Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2022 – 10:25 am BST

PDB ID	:	7Z2P
Title	:	Tubulin-nocodazole complex
Authors	:	Prota, A.E.; Muehlethaler, T.; Cavalli, A.; Steinmetz, M.O.
Deposited on	:	2022-02-28
Resolution	:	2.00 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

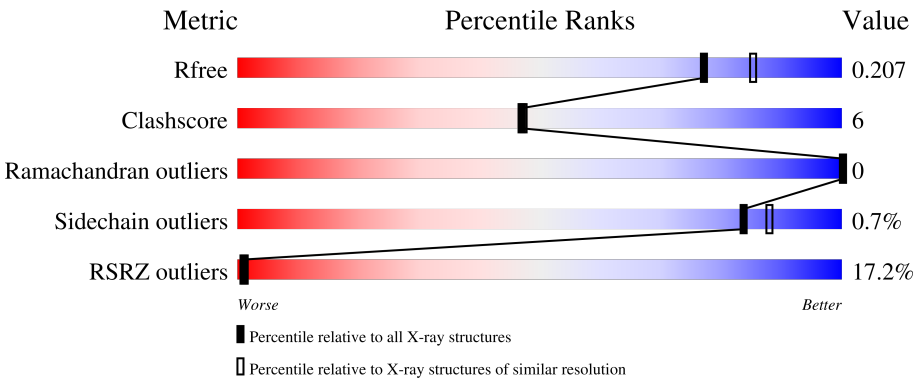
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	13% 85% 12% •
1	C	451	8% 82% 15% •
2	B	445	11% 80% 15% 5%
2	D	445	18% 79% 15% • 5%
3	E	143	16% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	35% 78% 12% 10%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18454 atoms, of which 22 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
			Total	C	N	O	S			
1	A	439	3462	2199	583	655	25	0	8	0
1	C	440	3473	2203	585	660	25	0	10	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	3339	2101	565	646	27	0	4	0
2	D	421	3320	2088	562	642	28	0	3	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1021	630	185	201	5	0	1	0

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

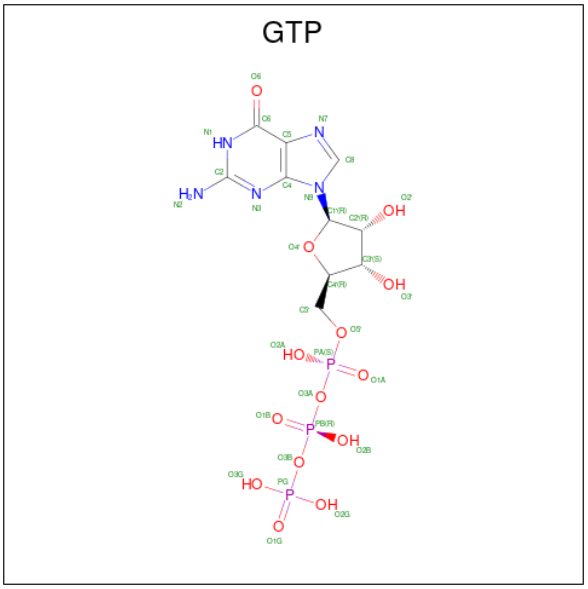
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	344	2818	1807	479	518	14	0	0	0

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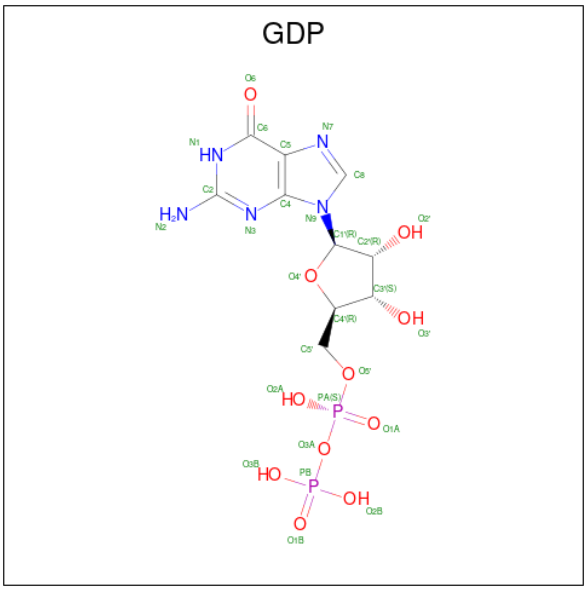
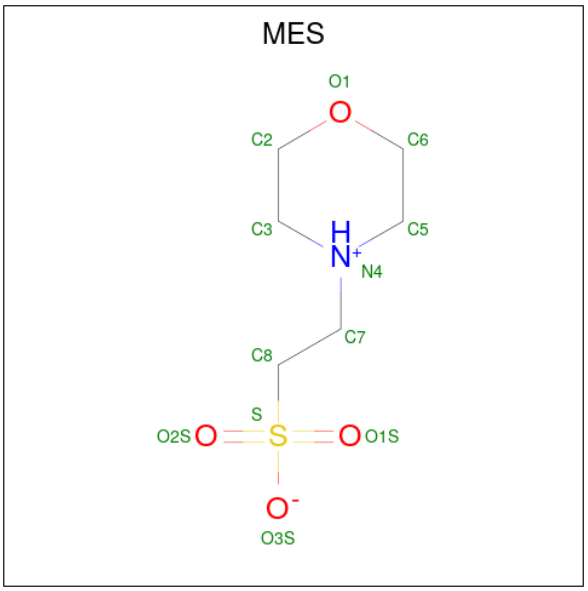
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



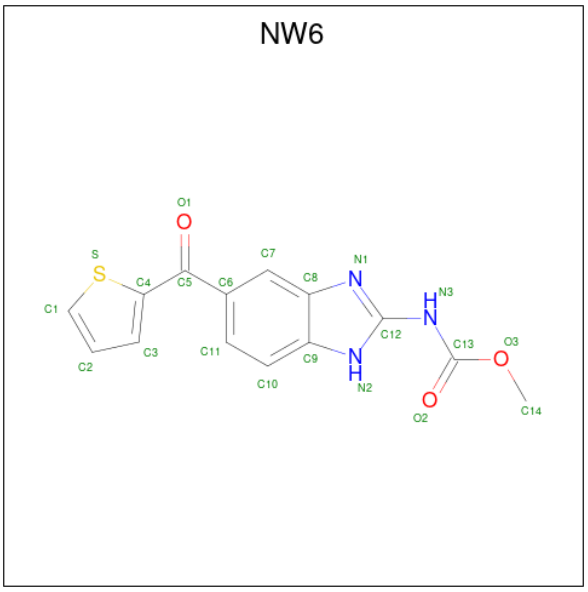
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
7	D	1	28	10	5	11	2	0	0

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



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

- Molecule 9 is nocodazole (three-letter code: NW6) (formula: $C_{14}H_{11}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
9	B	1	32	14	11	3	3	1	0	0

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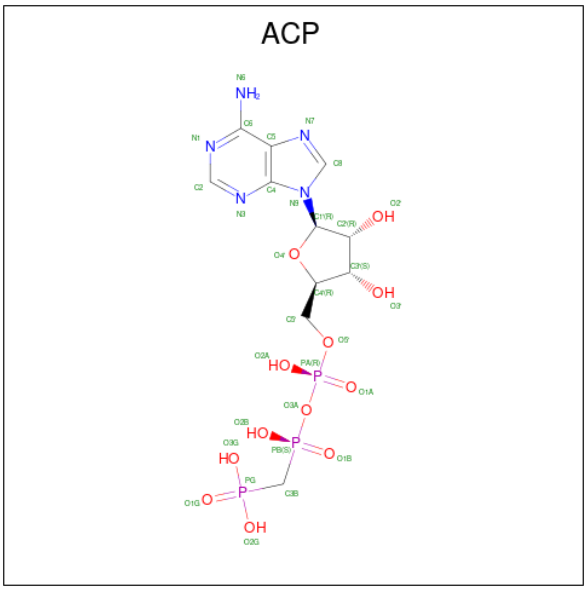
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
9	D	1	32	14	11	3	3	1	0	0

- Molecule 10 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
			Total	C	N	O	P		
10	F	1	31	11	5	12	3	0	0

- Molecule 11 is water.

