Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 10:27 AM EST

PDB ID	:	5SB8
Title	:	Tubulin-maytansinoid-3-complex
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Deposited on	:	2021-07-20
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

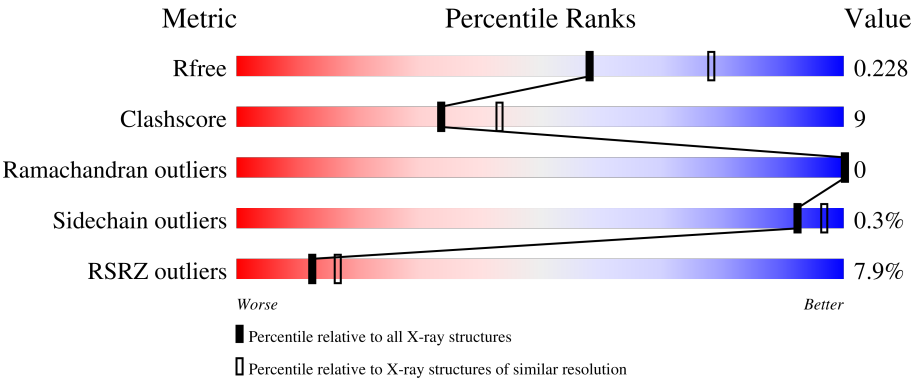
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	4% 78% 18% ·
1	C	451	80% 18% ·
2	B	445	2% 74% 21% 5%
2	D	445	7% 75% 21% ·
3	E	143	6% 73% 13% 14%

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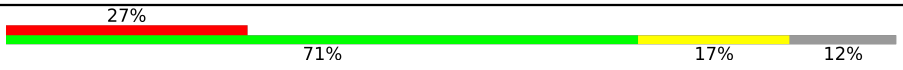
Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18058 atoms, of which 5 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
			3433	2172	583	656	22			
1	C	440	Total	C	N	O	S	0	3	0
			3461	2189	589	659	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	1	0
			3337	2097	571	643	26			
2	D	427	Total	C	N	O	S	1	0	0
			3348	2101	571	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
			1024	631	186	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

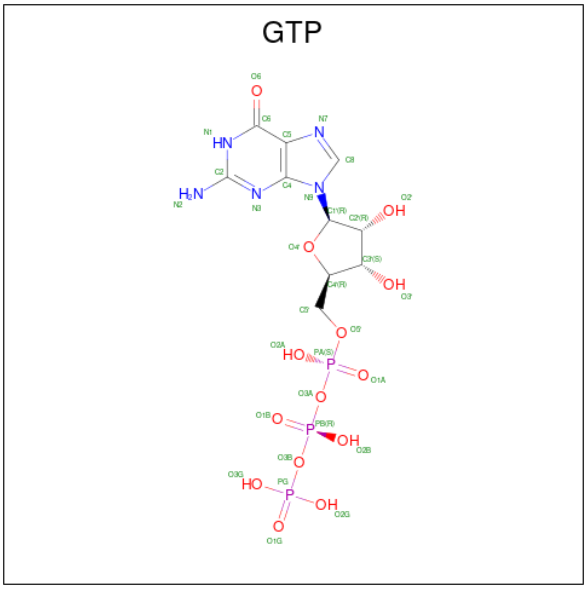
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	339	Total	C	N	O	S	0	0	0
			2780	1785	477	504	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 (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	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 (three-letter code: 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		

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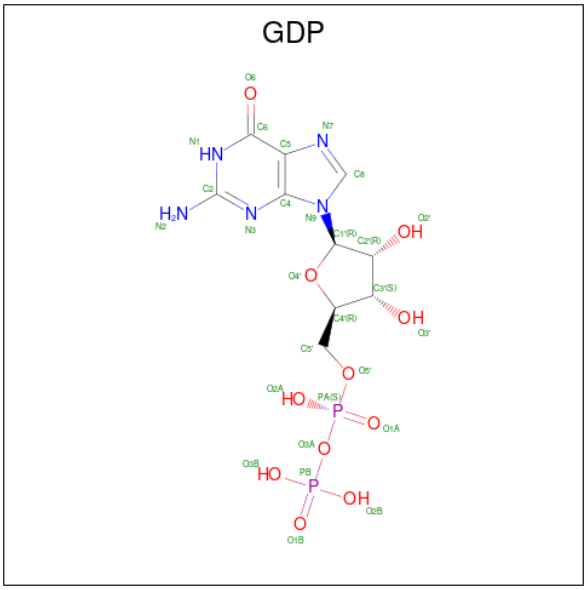
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

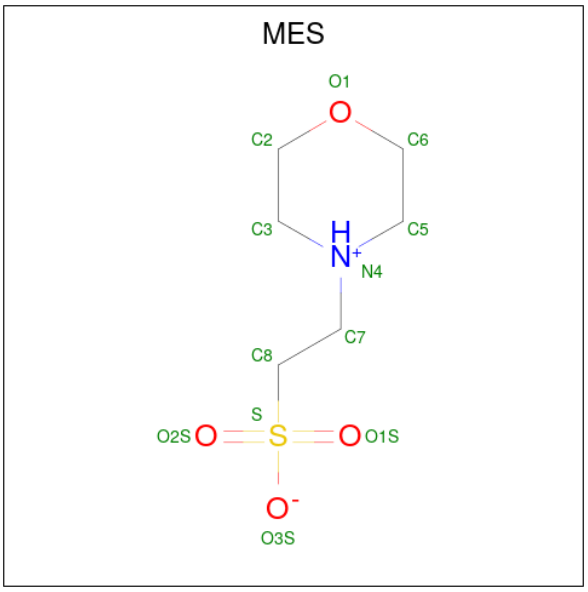
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



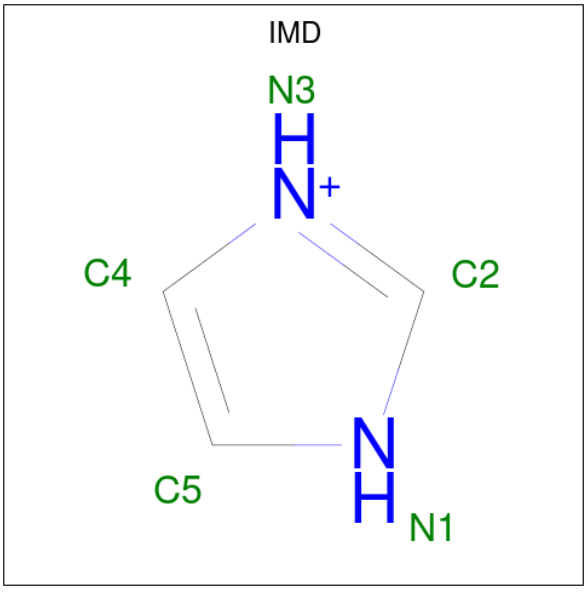
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

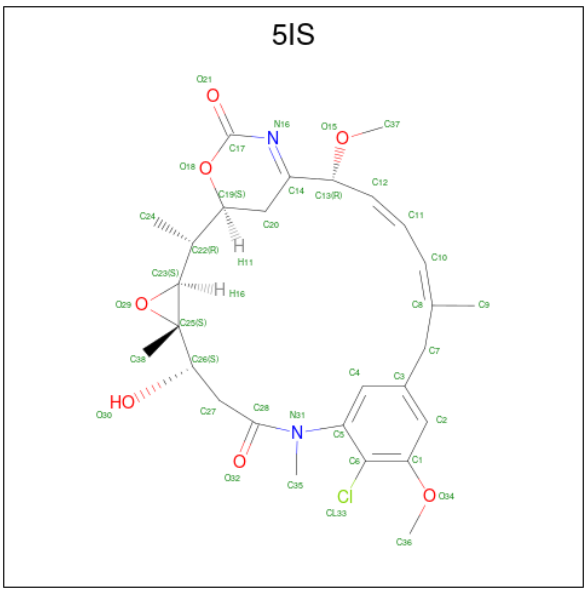
- Molecule 10 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

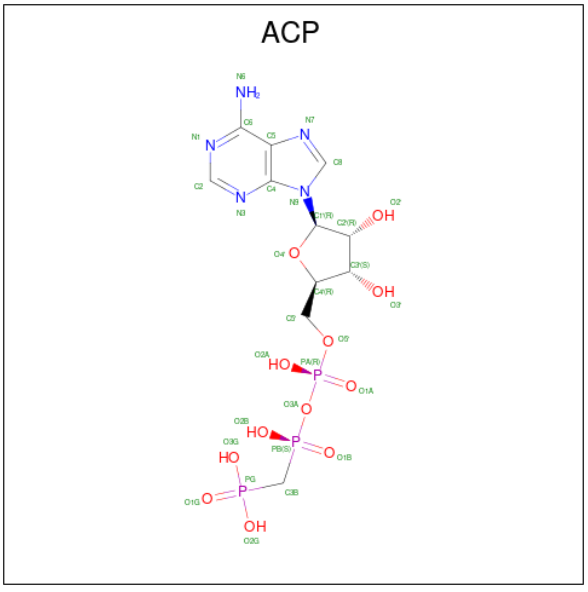
- Molecule 11 is (1S,2R,3S,5S,6S,16E,18E,20R)-11-chloro-6-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16,18,21-hexaene-8,23-dione (three-letter code: 5IS) (formula: $C_{28}H_{35}ClN_2O_7$) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	Cl	N	O	0	0
			38	28	1	2	7		

- 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.

