wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2026 – 05:45 pm GMT

PDB ID	:	9R2X / pdb_00009r2x
Title	:	T2R-TTL-compound 5 complex
Authors	:	Estevez-Gallego, J.; Steinmetz, M.O.; Komarov, I.V.; Spring, D.; Prota, A.E.
Deposited on	:	2025-05-01
Resolution	:	2.48 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 (i) 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 (i)) were used in the production of this report:

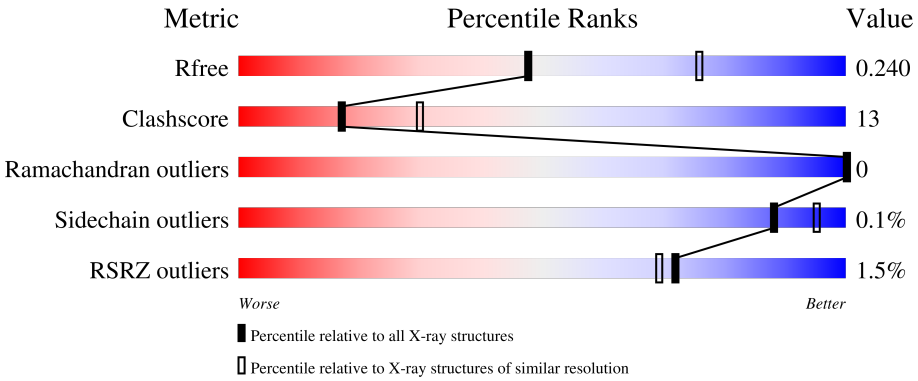
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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.



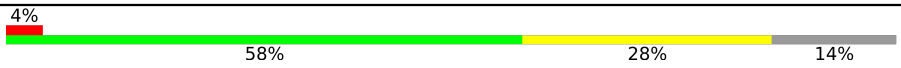
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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 <=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	70% 27% .
1	C	451	77% 21% .
2	B	445	71% 26% .
2	D	445	64% 30% 5%
3	E	143	3% 62% 24% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 17929 atoms, of which 73 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	11	0
			3463	2202	582	654	25			
1	C	440	Total	C	N	O	S	0	10	0
			3484	2207	586	667	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	10	0
			3434	2159	586	661	28			
2	D	422	Total	C	N	O	S	0	2	0
			3323	2089	563	643	28			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	437	ASP	-	insertion	UNP Q6B856
B	438	ALA	-	insertion	UNP Q6B856
B	439	THR	-	insertion	UNP Q6B856
B	440	ALA	-	insertion	UNP Q6B856
B	441	GLU	-	insertion	UNP Q6B856
B	442	TYR	-	insertion	UNP Q6B856
B	443	GLN	-	insertion	UNP Q6B856
B	444	GLN	-	insertion	UNP Q6B856
B	445	TYR	-	insertion	UNP Q6B856
B	446	GLN	-	insertion	UNP Q6B856
D	437	ASP	-	insertion	UNP Q6B856
D	438	ALA	-	insertion	UNP Q6B856
D	439	THR	-	insertion	UNP Q6B856
D	440	ALA	-	insertion	UNP Q6B856
D	441	GLU	-	insertion	UNP Q6B856
D	442	TYR	-	insertion	UNP Q6B856

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Chain	Residue	Modelled	Actual	Comment	Reference
D	443	GLN	-	insertion	UNP Q6B856
D	444	GLN	-	insertion	UNP Q6B856
D	445	TYR	-	insertion	UNP Q6B856
D	446	GLN	-	insertion	UNP Q6B856

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1023	631	184	203	5			

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 tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	330	Total	C	N	O	S	0	0	0
			2706	1742	460	490	14			

There are 39 discrepancies between the modelled and reference sequences:

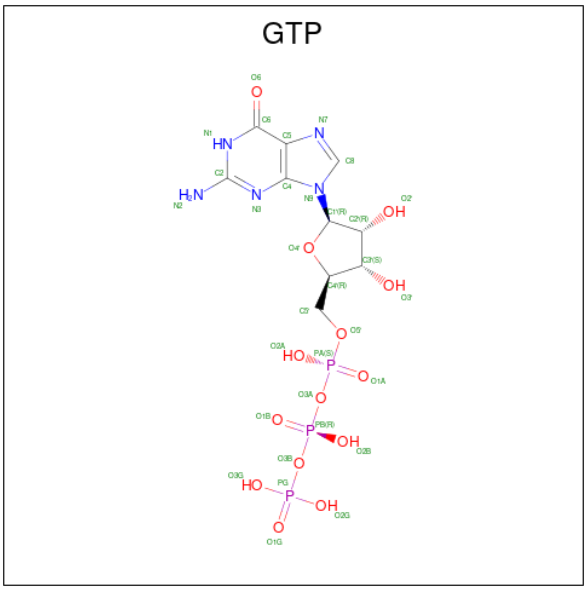
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion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

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Chain	Residue	Modelled	Actual	Comment	Reference
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: $C_{10}H_{16}N_5O_{14}P_3$).



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		

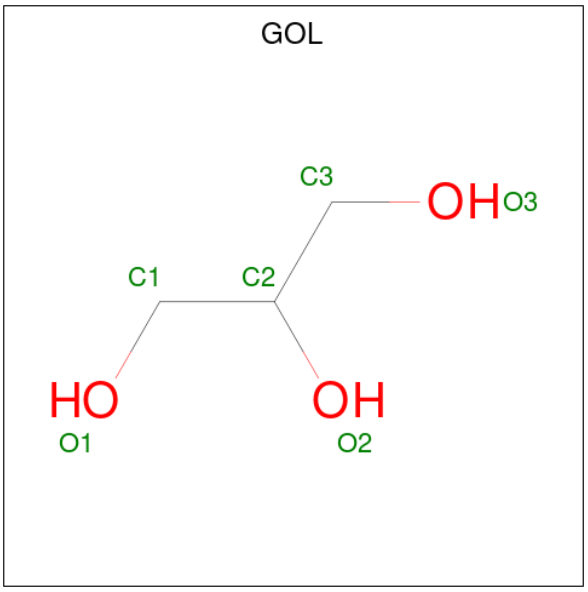
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

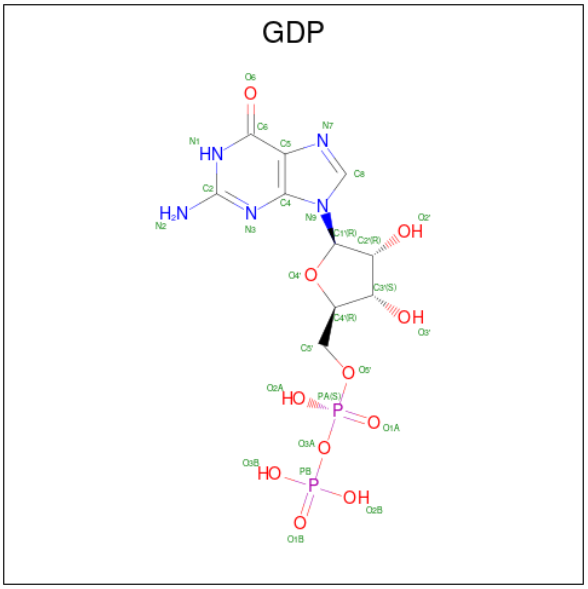
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



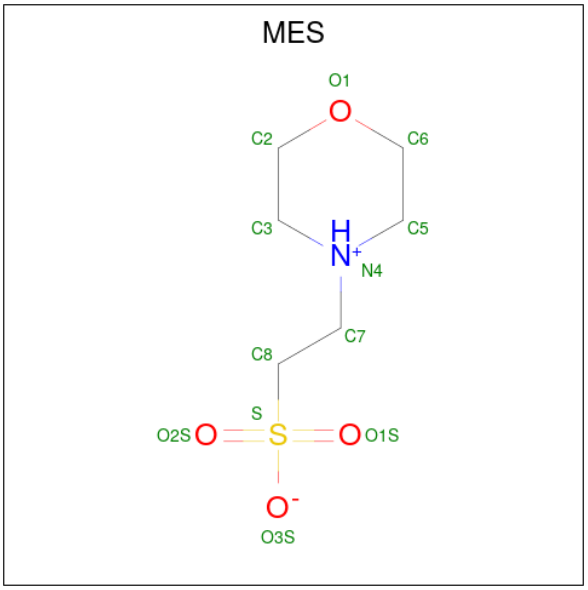
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

