Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 07:16 pm BST

PDB ID	:	8B7C
Title	:	Tubulin-maytansinoid-12 complex
Authors	:	Boiarska, Z.; Perez-Pena, H.; Abel, A.-C.; Marzullo, P.; Alvarez-Bernad, B.; Bonato, F.; Santini, B.; Horvath, D.; Lucena-Agell, D.; Vasile, F.; Sironi, M.; Diaz, J.F.; Steinmetz, M.O.; Prota, A.E.; Pieraccini, S.; Passarella, D.
Deposited on	:	2022-09-29
Resolution	:	1.90 Å(reported)

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

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

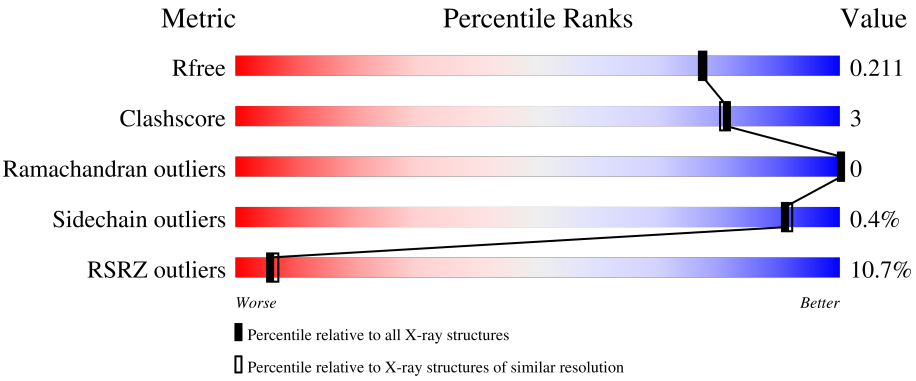
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	5% 90% 7% .
1	C	451	2% 92% 6% .
2	B	445	5% 86% 9% 5%
2	D	445	10% 90% 6% .

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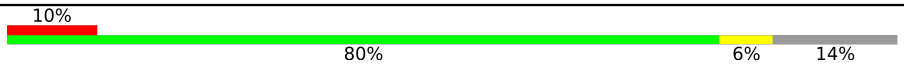
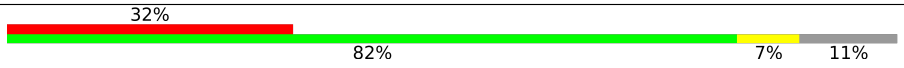
Mol	Chain	Length	Quality of chain
3	E	143	
4	F	384	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18822 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	438	Total	C	N	O	S	0	1	0
			3427	2169	582	653	23			
1	C	440	Total	C	N	O	S	0	7	0
			3468	2194	586	663	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	1	0
			3345	2102	572	644	27			
2	D	426	Total	C	N	O	S	0	1	0
			3354	2104	574	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	1	0
			1019	628	184	202	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

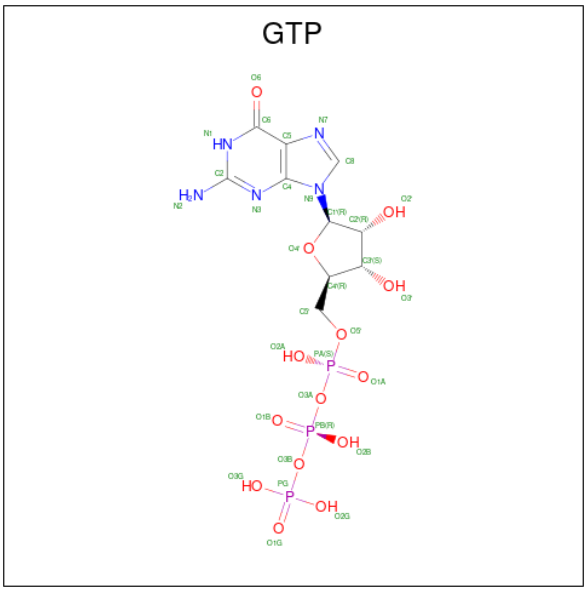
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	342	Total	C	N	O	S	0	1	0
			2804	1800	481	508	15			

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
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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: 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 (three-letter code: 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

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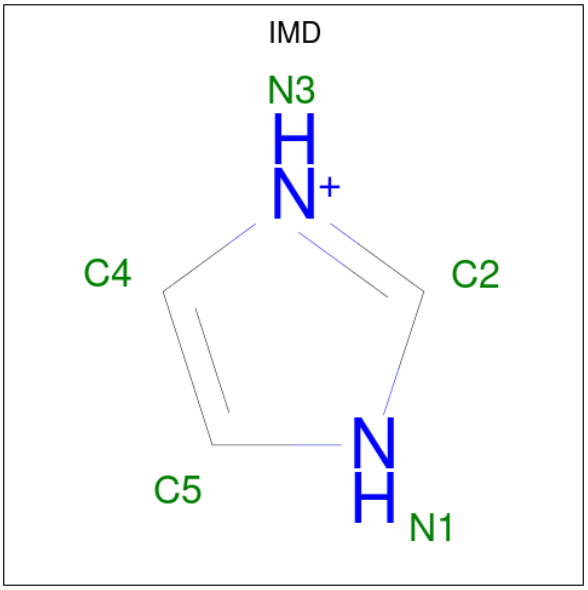
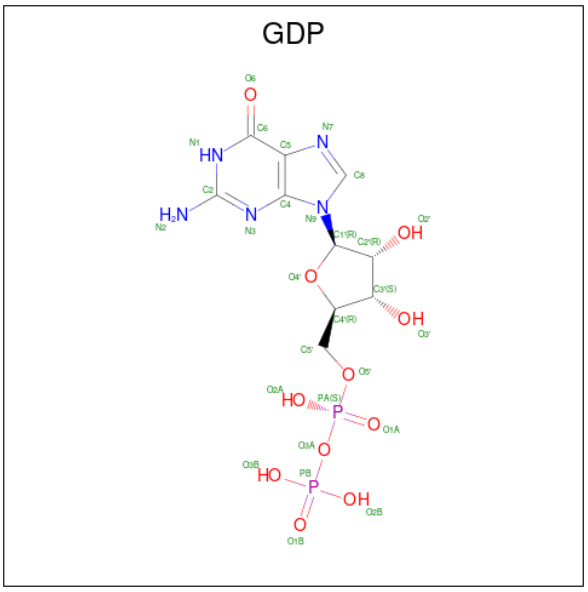
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0

- Molecule 8 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



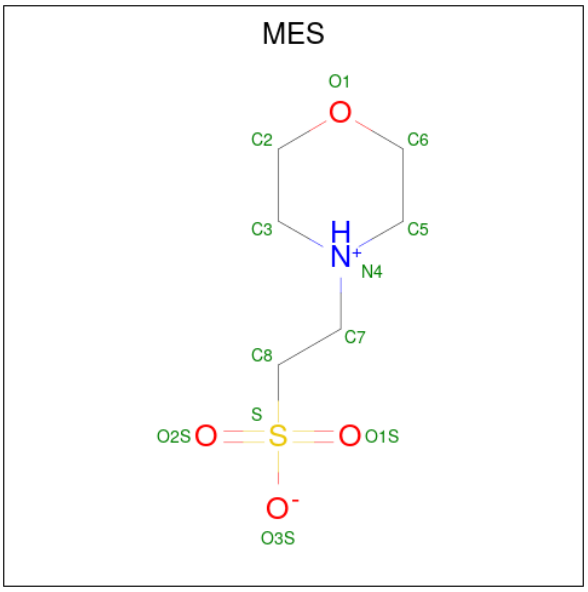
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N 5 3 2	0	0

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



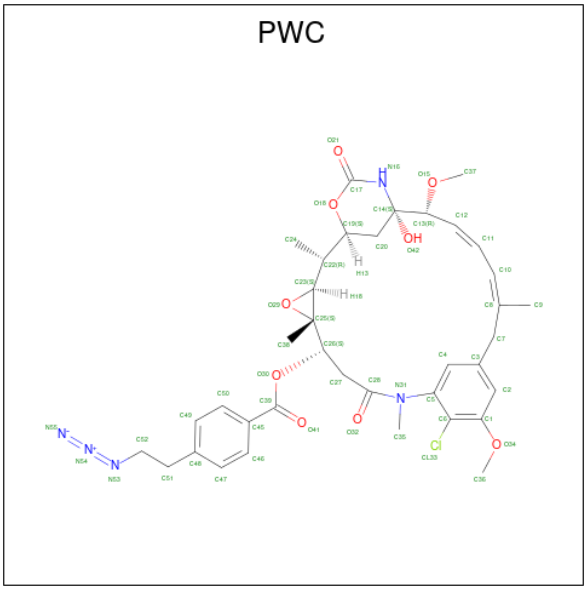
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



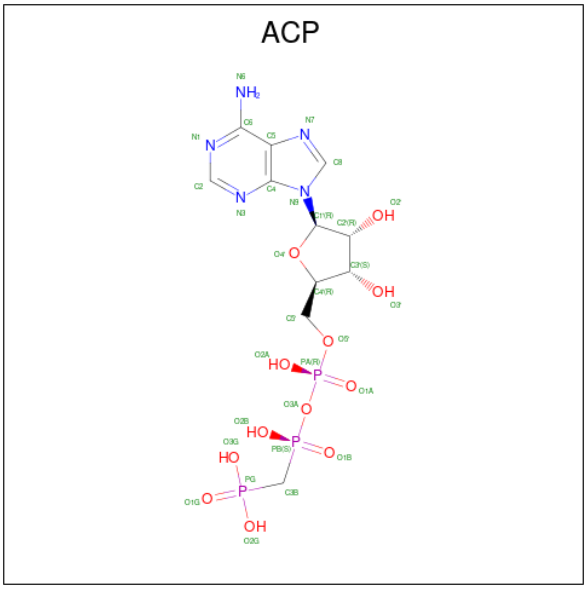
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is [(1 {S},2 {R},3 {S},5 {S},6 {S},16 {E},18 {E},20 {R},21 {S})-11-chloranyl-12,20-dimethoxy-2,5,9,16-tetramethyl-21-oxidanyl-8,23-bis(oxidanylidene)-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1^{10,14}.0^{3,5}]hexacosa-10(26),11,13,16,18-pentaen-6-yl] 4-[2-(2-azanylhydrazinyl)ethyl]benzoate (three-letter code: PWC) (formula: $C_{37}H_{44}ClN_5O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	Cl	N	O	0	0
			52	37	1	5	9		

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



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

- Molecule 13 is water.

