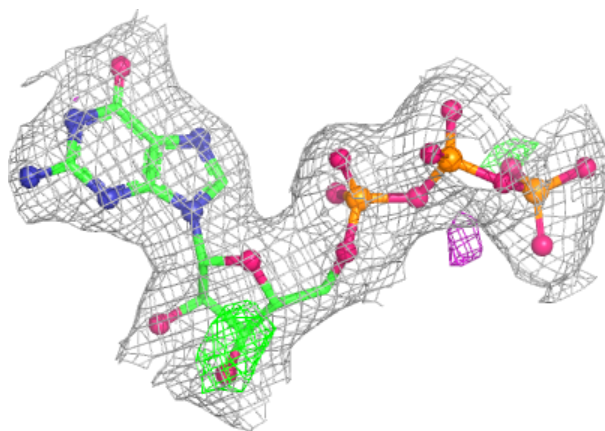
Electron density around GDP B 501:

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and green (positive)

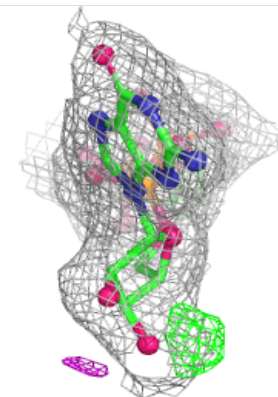
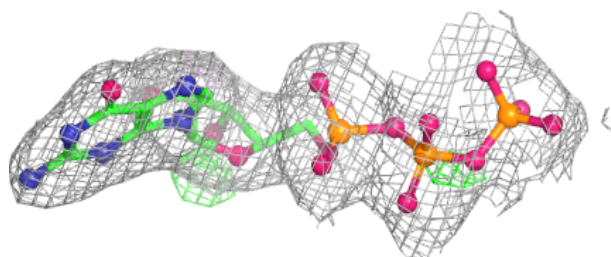
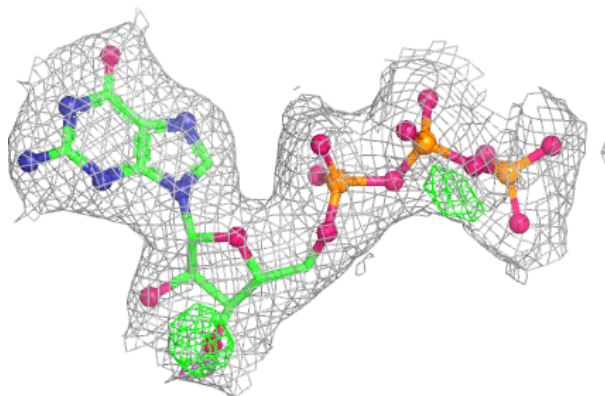


Electron density around GTP A 501:

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

There are no such residues in this entry.