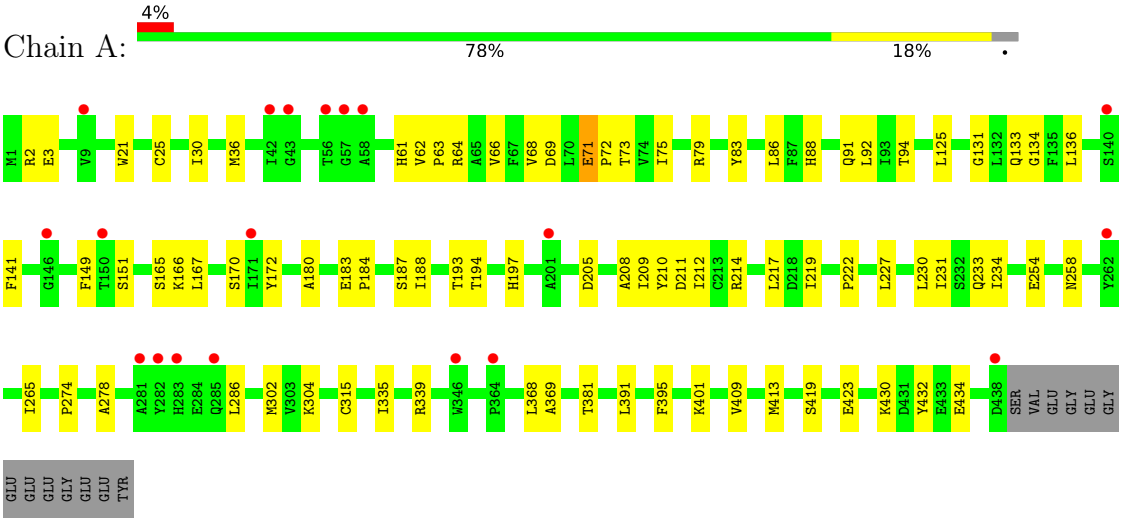
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	79	Total O 79 79	0	0
13	B	100	Total O 100 100	0	0
13	C	203	Total O 203 203	0	0
13	D	40	Total O 40 40	0	0
13	E	17	Total O 17 17	0	0
13	F	17	Total O 17 17	0	0

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.

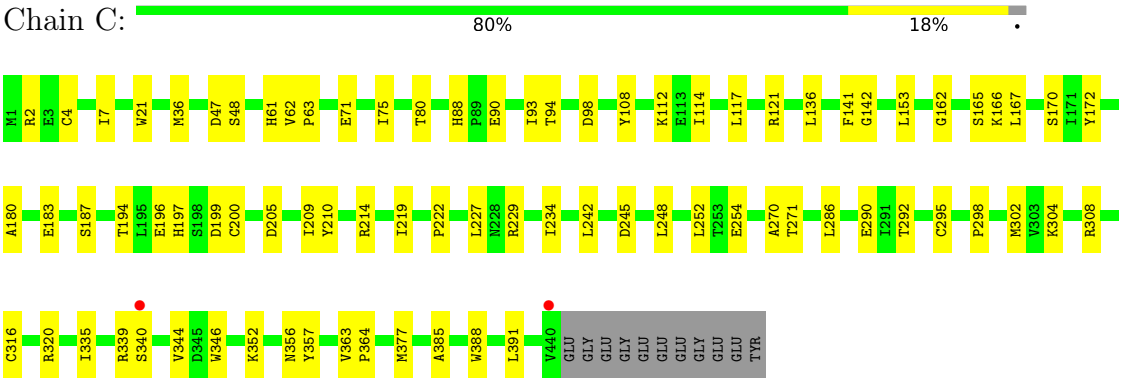
• Molecule 1: Tubulin alpha-1B chain

Chain A:



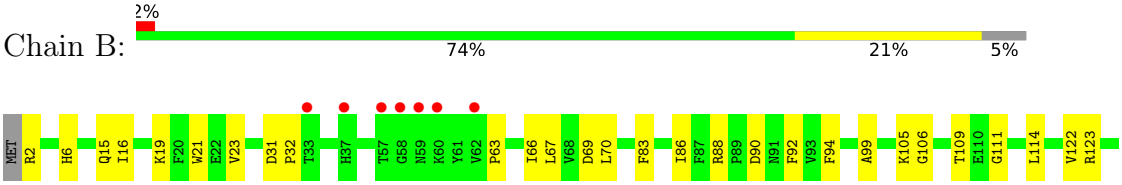
• Molecule 1: Tubulin alpha-1B chain

Chain C:



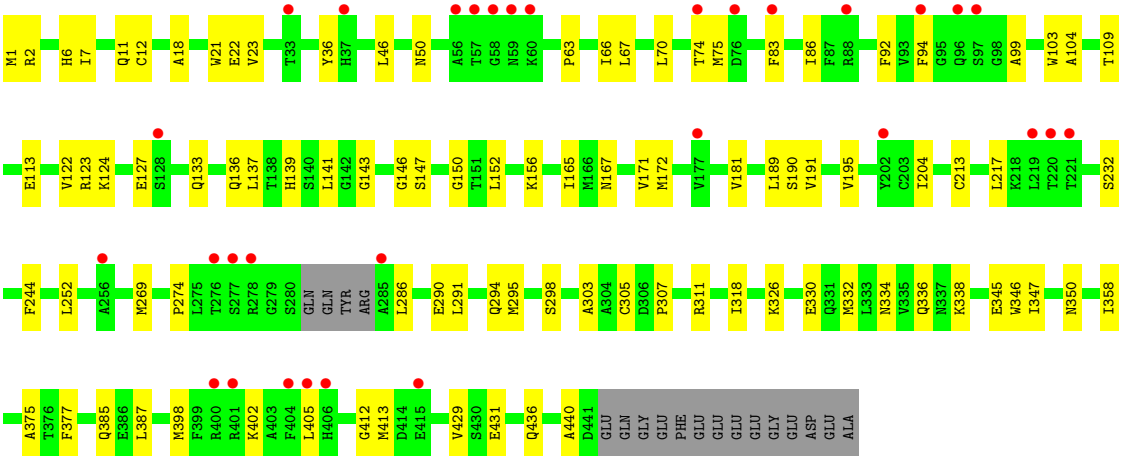
• Molecule 2: Tubulin beta-2B chain

Chain B:



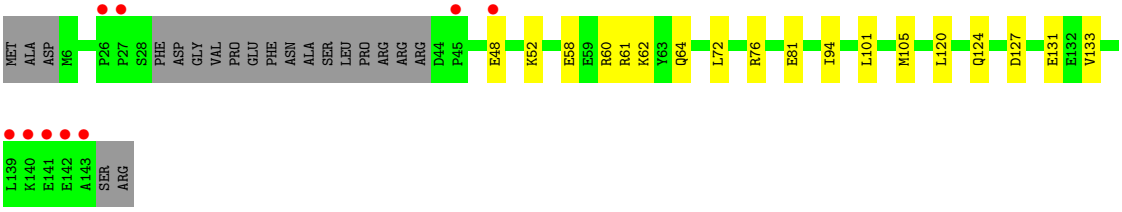
• Molecule 2: Tubulin beta-2B chain

Chain D:



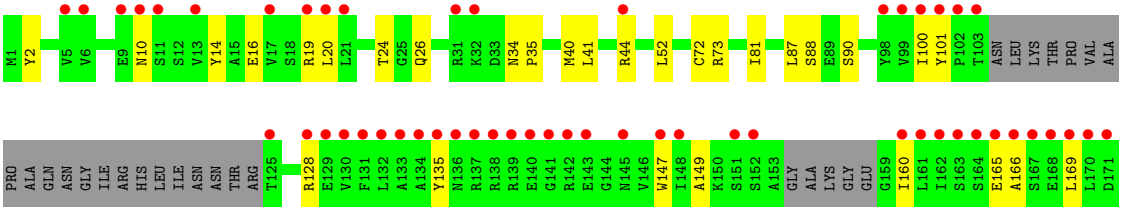
• Molecule 3: Stathmin-4

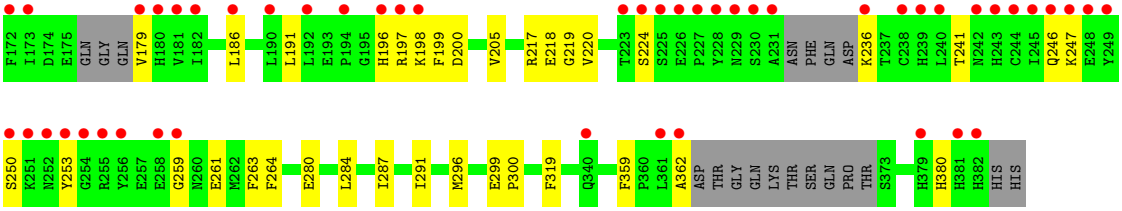
Chain E:



• Molecule 4: Tubulin-Tyrosine Ligase

Chain F:




F172 I173 D174 E175 GLN GLY GLN V179 H180 V181 I182 L186 L190 L191 L192 E193 P194 G195 H196 R197 K198 F199 D200 V205 R217 E218 G219 V220 T223 S224 S225 E226 P227 Y228 N229 S230 A231 ASN PHE GLN ASP K236 T237 C238 H239 L240 T241 N242 H243 C244 I245 Q246 K247 E248 Y249
S250 K251 N252 Y253 G254 R255 Y256 E257 E258 G259 N260 E261 M262 F263 F264 E280 L284 I287 I291 M296 E299 P300 F319 Q340 F359 P360 L361 A362 ASP THR GLY GLN LYS THR SER GLN PRO THR S373 H379 H380 H381 H382 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	104.66Å 157.49Å 181.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.30 49.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.66-2.30) 100.0 (49.66-2.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.193 , 0.230 0.191 , 0.228	Depositor DCC
R_{free} test set	6674 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.5	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	0.96	EDS
Total number of atoms	18058	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: GTP, 5IS, MES, ACP, MG, GDP, IMD, 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	0.24	0/3511	0.46	0/4766
1	C	0.24	0/3540	0.46	0/4806
2	B	0.24	0/3411	0.46	0/4619
2	D	0.24	0/3421	0.45	0/4633
3	E	0.23	0/1033	0.40	0/1371
4	F	0.23	0/2843	0.45	0/3838
All	All	0.24	0/17759	0.45	0/24033

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	3433	0	3339	54	0
1	C	3461	0	3367	59	0
2	B	3337	0	3215	68	0
2	D	3348	0	3227	64	0
3	E	1024	0	1035	11	0
4	F	2780	0	2751	42	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	1	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	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	12	0	12	2	0
10	B	5	5	5	0	0
11	D	38	0	0	0	0
12	F	31	0	14	2	0
13	A	79	0	0	0	0
13	B	100	0	0	3	0
13	C	203	0	0	4	0
13	D	40	0	0	1	0
13	E	17	0	0	1	0
13	F	17	0	0	0	0
All	All	18053	5	17013	295	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 9.