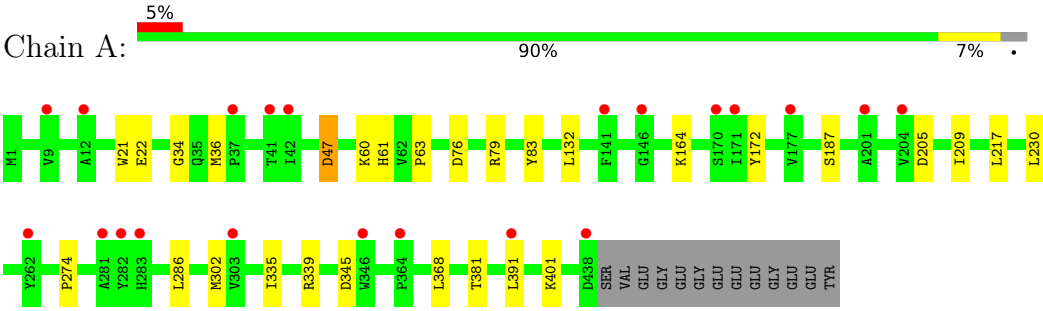
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	217	Total	O	0	0
			217	217		
13	B	244	Total	O	0	0
			244	244		
13	C	394	Total	O	0	0
			394	394		
13	D	168	Total	O	0	0
			168	168		
13	E	58	Total	O	0	0
			58	58		
13	F	95	Total	O	0	0
			95	95		

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.

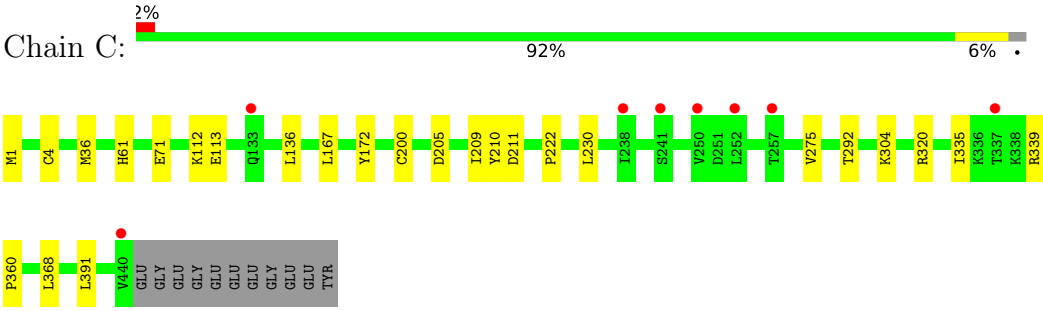
• Molecule 1: Tubulin alpha-1B chain

Chain A:



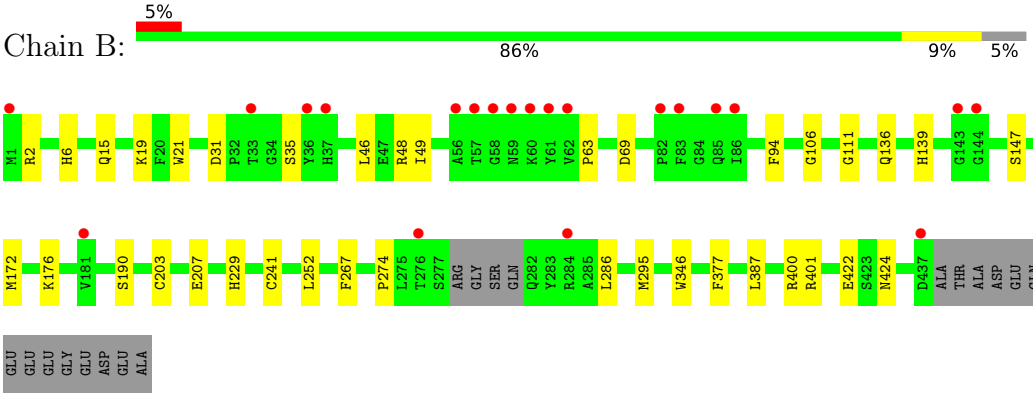
• Molecule 1: Tubulin alpha-1B chain

Chain C:



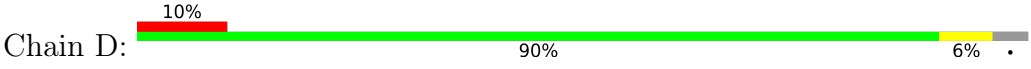
• Molecule 2: Tubulin beta-2B chain

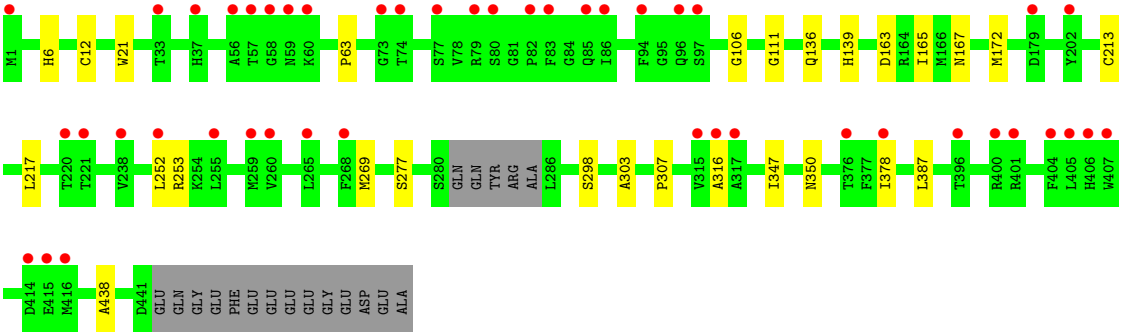
Chain B:



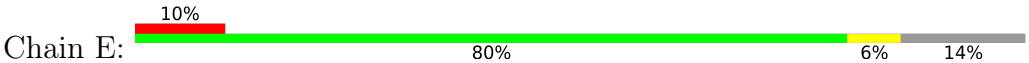
• Molecule 2: Tubulin beta-2B chain

Chain D:

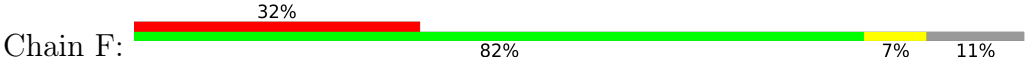


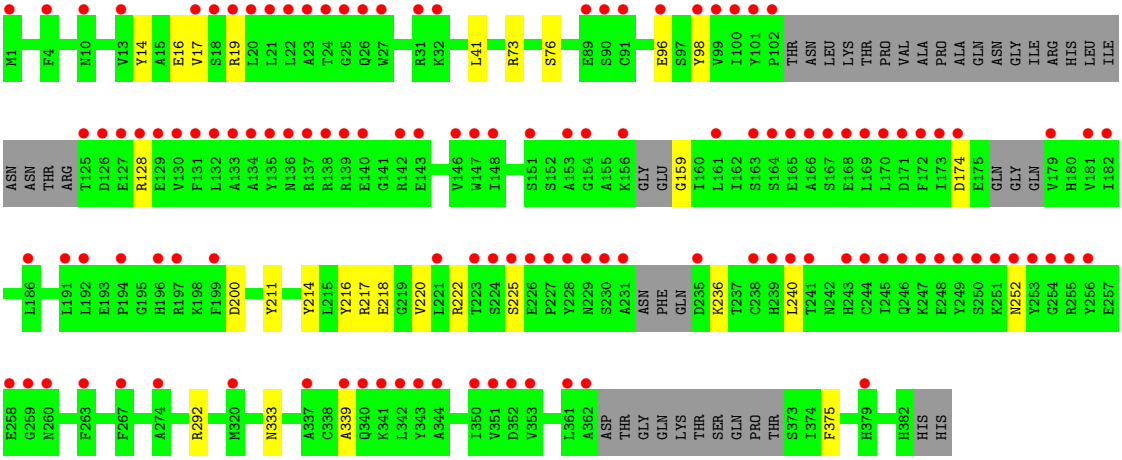


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.87Å 157.94Å 180.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 1.90 49.57 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.57-1.90) 99.9 (49.57-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.183 , 0.211 0.183 , 0.211	Depositor DCC
R_{free} test set	11763 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18822	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: MES, MG, PWC, ACP, IMD, GTP, GDP, CA

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	0.25	0/3508	0.43	0/4762
1	C	0.27	0/3564	0.44	0/4839
2	B	0.26	0/3419	0.43	0/4629
2	D	0.25	0/3427	0.42	0/4640
3	E	0.24	0/1030	0.34	0/1367
4	F	0.24	0/2870	0.40	0/3872
All	All	0.25	0/17818	0.42	0/24109

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	3427	0	3339	17	0
1	C	3468	0	3383	15	0
2	B	3345	0	3227	23	0
2	D	3354	0	3234	16	0
3	E	1019	0	1035	5	0
4	F	2804	0	2778	16	0
5	A	32	0	12	0	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
7	E	1	0	0	0	0
8	A	5	0	5	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	12	0	0
11	D	52	0	0	0	0
12	F	31	0	14	1	0
13	A	217	0	0	0	0
13	B	244	0	0	4	0
13	C	394	0	0	1	0
13	D	168	0	0	2	0
13	E	58	0	0	2	0
13	F	95	0	0	2	0
All	All	18822	0	17075	90	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 3.