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



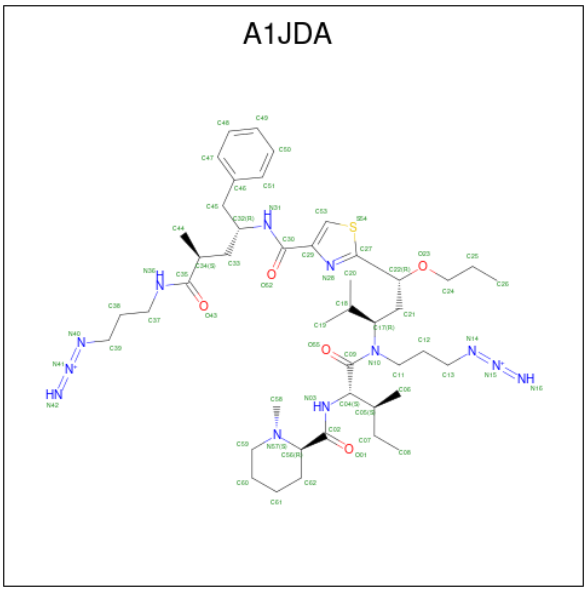
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



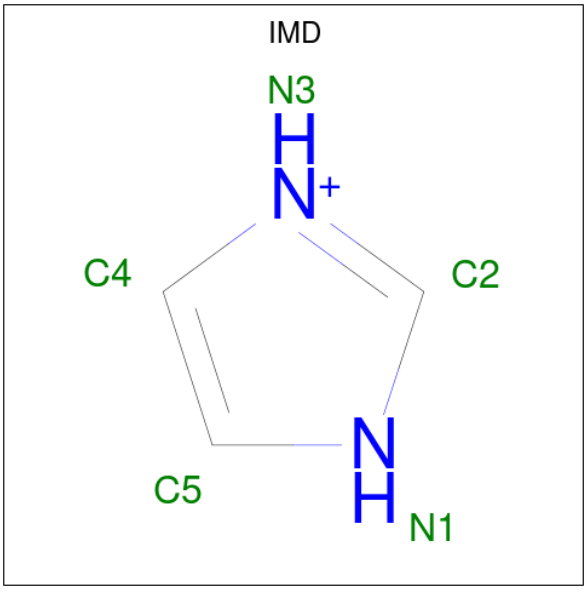
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is {N}-[(2 {R},4 {S})-5-[3-[(azanylidene-$l^{4}-azanylidene)amino]propylamino]-4-methyl-5-oxidanylidene-1-phenyl-pentan-2-yl]-2-[(1 {R},3 {R})-3-[3-[(azanylidene-$l^{4}-azanylidene)amino]propyl-[(2 {S},3 {S})-3-methyl-2-[[(2 {R})-1-methylpiperidin-2-yl]carbonylamino]pentanoyl]amino]-4-methyl-1-propoxy-pentyl]-1,3-thiazole-4-carboxamide (CCD ID: A1JDA) (formula: $C_{44}H_{72}N_{12}O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	S	0	0
			130	44	68	12	5	1		

- Molecule 12 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



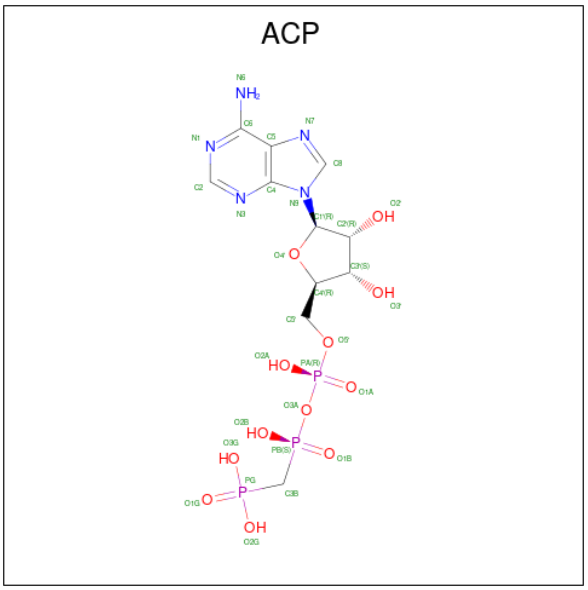
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	H	N	0	0
			10	3	5	2		
12	C	1	Total	C	N		0	0
			5	3	2			
12	C	1	Total	C	N		0	0
			5	3	2			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	E	1	Total C N 5 3 2	0	0

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	26	Total O 26 26	0	0
14	B	39	Total O 39 39	0	0
14	C	57	Total O 57 57	0	0
14	D	8	Total O 8 8	0	0
14	E	3	Total O 3 3	0	0
14	F	7	Total O 7 7	0	0

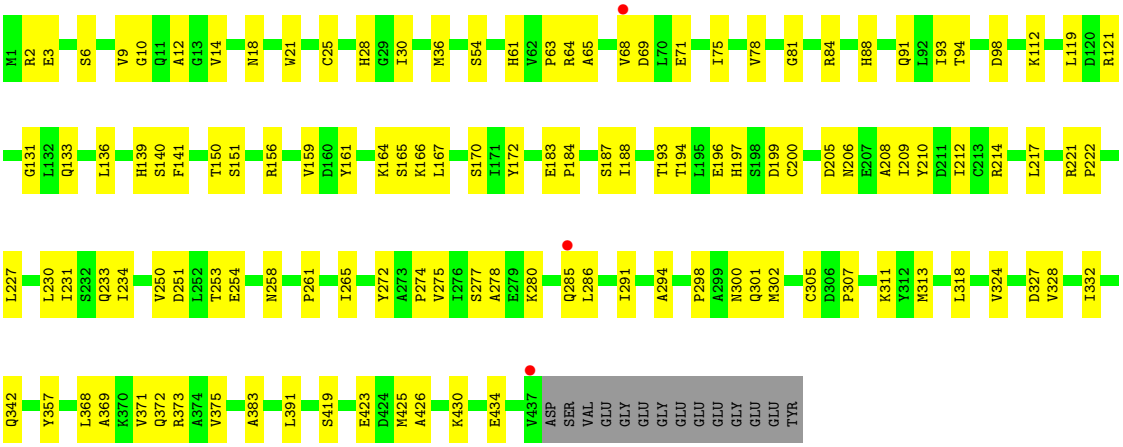
3 Residue-property plots (i)

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

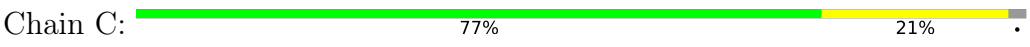
Chain A:





• Molecule 1: Tubulin alpha-1B chain

Chain C:



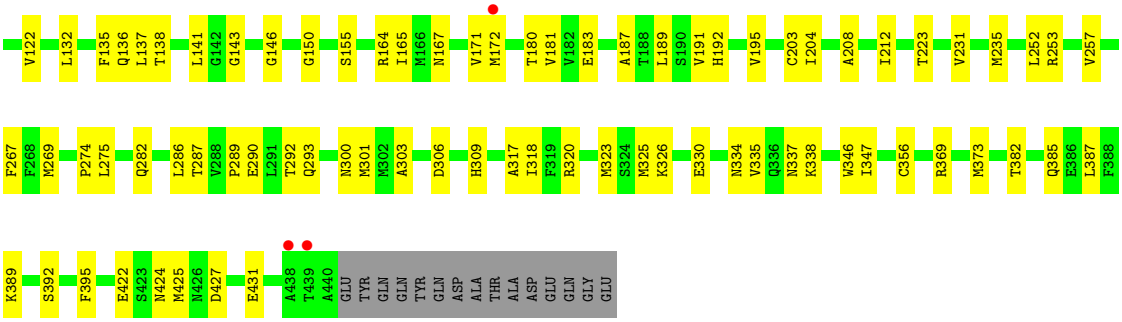


• Molecule 2: Tubulin beta-2B chain

Chain B:

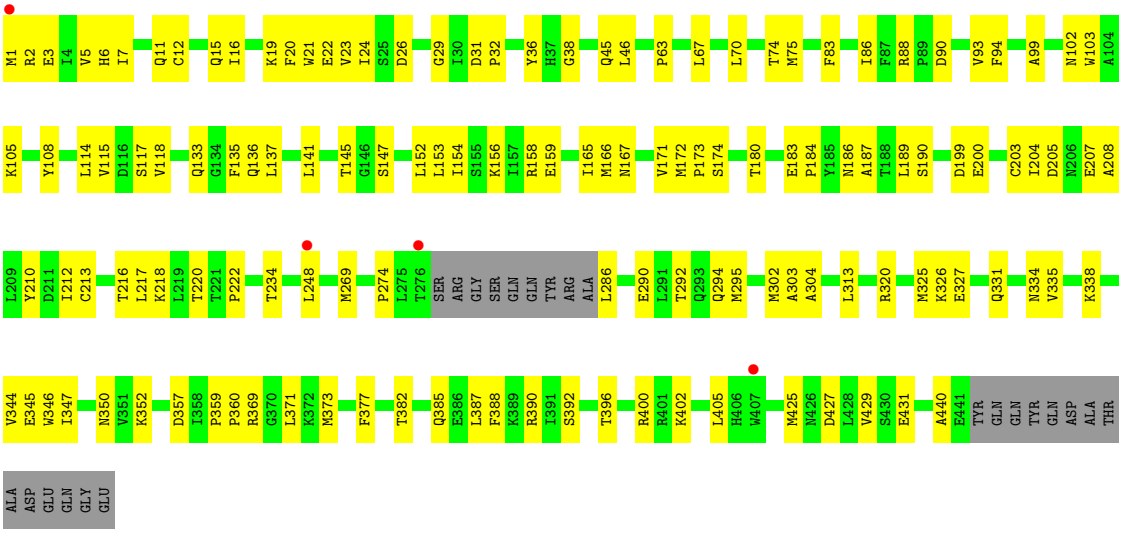






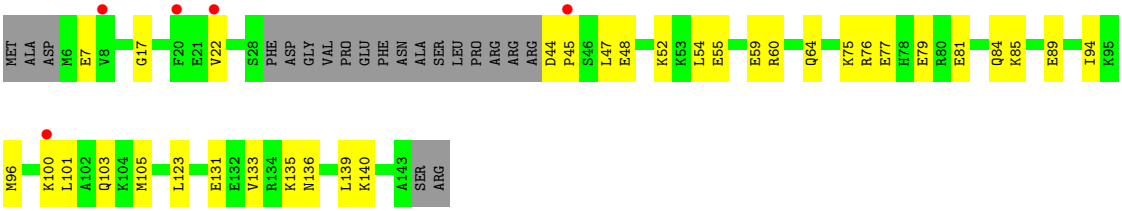
• Molecule 2: Tubulin beta-2B chain





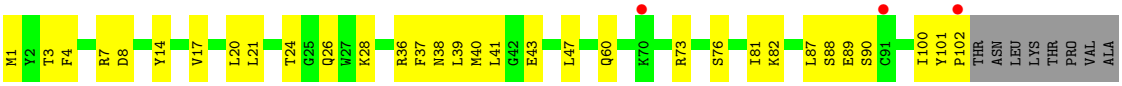
• Molecule 3: Stathmin-4

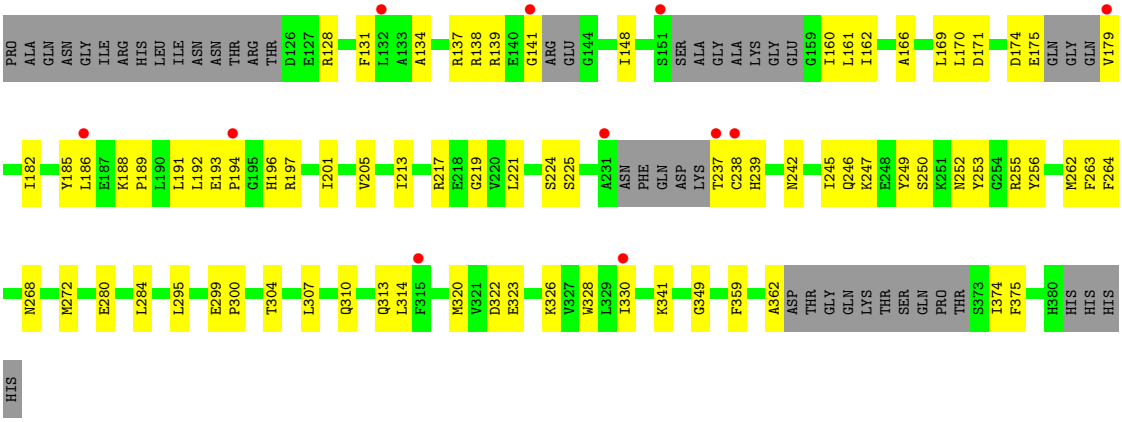




• Molecule 4: Tubulin tyrosine ligase






PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG THR D126 E127 R128 F131 L132 A133 A134 R137 R138 R139 E140 G141 ARG GLU G144 I148 S151 SER ALA GLY ALA LYS GLY GLU G159 I160 L161 I162 A166 L169 L170 D171 D174 E175 GLN GLY GLN V179
I182 Y185 L186 E187 K188 P189 L190 L191 L192 E193 P194 G195 H196 R197 I201 V205 I213 R217 E218 G219 V220 L221 S224 S225 A231 ASN PHE GLN ASP LYS T237 C238 H239 N242 I245 Q246 K247 E248 Y249 S250 K251 N252 Y253 G254 R255 Y256 M262 F263 F264
N268 M272 E280 L284 L295 E299 P300 T304 L307 Q310 Q313 L314 F315 M320 V321 D322 E323 K326 V327 W328 L329 I330 K341 G349 F359 A362 ASP THR GLY GLN LYS THR SER GLN PRO THR S373 I374 F375 H380 HIS HIS HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.84Å 155.89Å 183.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.40 – 2.48 50.40 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.40-2.48) 99.9 (50.40-2.48)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.199 , 0.240 0.199 , 0.240	Depositor DCC
R_{free} test set	5403 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17929	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1JDA, MES, CA, IMD, GDP, ACP, GOL, MG, GTP

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	0.07	0/3575	0.21	0/4854
1	C	0.07	0/3586	0.21	0/4869
2	B	0.07	0/3533	0.22	0/4784
2	D	0.06	0/3402	0.20	0/4608
3	E	0.05	0/1037	0.15	0/1376
4	F	0.05	0/2766	0.20	0/3733
All	All	0.06	0/17899	0.21	0/24224

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

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	3463	0	3416	94	0
1	C	3484	0	3407	71	0
2	B	3434	0	3340	83	0
2	D	3323	0	3208	100	0
3	E	1023	0	1042	25	0
4	F	2706	0	2680	86	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	3	0
8	B	6	0	8	1	0
8	C	6	0	8	0	0
9	B	28	0	12	2	0
9	D	28	0	12	2	0
10	B	12	0	13	0	0
11	B	62	68	0	1	0
12	C	15	5	15	4	0
12	E	5	0	5	0	0
13	F	31	0	14	0	0
14	A	26	0	0	1	0
14	B	39	0	0	2	0
14	C	57	0	0	2	0
14	D	8	0	0	0	0
14	E	3	0	0	1	0
14	F	7	0	0	1	0
All	All	17856	73	17228	444	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 13.