All (295) 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)
12:F:401:ACP:H5'1	12:F:401:ACP:H8	1.50	0.93
1:C:270:ALA:HB3	1:C:302[B]:MET:HG3	1.53	0.90
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.57	0.86
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.65	0.78
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.68	0.76
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.67	0.75
1:C:209:ILE:HD11	1:C:302[B]:MET:HE2	1.70	0.73
2:B:83:PHE:O	2:B:86:ILE:HG22	1.90	0.72
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.70	0.71
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.21	0.71
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.72	0.70
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.74	0.70
2:D:431:GLU:OE1	13:D:601:HOH:O	2.09	0.70
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.32	0.69
2:D:298:SER:HB3	2:D:307:PRO:HD2	1.76	0.68
2:D:1:MET:CE	2:D:50:ASN:HB2	2.23	0.67
2:D:181:VAL:HG22	2:D:398:MET:SD	2.34	0.67
2:D:136:GLN:HA	2:D:167:ASN:O	1.95	0.67
2:B:298:SER:HA	2:B:301:MET:CE	2.25	0.66
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.78	0.65
2:B:424:ASN:HB3	13:B:611:HOH:O	1.96	0.65
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.32	0.65
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.79	0.65
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.79	0.64
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.78	0.64
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.38	0.64
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.32	0.64
1:A:166:LYS:HE2	1:A:197:HIS:O	1.98	0.64
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.79	0.64
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.34	0.62
2:B:136:GLN:HA	2:B:167:ASN:O	1.98	0.62
2:B:2:ARG:HA	2:B:131:CYS:O	1.99	0.62
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.11	0.61
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.61
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.61
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.31	0.61
4:F:149:ALA:O	4:F:160:ILE:HG23	2.02	0.60
1:C:180:ALA:O	1:C:183:GLU:HG3	2.02	0.60
4:F:246:GLN:O	4:F:250:SER:HB3	2.01	0.60
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.83	0.60
2:D:1:MET:HE3	2:D:50:ASN:HB2	1.85	0.59
2:D:152:LEU:O	2:D:156:LYS:HG2	2.03	0.58
1:C:229:ARG:NH1	13:C:605:HOH:O	2.35	0.58
1:C:209:ILE:HD11	1:C:302[B]:MET:CE	2.33	0.58
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.85	0.58
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.86	0.58
1:C:48:SER:OG	1:C:245:ASP:HB2	2.03	0.58
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.86	0.57
2:D:11:GLN:HA	2:D:74:THR:HG21	1.86	0.57
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.85	0.57
2:B:123:ARG:O	2:B:127:GLU:HG3	2.05	0.57
2:B:298:SER:HA	2:B:301:MET:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.20	0.57
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.86	0.57
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.34	0.57
2:D:332:MET:O	2:D:336:GLN:HG3	2.05	0.57
2:D:147:SER:HB2	2:D:190:SER:OG	2.05	0.56
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.87	0.56
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.87	0.56
4:F:10:ASN:HB2	4:F:44:ARG:NH2	2.21	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.06	0.56
2:D:75:MET:SD	2:D:94:PHE:HB3	2.46	0.56
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.86	0.56
2:B:298:SER:HA	2:B:301:MET:HE1	1.87	0.56
1:C:271:THR:HG21	1:C:295:CYS:O	2.06	0.56
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.88	0.55
2:D:83:PHE:O	2:D:86:ILE:HG22	2.05	0.55
2:D:171:VAL:HA	2:D:204:ILE:O	2.07	0.55
2:D:191:VAL:O	2:D:195:VAL:HG23	2.07	0.55
1:C:340:SER:HA	13:C:625:HOH:O	2.05	0.55
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.87	0.55
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.71	0.55
1:C:88[A]:HIS:CE1	1:C:90:GLU:HG3	2.42	0.55
1:C:47:ASP:OD2	13:C:601:HOH:O	2.18	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.88	0.54
2:D:123:ARG:O	2:D:127:GLU:HG3	2.06	0.54
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.88	0.54
2:B:248:LEU:HD21	2:B:352:LYS:CB	2.37	0.54
13:B:677:HOH:O	1:C:2:ARG:HD2	2.08	0.54
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.23	0.54
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.90	0.54
2:D:290:GLU:O	2:D:294:GLN:HG3	2.08	0.54
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.38	0.54
2:B:2:ARG:HB3	2:B:133:GLN:HG3	1.89	0.54
3:E:120:LEU:O	3:E:124:GLN:HG3	2.08	0.54
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.90	0.53
4:F:40:MET:HE3	4:F:52:LEU:HD21	1.89	0.53
1:A:409:VAL:HA	1:A:413:MET:O	2.09	0.53
2:B:141:LEU:HD12	2:B:172:MET:SD	2.48	0.53
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.09	0.53
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.91	0.52
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.74	0.52
2:D:7:ILE:O	2:D:137:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.92	0.52
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.10	0.52
1:C:166:LYS:HE2	1:C:197:HIS:O	2.10	0.52
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.45	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.45	0.52
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.44	0.52
3:E:81:GLU:OE1	13:E:201:HOH:O	2.19	0.52
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.46	0.51
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.46	0.51
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.46	0.51
2:D:326:LYS:O	2:D:330:GLU:HG3	2.11	0.51
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.91	0.51
2:B:15:GLN:O	2:B:19:LYS:HG2	2.10	0.51
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.46	0.51
1:A:75:ILE:HB	1:A:94:THR:CG2	2.40	0.51
1:A:25:CYS:HB3	1:A:30:ILE:O	2.11	0.51
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.51	0.51
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.93	0.51
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.45	0.50
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.50
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.26	0.50
1:A:83:TYR:HB3	1:A:86:LEU:HD12	1.93	0.50
2:B:390:ARG:NE	13:B:602:HOH:O	2.43	0.50
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.39	0.50
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.47	0.50
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.47	0.50
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.47	0.50
1:A:187:SER:CB	1:A:391:LEU:HD21	2.42	0.49
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.49
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.93	0.49
4:F:160:ILE:O	4:F:236:LYS:NZ	2.43	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.49
1:A:209:ILE:HD11	1:A:302:MET:SD	2.52	0.49
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.94	0.49
4:F:160:ILE:HD12	4:F:160:ILE:N	2.27	0.49
1:A:2:ARG:HB2	1:A:133:GLN:CG	2.43	0.49
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.12	0.49
2:B:295:MET:CG	2:B:377:PHE:HB2	2.42	0.49
1:C:80:THR:HG22	1:C:80:THR:O	2.12	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.49
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.48	0.48
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.95	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.48
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.13	0.48
2:B:199:ASP:OD1	9:B:504:MES:H62	2.13	0.48
4:F:88:SER:OG	4:F:90:SER:O	2.32	0.48
4:F:198:LYS:HG2	4:F:199:PHE:H	1.77	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.48
2:D:311:ARG:NH1	2:D:436:GLN:O	2.47	0.48
1:A:214:ARG:HG2	1:A:219:ILE:O	2.13	0.48
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.41	0.48
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.41	0.47
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.95	0.47
3:E:60:ARG:O	3:E:64:GLN:HG3	2.14	0.47
4:F:87:LEU:O	4:F:88:SER:OG	2.29	0.47
2:B:389:LYS:O	2:B:393:GLU:HG3	2.14	0.47
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.44	0.47
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.49	0.47
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.30	0.47
2:B:67:LEU:N	2:B:67:LEU:HD12	2.29	0.47
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.44	0.47
2:D:146:GLY:O	2:D:150:GLY:HA3	2.14	0.47
1:A:2:ARG:HB3	1:A:131:GLY:O	2.15	0.47
2:B:248:LEU:CD2	2:B:352:LYS:HB3	2.45	0.47
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.49	0.47
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.46	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.47
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.96	0.47
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.50	0.47
4:F:296:MET:SD	4:F:380:HIS:HB2	2.54	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.96	0.46
1:C:242:LEU:HD11	1:C:252:LEU:CB	2.44	0.46
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.49	0.46
4:F:259:GLY:O	4:F:261:GLU:HG3	2.16	0.46
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.50	0.46
1:C:270:ALA:CB	1:C:302[B]:MET:HG3	2.35	0.46
1:C:234:ILE:HD12	1:C:234:ILE:N	2.31	0.46
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.98	0.46
1:A:75:ILE:HB	1:A:94:THR:HG21	1.97	0.46
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.50	0.46
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:SER:HA	1:C:199:ASP:OD2	2.16	0.46
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.98	0.46
4:F:186:LEU:HG	12:F:401:ACP:N1	2.32	0.45
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.97	0.45
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.52	0.45
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.47	0.45
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.16	0.45
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.98	0.45
1:A:227:LEU:O	1:A:231:ILE:HG13	2.17	0.45
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.46	0.45
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.32	0.45
2:D:18:ALA:O	2:D:22:GLU:HG3	2.16	0.45
1:A:180:ALA:O	1:A:183:GLU:HG3	2.16	0.45
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.45
2:B:318:ILE:N	2:B:318:ILE:HD12	2.31	0.45
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.82	0.45
4:F:247:LYS:HA	4:F:253:TYR:CD2	2.52	0.45
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.52	0.45
2:D:295:MET:CE	2:D:377:PHE:HB2	2.43	0.45
2:D:303:ALA:O	2:D:305:CYS:N	2.50	0.45
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.99	0.44
2:B:164:ARG:O	9:B:504:MES:H71	2.18	0.44
2:B:276:THR:HG21	2:B:282:GLN:HA	1.99	0.44
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.35	0.44
1:C:214:ARG:HG2	1:C:219:ILE:O	2.18	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.44
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.99	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:D:104:ALA:HB2	2:D:413:MET:SD	2.58	0.44
2:D:109:THR:O	2:D:113:GLU:HG2	2.17	0.44
4:F:197:ARG:HB2	4:F:224:SER:O	2.18	0.44
1:A:430:LYS:O	1:A:434:GLU:HG3	2.17	0.44
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.99	0.44
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.44
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.53	0.44
1:C:88[A]:HIS:HE1	1:C:90:GLU:HG3	1.80	0.44
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.99	0.44
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.18	0.44
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.18	0.44
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.52	0.44
2:D:387:LEU:HD23	2:D:387:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.58	0.43
2:D:213:CYS:HA	2:D:217:LEU:HD12	1.99	0.43
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.54	0.43
3:E:127:ASP:O	3:E:131:GLU:HG2	2.18	0.43
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.18	0.43
2:D:7:ILE:O	2:D:137:LEU:HA	2.18	0.43
2:B:137:LEU:HD23	2:B:154:ILE:HD11	2.00	0.43
2:D:66:ILE:HD12	2:D:122:VAL:HG22	2.01	0.43
2:B:317:ALA:C	2:B:318:ILE:HD12	2.39	0.43
2:B:323:MET:HB3	2:B:373:MET:HE2	2.01	0.43
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.53	0.43
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.99	0.43
3:E:58:GLU:HG2	3:E:62:LYS:HE3	2.00	0.43
1:A:419:SER:O	1:A:423[A]:GLU:HG3	2.19	0.43
4:F:147:TRP:HB2	4:F:169:LEU:HD11	2.00	0.43
2:B:105:LYS:HA	2:B:109:THR:OG1	2.19	0.43
1:C:242:LEU:HD11	1:C:252:LEU:HB3	2.01	0.43
4:F:26:GLN:HE22	4:F:362:ALA:H	1.66	0.43
2:B:301:MET:HE1	2:B:307:PRO:CG	2.49	0.42
1:C:108:TYR:O	1:C:112:LYS:HG2	2.19	0.42
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.01	0.42
1:A:151:SER:HB2	1:A:193:THR:OG1	2.20	0.42
2:D:274:PRO:HB3	2:D:286:LEU:HD22	2.02	0.42
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.18	0.42
1:A:71:GLU:HG2	1:A:72:PRO:N	2.33	0.42
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.54	0.42
1:A:62:VAL:HG13	1:A:86:LEU:O	2.19	0.42
2:B:316:ALA:HB3	2:B:378:ILE:HB	2.01	0.42
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.32	0.42
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.02	0.42
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.44	0.42
1:C:196:GLU:HG2	13:C:649:HOH:O	2.19	0.42
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.82	0.42
2:D:141:LEU:HA	2:D:147:SER:HB3	2.01	0.42
1:C:62:VAL:HG11	1:C:88[B]:HIS:CD2	2.55	0.41
2:D:412:GLY:C	3:E:133:VAL:HG13	2.40	0.41
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.02	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.41
2:B:329:ASP:O	2:B:333:LEU:HG	2.20	0.41
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:GLN:HG2	2:B:436:GLN:O	2.20	0.41
1:C:194:THR:O	1:C:194:THR:HG22	2.20	0.41
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.55	0.41
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.56	0.41
1:A:208:ALA:O	1:A:212:ILE:HG13	2.21	0.41
1:C:316:CYS:O	1:C:377:MET:HG3	2.21	0.41
2:D:124:LYS:C	2:D:124:LYS:HD3	2.40	0.41
4:F:72:CYS:O	4:F:73:ARG:HD2	2.20	0.41
3:E:101:LEU:O	3:E:105:MET:HG2	2.19	0.41
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.21	0.41
1:A:136:LEU:HD22	1:A:167:LEU:HB2	2.03	0.41
1:A:66:VAL:HG23	1:A:125:LEU:HD12	2.03	0.41
1:C:187:SER:CB	1:C:391:LEU:HD21	2.51	0.41
3:E:48:GLU:HG2	3:E:52:LYS:HE3	2.02	0.41
4:F:19:ARG:O	4:F:19:ARG:HD2	2.21	0.41
4:F:135:TYR:OH	4:F:165:GLU:HA	2.21	0.41
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.56	0.41
2:D:291:LEU:HG	2:D:375:ALA:HB2	2.03	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.40
1:A:183:GLU:N	1:A:184:PRO:CD	2.84	0.40
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.50	0.40
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.19	0.40
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.51	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.40
2:B:269:MET:HE3	2:B:301:MET:SD	2.61	0.40
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.36	0.40
1:A:194:THR:O	1:A:194:THR:HG22	2.21	0.40
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.02	0.40
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.56	0.40
2:B:70:LEU:HD12	2:B:99:ALA:HB2	2.03	0.40
2:B:114:LEU:HG	2:B:114:LEU:O	2.22	0.40
2:B:187:ALA:O	2:B:191:VAL:HG23	2.21	0.40
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.54	0.40
1:A:134:GLY:HA3	1:A:165:SER:O	2.22	0.40
2:B:235:MET:HE2	2:B:235:MET:HB3	1.93	0.40
1:C:205:ASP:OD2	1:C:304:LYS:HG3	2.22	0.40
4:F:20:LEU:O	4:F:24:THR:HG23	2.22	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	441/451 (98%)	431 (98%)	10 (2%)	0	100	100
2	B	419/445 (94%)	410 (98%)	9 (2%)	0	100	100
2	D	423/445 (95%)	415 (98%)	8 (2%)	0	100	100
3	E	120/143 (84%)	118 (98%)	2 (2%)	0	100	100
4	F	327/384 (85%)	316 (97%)	11 (3%)	0	100	100
All	All	2167/2319 (93%)	2118 (98%)	49 (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%)	367 (99%)	3 (1%)	81	91
1	C	374/379 (99%)	373 (100%)	1 (0%)	92	97
2	B	367/383 (96%)	366 (100%)	1 (0%)	92	97
2	D	368/383 (96%)	367 (100%)	1 (0%)	92	97
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	305/342 (89%)	305 (100%)	0	100	100
All	All	1895/1993 (95%)	1889 (100%)	6 (0%)	92	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	315	CYS
1	A	381	THR
2	B	139	HIS
1	C	71	GLU
2	D	139	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 16 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
8	GDP	B	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.89	7 (22%)
11	5IS	D	503	-	40,41,41	2.88	6 (15%)	40,61,61	2.07	12 (30%)
5	GTP	A	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.75	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	ACP	F	401	6	27,33,33	1.98	7 (25%)	32,52,52	1.38	4 (12%)
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.94	8 (25%)
10	IMD	B	505	-	3,5,5	0.40	0	4,5,5	0.59	0
5	GTP	C	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.72	6 (18%)
9	MES	B	504	-	12,12,12	2.19	1 (8%)	14,16,16	1.99	5 (35%)