All (90) 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:B:229:HIS:ND1	13:B:605:HOH:O	2.29	0.65
1:A:132:LEU:O	1:A:164:LYS:NZ	2.32	0.62
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.32	0.62
1:C:1:MET:O	13:C:601:HOH:O	2.16	0.61
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.60
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.84	0.60
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.85	0.58
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.86	0.58
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.85	0.57
3:E:44:ASP:N	13:E:304:HOH:O	2.37	0.56
4:F:159:GLY:N	13:F:501:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.24	0.55
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.88	0.54
2:B:2:ARG:NH1	13:B:610:HOH:O	2.38	0.54
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.48	0.53
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.91	0.52
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.92	0.52
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.92	0.51
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.93	0.50
3:E:85:LYS:NZ	13:E:306:HOH:O	2.43	0.50
4:F:292:ARG:NH2	13:F:503:HOH:O	2.40	0.50
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.92	0.50
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.93	0.49
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.43	0.49
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.49
4:F:333:ASN:ND2	12:F:401:ACP:O3G	2.40	0.49
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.46	0.49
2:B:147:SER:OG	2:B:190:SER:OG	2.27	0.49
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.45	0.49
1:A:47:ASP:N	1:A:47:ASP:OD1	2.47	0.48
2:B:136:GLN:HA	2:B:167:ASN:O	2.14	0.48
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.96	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.14	0.48
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.44	0.47
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.96	0.47
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.49	0.46
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.97	0.46
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.45
4:F:14:TYR:HA	4:F:17:VAL:HB	1.98	0.45
2:B:147:SER:HG	2:B:190:SER:HG	1.58	0.45
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.29	0.45
2:D:136:GLN:HA	2:D:167:ASN:O	2.17	0.45
2:D:438:ALA:O	13:D:602:HOH:O	2.20	0.45
2:B:31:ASP:OD1	2:B:35:SER:N	2.41	0.45
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.44
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.00	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.00	0.44
4:F:200:ASP:OD2	4:F:222:ARG:NH2	2.51	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.43
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.33	0.43
3:E:135:LYS:HE2	3:E:139:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:ARG:HB2	4:F:76:SER:HB2	1.99	0.43
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.00	0.43
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.99	0.43
2:B:422:GLU:HG3	13:B:602:HOH:O	2.18	0.43
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.43
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.54	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.00	0.43
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.43
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.99	0.43
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.43
2:D:298:SER:HB3	2:D:307:PRO:HD2	2.01	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.42
2:D:167:ASN:ND2	13:D:611:HOH:O	2.52	0.42
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.42
2:D:217:LEU:HA	2:D:277:SER:HB3	2.01	0.42
2:B:46:LEU:HA	2:B:49:ILE:HB	2.00	0.42
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.01	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.42
4:F:220:VAL:HG11	4:F:339:ALA:HB2	2.02	0.42
2:B:48:ARG:NH2	2:B:241:CYS:O	2.52	0.42
4:F:225:SER:HB2	4:F:252:ASN:HB2	2.01	0.42
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.60	0.42
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.55	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.55	0.41
2:B:424:ASN:HB3	13:B:626:HOH:O	2.21	0.41
2:D:316:ALA:HB3	2:D:378:ILE:HB	2.03	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.41
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.56	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.41
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.03	0.41
1:A:209:ILE:HD11	1:A:302:MET:SD	2.60	0.41
2:D:163:ASP:O	2:D:253:ARG:NH2	2.54	0.41
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.40
2:B:15:GLN:O	2:B:19:LYS:HG2	2.22	0.40
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.03	0.40
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.03	0.40

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	437/451 (97%)	428 (98%)	9 (2%)	0	100	100
1	C	445/451 (99%)	436 (98%)	9 (2%)	0	100	100
2	B	420/445 (94%)	414 (99%)	6 (1%)	0	100	100
2	D	423/445 (95%)	416 (98%)	7 (2%)	0	100	100
3	E	120/143 (84%)	120 (100%)	0	0	100	100
4	F	331/384 (86%)	323 (98%)	8 (2%)	0	100	100
All	All	2176/2319 (94%)	2137 (98%)	39 (2%)	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	370/379 (98%)	368 (100%)	2 (0%)	88	89
1	C	378/379 (100%)	377 (100%)	1 (0%)	92	93
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	93
2	D	369/383 (96%)	368 (100%)	1 (0%)	92	93
3	E	111/127 (87%)	110 (99%)	1 (1%)	78	79
4	F	307/342 (90%)	306 (100%)	1 (0%)	92	93
All	All	1903/1993 (96%)	1896 (100%)	7 (0%)	91	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	381	THR
2	B	139	HIS
1	C	71	GLU
2	D	139	HIS
3	E	140	LYS
4	F	211	TYR

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

Mol	Chain	Res	Type
1	A	301	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\#\|Z\|>2$
11	PWC	D	503	-	53,56,56	4.70	36 (67%)	63,82,82	1.56	16 (25%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.31	5 (15%)
12	ACP	F	401	6	27,33,33	1.97	7 (25%)	32,52,52	1.23	4 (12%)
8	IMD	A	504	-	3,5,5	0.41	0	4,5,5	0.57	0
10	MES	B	504	-	12,12,12	2.16	1 (8%)	14,16,16	2.10	4 (28%)
9	GDP	B	501	6	24,30,30	0.92	1 (4%)	30,47,47	1.05	3 (10%)
5	GTP	A	501	6	26,34,34	1.09	2 (7%)	32,54,54	1.34	5 (15%)
9	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.14	3 (10%)

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
11	PWC	D	503	-	-	11/54/81/81	0/3/5/5
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
12	ACP	F	401	6	-	3/15/38/38	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	IMD	A	504	-	-	-	0/1/1/1
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	PWC	N54-N53	10.35	1.50	1.23
11	D	503	PWC	O41-C39	9.27	1.48	1.22
11	D	503	PWC	C7-C8	8.68	1.62	1.51
11	D	503	PWC	C7-C3	8.05	1.64	1.51
11	D	503	PWC	O21-C17	7.76	1.36	1.21
11	D	503	PWC	C5-C6	7.48	1.47	1.40
11	D	503	PWC	O34-C1	7.48	1.49	1.37
10	B	504	MES	C8-S	-7.22	1.67	1.77
11	D	503	PWC	C6-CL33	7.04	1.88	1.72
11	D	503	PWC	C27-C26	7.03	1.62	1.52
11	D	503	PWC	O29-C23	6.06	1.52	1.45
11	D	503	PWC	C45-C39	5.89	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PG-O1G	5.48	1.61	1.50
11	D	503	PWC	O29-C25	5.43	1.52	1.45
11	D	503	PWC	C4-C3	5.21	1.48	1.39
11	D	503	PWC	C14-N16	5.01	1.53	1.46
11	D	503	PWC	C22-C19	5.01	1.66	1.53
11	D	503	PWC	C4-C5	4.99	1.47	1.39
11	D	503	PWC	C2-C3	4.91	1.47	1.39
11	D	503	PWC	C2-C1	4.90	1.47	1.38
11	D	503	PWC	C47-C46	4.84	1.47	1.38
11	D	503	PWC	C38-C25	4.82	1.63	1.52
11	D	503	PWC	C35-N31	4.76	1.54	1.46
11	D	503	PWC	C46-C45	4.68	1.47	1.39
11	D	503	PWC	C50-C49	4.67	1.47	1.38
11	D	503	PWC	C50-C45	4.66	1.47	1.39
11	D	503	PWC	O42-C14	4.45	1.48	1.41
11	D	503	PWC	C1-C6	4.37	1.47	1.40
11	D	503	PWC	C25-C23	4.31	1.52	1.47
11	D	503	PWC	O18-C19	4.24	1.52	1.46
12	F	401	ACP	PB-O1B	4.12	1.61	1.51
11	D	503	PWC	C47-C48	4.10	1.47	1.38
5	C	501	GTP	C5-C6	-4.02	1.39	1.47
11	D	503	PWC	C51-C48	3.97	1.63	1.51
11	D	503	PWC	C9-C8	3.82	1.60	1.50
11	D	503	PWC	C49-C48	3.79	1.47	1.38
5	A	501	GTP	C5-C6	-3.77	1.39	1.47
12	F	401	ACP	PB-O2B	-3.46	1.48	1.56
12	F	401	ACP	PB-O3A	3.12	1.61	1.58
12	F	401	ACP	PG-O2G	-2.88	1.48	1.54
11	D	503	PWC	C25-C26	2.78	1.62	1.54
12	F	401	ACP	PG-O3G	2.73	1.61	1.54
11	D	503	PWC	C22-C23	2.73	1.61	1.55
12	F	401	ACP	C5-C4	2.42	1.47	1.40
11	D	503	PWC	O15-C37	2.29	1.50	1.42
9	D	501	GDP	C6-N1	-2.25	1.34	1.37
9	B	501	GDP	C6-N1	-2.24	1.34	1.37
5	C	501	GTP	C2-N3	2.13	1.38	1.33
5	A	501	GTP	C2-N3	2.08	1.38	1.33
11	D	503	PWC	O34-C36	2.05	1.48	1.42