The worst 5 of 444 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)
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.42	1.02
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.41	0.99
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.41	0.98
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.47	0.97
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.48	0.92

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	446/451 (99%)	428 (96%)	18 (4%)	0	100	100
1	C	448/451 (99%)	438 (98%)	10 (2%)	0	100	100
2	B	438/445 (98%)	426 (97%)	12 (3%)	0	100	100
2	D	420/445 (94%)	404 (96%)	16 (4%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	316/384 (82%)	296 (94%)	20 (6%)	0	100	100
All	All	2189/2319 (94%)	2111 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	379/379 (100%)	379 (100%)	0	100	100
1	C	381/379 (100%)	380 (100%)	1 (0%)	86	93
2	B	381/383 (100%)	381 (100%)	0	100	100
2	D	367/383 (96%)	367 (100%)	0	100	100
3	E	112/127 (88%)	112 (100%)	0	100	100
4	F	297/342 (87%)	297 (100%)	0	100	100
All	All	1917/1993 (96%)	1916 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	71	GLU

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

Mol	Chain	Res	Type
2	D	102	ASN
2	D	300	ASN
4	F	333	ASN
3	E	18	GLN
2	D	294	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
5	GTP	C	502	6	30,34,34	0.82	1 (3%)	46,54,54	1.69	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	A1JDA	B	506	-	61,64,64	1.43	8 (13%)	69,83,83	1.57	13 (18%)
8	GOL	A	504	-	5,5,5	0.33	0	5,5,5	0.37	0
8	GOL	A	506	-	5,5,5	0.33	0	5,5,5	0.41	0
9	GDP	B	501	-	28,30,30	1.14	3 (10%)	44,47,47	1.72	6 (13%)
12	IMD	C	507	-	5,5,5	0.30	0	5,5,5	0.73	0
8	GOL	B	505	-	5,5,5	0.33	0	5,5,5	0.34	0
12	IMD	E	201	-	5,5,5	0.30	0	5,5,5	0.79	0
10	MES	B	503	-	12,12,12	1.12	1 (8%)	14,16,16	0.90	0
13	ACP	F	501	6	30,33,33	2.14	2 (6%)	45,52,52	0.91	3 (6%)
8	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.39	0
12	IMD	C	501	-	5,5,5	0.29	0	5,5,5	0.80	0
5	GTP	A	501	6	30,34,34	0.83	1 (3%)	46,54,54	1.68	10 (21%)
9	GDP	D	501	6	28,30,30	1.14	3 (10%)	44,47,47	1.80	7 (15%)
8	GOL	C	506	-	5,5,5	0.33	0	5,5,5	0.37	0
12	IMD	C	505	-	5,5,5	0.29	0	5,5,5	0.78	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	GTP	C	502	6	-	10/22/38/38	0/3/3/3
11	A1JDA	B	506	-	-	14/74/86/86	0/3/3/3
8	GOL	A	504	-	-	0/4/4/4	-
8	GOL	A	506	-	-	0/4/4/4	-
9	GDP	B	501	-	-	6/16/32/32	0/3/3/3
12	IMD	C	507	-	-	-	0/1/1/1
8	GOL	B	505	-	-	0/4/4/4	-
12	IMD	E	201	-	-	-	0/1/1/1
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
13	ACP	F	501	6	-	5/19/38/38	0/3/3/3
8	GOL	A	505	-	-	1/4/4/4	-
12	IMD	C	501	-	-	-	0/1/1/1
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
9	GDP	D	501	6	-	2/16/32/32	0/3/3/3
8	GOL	C	506	-	-	0/4/4/4	-
12	IMD	C	505	-	-	-	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	501	ACP	PB-O3A	10.85	1.70	1.58
11	B	506	A1JDA	C33-C34	-7.27	1.34	1.54
9	D	501	GDP	C5-C4	3.12	1.47	1.38
9	B	501	GDP	C5-C4	3.07	1.47	1.38
10	B	503	MES	C8-S	2.93	1.81	1.77

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	501	GDP	C5-C4-N3	-5.93	118.83	128.46
9	B	501	GDP	C5-C4-N3	-5.77	119.11	128.46
11	B	506	A1JDA	C44-C34-C35	5.01	117.48	109.42
5	A	501	GTP	C5-C4-N3	-4.91	120.49	128.46
9	D	501	GDP	C2-N3-C4	4.80	120.85	112.30

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

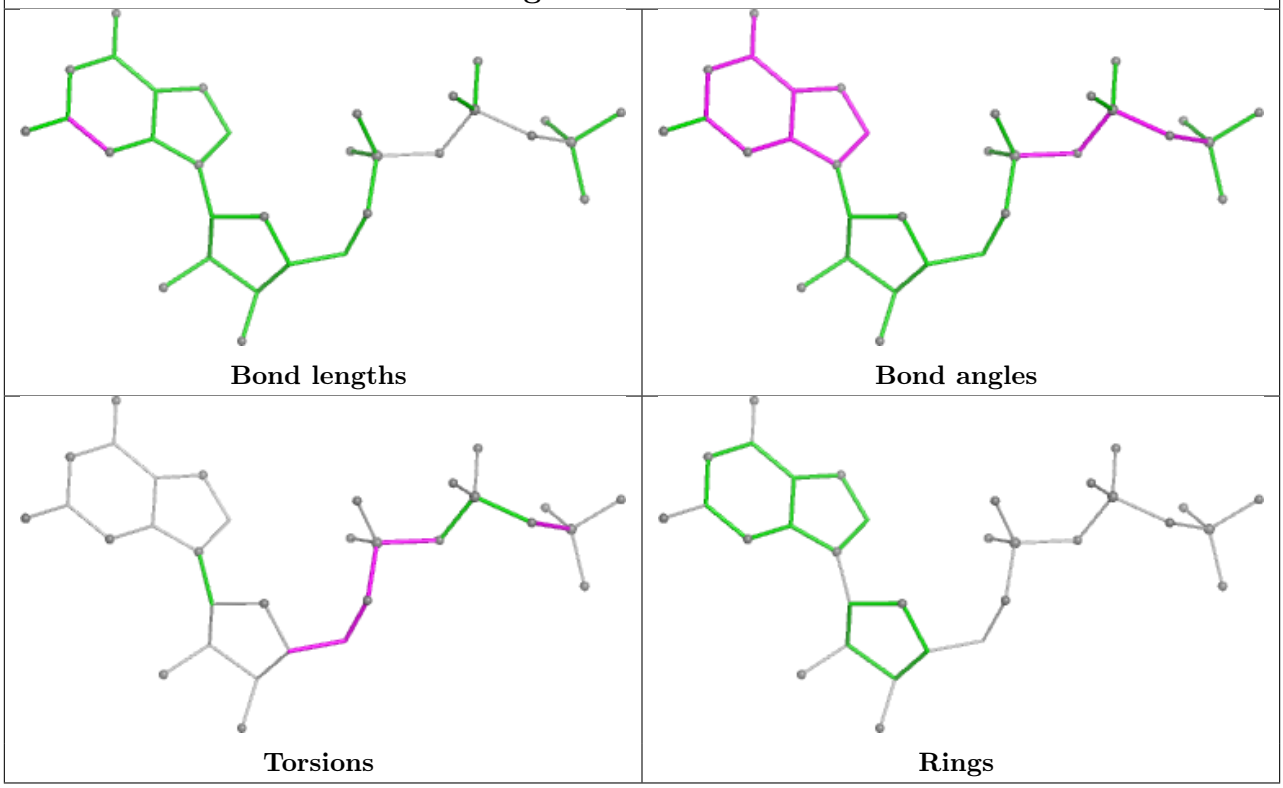
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	506	A1JDA	1	0
8	A	504	GOL	1	0
9	B	501	GDP	2	0
12	C	507	IMD	3	0
8	B	505	GOL	1	0
8	A	505	GOL	2	0
5	A	501	GTP	1	0
9	D	501	GDP	2	0
12	C	505	IMD	1	0

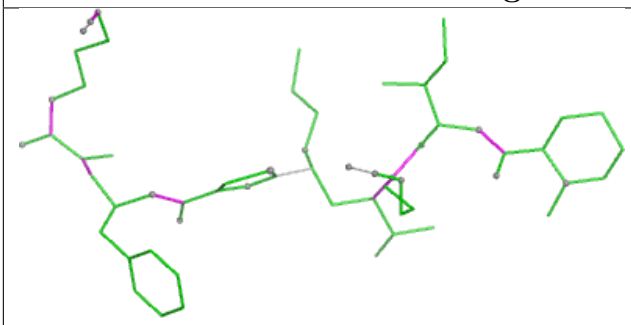
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