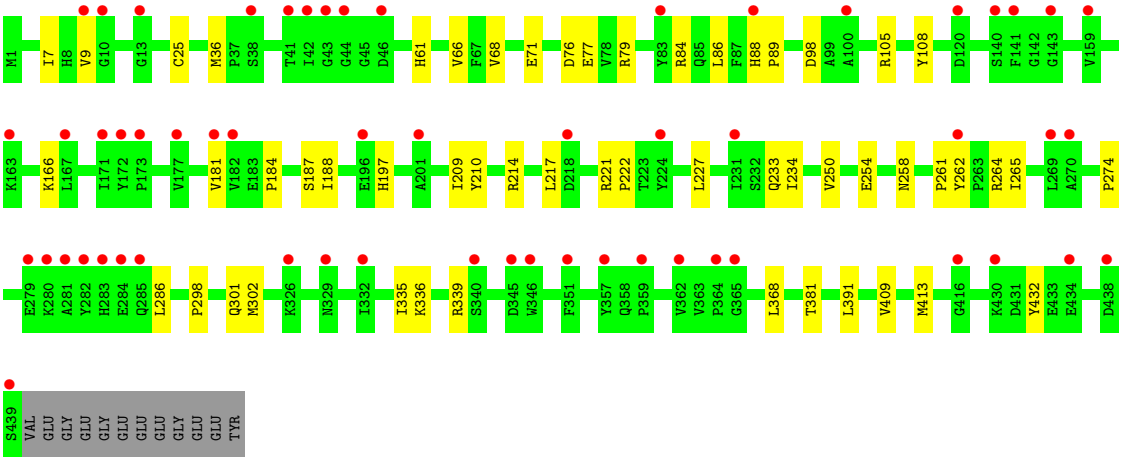
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	150	150	150	0	0
11	B	169	169	169	0	0
11	C	280	280	280	0	0
11	D	85	85	85	0	0
11	E	34	34	34	0	0
11	F	59	59	59	0	0

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.

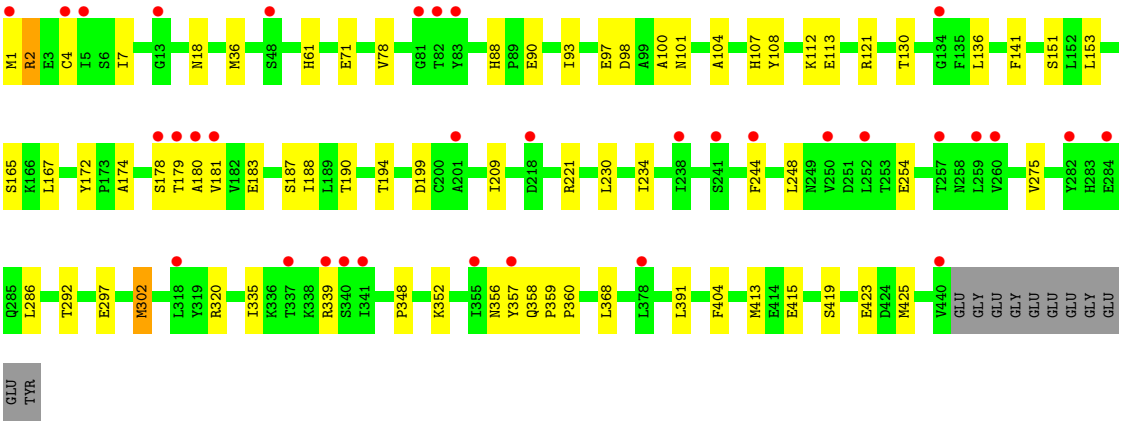
• Molecule 1: Tubulin alpha-1B chain

Chain A:



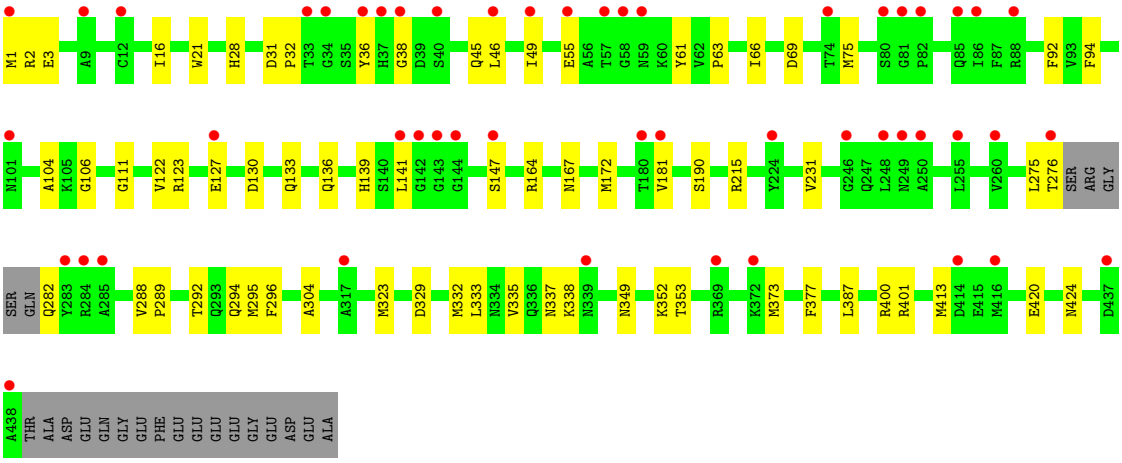
• Molecule 1: Tubulin alpha-1B chain

Chain C:



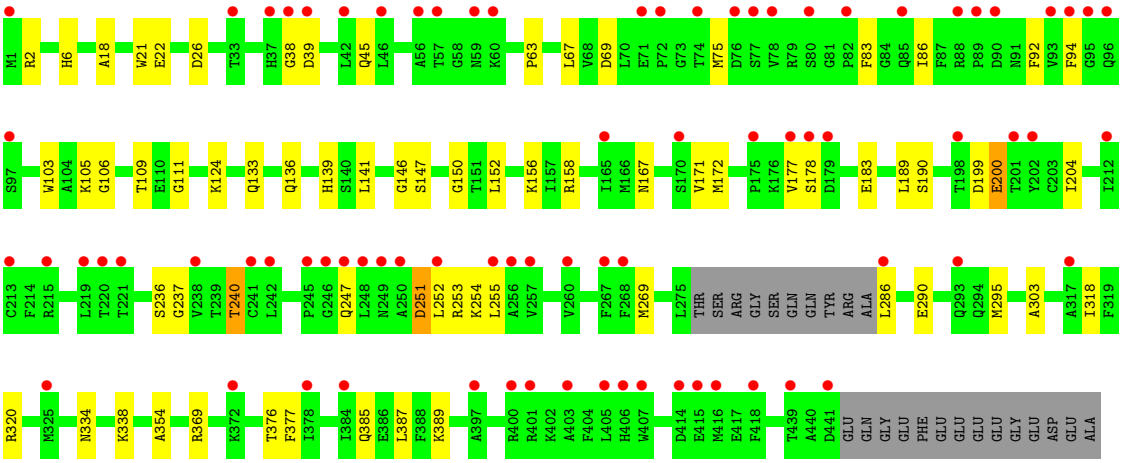
• Molecule 2: Tubulin beta-2B chain

Chain B:



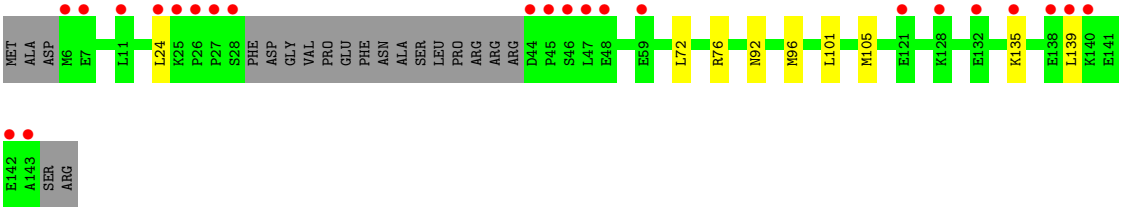
- Molecule 2: Tubulin beta-2B chain

Chain D:



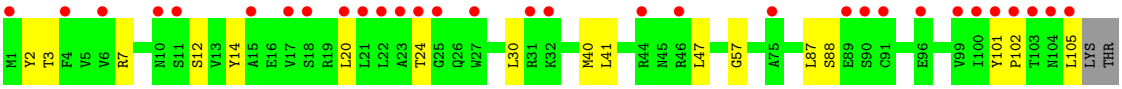
- Molecule 3: Stathmin-4

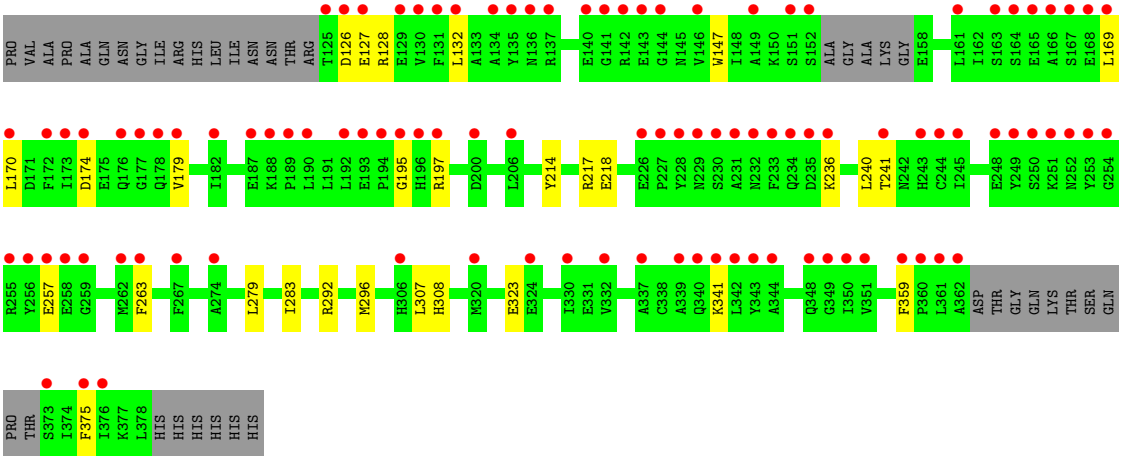
Chain E:



- Molecule 4: Tubulin beta-2B chain

Chain F:




PRO VAL ALA PRO ALA GLN ASN GLY ILE ARG HIS LEU ILE ASN ASN THR ARG T125 D126 E127 R128 E129 V130 F131 L132 A133 A134 Y135 N136 R137 E140 G141 R142 E143 G144 N145 V146 W147 I148 A149 K150 S151 S152 ALA GLY ALA LYS GLY E158 L161 I162 S163 S164 E165 A166 S167 E168 L169
L170 D171 F172 I173 D174 E175 Q176 G177 Q178 V179 I182 E187 K188 P189 L190 L191 L192 E193 P194 G195 H196 R197 D200 L206 Y214 R217 E218 E226 P227 Y228 N229 S230 A231 N232 F233 Q234 D235 K236 L240 T241 N242 H243 C244 I245 E248 Y249 S250 K251 N252 Y253 G254
R255 Y256 E257 E258 G259 M262 F263 F267 A274 L279 I283 R292 M296 H306 L307 H308 M320 E323 E324 I330 E331 V332 A337 C338 A339 Q340 K341 L342 Y343 A344 Q348 G349 I350 V351 F359 P360 L361 A362 ASP THR GLY GLN LYS THR SER GLN
PRO THR S373 I374 F375 I376 K377 L378 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.73Å 158.09Å 179.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.00 49.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.37-2.00) 99.8 (49.37-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.178 , 0.209 0.176 , 0.207	Depositor DCC
R_{free} test set	10017 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18454	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, GDP, MG, NW6, MES, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.26	0/3564	0.49	0/4839
1	C	0.28	0/3582	0.50	0/4865
2	B	0.27	0/3425	0.49	0/4639
2	D	0.26	0/3402	0.49	0/4608
3	E	0.26	0/1033	0.43	0/1371
4	F	0.25	0/2880	0.47	0/3890
All	All	0.27	0/17886	0.48	0/24212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3462	0	3406	36	0
1	C	3473	0	3412	49	0
2	B	3339	0	3224	51	0
2	D	3320	0	3208	51	0
3	E	1021	0	1036	7	0
4	F	2818	0	2789	29	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	B	28	0	12	0	0
7	D	28	0	12	0	0
8	B	12	0	12	1	0
8	D	12	0	12	3	0
9	B	21	11	0	0	0
9	D	21	11	0	4	0
10	F	31	0	14	1	0
11	A	150	0	0	3	0
11	B	169	0	0	6	0
11	C	280	0	0	6	0
11	D	85	0	0	0	0
11	E	34	0	0	1	0
11	F	59	0	0	1	0
All	All	18432	22	17161	214	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 6.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:GLN:HE21	2:D:354:ALA:HA	1.41	0.84
1:A:77:GLU:OE1	11:A:601:HOH:O	1.99	0.81
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.63	0.80
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.63	0.80
2:D:167:ASN:OD1	2:D:200:GLU:HG3	1.82	0.79
2:D:236:SER:O	2:D:240:THR:HG22	1.82	0.78
1:C:339:ARG:O	11:C:601:HOH:O	2.03	0.76
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.70	0.73
2:D:247:GLN:NE2	2:D:354:ALA:HA	2.04	0.73
1:C:101:ASN:ND2	1:C:180:ALA:HB2	2.04	0.73
2:D:255:LEU:HD13	9:D:504:NW6:C8	2.20	0.72
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.30	0.71
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.72	0.71
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:GLY:O	2:D:240:THR:HG23	1.92	0.70
2:B:1:MET:HG3	2:B:130:ASP:OD2	1.91	0.69
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.74	0.69
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.28	0.68
2:D:147[B]:SER:HG	2:D:190:SER:HG	1.26	0.68
2:B:294:GLN:OE1	11:B:601:HOH:O	2.11	0.67
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.34	0.67
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.30	0.66
2:B:329:ASP:O	2:B:333:LEU:HG	1.95	0.66
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.76	0.66
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.26	0.65
1:C:360:PRO:HB2	11:C:807:HOH:O	1.97	0.65
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.79	0.65
2:B:420:GLU:OE1	11:B:602:HOH:O	2.14	0.64
2:B:323:MET:HB3	2:B:373:MET:HE1	1.81	0.63
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.34	0.62
1:C:286:LEU:HB2	11:C:621:HOH:O	1.98	0.62
1:C:178:SER:HB2	1:C:183:GLU:OE1	2.00	0.62
2:B:323:MET:HB3	2:B:373:MET:CE	2.30	0.61
2:D:167:ASN:ND2	2:D:252:LEU:HD22	2.14	0.61
2:B:332:MET:HG3	2:B:353:THR:HG21	1.82	0.61
1:C:179:THR:HG22	11:C:837:HOH:O	2.00	0.60
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.83	0.59
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.37	0.59
2:D:2:ARG:HB3	2:D:133:GLN:HE21	1.68	0.59
2:D:318:ILE:CG2	2:D:376:THR:HB	2.32	0.59
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.84	0.59
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.85	0.59
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.85	0.59
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.85	0.58
2:B:1:MET:HB2	2:B:3:GLU:OE2	2.03	0.58
3:E:72:LEU:O	3:E:76:ARG:HG2	2.03	0.58
2:B:181:VAL:HG12	1:C:348[A]:PRO:HG2	1.86	0.58
4:F:241:THR:OG1	10:F:401:ACP:O3'	2.19	0.58
2:D:2:ARG:HB3	2:D:133:GLN:NE2	2.19	0.57
2:B:141:LEU:HD12	2:B:172:MET:SD	2.44	0.57
2:D:255:LEU:HB3	9:D:504:NW6:C10	2.35	0.56
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.20	0.56
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.86	0.56
4:F:126:ASP:OD1	4:F:127:GLU:N	2.39	0.56
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:ASN:OD1	2:B:338:LYS:N	2.38	0.56
1:C:415:GLU:OE2	11:C:602:HOH:O	2.18	0.56
2:D:240:THR:OG1	2:D:318:ILE:HD11	2.05	0.56
1:C:320:ARG:HA	1:C:356:ASN:O	2.06	0.56
1:C:359:PRO:HB2	11:C:667:HOH:O	2.06	0.55
2:D:106:GLY:O	2:D:111:GLY:HA3	2.06	0.55
1:C:174:ALA:O	1:C:178:SER:HB3	2.07	0.55
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.89	0.55
2:D:69:ASP:O	2:D:94:PHE:HA	2.06	0.55
4:F:40:MET:HE2	4:F:47:LEU:HG	1.89	0.55
2:B:69:ASP:O	2:B:94:PHE:HA	2.07	0.54
2:D:177:VAL:HG12	2:D:177:VAL:O	2.06	0.54
2:B:215:ARG:NH1	11:B:606:HOH:O	2.40	0.54
3:E:135:LYS:NZ	3:E:139:LEU:HD11	2.22	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.53
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.43	0.53
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.38	0.53
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.36	0.52
2:B:2:ARG:HA	2:B:133:GLN:HG3	1.92	0.52
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.92	0.52
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.09	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.45	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.45	0.52
2:B:282:GLN:N	11:B:609:HOH:O	2.43	0.52
2:D:124:LYS:C	2:D:124:LYS:HD3	2.30	0.52
1:A:261:PRO:HD2	11:A:710:HOH:O	2.10	0.51
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.38	0.51
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.10	0.51
1:A:264:ARG:NH1	11:A:604:HOH:O	2.31	0.51
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.51
2:D:83:PHE:O	2:D:86:ILE:HG22	2.10	0.51
2:D:152:LEU:O	2:D:156:LYS:HG2	2.10	0.51
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.51
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.93	0.51
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.46	0.50
2:D:141:LEU:HD12	2:D:172:MET:SD	2.50	0.50
2:B:333:LEU:CD1	4:F:57:GLY:HA3	2.41	0.50
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.52	0.50
2:D:158:ARG:NE	8:D:503:MES:O1	2.43	0.50
2:D:240:THR:HG21	2:D:320:ARG:HD2	1.94	0.50
4:F:323:GLU:OE2	11:F:501:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:PHE:CG	2:B:335:VAL:HG11	2.46	0.50
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.46	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.12	0.50
1:C:234:ILE:HD13	1:C:302:MET:SD	2.52	0.50
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.94	0.49
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.95	0.49
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.47	0.49
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.95	0.49
2:B:292:THR:HG22	2:B:335:VAL:CG2	2.40	0.49
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.48	0.49
3:E:135:LYS:HZ2	3:E:139:LEU:HD11	1.78	0.49
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.13	0.48
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.95	0.48
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.43	0.48
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.44	0.48
2:B:304:ALA:N	11:B:611:HOH:O	2.46	0.48
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.49	0.48
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.48	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.43	0.48
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.14	0.48
1:C:97:GLU:OE2	2:D:253:ARG:NH1	2.47	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.48
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.95	0.47
1:C:297:GLU:OE2	1:C:339:ARG:NH2	2.36	0.47
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.95	0.47
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.95	0.47
1:A:79:ARG:O	1:A:84:ARG:HB2	2.14	0.47
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.30	0.47
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.97	0.47
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.46
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.46
1:C:108:TYR:O	1:C:112:LYS:HG2	2.16	0.46
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.80	0.46
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	1.98	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.15	0.46
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.46
2:B:2:ARG:CA	2:B:133:GLN:HG3	2.45	0.46
1:C:1:MET:HG2	1:C:130:THR:OG1	2.15	0.46
4:F:236:LYS:HB3	4:F:240:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165[B]:SER:HA	1:C:199:ASP:OD2	2.15	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.96	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.98	0.45
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.50	0.45
1:C:419:SER:O	1:C:423:GLU:HG3	2.17	0.45
2:D:105:LYS:HA	2:D:109:THR:OG1	2.17	0.45
2:B:349:ASN:O	2:B:352:LYS:HE2	2.17	0.45
2:D:167:ASN:HD21	2:D:252:LEU:HD22	1.80	0.45
2:D:158:ARG:HE	8:D:503:MES:C2	2.30	0.45
2:B:424:ASN:HB3	11:B:621:HOH:O	2.17	0.45
1:C:165[A]:SER:HA	1:C:199:ASP:OD2	2.16	0.45
1:C:112:LYS:HE2	11:E:233:HOH:O	2.16	0.45
2:D:178:SER:OG	2:D:183:GLU:OE2	2.29	0.45
1:C:100:ALA:HA	2:D:254:LYS:CG	2.47	0.45
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.99	0.45
2:B:28:HIS:HB3	2:B:49:ILE:HD13	1.99	0.45
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.81	0.44
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.48	0.44
1:C:2:ARG:HD2	1:C:2:ARG:N	2.32	0.44
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.52	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.44
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.53	0.44
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.81	0.44
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.00	0.43
2:D:255:LEU:HB3	9:D:504:NW6:C9	2.48	0.43
4:F:263:PHE:CE2	4:F:341:LYS:HE2	2.53	0.43
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	2.00	0.43
4:F:292:ARG:O	4:F:296:MET:HG2	2.18	0.43
2:D:199:ASP:OD1	8:D:503:MES:H62	2.18	0.43
4:F:87:LEU:O	4:F:88:SER:OG	2.25	0.43
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.53	0.43
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.49	0.43
2:B:323:MET:HB3	2:B:373:MET:HE2	2.01	0.43
2:B:181:VAL:HG12	1:C:348[A]:PRO:CG	2.47	0.43
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.01	0.43
2:B:275:LEU:O	2:B:276:THR:C	2.57	0.42
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.42
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.18	0.42
3:E:101:LEU:O	3:E:105:MET:HG2	2.20	0.42
2:B:123:ARG:O	2:B:127:GLU:HG3	2.19	0.42
2:D:255:LEU:HD13	9:D:504:NW6:C9	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:20:LEU:O	4:F:24:THR:HG23	2.19	0.42
3:E:92:ASN:O	3:E:96:MET:HG2	2.20	0.42
2:B:288:VAL:N	2:B:289:PRO:CD	2.83	0.42
2:D:251:ASP:OD1	2:D:251:ASP:C	2.57	0.42
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.54	0.42
2:D:18:ALA:O	2:D:22:GLU:HG3	2.19	0.42
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.55	0.42
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.20	0.42
4:F:3:THR:HB	4:F:30:LEU:HD11	2.02	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.41
2:B:55:GLU:HG2	2:B:61:TYR:CE2	2.55	0.41
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.03	0.41
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.84	0.41
1:C:141:PHE:HB3	1:C:187:SER:OG	2.19	0.41
1:C:181[B]:VAL:HG11	1:C:404:PHE:CZ	2.56	0.41
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.02	0.41
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.85	0.41
1:A:184:PRO:O	1:A:188:ILE:HD13	2.20	0.41
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.34	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
1:A:187:SER:CB	1:A:391:LEU:HD21	2.51	0.41
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.03	0.41
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.03	0.40
2:B:164:ARG:O	8:B:503:MES:H31	2.22	0.40
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.85	0.40
2:D:385:GLN:OE1	2:D:389:LYS:HE3	2.21	0.40
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.47	0.40
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.21	0.40
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.56	0.40
2:D:146:GLY:O	2:D:150:GLY:HA3	2.21	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	445/451 (99%)	437 (98%)	8 (2%)	0	100	100
1	C	448/451 (99%)	441 (98%)	7 (2%)	0	100	100
2	B	423/445 (95%)	418 (99%)	5 (1%)	0	100	100
2	D	420/445 (94%)	409 (97%)	11 (3%)	0	100	100
3	E	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
4	F	336/384 (88%)	328 (98%)	8 (2%)	0	100	100
All	All	2192/2319 (94%)	2150 (98%)	42 (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	378/379 (100%)	374 (99%)	4 (1%)	73	78
1	C	381/379 (100%)	378 (99%)	3 (1%)	81	86
2	B	369/383 (96%)	368 (100%)	1 (0%)	92	95
2	D	367/383 (96%)	362 (99%)	5 (1%)	67	72
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	310/342 (91%)	309 (100%)	1 (0%)	92	95
All	All	1916/1993 (96%)	1902 (99%)	14 (1%)	84	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	221	ARG
1	A	262	TYR
1	A	381	THR
2	B	139	HIS
1	C	2	ARG
1	C	221	ARG
1	C	302	MET
2	D	39	ASP
2	D	139	HIS
2	D	200	GLU
2	D	240	THR
2	D	251	ASP
4	F	12	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	356	ASN
2	D	15	GLN
2	D	247	GLN
3	E	92	ASN