All (40) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	504	MES	O1S-S-C8	5.19	113.17	106.92
11	D	503	PWC	O30-C39-C45	4.58	119.31	111.92
11	D	503	PWC	O34-C1-C6	4.08	120.37	115.53
10	B	504	MES	C5-N4-C3	3.24	116.12	108.83
5	A	501	GTP	C8-N7-C5	3.09	108.88	102.99
12	F	401	ACP	N3-C2-N1	-2.99	124.00	128.68
5	C	501	GTP	C5-C6-N1	2.97	119.19	113.95
5	C	501	GTP	C8-N7-C5	2.97	108.64	102.99
9	D	501	GDP	PA-O3A-PB	-2.95	122.69	132.83
5	A	501	GTP	C5-C6-N1	2.93	119.12	113.95
12	F	401	ACP	C3'-C2'-C1'	2.90	105.34	100.98
10	B	504	MES	C7-N4-C5	2.89	118.63	111.23
5	A	501	GTP	PA-O3A-PB	-2.79	123.27	132.83
12	F	401	ACP	PB-O3A-PA	-2.71	123.98	132.56
11	D	503	PWC	C10-C11-C12	-2.67	118.06	124.53
5	C	501	GTP	PA-O3A-PB	-2.65	123.72	132.83
11	D	503	PWC	C36-O34-C1	-2.61	113.59	117.53
11	D	503	PWC	C27-C26-C25	-2.59	109.15	114.60
11	D	503	PWC	O34-C1-C2	-2.57	119.69	124.12
10	B	504	MES	C6-C5-N4	-2.57	106.21	110.10
5	C	501	GTP	PB-O3B-PG	-2.55	124.06	132.83
5	A	501	GTP	C2-N1-C6	-2.55	120.41	125.10
12	F	401	ACP	C4-C5-N7	-2.54	106.75	109.40
11	D	503	PWC	C24-C22-C23	-2.45	107.26	112.55
11	D	503	PWC	O30-C26-C25	2.43	110.97	105.48
11	D	503	PWC	C19-O18-C17	-2.43	114.85	121.06
5	C	501	GTP	C2-N1-C6	-2.41	120.66	125.10
9	B	501	GDP	C5-C6-N1	2.38	118.16	113.95
5	A	501	GTP	PB-O3B-PG	-2.36	124.73	132.83
11	D	503	PWC	C9-C8-C7	2.36	119.86	114.88
9	D	501	GDP	C8-N7-C5	2.34	107.45	102.99
9	B	501	GDP	PA-O3A-PB	-2.27	125.03	132.83
9	D	501	GDP	C5-C6-N1	2.27	117.95	113.95
9	B	501	GDP	C8-N7-C5	2.24	107.26	102.99
11	D	503	PWC	C4-C5-C6	-2.17	119.77	122.53
11	D	503	PWC	C26-O30-C39	2.11	121.31	117.55
11	D	503	PWC	O18-C17-N16	2.09	122.68	118.78
11	D	503	PWC	C35-N31-C5	2.06	119.60	116.72
11	D	503	PWC	C24-C22-C19	-2.05	108.43	111.43
11	D	503	PWC	C38-C25-C26	2.01	120.07	114.51

There are no chirality outliers.

All (40) torsion outliers are listed below:

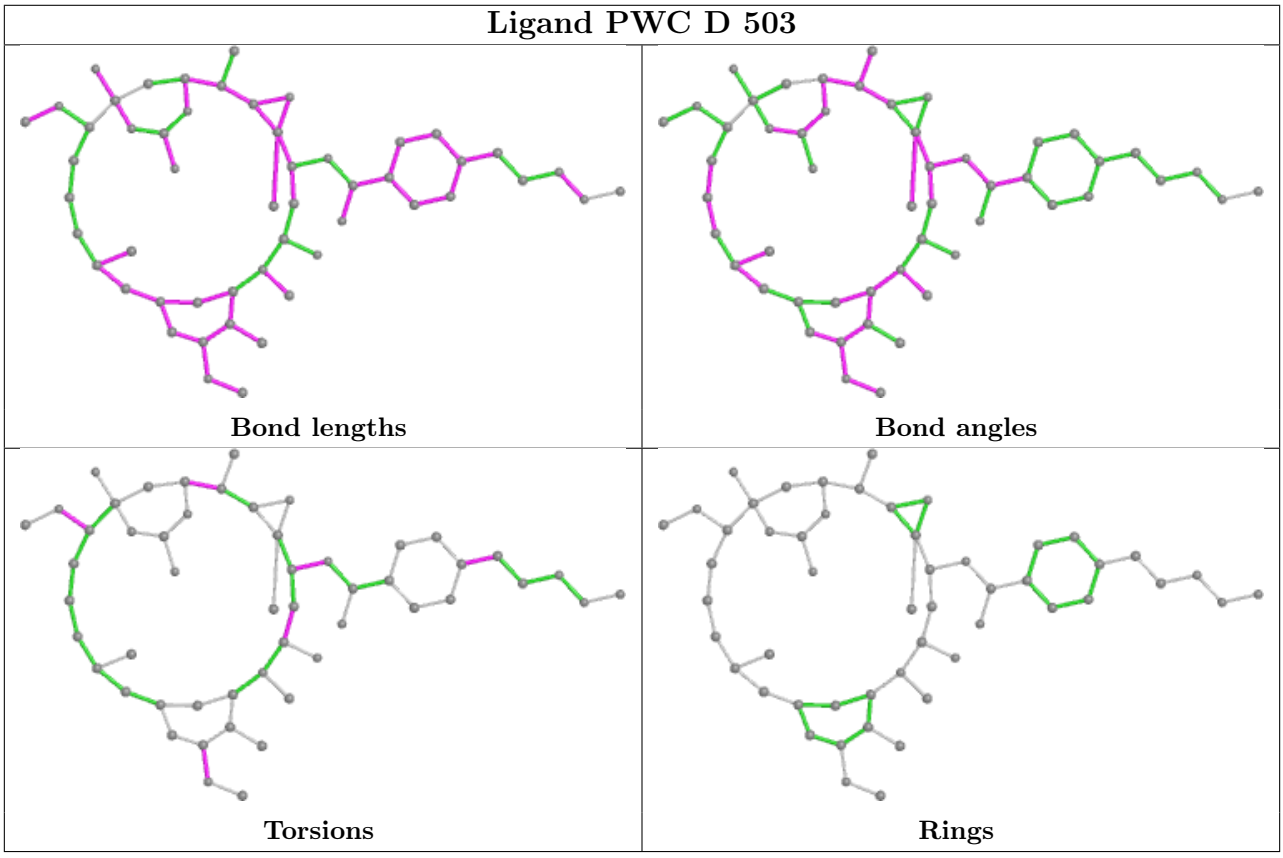
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O2S
10	B	504	MES	C7-C8-S-O3S
11	D	503	PWC	C12-C13-O15-C37
11	D	503	PWC	C6-C1-O34-C36
11	D	503	PWC	C25-C26-O30-C39
12	F	401	ACP	C5'-O5'-PA-O3A
11	D	503	PWC	C2-C1-O34-C36
11	D	503	PWC	C27-C26-O30-C39
11	D	503	PWC	C14-C13-O15-C37
5	A	501	GTP	PB-O3B-PG-O1G
9	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O1S
11	D	503	PWC	C20-C19-C22-C24
5	C	501	GTP	PB-O3A-PA-O2A
11	D	503	PWC	C49-C48-C51-C52
11	D	503	PWC	C47-C48-C51-C52
5	C	501	GTP	PB-O3B-PG-O1G
11	D	503	PWC	C26-C27-C28-O32
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
11	D	503	PWC	C26-C27-C28-N31

There are no ring outliers.

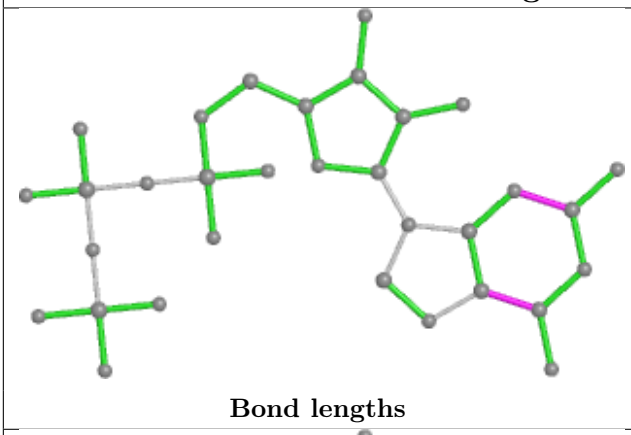
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	1	0
9	D	501	GDP	1	0

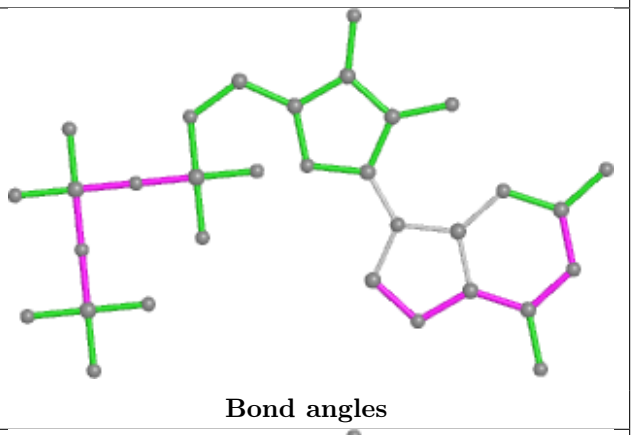
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