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
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	5IS	D	503	-	-	11/40/64/64	0/2/4/4
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
12	ACP	F	401	6	-	6/15/38/38	0/3/3/3
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
10	IMD	B	505	-	-	-	0/1/1/1
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	5IS	C20-C14	-13.16	1.34	1.50
11	D	503	5IS	C14-N16	9.60	1.44	1.28
9	B	504	MES	C8-S	-7.31	1.67	1.77
12	F	401	ACP	PG-O1G	5.43	1.61	1.50
8	D	501	GDP	C5-C6	4.20	1.48	1.41
8	B	501	GDP	C5-C6	4.15	1.48	1.41
12	F	401	ACP	PB-O1B	4.15	1.61	1.51
11	D	503	5IS	O29-C23	-3.69	1.40	1.45
11	D	503	5IS	C25-C23	3.61	1.51	1.47
12	F	401	ACP	PB-O2B	-3.46	1.48	1.56
12	F	401	ACP	PB-O3A	3.34	1.62	1.58
5	A	501	GTP	C6-N1	3.09	1.38	1.33
5	C	501	GTP	C6-N1	3.04	1.38	1.33
12	F	401	ACP	PG-O2G	-2.86	1.48	1.54
11	D	503	5IS	C5-N31	-2.84	1.40	1.44
12	F	401	ACP	PG-O3G	2.80	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	5IS	C17-N16	2.71	1.41	1.34
12	F	401	ACP	C5-C4	2.48	1.47	1.40
8	D	501	GDP	C5-C4	2.45	1.47	1.40
8	B	501	GDP	C5-C4	2.39	1.47	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	503	5IS	C25-O29-C23	6.06	64.43	60.79
11	D	503	5IS	C6-C5-N31	5.36	126.21	120.71
5	A	501	GTP	N3-C2-N1	-5.35	120.08	127.22
5	C	501	GTP	N3-C2-N1	-5.18	120.31	127.22
8	B	501	GDP	C2-N3-C4	4.87	120.92	115.36
8	D	501	GDP	C2-N3-C4	4.85	120.90	115.36
11	D	503	5IS	O29-C25-C23	-4.43	56.41	59.38
9	B	504	MES	C5-N4-C3	4.29	118.48	108.83
5	A	501	GTP	C2-N3-C4	4.11	120.05	115.36
8	B	501	GDP	C2-N1-C6	4.06	122.38	115.93
8	D	501	GDP	C2-N1-C6	4.05	122.36	115.93
8	D	501	GDP	C5-C6-N1	-4.02	117.93	123.43
8	B	501	GDP	C5-C6-N1	-3.99	117.98	123.43
11	D	503	5IS	C20-C14-C13	3.97	127.49	116.61
5	C	501	GTP	C2-N3-C4	3.97	119.89	115.36
8	B	501	GDP	C4-C5-C6	-3.89	117.08	120.80
12	F	401	ACP	C3'-C2'-C1'	3.77	106.66	100.98
8	D	501	GDP	C4-C5-C6	-3.71	117.25	120.80
11	D	503	5IS	C19-C20-C14	3.57	122.25	112.00
9	B	504	MES	O1S-S-C8	3.35	110.95	106.92
8	B	501	GDP	N3-C2-N1	-3.33	122.79	127.22
5	C	501	GTP	PA-O3A-PB	-3.26	121.64	132.83
8	D	501	GDP	N3-C2-N1	-3.25	122.88	127.22
5	A	501	GTP	PA-O3A-PB	-3.21	121.81	132.83
8	D	501	GDP	PA-O3A-PB	-3.16	121.99	132.83
12	F	401	ACP	N3-C2-N1	-3.05	123.91	128.68
5	A	501	GTP	C5-C6-N1	-2.95	119.39	123.43
5	C	501	GTP	C5-C6-N1	-2.95	119.40	123.43
5	C	501	GTP	PB-O3B-PG	-2.84	123.07	132.83
11	D	503	5IS	C27-C28-N31	-2.82	115.71	118.89
8	B	501	GDP	PA-O3A-PB	-2.81	123.17	132.83
8	D	501	GDP	C4-C5-N7	-2.76	106.53	109.40
12	F	401	ACP	PB-O3A-PA	-2.69	124.03	132.56
8	B	501	GDP	C4-C5-N7	-2.66	106.62	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	GTP	C2-N1-C6	2.65	120.14	115.93
8	D	501	GDP	C3'-C2'-C1'	2.63	104.94	100.98
5	C	501	GTP	C2-N1-C6	2.62	120.09	115.93
5	A	501	GTP	PB-O3B-PG	-2.59	123.95	132.83
9	B	504	MES	C7-N4-C5	2.53	117.71	111.23
9	B	504	MES	C6-C5-N4	-2.52	106.28	110.10
12	F	401	ACP	C4-C5-N7	-2.41	106.89	109.40
9	B	504	MES	O3S-S-C8	2.22	109.36	105.77
11	D	503	5IS	C4-C5-C6	-2.20	119.72	122.53
11	D	503	5IS	O34-C1-C6	2.17	118.11	115.53
11	D	503	5IS	O29-C25-C38	2.17	117.28	114.17
11	D	503	5IS	C5-C6-CL33	2.17	122.40	120.09
11	D	503	5IS	O34-C1-C2	-2.17	120.39	124.12
11	D	503	5IS	O18-C19-C22	2.01	109.93	105.76

There are no chirality outliers.