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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
9	NW6	D	504	-	23,23,23	1.86	4 (17%)	20,32,32	1.62	5 (25%)
7	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.10	3 (10%)
9	NW6	B	504	-	23,23,23	1.74	5 (21%)	20,32,32	1.70	5 (25%)
5	GTP	A	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.30	5 (15%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.32	5 (15%)
7	GDP	B	501	6	24,30,30	0.94	2 (8%)	30,47,47	1.12	4 (13%)
8	MES	D	503	-	12,12,12	2.18	1 (8%)	14,16,16	1.96	6 (42%)
8	MES	B	503	-	12,12,12	1.96	1 (8%)	14,16,16	1.89	3 (21%)
10	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.37	4 (12%)

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
9	NW6	D	504	-	-	0/8/14/14	0/3/3/3
7	GDP	D	501	6	-	4/12/32/32	0/3/3/3
9	NW6	B	504	-	-	0/8/14/14	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
7	GDP	B	501	6	-	5/12/32/32	0/3/3/3
8	MES	D	503	-	-	4/6/14/14	0/1/1/1
8	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	ACP	F	401	6	-	3/15/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	MES	C8-S	-7.28	1.67	1.77
8	B	503	MES	C8-S	-6.51	1.68	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	504	NW6	C12-N2	4.92	1.41	1.34
9	B	504	NW6	C12-N2	4.46	1.41	1.34
9	D	504	NW6	C12-N3	4.08	1.44	1.38
5	A	501	GTP	C5-C6	-4.00	1.39	1.47
5	C	501	GTP	C5-C6	-3.91	1.39	1.47
9	B	504	NW6	C12-N3	3.37	1.43	1.38
9	D	504	NW6	C13-N3	3.13	1.42	1.36
10	F	401	ACP	PG-O3G	2.96	1.61	1.54
10	F	401	ACP	PG-O2G	2.87	1.61	1.54
10	F	401	ACP	PB-O3A	2.58	1.61	1.58
10	F	401	ACP	C5-C4	2.54	1.47	1.40
9	B	504	NW6	C13-N3	2.53	1.41	1.36
9	D	504	NW6	C11-C6	2.31	1.43	1.39
7	D	501	GDP	C6-N1	-2.30	1.34	1.37
9	B	504	NW6	C11-C6	2.29	1.43	1.39
7	B	501	GDP	O4'-C1'	2.22	1.44	1.41
7	B	501	GDP	C6-N1	-2.18	1.34	1.37
10	F	401	ACP	PB-O2B	2.17	1.61	1.56
5	C	501	GTP	C2-N3	2.08	1.38	1.33
9	B	504	NW6	C12-N1	-2.07	1.31	1.34
5	A	501	GTP	C2-N3	2.00	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	503	MES	C5-N4-C3	4.30	118.50	108.83
9	B	504	NW6	C11-C10-C9	-3.78	116.08	120.84
10	F	401	ACP	PB-O3A-PA	-3.64	121.00	132.56
9	D	504	NW6	C11-C10-C9	-3.62	116.28	120.84
8	D	503	MES	C5-N4-C3	3.34	116.35	108.83
8	D	503	MES	O2S-S-C8	3.29	110.88	106.92
9	B	504	NW6	C12-N3-C13	-3.19	122.96	127.67
8	B	503	MES	O1S-S-C8	3.11	110.65	106.92
10	F	401	ACP	C3'-C2'-C1'	3.10	105.64	100.98
10	F	401	ACP	N3-C2-N1	-3.07	123.89	128.68
5	C	501	GTP	C8-N7-C5	3.04	108.79	102.99
5	A	501	GTP	C8-N7-C5	3.04	108.78	102.99
5	A	501	GTP	C5-C6-N1	2.90	119.08	113.95
5	C	501	GTP	C5-C6-N1	2.89	119.05	113.95
9	D	504	NW6	O3-C13-N3	2.85	113.24	109.25
7	D	501	GDP	PA-O3A-PB	-2.85	123.06	132.83
8	D	503	MES	C6-C5-N4	-2.81	105.84	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	503	MES	O3S-S-C8	2.71	110.15	105.77
9	B	504	NW6	C12-N2-C9	-2.59	103.15	106.73
10	F	401	ACP	C4-C5-N7	-2.56	106.73	109.40
5	A	501	GTP	C2-N1-C6	-2.56	120.38	125.10
7	B	501	GDP	C5-C6-N1	2.55	118.46	113.95
9	B	504	NW6	C12-N1-C8	-2.53	103.24	106.73
5	A	501	GTP	PB-O3B-PG	-2.52	124.18	132.83
5	C	501	GTP	C2-N1-C6	-2.50	120.50	125.10
5	C	501	GTP	PA-O3A-PB	-2.47	124.34	132.83
5	C	501	GTP	PB-O3B-PG	-2.44	124.44	132.83
9	D	504	NW6	C12-N2-C9	-2.35	103.48	106.73
5	A	501	GTP	PA-O3A-PB	-2.34	124.78	132.83
7	D	501	GDP	C8-N7-C5	2.34	107.45	102.99
9	B	504	NW6	O3-C13-N3	2.32	112.50	109.25
7	B	501	GDP	O6-C6-C5	-2.29	119.89	124.37
7	D	501	GDP	C5-C6-N1	2.23	117.89	113.95
8	D	503	MES	O1S-S-C8	2.21	109.58	106.92
7	B	501	GDP	PA-O3A-PB	-2.21	125.24	132.83
9	D	504	NW6	O3-C13-O2	-2.16	121.40	124.58
7	B	501	GDP	C8-N7-C5	2.15	107.09	102.99
8	D	503	MES	C7-N4-C5	2.15	116.74	111.23
8	D	503	MES	O3S-S-C8	2.12	109.19	105.77
9	D	504	NW6	C12-N1-C8	-2.06	103.89	106.73

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
7	D	501	GDP	C5'-O5'-PA-O1A
8	D	503	MES	C8-C7-N4-C5
8	D	503	MES	C7-C8-S-O1S
8	D	503	MES	C7-C8-S-O3S
10	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3B-PG-O1G
7	D	501	GDP	C5'-O5'-PA-O2A
10	F	401	ACP	C5'-O5'-PA-O1A