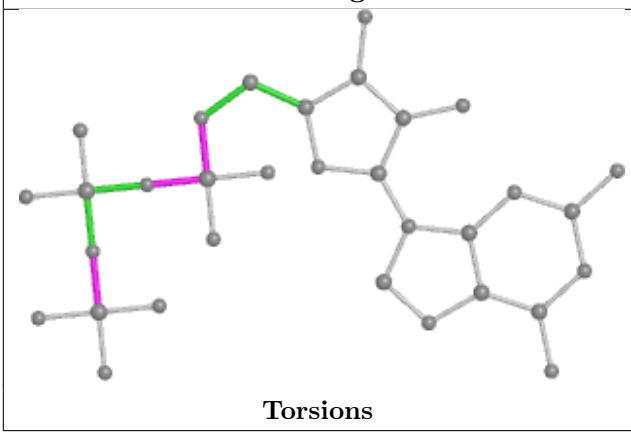
Ligand GTP C 501



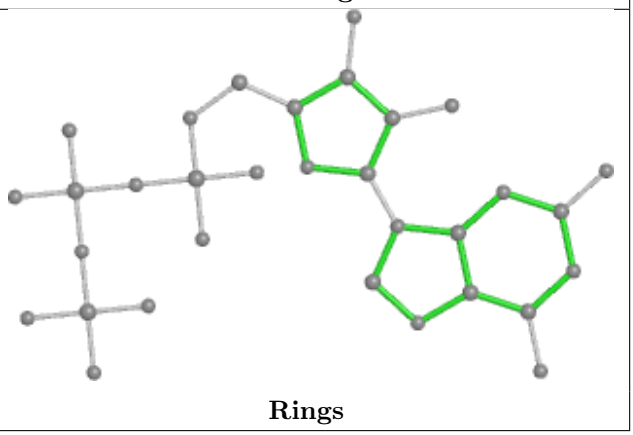
Bond lengths



Bond angles

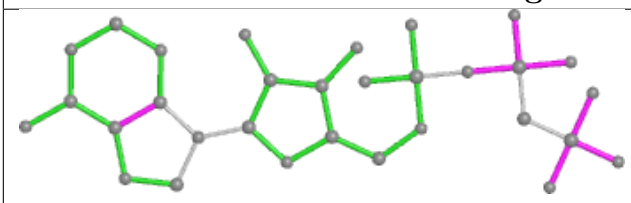


Torsions

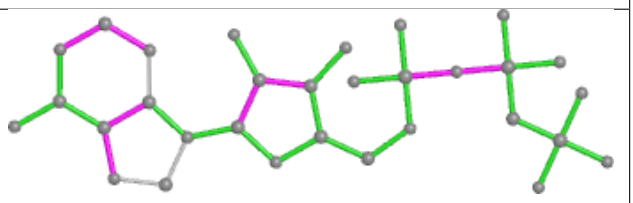


Rings

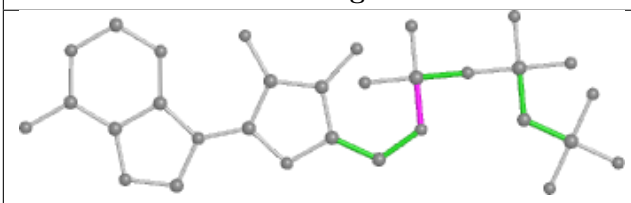
Ligand ACP F 401



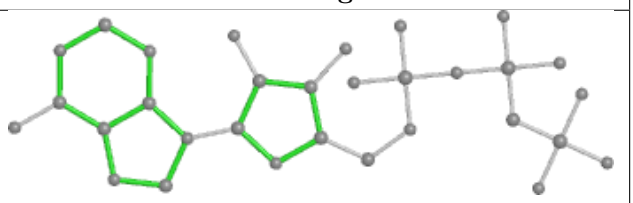
Bond lengths



Bond angles

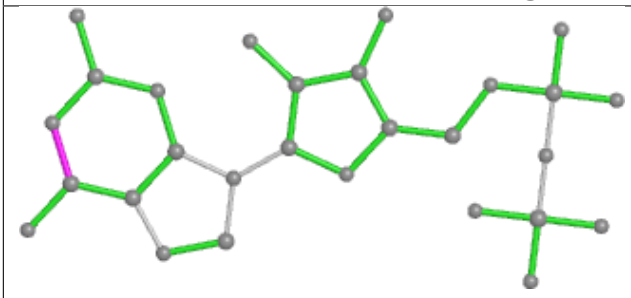


Torsions

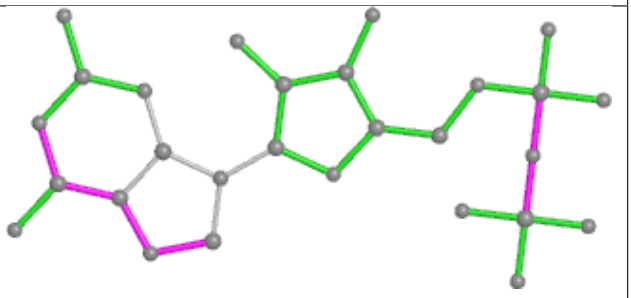


Rings

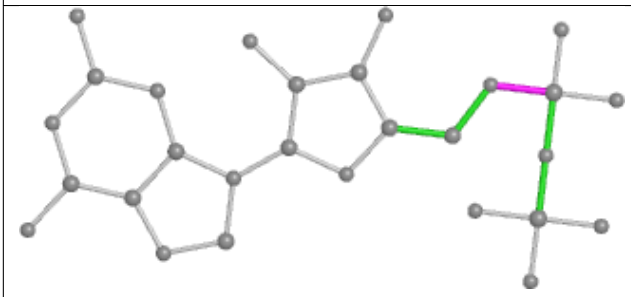
Ligand GDP B 501



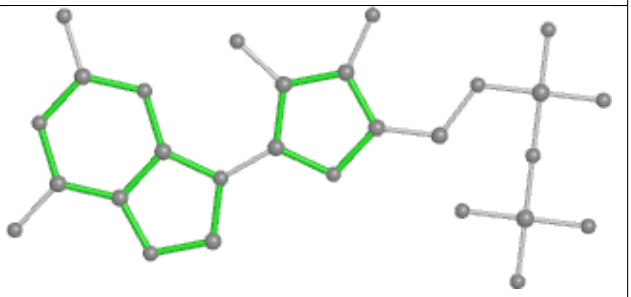
Bond lengths



Bond angles

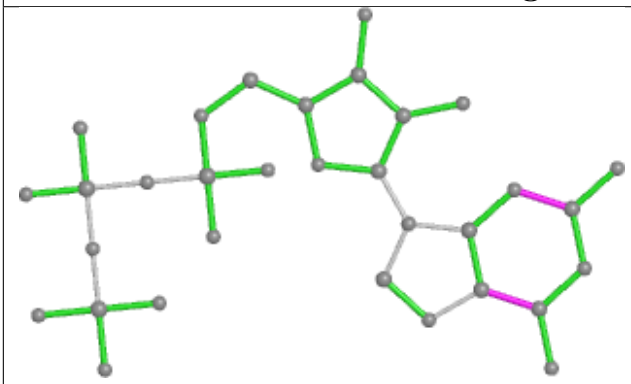


Torsions

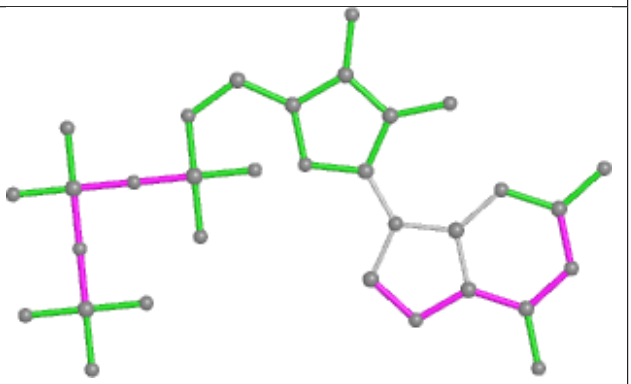


Rings

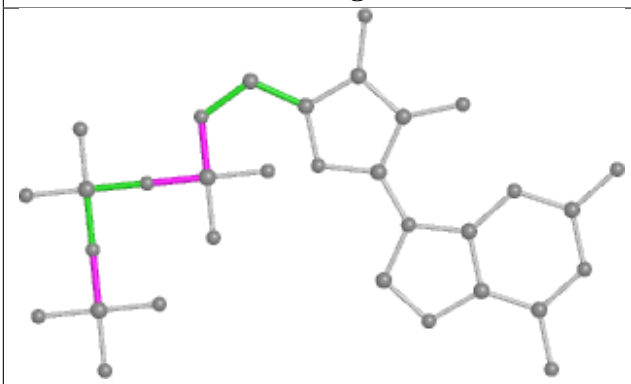
Ligand GTP A 501



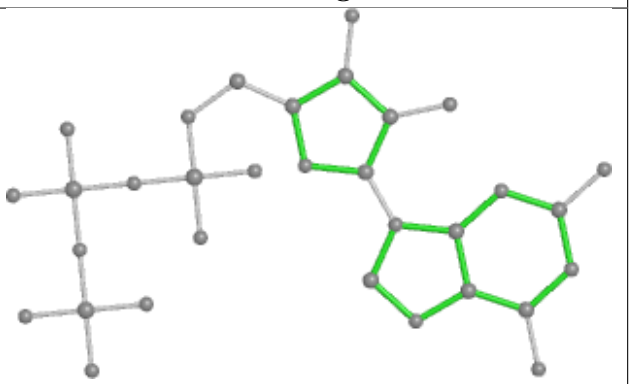
Bond lengths



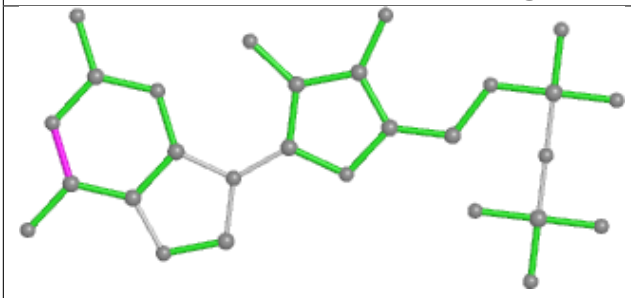
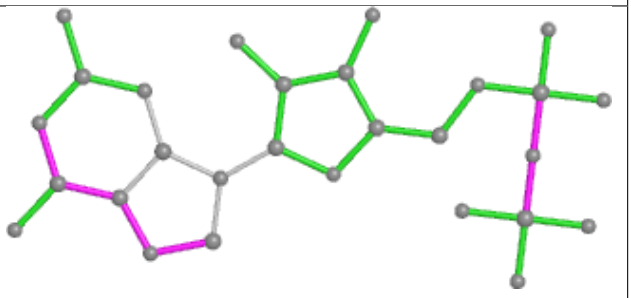
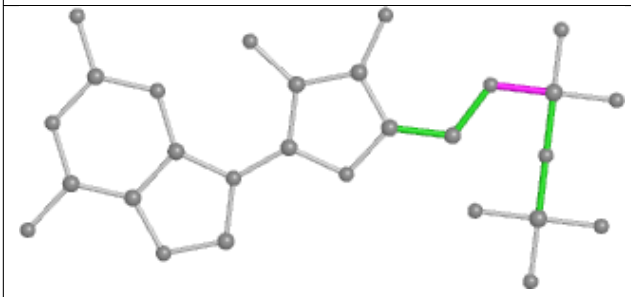
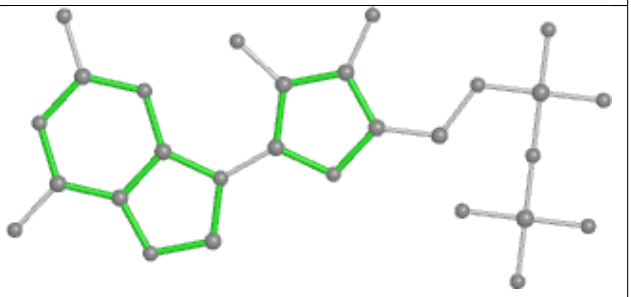
Bond angles



Torsions



Rings

Ligand GDP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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

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	438/451 (97%)	0.36	21 (4%) 30 33	32, 49, 82, 154	0
1	C	440/451 (97%)	0.10	9 (2%) 65 68	26, 38, 64, 101	0
2	B	423/445 (95%)	0.31	21 (4%) 28 32	29, 47, 83, 128	0
2	D	426/445 (95%)	0.56	46 (10%) 5 6	32, 55, 90, 132	0
3	E	123/143 (86%)	0.49	14 (11%) 5 5	38, 61, 101, 137	0
4	F	342/384 (89%)	1.50	124 (36%) 0 0	41, 72, 138, 178	0
All	All	2192/2319 (94%)	0.52	235 (10%) 6 6	26, 51, 98, 178	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	8.3
4	F	89	GLU	7.6
1	A	282	TYR	7.5
4	F	250	SER	7.5
4	F	132	LEU	7.4
4	F	169	LEU	7.2
4	F	135	TYR	7.0
4	F	251	LYS	6.9
4	F	20	LEU	6.9
4	F	142	ARG	6.8
4	F	166	ALA	6.6
4	F	249	TYR	6.6
4	F	253	TYR	6.5
4	F	99	VAL	6.4
4	F	131	PHE	6.4
2	D	57	THR	6.2
4	F	161	LEU	6.2
4	F	173	ILE	6.2
4	F	362	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
4	F	134	ALA	6.1
2	B	59	ASN	5.8
4	F	170	LEU	5.7
4	F	100	ILE	5.6
3	E	139	LEU	5.6
4	F	259	GLY	5.6
2	B	1	MET	5.4
4	F	248	GLU	5.2
4	F	244	CYS	5.2
3	E	26	PRO	5.1
2	B	57	THR	5.1
4	F	361	LEU	5.0
4	F	101	TYR	4.9
4	F	182	ILE	4.8
4	F	256	TYR	4.7
3	E	143	ALA	4.7
4	F	245	ILE	4.6
4	F	252	ASN	4.6
4	F	254	GLY	4.6
2	D	94	PHE	4.5
1	A	262	TYR	4.5
4	F	22	LEU	4.5
1	A	42	ILE	4.5
3	E	142	GLU	4.3
1	C	340	SER	4.3
4	F	129	GLU	4.3
2	D	400	ARG	4.2
4	F	194	PRO	4.2
1	C	440	VAL	4.1
2	B	37	HIS	4.0
4	F	21	LEU	4.0
4	F	240	LEU	3.9
4	F	25	GLY	3.9
3	E	27	PRO	3.9
4	F	165	GLU	3.8
4	F	239	HIS	3.8
2	B	58	GLY	3.8
4	F	179	VAL	3.8
4	F	139	ARG	3.8
4	F	136	ASN	3.7
2	B	33	THR	3.7
4	F	24	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	268	PHE	3.7
1	A	171	ILE	3.6
4	F	17	VAL	3.6
4	F	339	ALA	3.6
2	D	97	SER	3.6
4	F	243	HIS	3.5
4	F	13	VAL	3.5
4	F	344	ALA	3.5
2	B	82	PRO	3.5