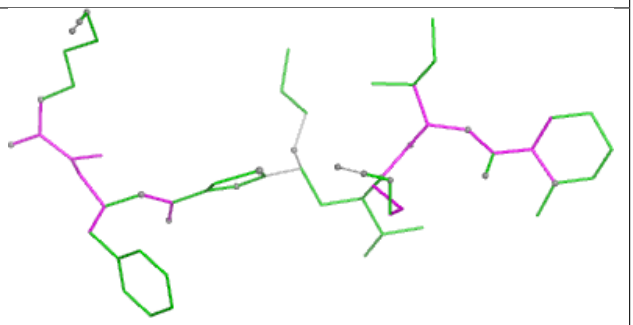
Ligand GTP C 502



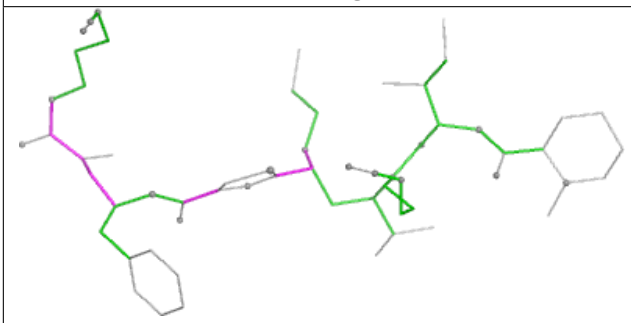
Ligand A1JDA B 506



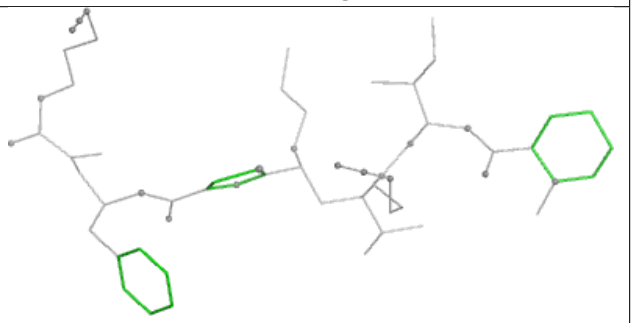
Bond lengths



Bond angles

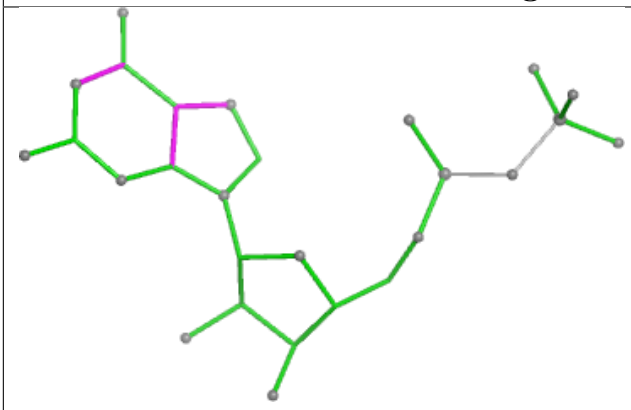


Torsions

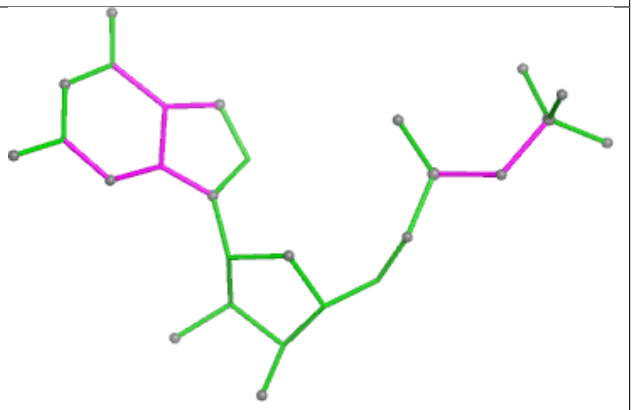


Rings

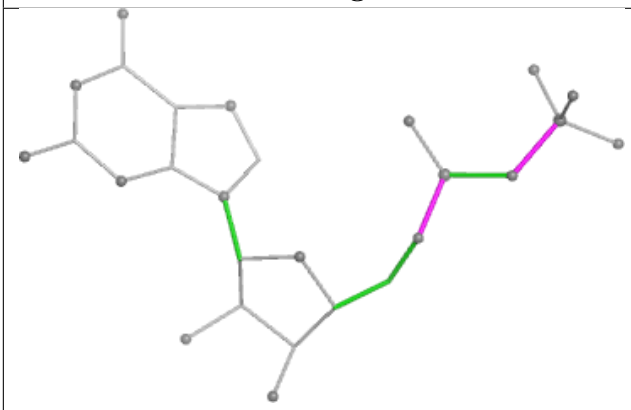
Ligand GDP B 501



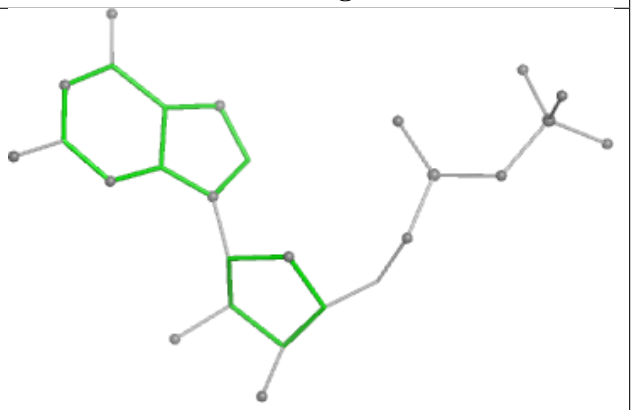
Bond lengths



Bond angles

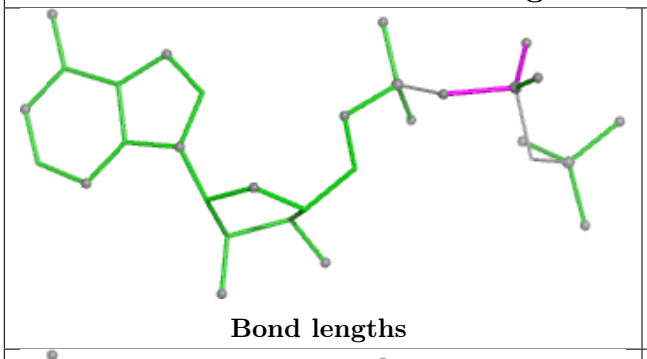


Torsions

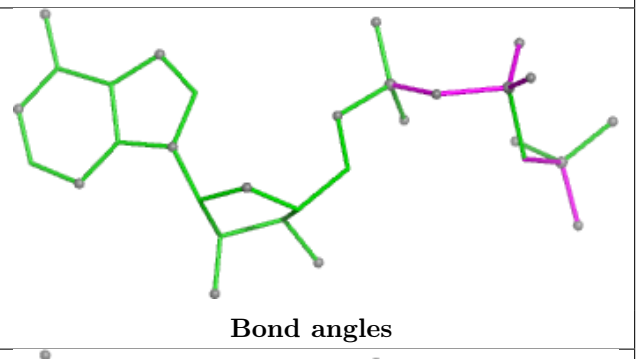


Rings

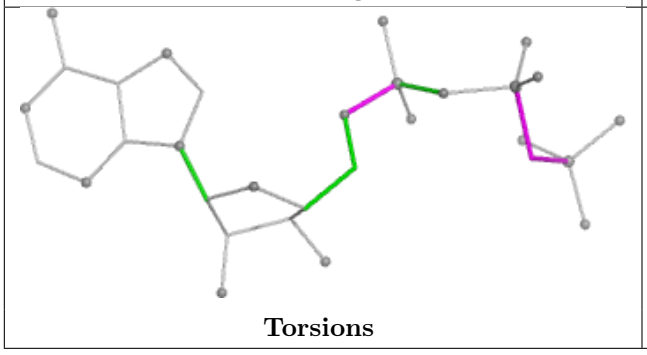
Ligand ACP F 501



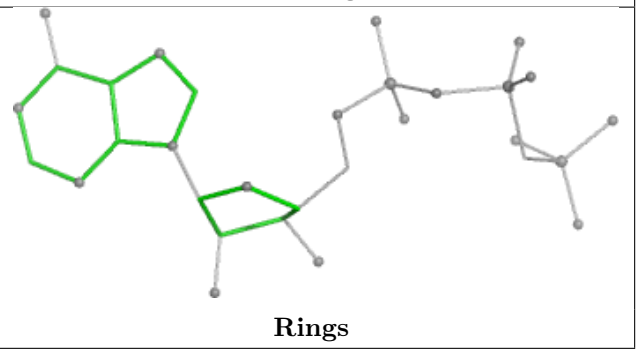
Bond lengths



Bond angles

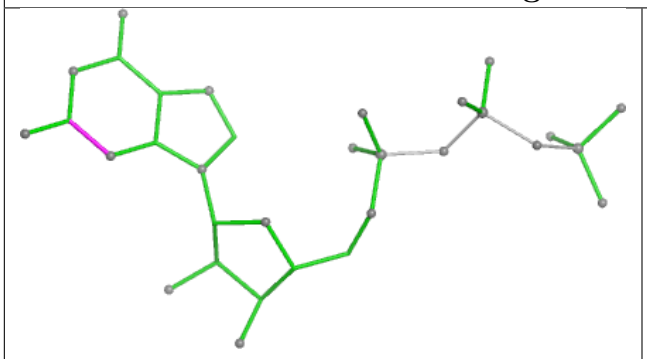


Torsions

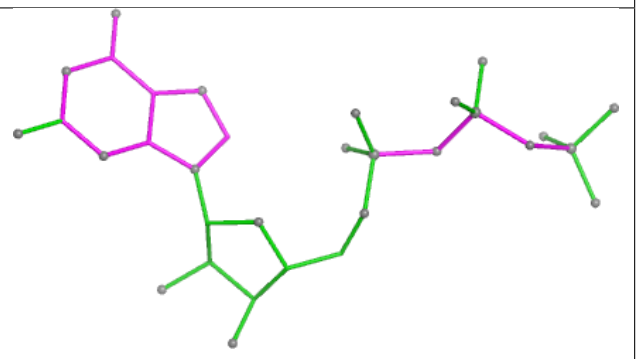


Rings

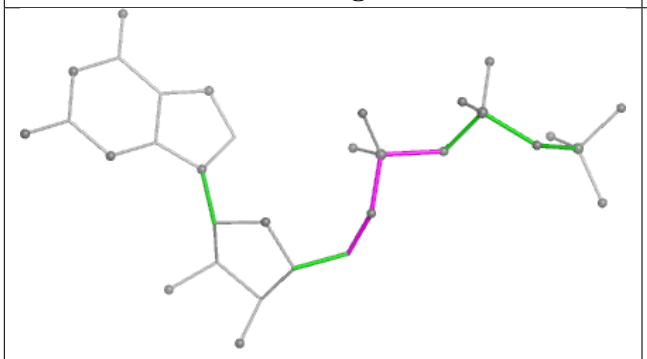
Ligand GTP A 501



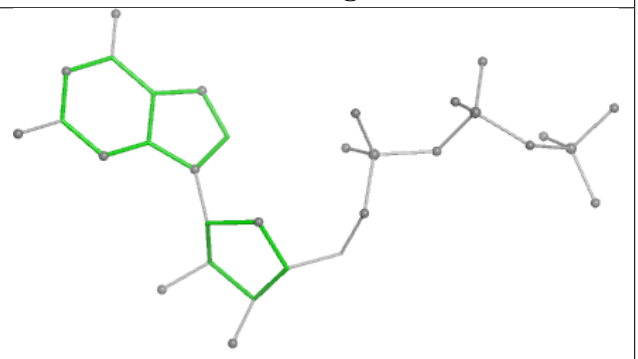