All (39) 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
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	PA-O3A-PB-O3B
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
11	D	503	5IS	C11-C12-C13-C14
11	D	503	5IS	C14-C13-O15-C37
11	D	503	5IS	C6-C1-O34-C36
11	D	503	5IS	C20-C19-C22-C24
11	D	503	5IS	O18-C19-C22-C24
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
11	D	503	5IS	C2-C1-O34-C36
12	F	401	ACP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O2S
11	D	503	5IS	C23-C25-C26-O30
11	D	503	5IS	O18-C19-C22-C23
9	B	504	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3A-PA-O2A
11	D	503	5IS	C26-C27-C28-N31
5	C	501	GTP	C4'-C5'-O5'-PA
11	D	503	5IS	C26-C27-C28-O32
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
12	F	401	ACP	PB-O3A-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
11	D	503	5IS	O29-C25-C26-O30

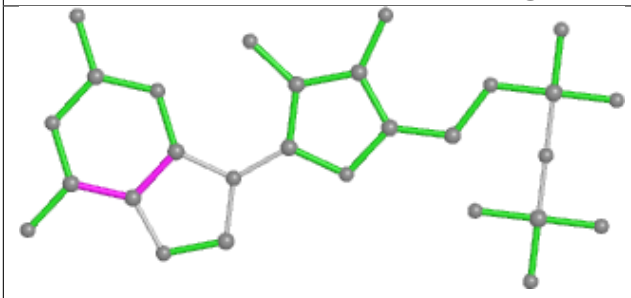
There are no ring outliers.

4 monomers are involved in 6 short contacts:

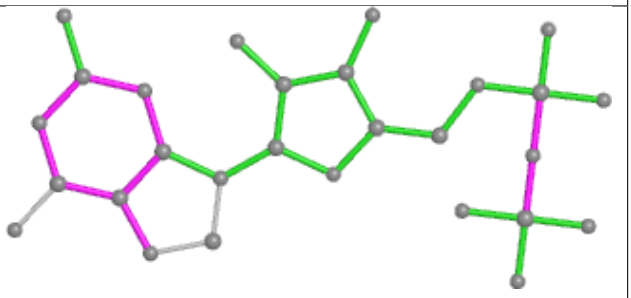
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	2	0
8	D	501	GDP	1	0
5	C	501	GTP	1	0
9	B	504	MES	2	0

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 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.

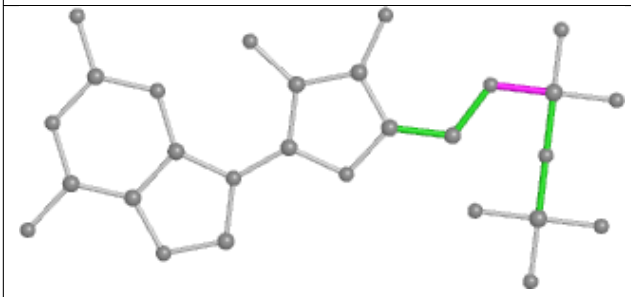
Ligand GDP B 501



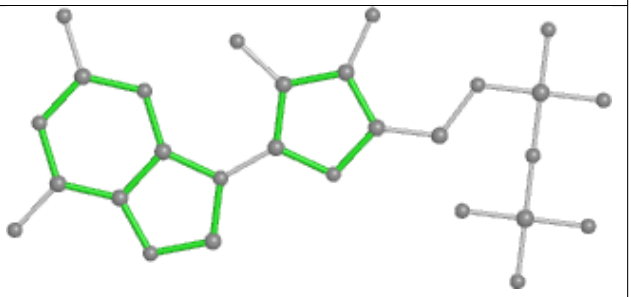
Bond lengths



Bond angles

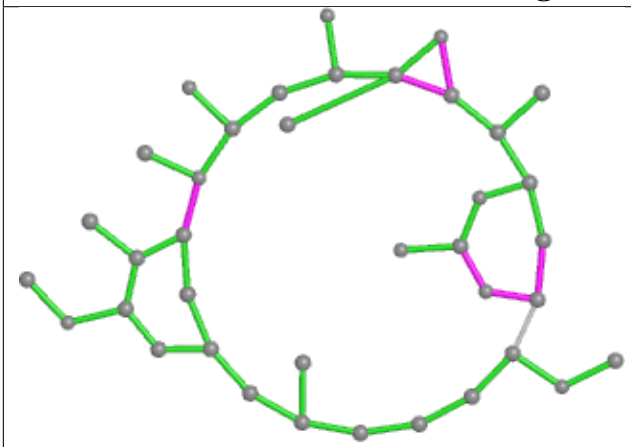


Torsions



Rings

Ligand 5IS D 503



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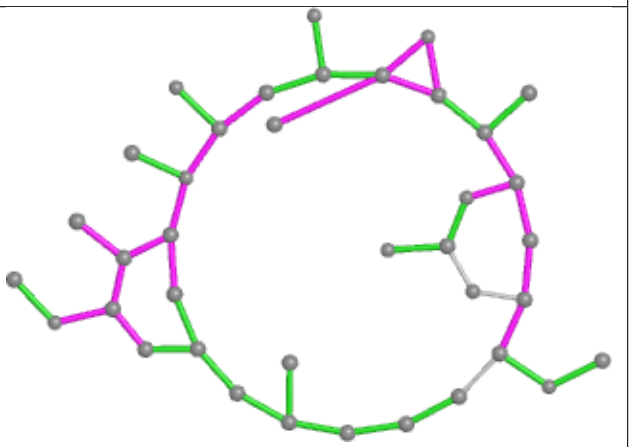
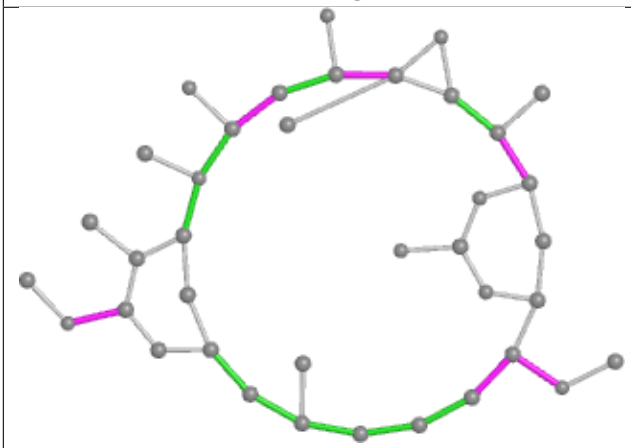


Bond angles



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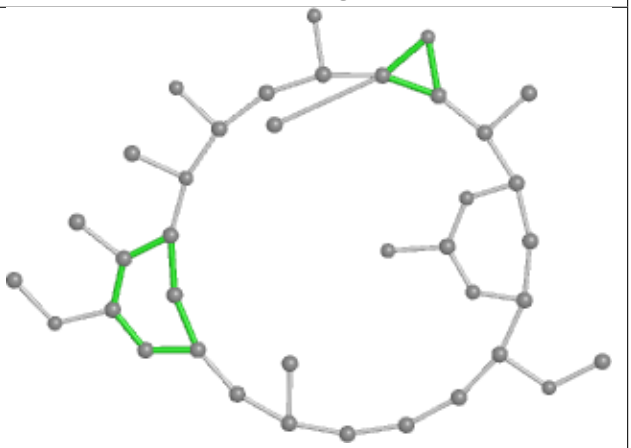
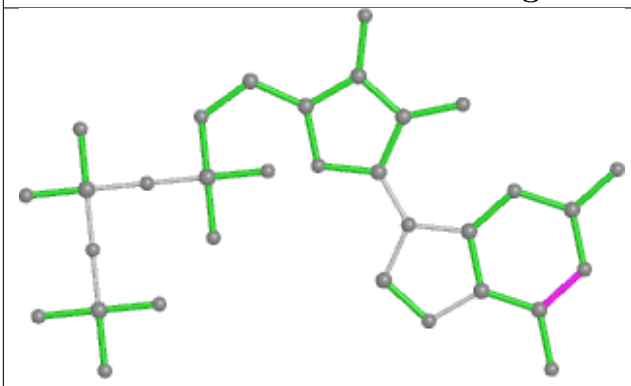
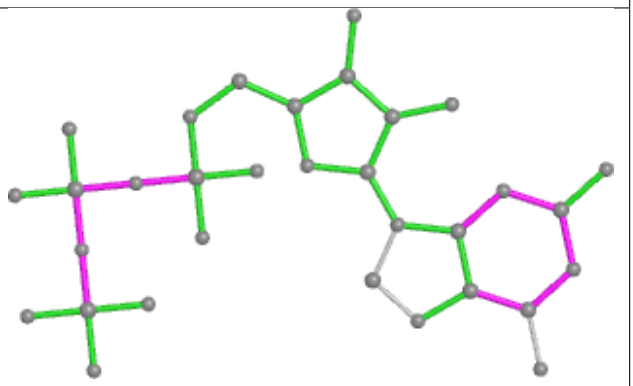