4	F	133	ALA	3.4
2	D	85	GLN	3.4
4	F	192	LEU	3.4
4	F	167	SER	3.3
4	F	138	ARG	3.3
4	F	227	PRO	3.3
4	F	255	ARG	3.3
2	D	59	ASN	3.3
2	D	37	HIS	3.3
4	F	353	VAL	3.3
2	D	317	ALA	3.3
4	F	23	ALA	3.3
4	F	125	THR	3.3
3	E	135	LYS	3.2
4	F	154	GLY	3.2
4	F	225	SER	3.2
4	F	172	PHE	3.2
2	D	220	THR	3.2
1	A	281	ALA	3.2
4	F	27	TRP	3.2
4	F	223	THR	3.2
1	A	177	VAL	3.1
2	D	405	LEU	3.1
2	D	406	HIS	3.1
4	F	342	LEU	3.1
4	F	26	GLN	3.1
4	F	343	TYR	3.1
2	B	276	THR	3.0
4	F	19	ARG	3.0
4	F	231	ALA	3.0
4	F	258	GLU	3.0
2	B	437	ASP	3.0
4	F	340	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	140	LYS	3.0
4	F	228	TYR	3.0
2	D	401	ARG	2.9
1	A	37	PRO	2.9
4	F	230	SER	2.9
4	F	168	GLU	2.9
4	F	126	ASP	2.9
2	D	82	PRO	2.9
4	F	102	PRO	2.9
1	C	337	THR	2.9
4	F	10	ASN	2.9
2	D	202	TYR	2.9
2	B	284	ARG	2.9
1	A	346	TRP	2.8
2	D	376	THR	2.8
4	F	143	GLU	2.8
4	F	229	ASN	2.8
2	D	33	THR	2.8
2	D	260	VAL	2.8
3	E	141	GLU	2.8
2	B	56	ALA	2.7
4	F	199	PHE	2.7
2	D	77	SER	2.7
4	F	263	PHE	2.7
1	C	252	LEU	2.7
2	D	1	MET	2.7
3	E	45	PRO	2.7
4	F	32	LYS	2.7
4	F	246	GLN	2.7
4	F	379	HIS	2.7
4	F	18	SER	2.7
2	D	83	PHE	2.6
2	D	73	GLY	2.6
1	A	41	THR	2.6
2	D	404	PHE	2.6
4	F	247	LYS	2.6
4	F	352	ASP	2.6
3	E	28	SER	2.6
4	F	163	SER	2.6
4	F	186	LEU	2.6
3	E	6	MET	2.6
4	F	238	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	86	ILE	2.6
2	D	58	GLY	2.6
4	F	181	VAL	2.6
2	D	259	MET	2.5
2	D	80	SER	2.5
2	D	56	ALA	2.5
1	A	12	ALA	2.5
3	E	138	GLU	2.5
1	A	146	GLY	2.5
4	F	90	SER	2.5
4	F	226	GLU	2.5
2	D	407	TRP	2.5
4	F	98	TYR	2.5
4	F	151	SER	2.5
2	B	143	GLY	2.4
2	D	378	ILE	2.4
2	D	265	LEU	2.4
4	F	196	HIS	2.4
4	F	147	TRP	2.4
2	B	36	TYR	2.4
2	D	74	THR	2.4
1	C	250	VAL	2.4
4	F	1	MET	2.4
4	F	241	THR	2.4
2	B	144	GLY	2.4
4	F	174	ASP	2.4
4	F	337	ALA	2.4
4	F	140	GLU	2.3
4	F	267	PHE	2.3
1	A	9	VAL	2.3
4	F	164	SER	2.3
4	F	351	VAL	2.3
2	B	61	TYR	2.3
2	B	181	VAL	2.3
4	F	148	ILE	2.3
1	A	438	ASP	2.3
4	F	96	GLU	2.3
2	B	62	VAL	2.3
2	D	415	GLU	2.3
2	D	79	ARG	2.3
2	D	316	ALA	2.3
2	D	221	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	156	LYS	2.3
4	F	320	MET	2.3
1	A	303	VAL	2.3
2	B	60	LYS	2.3
4	F	171	ASP	2.3
2	D	252	LEU	2.2
2	B	83	PHE	2.2
4	F	128	ARG	2.2
1	A	283	HIS	2.2
2	B	86	ILE	2.2
3	E	24	LEU	2.2
2	D	179	ASP	2.2
4	F	224	SER	2.2
1	A	201	ALA	2.2
1	A	204	VAL	2.2
1	C	238	ILE	2.2
4	F	91	CYS	2.2
4	F	274	ALA	2.2
2	D	315	VAL	2.2
1	A	391	LEU	2.1
1	C	257	THR	2.1
4	F	127	GLU	2.1
4	F	197	ARG	2.1
3	E	136	ASN	2.1
4	F	153	ALA	2.1
4	F	235	ASP	2.1
4	F	341	LYS	2.1
4	F	4	PHE	2.1
4	F	146	VAL	2.1
4	F	137	ARG	2.1
4	F	221	LEU	2.1
1	C	133	GLN	2.1
1	A	364	PRO	2.1
2	D	96	GLN	2.1
2	D	238	VAL	2.1
2	D	414	ASP	2.1
4	F	350	ILE	2.1
2	D	60	LYS	2.1
2	D	416	MET	2.0
1	A	170	SER	2.0
1	C	241	SER	2.0
2	B	85	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	260	ASN	2.0
4	F	31	ARG	2.0
2	D	255	LEU	2.0
4	F	191	LEU	2.0
1	A	141	PHE	2.0
2	D	396	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