Bond lengths



Bond angles

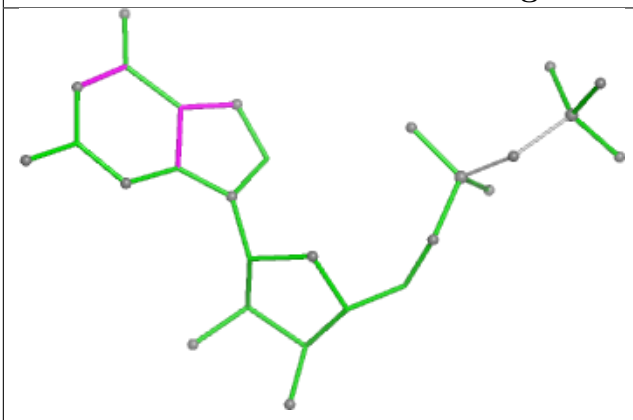


Torsions

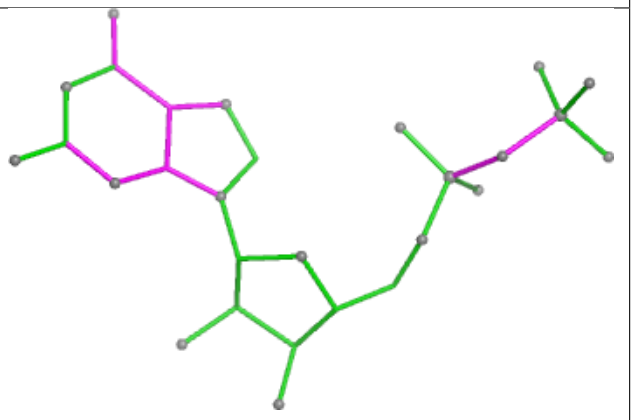


Rings

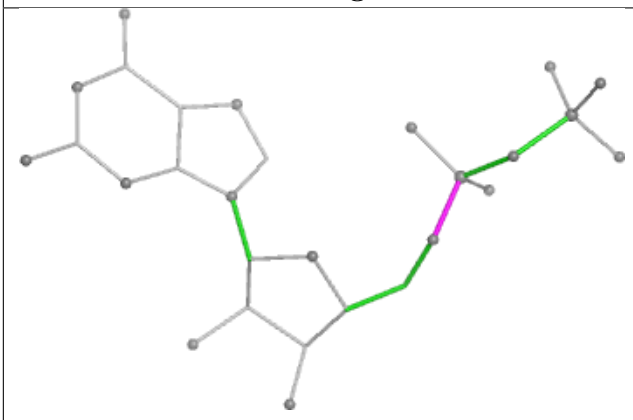
Ligand GDP D 501



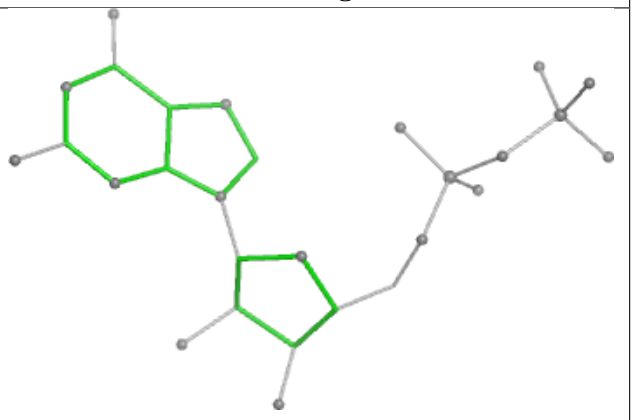
Bond lengths



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	437/451 (96%)	0.11	3 (0%)	84	82	36, 77, 111, 158	11 (2%)
1	C	440/451 (97%)	-0.11	1 (0%)	91	90	29, 65, 90, 130	10 (2%)
2	B	430/445 (96%)	-0.07	5 (1%)	76	74	31, 67, 108, 175	11 (2%)
2	D	422/445 (94%)	0.16	4 (0%)	81	79	49, 89, 126, 172	5 (1%)
3	E	123/143 (86%)	0.30	5 (4%)	41	37	40, 89, 127, 155	2 (1%)
4	F	330/384 (85%)	0.36	14 (4%)	40	36	66, 100, 153, 181	0
All	All	2182/2319 (94%)	0.09	32 (1%)	72	69	29, 79, 129, 181	39 (1%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	237	THR	5.4
1	A	437	VAL	4.2
1	C	440	VAL	3.8
4	F	330	ILE	3.7
4	F	238	CYS	3.2