Rings

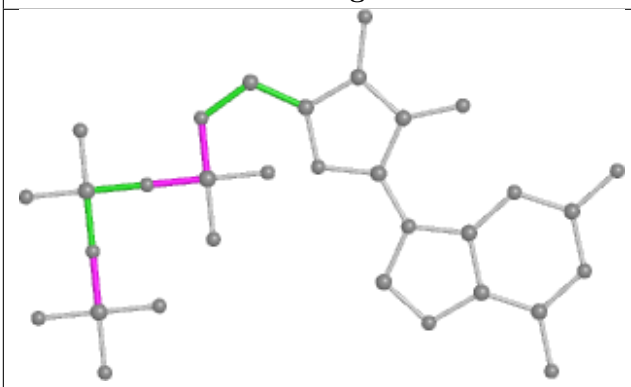
Ligand GTP A 501



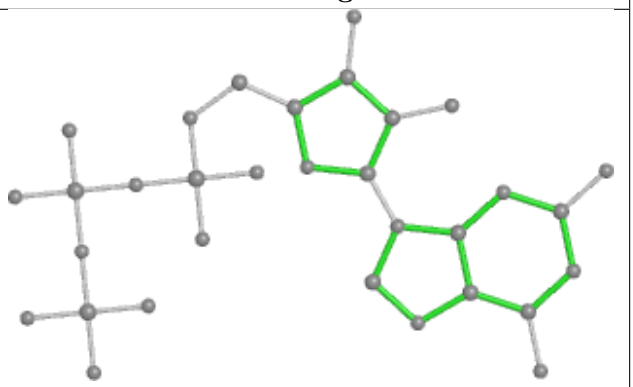
Bond lengths



Bond angles

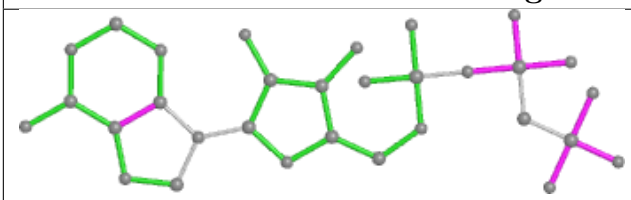


Torsions

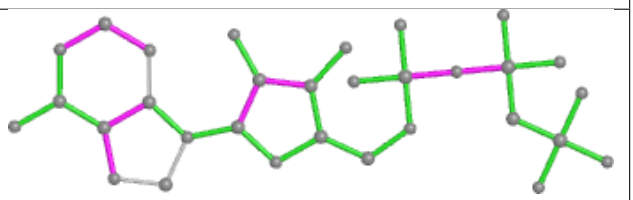


Rings

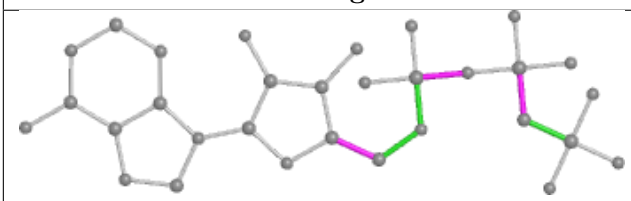
Ligand ACP F 401



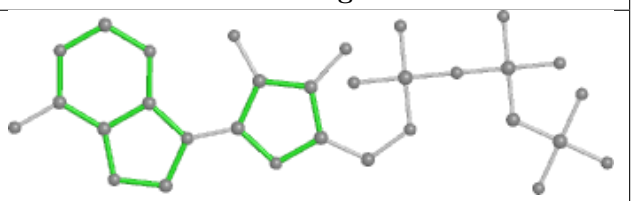
Bond lengths



Bond angles

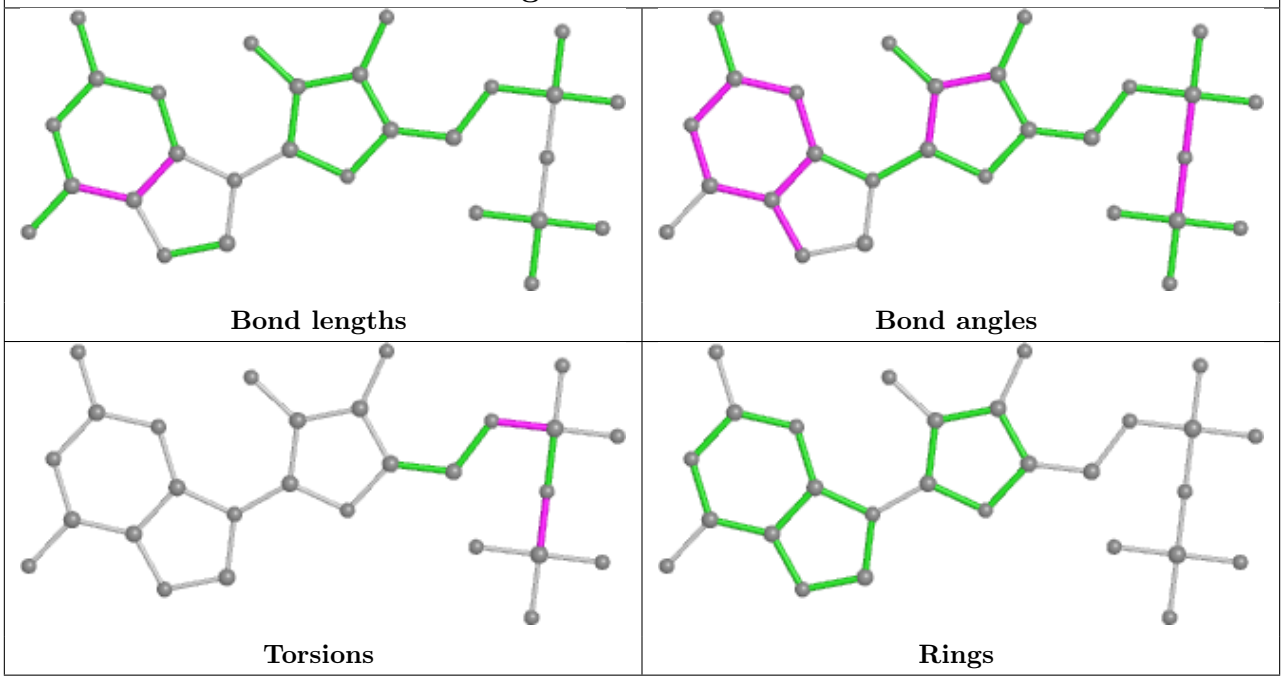


Torsions

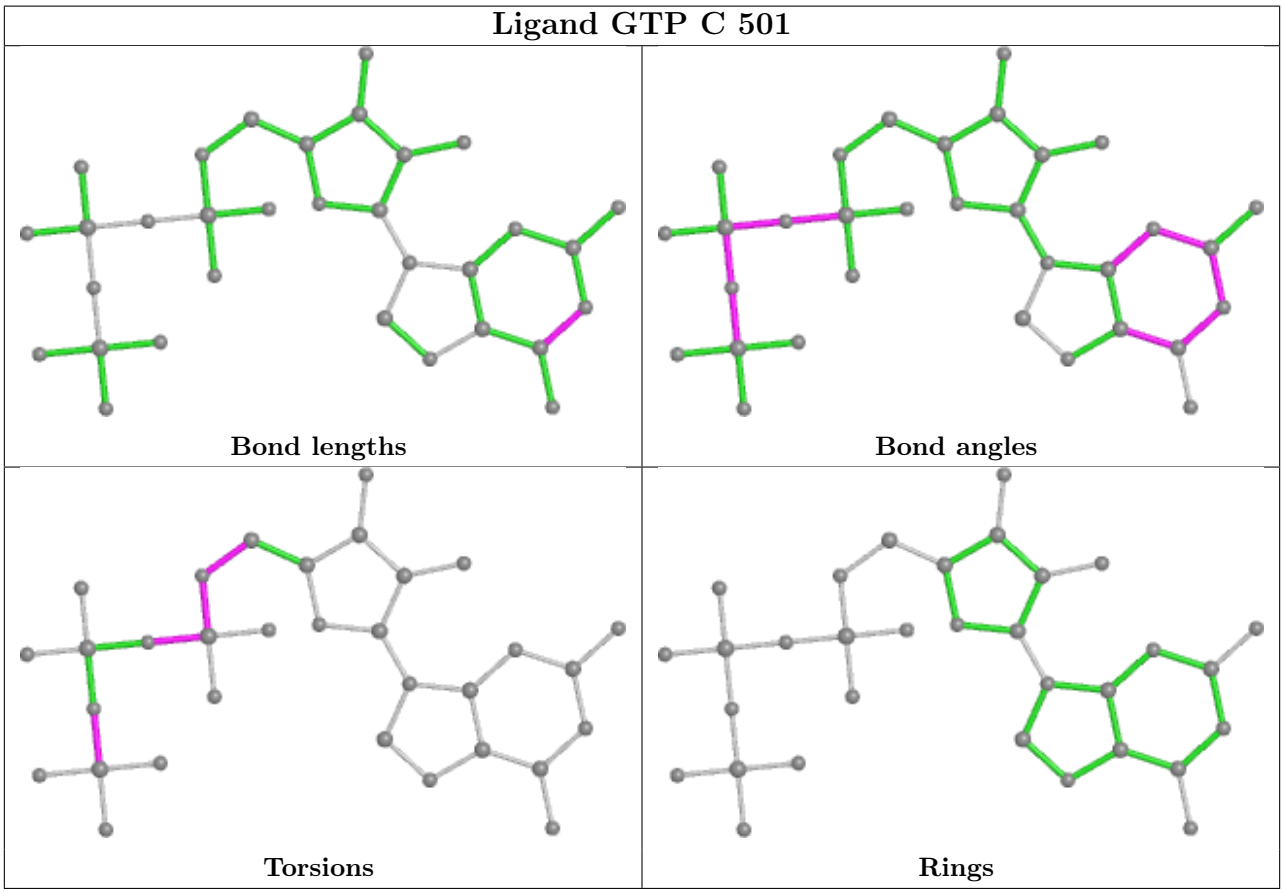


Rings

Ligand GDP D 501



Ligand GTP C 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.19	19 (4%) 35 42	40, 58, 88, 135	0
1	C	440/451 (97%)	-0.07	2 (0%) 91 94	34, 46, 71, 106	0
2	B	422/445 (94%)	0.06	10 (2%) 59 66	36, 54, 87, 141	1 (0%)
2	D	427/445 (95%)	0.36	31 (7%) 15 20	43, 68, 106, 129	2 (0%)
3	E	123/143 (86%)	0.36	9 (7%) 15 20	50, 71, 105, 146	0
4	F	339/384 (88%)	1.28	102 (30%) 0 0	53, 82, 144, 180	0
All	All	2189/2319 (94%)	0.33	173 (7%) 12 17	34, 61, 111, 180	3 (0%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.3
4	F	169	LEU	9.1
4	F	161	LEU	9.0
4	F	251	LYS	7.6
4	F	244	CYS	7.3
4	F	170	LEU	7.1
4	F	134	ALA	7.1
4	F	182	ILE	6.8
4	F	133	ALA	6.6
4	F	249	TYR	6.6
4	F	250	SER	6.5
4	F	130	VAL	6.5
4	F	253	TYR	6.2
4	F	103	THR	6.2
4	F	135	TYR	5.9
3	E	27	PRO	5.9
2	D	57	THR	5.8
4	F	132	LEU	5.5
4	F	166	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	5.4
4	F	100	ILE	5.4
2	B	59	ASN	5.3
4	F	136	ASN	5.2
4	F	254	GLY	5.2
4	F	131	PHE	5.1
2	B	57	THR	5.1
1	A	282	TYR	5.0
3	E	139	LEU	5.0
4	F	240	LEU	5.0
4	F	181	VAL	4.9
4	F	179	VAL	4.9
3	E	26	PRO	4.8
4	F	164	SER	4.8
4	F	101	TYR	4.8
4	F	165	GLU	4.8
4	F	137	ARG	4.6
4	F	143	GLU	4.5
4	F	163	SER	4.5
4	F	252	ASN	4.5
4	F	243	HIS	4.4
4	F	259	GLY	4.4
4	F	138	ARG	4.3
2	D	405	LEU	4.2
3	E	142	GLU	4.2
4	F	125	THR	4.1
4	F	129	GLU	4.0
4	F	239	HIS	4.0
4	F	142	ARG	4.0
4	F	167	SER	4.0
4	F	140	GLU	3.9
4	F	225	SER	3.9
4	F	147	TRP	3.9
4	F	21	LEU	3.9
4	F	162	ILE	3.9
2	D	285	ALA	3.9
2	D	277	SER	3.8
4	F	141	GLY	3.8
4	F	247	LYS	3.8
4	F	20	LEU	3.8
4	F	245	ILE	3.7
2	B	33	THR	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	139	ARG	3.6
4	F	256	TYR	3.6
4	F	6	VAL	3.5
4	F	246	GLN	3.5
2	B	284	ARG	3.4
4	F	17	VAL	3.4
2	D	276	THR	3.4
4	F	145	ASN	3.4
3	E	143	ALA	3.3
1	A	281	ALA	3.3
4	F	19	ARG	3.3
2	D	400	ARG	3.3
4	F	362	ALA	3.3
4	F	231	ALA	3.2
4	F	102	PRO	3.2
2	B	276	THR	3.2
2	D	37	HIS	3.2
4	F	255	ARG	3.2
2	D	96	GLN	3.1
4	F	242	ASN	3.1
2	D	94	PHE	3.1
1	A	42	ILE	3.0
2	D	83	PHE	3.0
4	F	168	GLU	3.0
4	F	224	SER	3.0
4	F	236	LYS	3.0
2	B	37	HIS	3.0