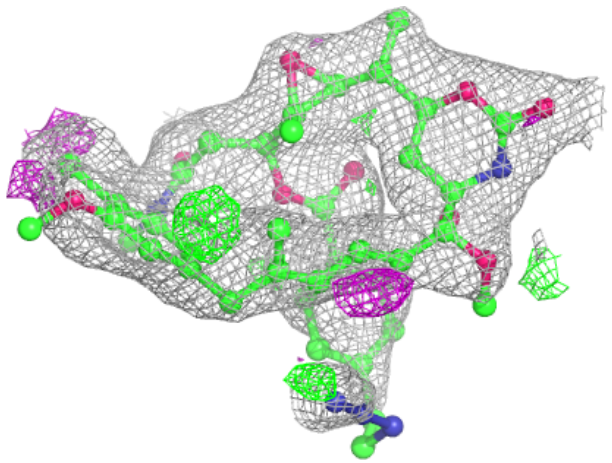
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

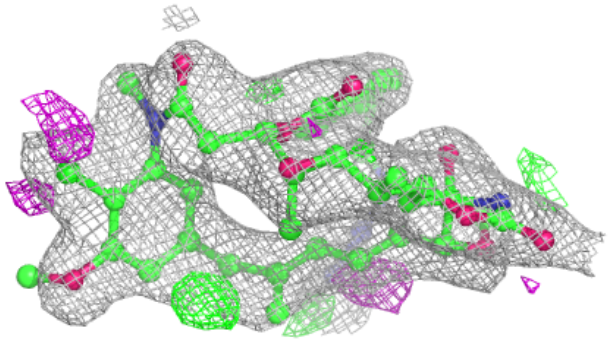
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	E	201	1/1	0.76	0.14	106,106,106,106	0
7	CA	B	503	1/1	0.79	0.07	87,87,87,87	0
8	IMD	A	504	5/5	0.87	0.11	65,67,72,74	0
6	MG	F	402	1/1	0.88	0.05	69,69,69,69	0
11	PWC	D	503	52/52	0.89	0.22	46,69,95,102	0
6	MG	D	502	1/1	0.90	0.12	61,61,61,61	0
12	ACP	F	401	31/31	0.91	0.14	63,76,98,99	0
7	CA	A	503	1/1	0.95	0.06	61,61,61,61	0
10	MES	B	504	12/12	0.95	0.11	38,49,62,63	0
9	GDP	D	501	28/28	0.96	0.10	43,50,60,68	0
9	GDP	B	501	28/28	0.98	0.16	27,34,40,41	0
6	MG	A	502	1/1	0.98	0.13	34,34,34,34	0
6	MG	C	502	1/1	0.98	0.12	29,29,29,29	0
5	GTP	A	501	32/32	0.98	0.17	27,33,38,39	0
5	GTP	C	501	32/32	0.98	0.14	24,30,32,33	0
7	CA	C	503	1/1	0.99	0.05	47,47,47,47	0
6	MG	B	502	1/1	0.99	0.17	26,26,26,26	0

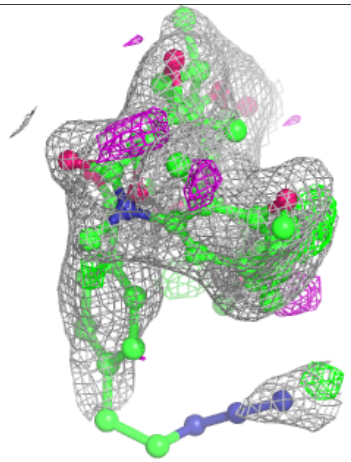
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PWC D 503:

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

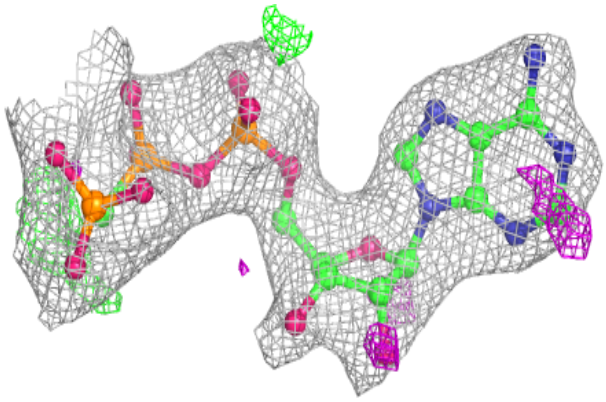


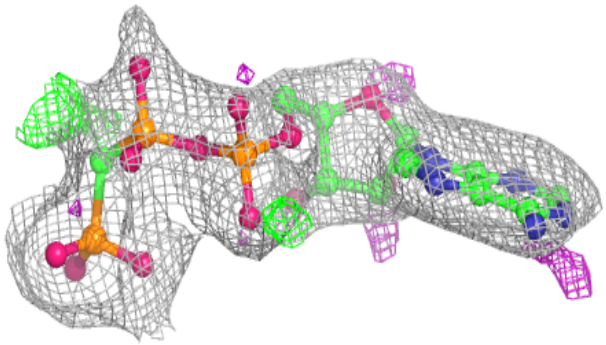


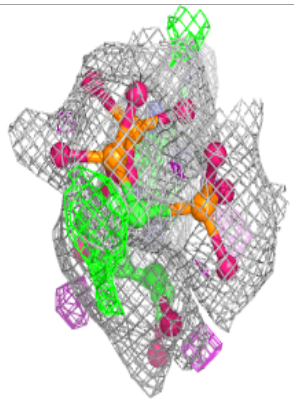


Electron density around ACP F 401:

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

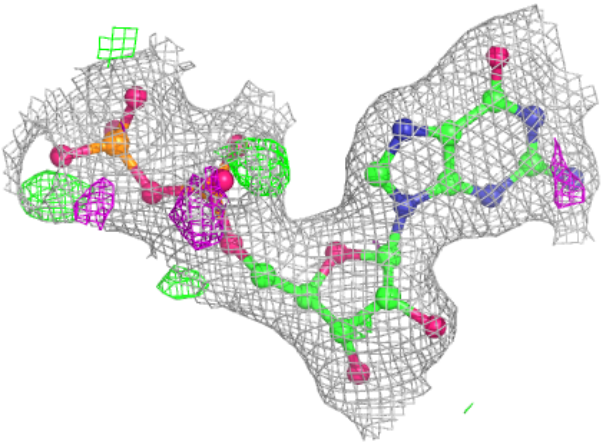


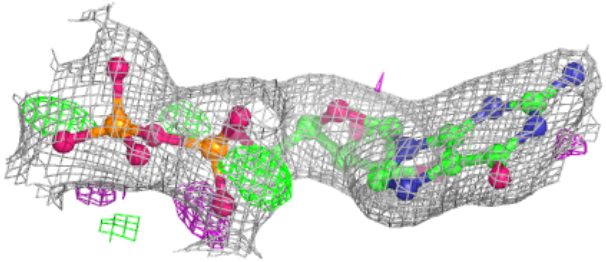


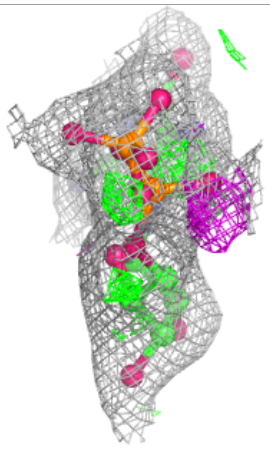


Electron density around GDP D 501:

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

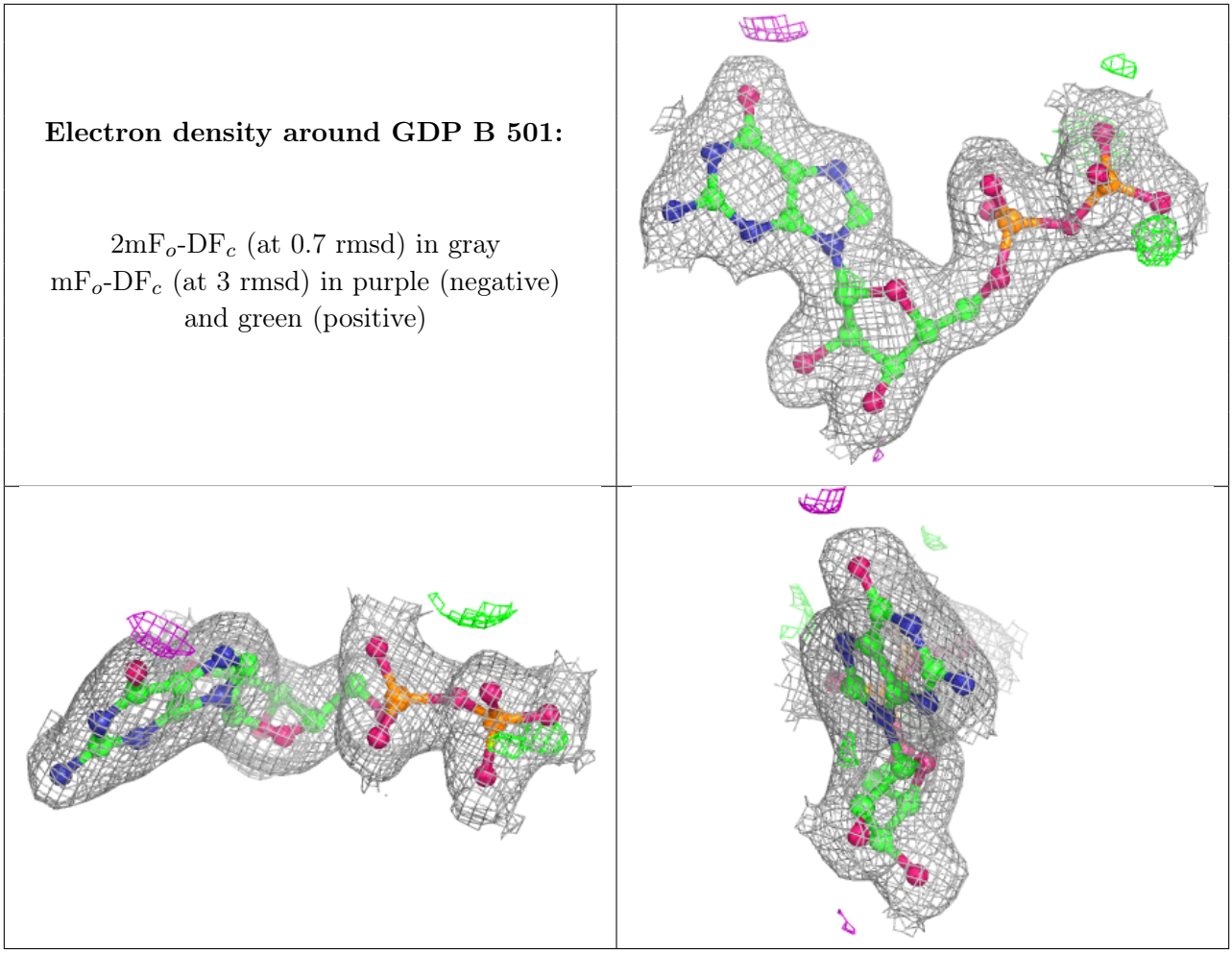






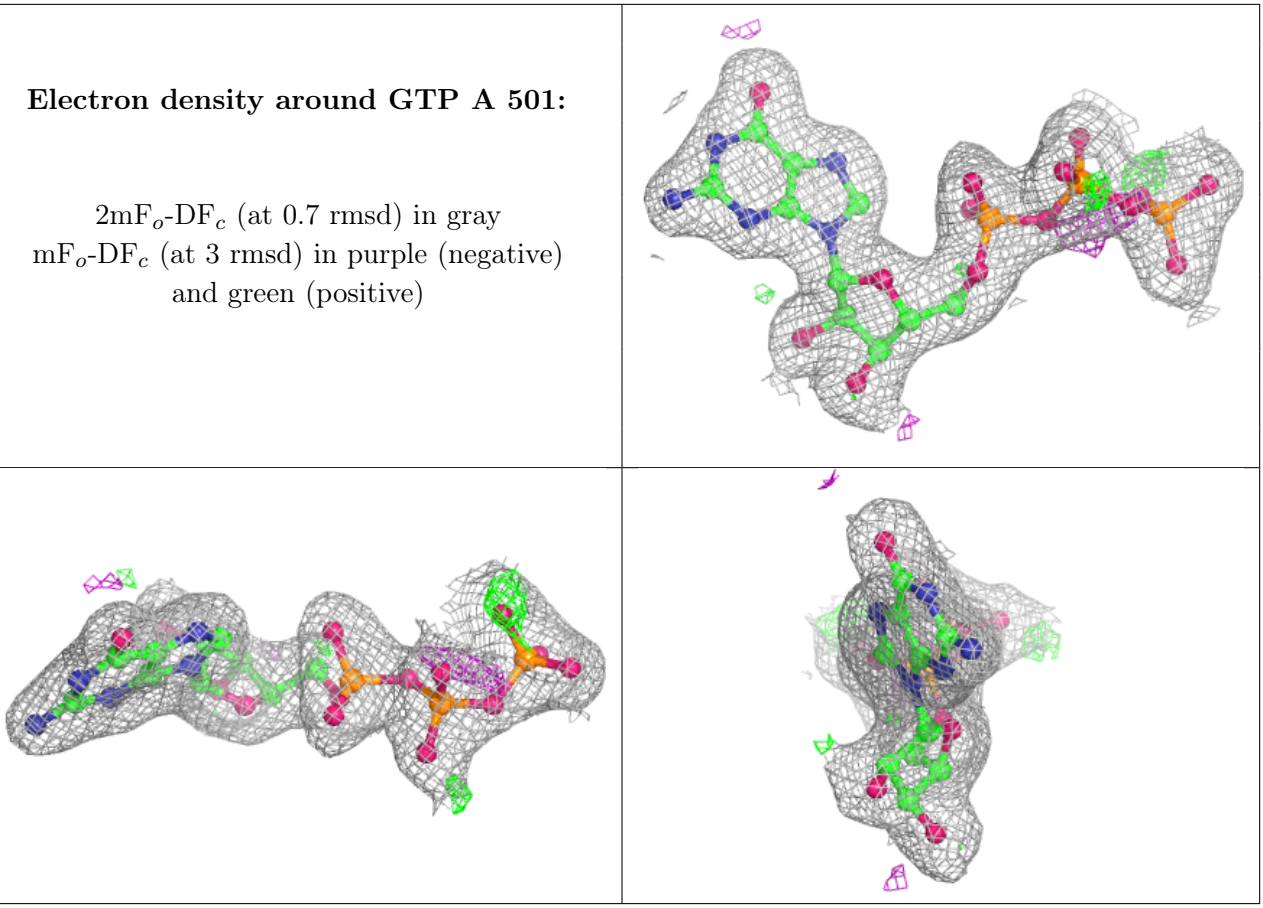
Electron density around GDP B 501:

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



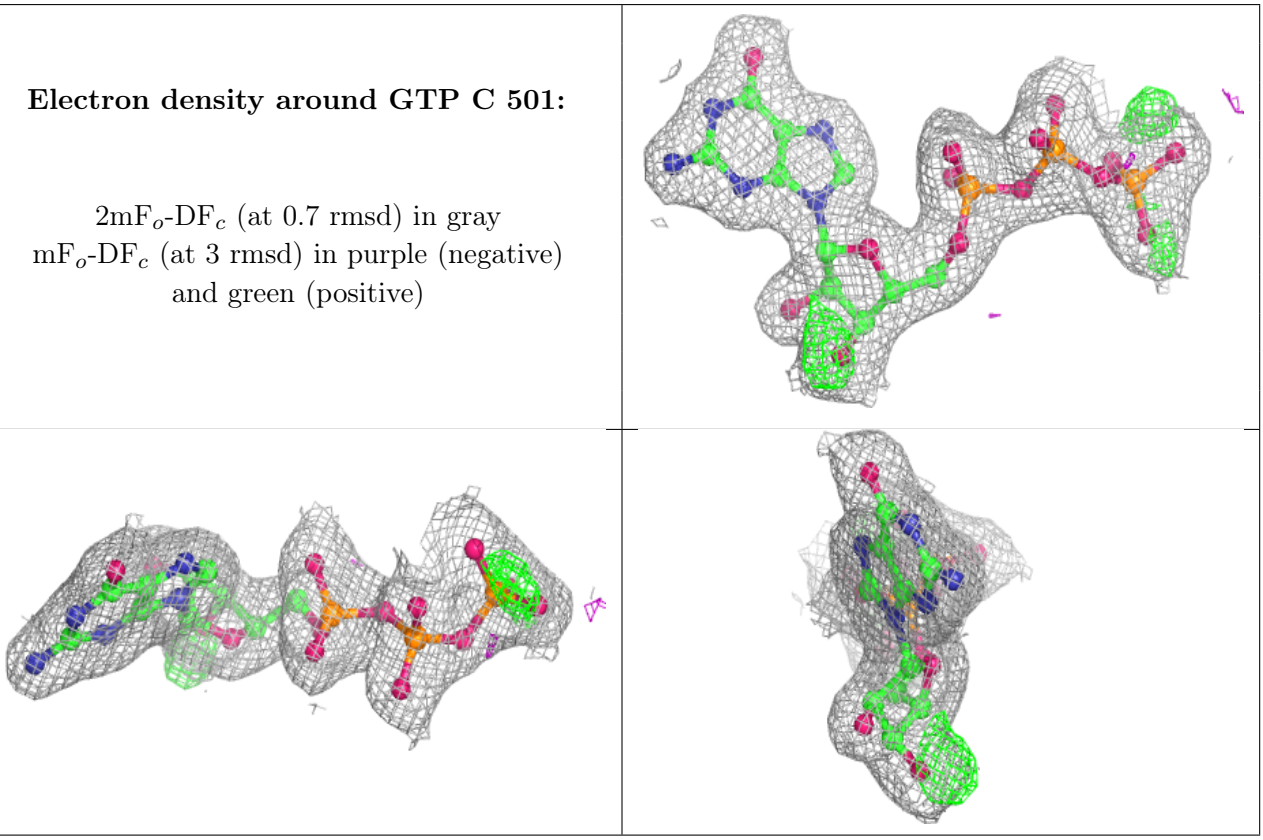
Electron density around GTP A 501:

$2mF_o$-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 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.