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

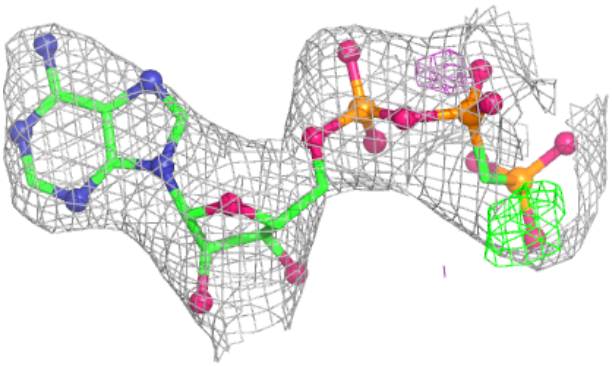
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

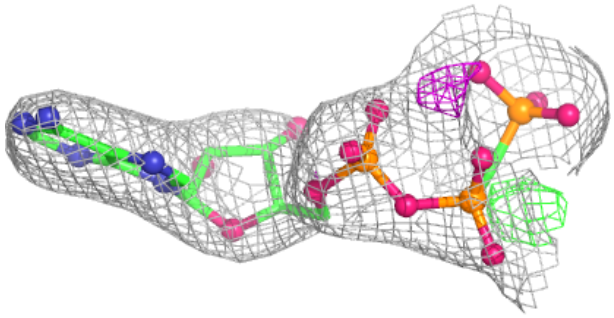
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	IMD	E	201	5/5	0.71	0.34	92,94,103,106	0
8	GOL	A	504	6/6	0.73	0.19	92,98,106,112	0
8	GOL	B	505	6/6	0.80	0.12	92,96,97,108	0
12	IMD	C	501	5/5	0.81	0.18	86,97,113,116	0
6	MG	F	502	1/1	0.81	0.10	96,96,96,96	0
12	IMD	C	507	5/5	0.82	0.29	71,73,97,98	0
6	MG	D	502	1/1	0.87	0.11	90,90,90,90	0
8	GOL	A	506	6/6	0.88	0.12	73,79,87,91	0
8	GOL	A	505	6/6	0.89	0.15	80,87,107,119	0
13	ACP	F	501	31/31	0.89	0.09	97,111,129,138	0
8	GOL	C	506	6/6	0.91	0.10	77,90,93,95	0
11	A1JDA	B	506	62/62	0.92	0.11	51,74,128,143	0
6	MG	B	502	1/1	0.92	0.12	67,67,67,67	0
12	IMD	C	505	5/5	0.92	0.13	77,78,93,102	0
9	GDP	D	501	28/28	0.93	0.09	73,85,100,122	0
7	CA	B	504	1/1	0.95	0.06	112,112,112,112	0
10	MES	B	503	12/12	0.95	0.08	65,70,78,93	0
9	GDP	B	501	28/28	0.96	0.07	44,54,66,74	0
5	GTP	A	501	32/32	0.97	0.07	50,62,71,77	0
5	GTP	C	502	32/32	0.98	0.06	47,56,68,81	0
7	CA	C	504	1/1	0.99	0.03	86,86,86,86	0
7	CA	A	503	1/1	0.99	0.03	104,104,104,104	0
6	MG	C	503	1/1	0.99	0.04	61,61,61,61	0
6	MG	A	502	1/1	1.00	0.01	52,52,52,52	0

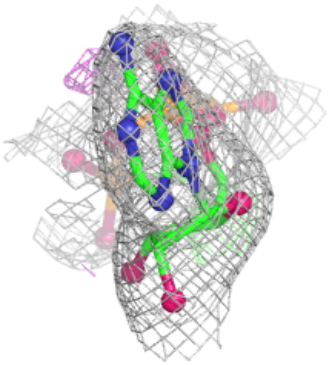
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 501:

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

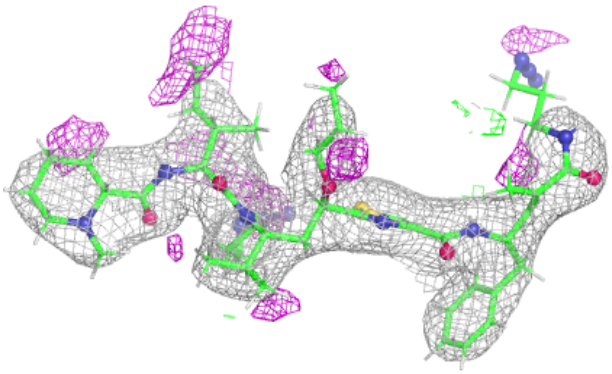


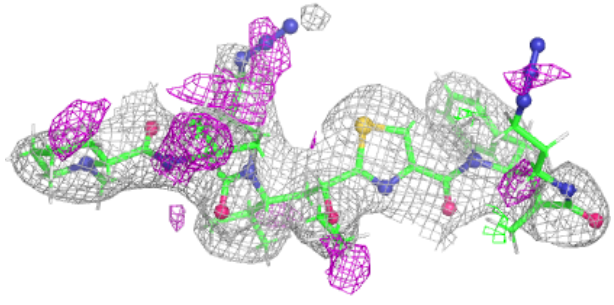


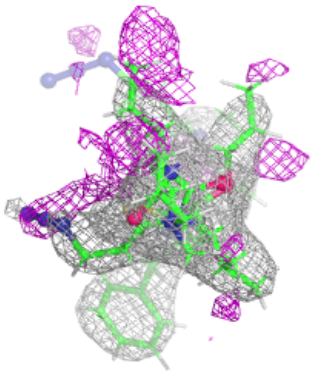


Electron density around A1JDA B 506:

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

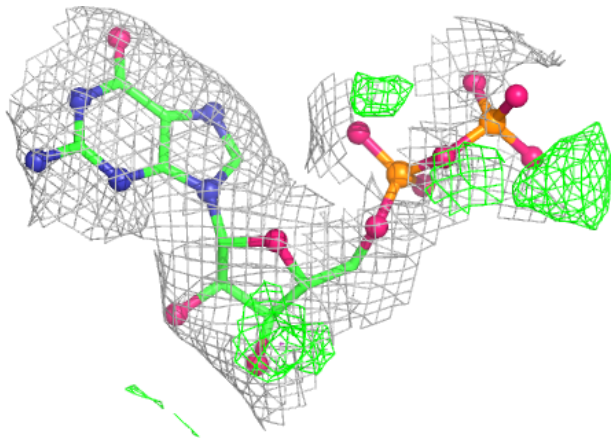


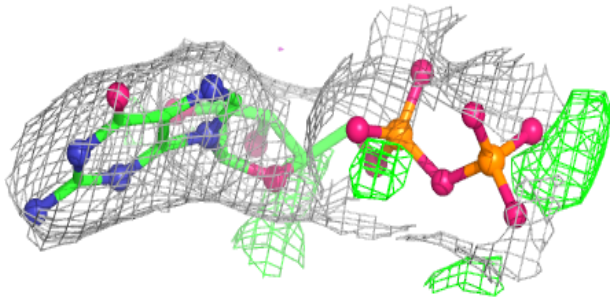


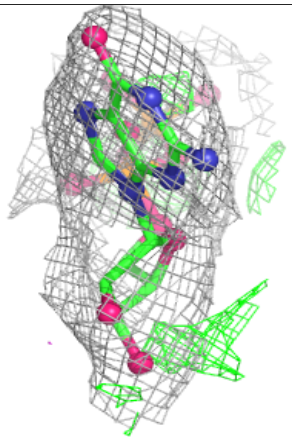


Electron density around GDP D 501:

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

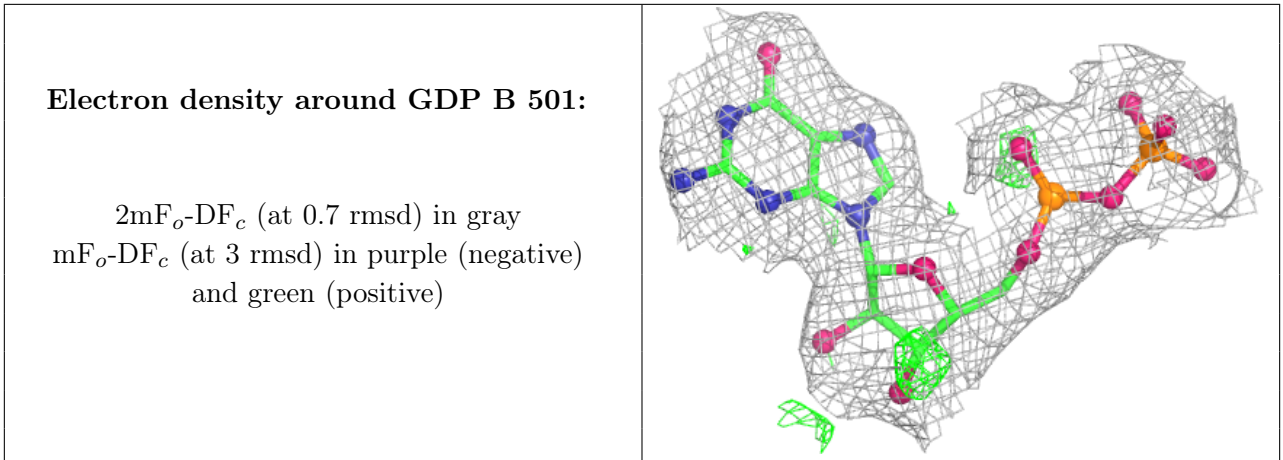






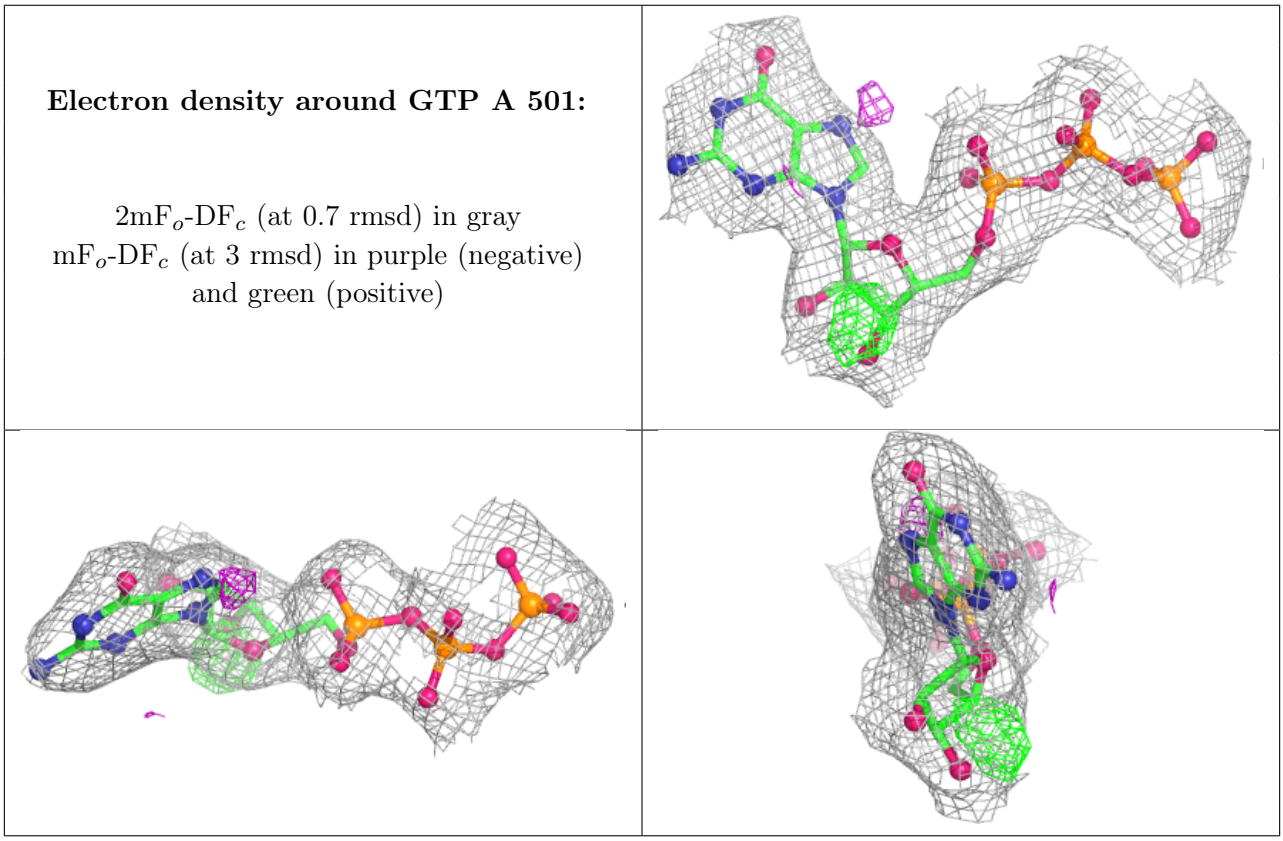
Electron density around GDP B 501:

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



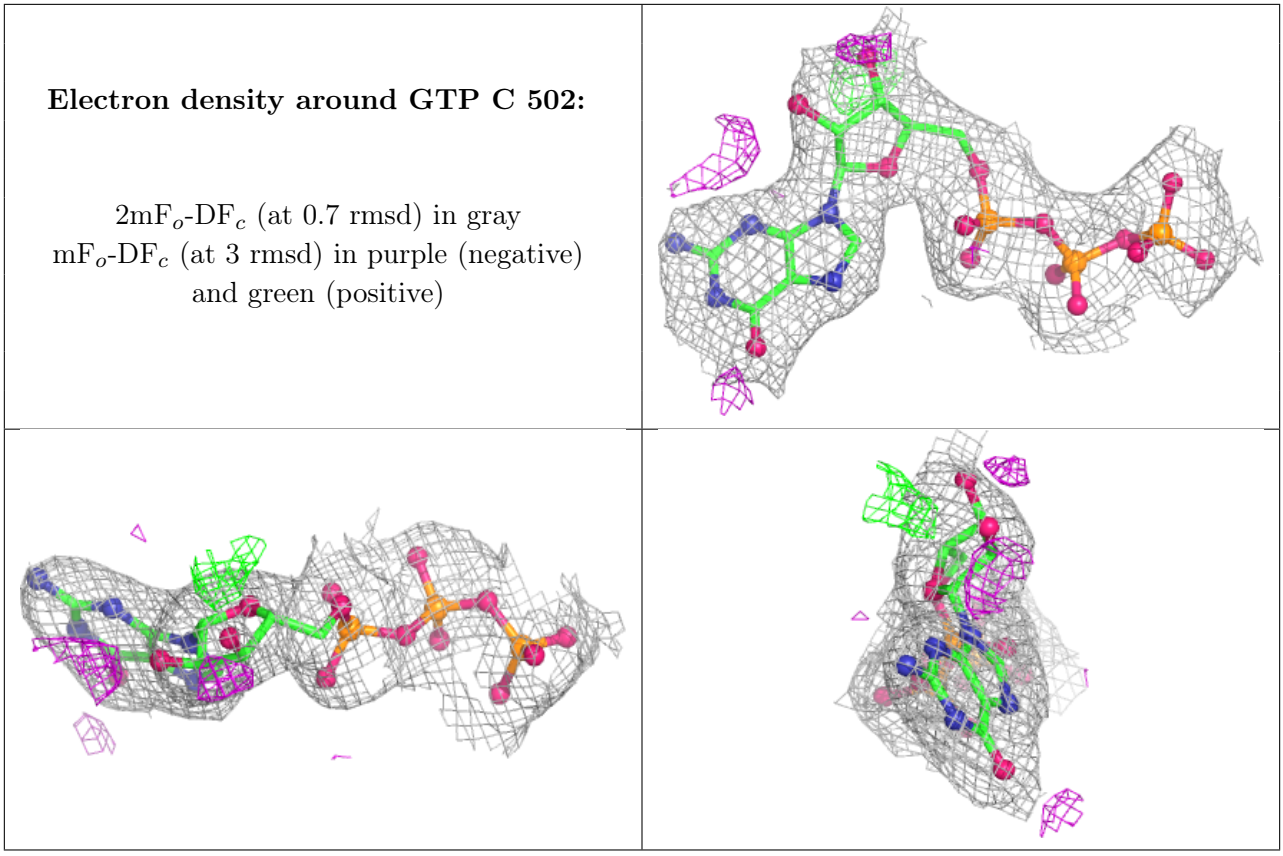
Electron density around GTP A 501:

$2mF_o$-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 502:

$2mF_o$-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.