4	F	248	GLU	3.0
4	F	172	PHE	3.0
3	E	140	LYS	2.9
2	B	58	GLY	2.9
2	D	58	GLY	2.9
2	B	60	LYS	2.9
4	F	99	VAL	2.9
1	A	346	TRP	2.9
4	F	148	ILE	2.8
1	A	364	PRO	2.8
4	F	180	HIS	2.8
4	F	340	GLN	2.8
2	D	401	ARG	2.7
2	B	62	VAL	2.7
4	F	226	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	192	LEU	2.7
4	F	196	HIS	2.7
4	F	228	TYR	2.6
4	F	10	ASN	2.6
4	F	186	LEU	2.6
2	D	97	SER	2.6
4	F	382	HIS	2.6
2	D	221	THR	2.6
1	C	340	SER	2.6
2	D	76	ASP	2.6
3	E	45	PRO	2.6
4	F	190	LEU	2.6
3	E	48	GLU	2.6
4	F	230	SER	2.5
4	F	98	TYR	2.5
4	F	258	GLU	2.5
2	D	406	HIS	2.5
1	A	57	GLY	2.5
4	F	361	LEU	2.5
2	D	59	ASN	2.5
1	A	56	THR	2.5
4	F	44	ARG	2.5
2	D	415	GLU	2.4
1	A	171	ILE	2.4
1	A	146	GLY	2.4
2	D	128	SER	2.4
4	F	152	SER	2.4
4	F	229	ASN	2.4
2	D	278	ARG	2.4
4	F	31	ARG	2.3
4	F	197	ARG	2.3
4	F	223	THR	2.3
4	F	171	ASP	2.3
2	D	219	LEU	2.3
4	F	379	HIS	2.3
4	F	128	ARG	2.3
4	F	194	PRO	2.3
4	F	5	VAL	2.3
4	F	198	LYS	2.3
4	F	381	HIS	2.2
2	B	437	ASP	2.2
4	F	151	SER	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	160	ILE	2.2
2	D	60	LYS	2.2
1	A	285	GLN	2.2
4	F	11	SER	2.2
1	A	283	HIS	2.2
1	A	9	VAL	2.1
4	F	13	VAL	2.1
1	A	438	ASP	2.1
2	D	177	VAL	2.1
2	D	88	ARG	2.1
2	D	202	TYR	2.1
4	F	238	CYS	2.1
2	D	56	ALA	2.1
1	C	440	VAL	2.1
1	A	43	GLY	2.1
1	A	140	SER	2.1
4	F	32	LYS	2.1
2	D	404	PHE	2.1
4	F	227	PRO	2.1
1	A	58	ALA	2.0
3	E	141	GLU	2.0
4	F	9	GLU	2.0
2	D	33	THR	2.0
2	D	74	THR	2.0
2	D	220	THR	2.0
1	A	201	ALA	2.0
2	D	256	ALA	2.0
1	A	150	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,

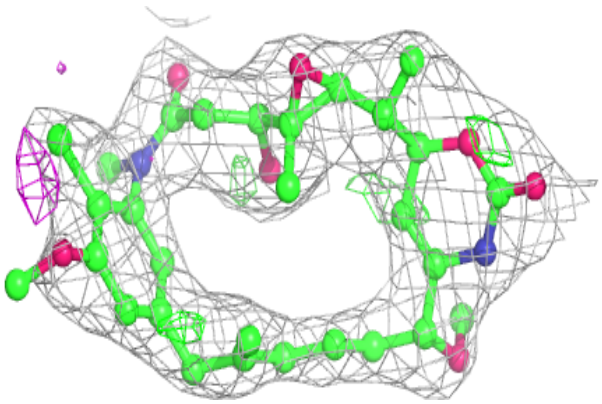
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

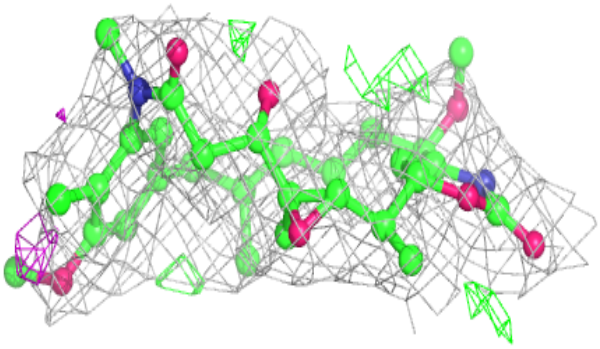
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	502	1/1	0.73	0.10	77,77,77,77	0
10	IMD	B	505	5/5	0.78	0.15	82,86,103,103	0
6	MG	F	402	1/1	0.83	0.13	92,92,92,92	0
11	5IS	D	503	38/38	0.83	0.24	65,86,97,107	0
12	ACP	F	401	31/31	0.88	0.20	91,99,112,116	0
7	CA	B	503	1/1	0.92	0.27	97,97,97,97	0
8	GDP	D	501	28/28	0.95	0.13	60,67,84,96	0
6	MG	C	502	1/1	0.96	0.12	35,35,35,35	0
7	CA	C	503	1/1	0.96	0.07	63,63,63,63	0
7	CA	A	503	1/1	0.97	0.03	77,77,77,77	0
6	MG	A	502	1/1	0.97	0.17	38,38,38,38	0
9	MES	B	504	12/12	0.97	0.13	42,49,59,61	0
5	GTP	A	501	32/32	0.98	0.21	35,44,52,56	0
6	MG	B	502	1/1	0.98	0.19	35,35,35,35	0
8	GDP	B	501	28/28	0.98	0.17	35,41,46,52	0
5	GTP	C	501	32/32	0.98	0.16	31,37,43,44	0

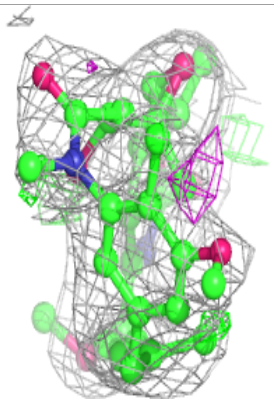
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5IS 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)