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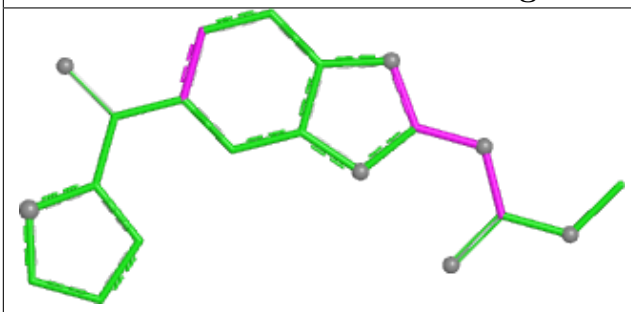
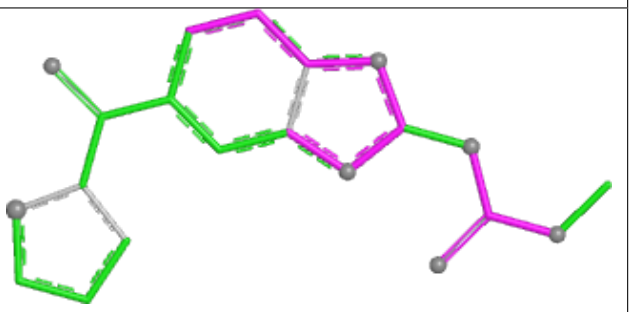
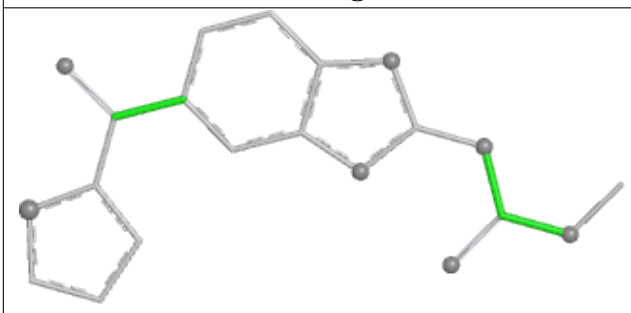
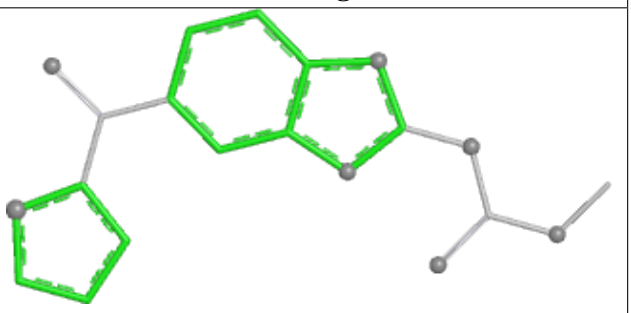
Mol	Chain	Res	Type	Atoms
10	F	401	ACP	C5'-O5'-PA-O2A
8	D	503	MES	C7-C8-S-O2S
7	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O3A
7	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
7	B	501	GDP	PB-O3A-PA-O1A
7	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA

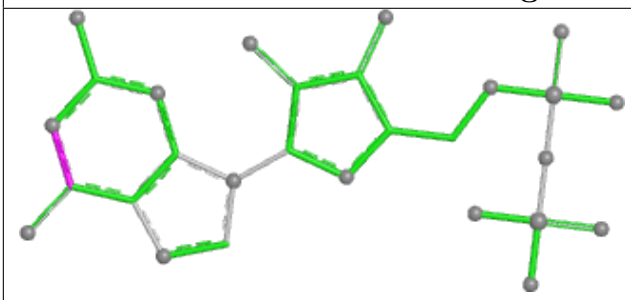
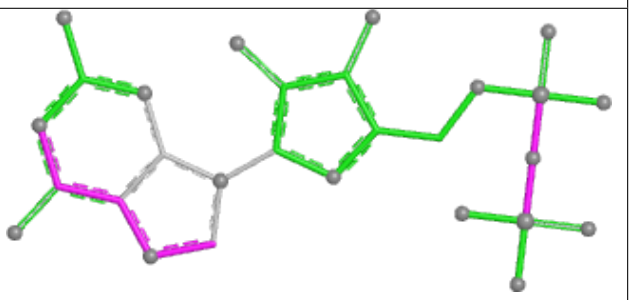
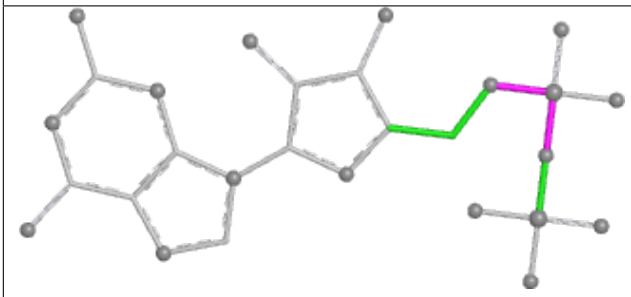
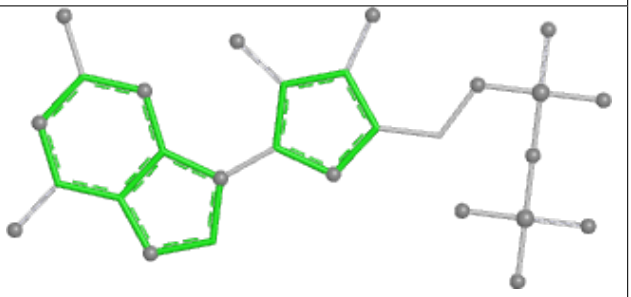
There are no ring outliers.

4 monomers are involved in 9 short contacts:

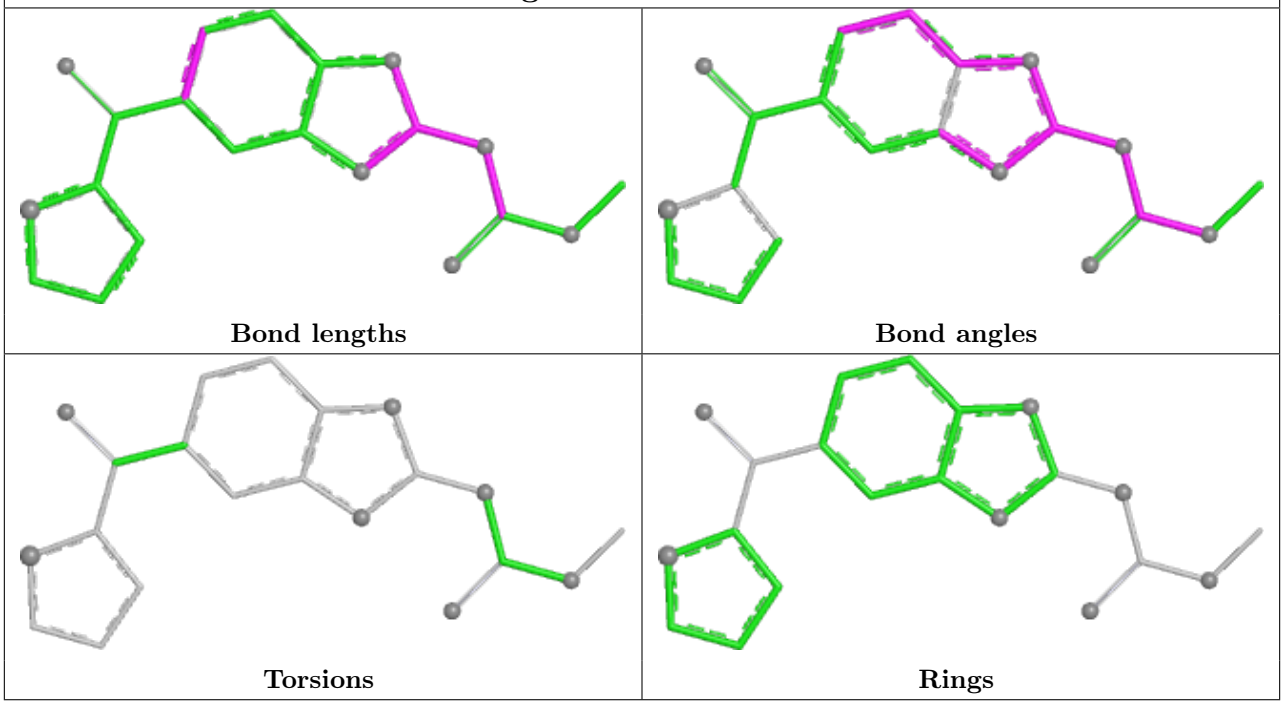
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	504	NW6	4	0
8	D	503	MES	3	0
8	B	503	MES	1	0
10	F	401	ACP	1	0

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.