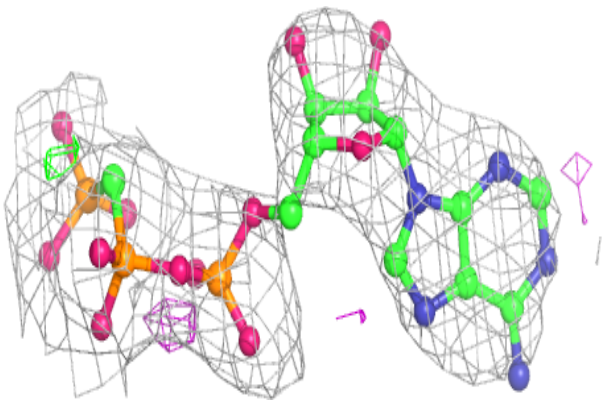


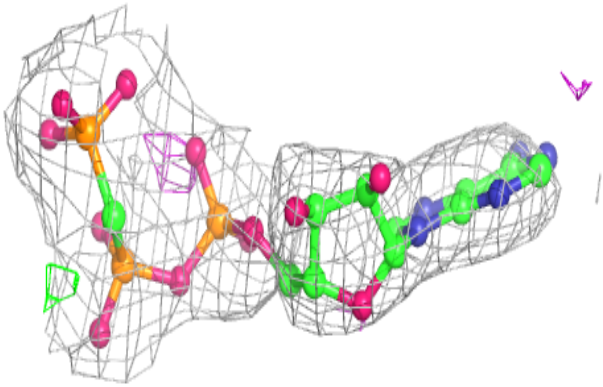


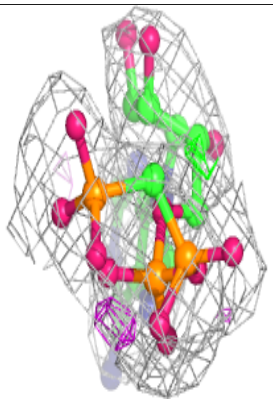


Electron density around ACP F 401:

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

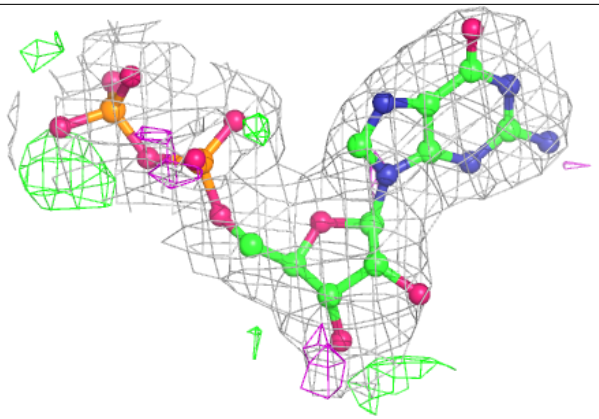


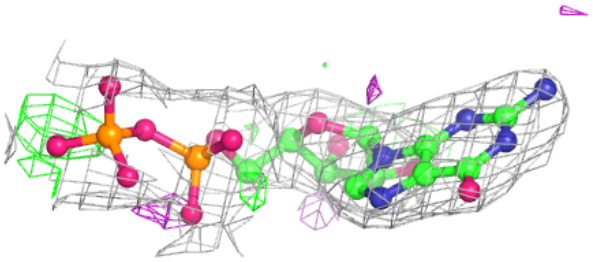


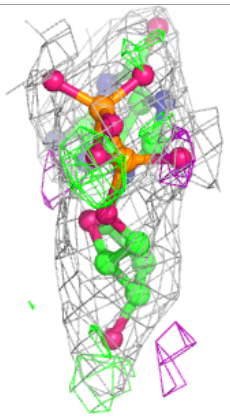


Electron density around GDP D 501:

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

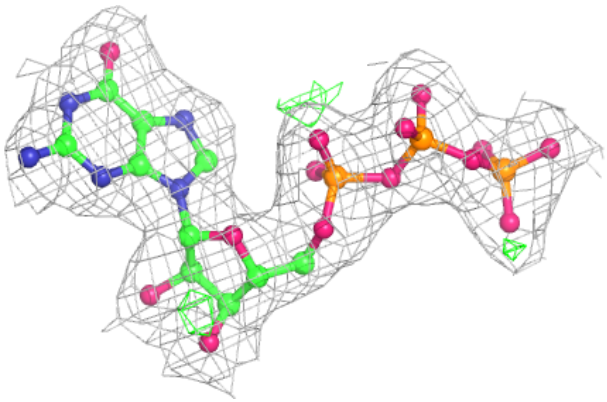


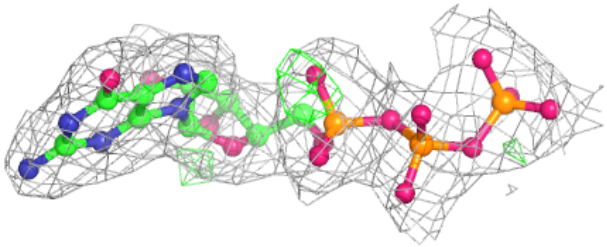


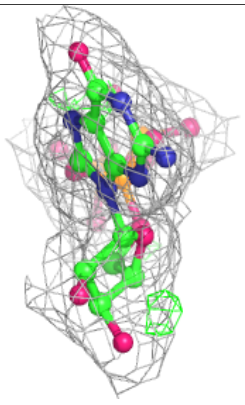


Electron density around GTP A 501:

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

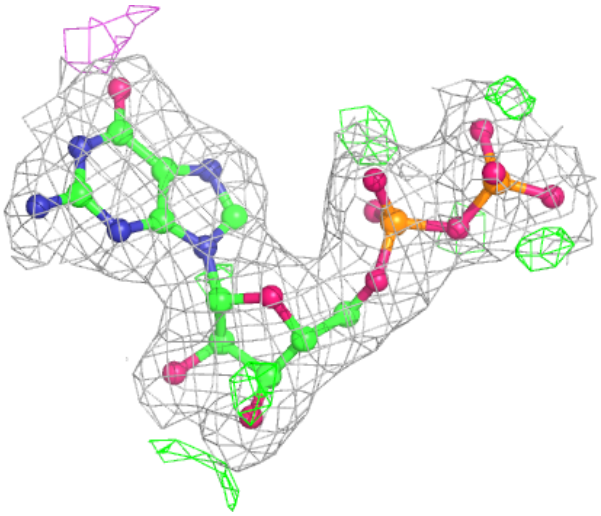


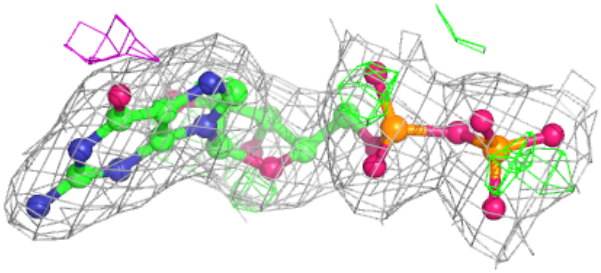


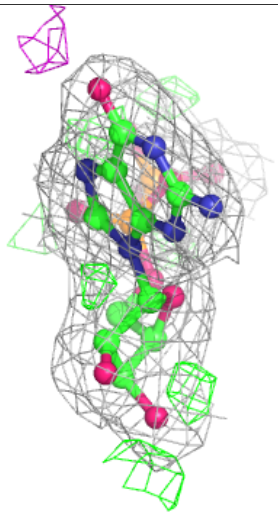


Electron density around GDP B 501:

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

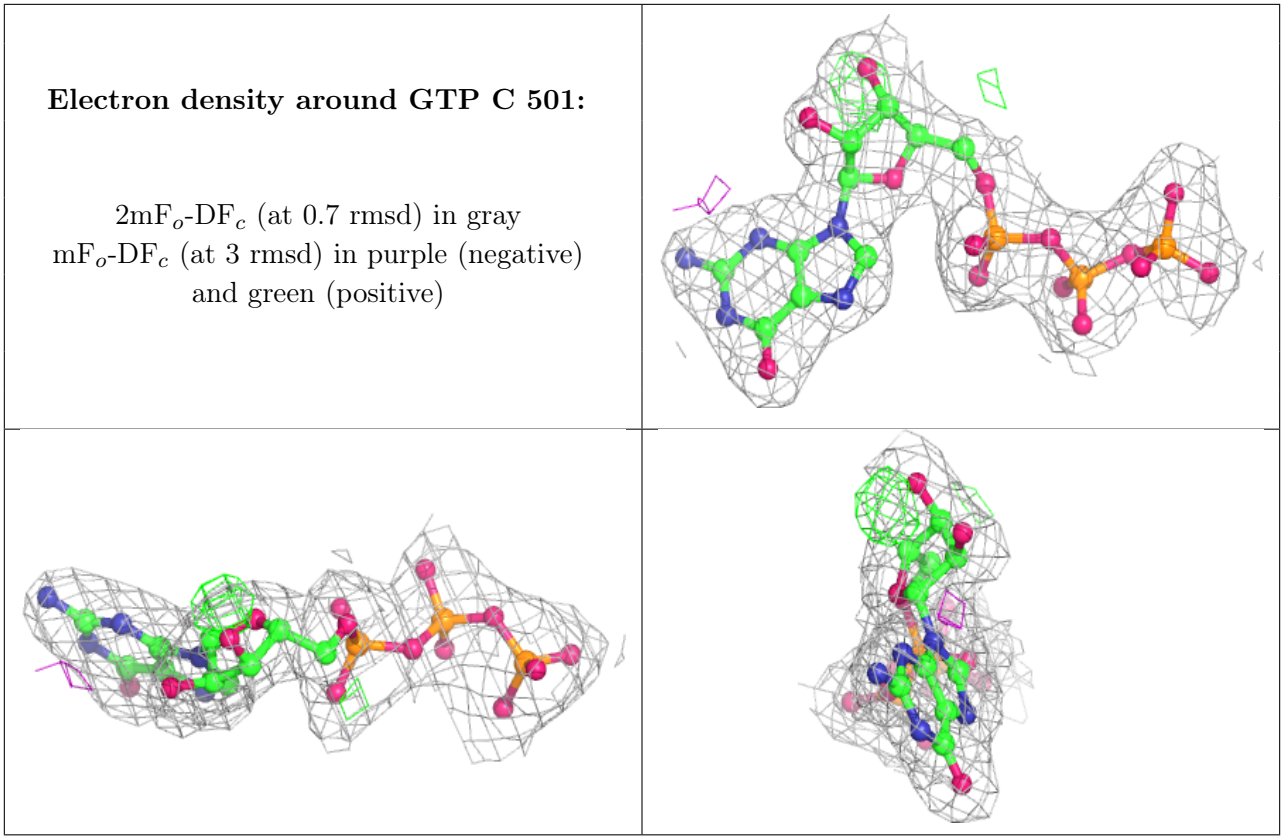






Electron density around GTP C 501:

$2mF_o$-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.