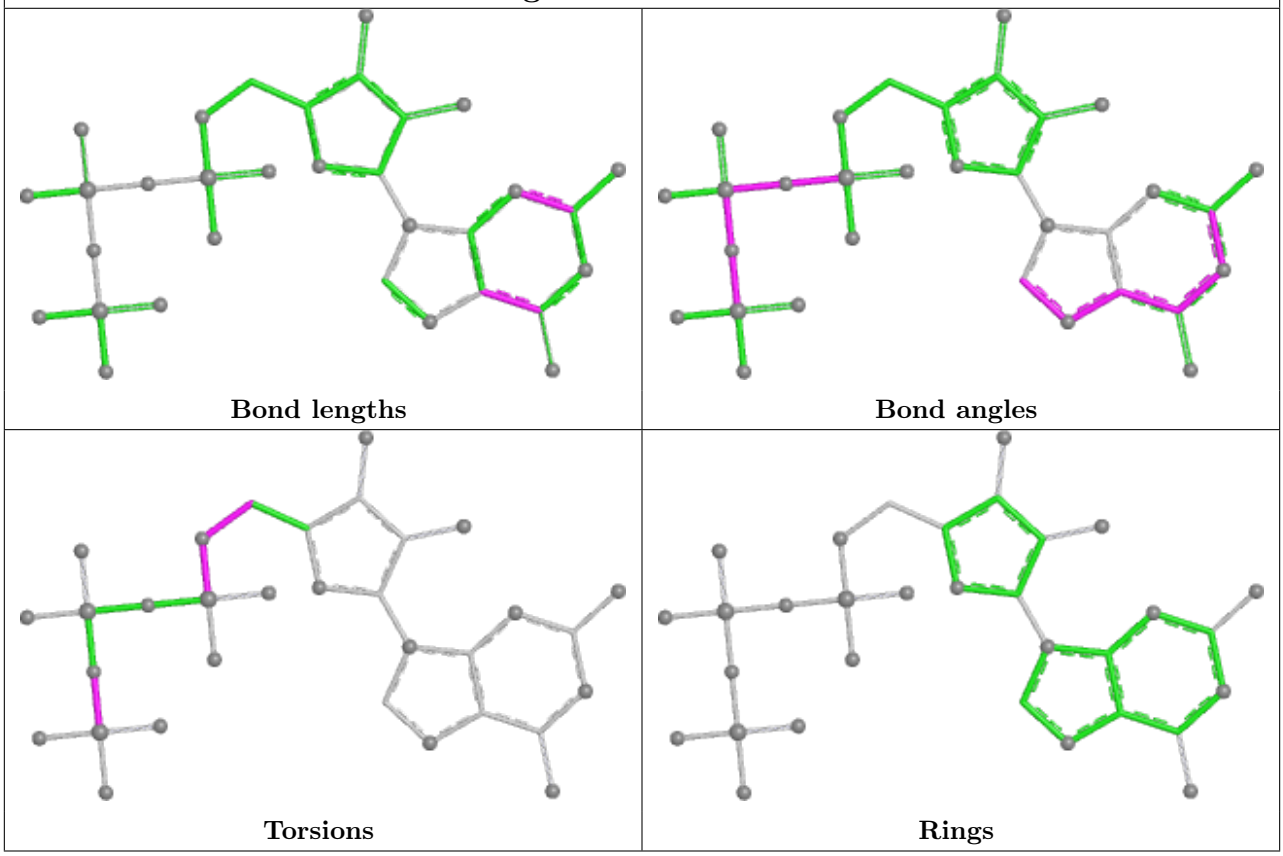
Ligand NW6 D 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

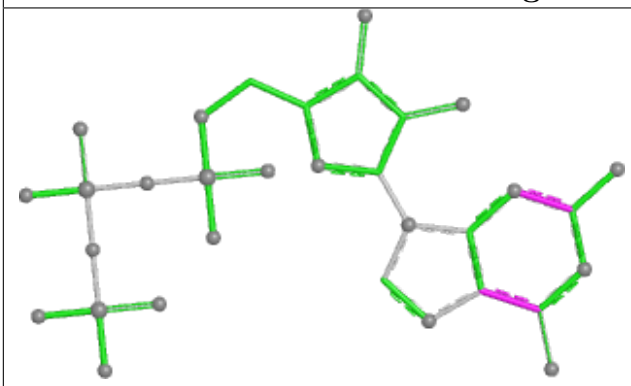
Ligand NW6 B 504



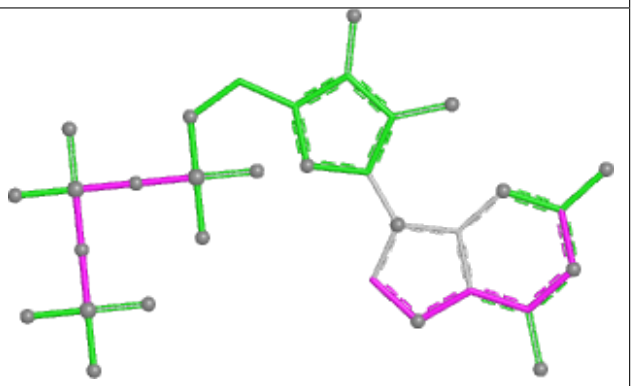
Ligand GTP A 501



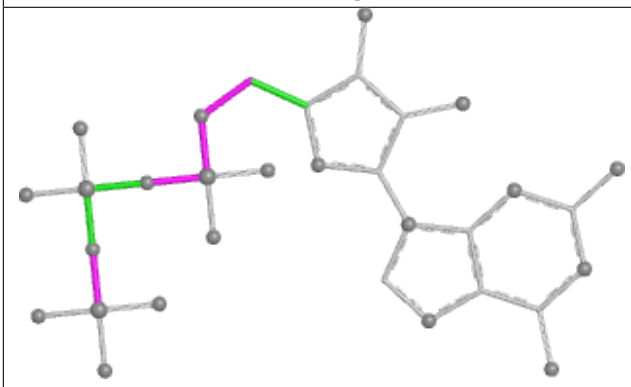
Ligand GTP C 501



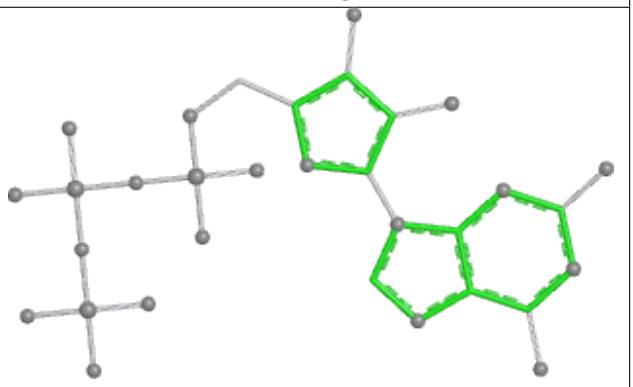
Bond lengths



Bond angles

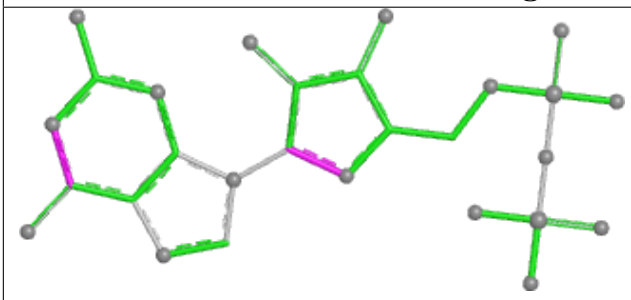


Torsions

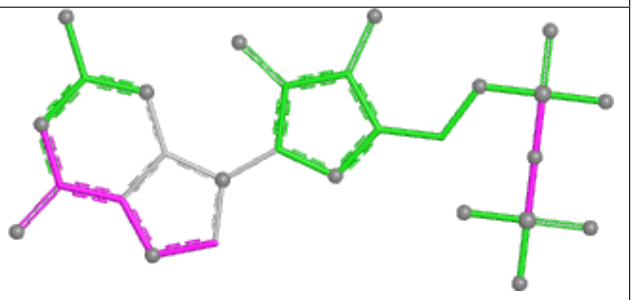


Rings

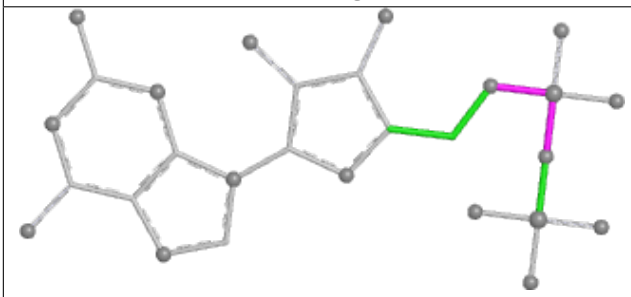
Ligand GDP B 501



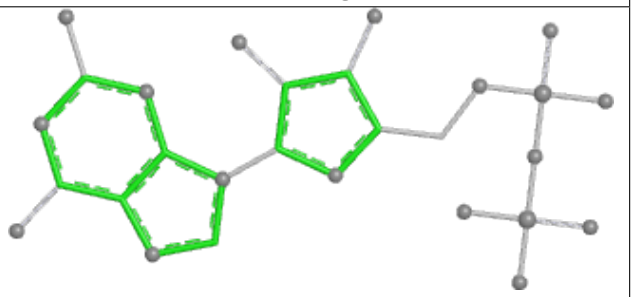
Bond lengths



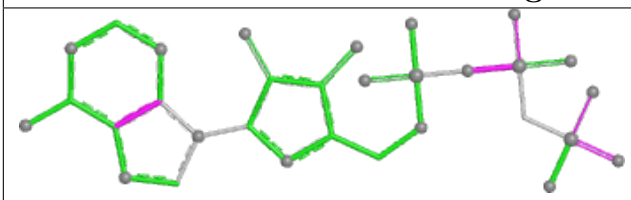
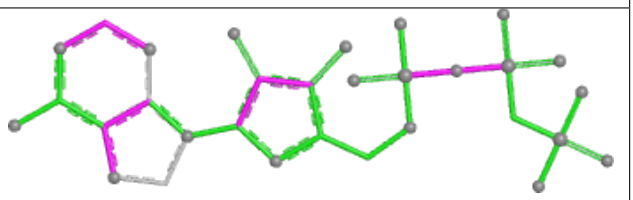
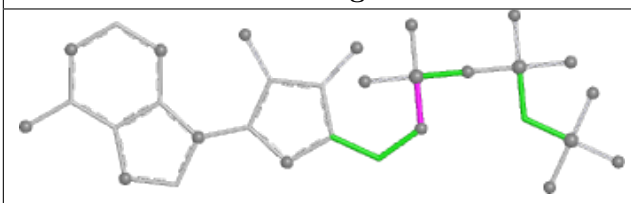
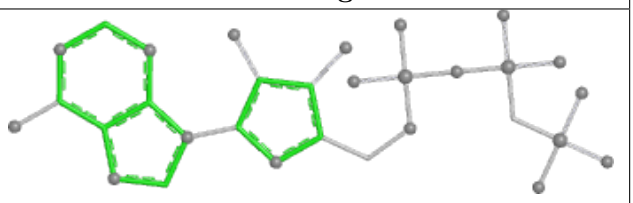
Bond angles



Torsions



Rings

Ligand ACP F 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	439/451 (97%)	0.93	57 (12%)	3	3	28, 44, 71, 130	0
1	C	440/451 (97%)	0.75	34 (7%)	13	12	23, 34, 57, 89	0
2	B	423/445 (95%)	0.96	50 (11%)	4	4	24, 40, 70, 110	0
2	D	421/445 (94%)	1.16	79 (18%)	1	1	29, 50, 79, 133	0
3	E	123/143 (86%)	1.13	23 (18%)	1	1	31, 55, 93, 113	0
4	F	344/384 (89%)	1.98	134 (38%)	0	0	36, 68, 124, 148	0
All	All	2190/2319 (94%)	1.12	377 (17%)	1	1	23, 45, 91, 148	0

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	249	ASN	12.3
4	F	89	GLU	11.1
4	F	169	LEU	10.4
4	F	104	ASN	10.3
1	C	440	VAL	10.2
3	E	143	ALA	10.1
4	F	173	ILE	9.5
4	F	130	VAL	9.4
4	F	20	LEU	9.0
1	A	282	TYR	8.8
4	F	103	THR	8.8
2	B	59	ASN	8.3
4	F	251	LYS	8.2
3	E	26	PRO	8.1
2	D	250	ALA	7.9
4	F	129	GLU	7.8
4	F	99	VAL	7.8
4	F	176	GLN	7.8
4	F	250	SER	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	439	SER	7.4
2	B	1	MET	7.4
4	F	135	TYR	7.4
4	F	253	TYR	7.3
4	F	131	PHE	7.3
4	F	361	LEU	6.8
4	F	179	VAL	6.7
2	B	58	GLY	6.7
4	F	249	TYR	6.7
2	D	246	GLY	6.7
2	B	276	THR	6.6
4	F	362	ALA	6.4
2	D	56	ALA	6.2
3	E	139	LEU	6.2
1	C	340	SER	6.2
2	B	82	PRO	6.1
4	F	100	ILE	6.0
4	F	17	VAL	6.0
4	F	234	GLN	5.9
4	F	90	SER	5.8
2	D	247	GLN	5.7
3	E	27	PRO	5.7
4	F	227	PRO	5.7
1	C	179	THR	5.6
4	F	132	LEU	5.5
4	F	137	ARG	5.4
1	A	346	TRP	5.4
2	D	37	HIS	5.2
4	F	24	THR	5.2
2	D	57	THR	5.1
2	D	400	ARG	5.0
2	D	220	THR	5.0
2	B	285	ALA	5.0
4	F	151	SER	5.0
4	F	165	GLU	4.9
2	D	82	PRO	4.8
4	F	164	SER	4.8
4	F	263	PHE	4.8
1	A	262	TYR	4.8
3	E	6	MET	4.8
4	F	126	ASP	4.8
4	F	350	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
3	E	132	GLU	4.7
4	F	339	ALA	4.7
2	D	77	SER	4.7
4	F	140	GLU	4.7
4	F	167	SER	4.7
1	A	281	ALA	4.6
4	F	136	ASN	4.6
4	F	236	LYS	4.5
4	F	1	MET	4.5
4	F	25	GLY	4.5
4	F	142	ARG	4.5
4	F	18	SER	4.5
4	F	105	LEU	4.5
4	F	22	LEU	4.5
4	F	254	GLY	4.3
2	D	179	ASP	4.3
4	F	178	GLN	4.3
2	B	437	ASP	4.3
4	F	267	PHE	4.2
1	C	341	ILE	4.2
2	D	59	ASN	4.2
1	A	364	PRO	4.2
1	A	280	LYS	4.2
4	F	11	SER	4.2
4	F	344	ALA	4.2
2	D	85	GLN	4.2
2	B	57	THR	4.2
4	F	168	GLU	4.2
1	A	46	ASP	4.2
4	F	231	ALA	4.2
4	F	182	ILE	4.1
4	F	46	ARG	4.1
1	A	362	VAL	4.1
1	C	357	TYR	4.1
4	F	143	GLU	4.1
2	B	249	ASN	4.1
4	F	172	PHE	4.1
4	F	152	SER	4.0
4	F	161	LEU	4.0
4	F	21	LEU	4.0
4	F	244	CYS	3.9
2	D	325	MET	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	248	LEU	3.9
4	F	243	HIS	3.8
4	F	170	LEU	3.8
4	F	187	GLU	3.7
3	E	142	GLU	3.7
4	F	101	TYR	3.7
4	F	233	PHE	3.7
1	A	365	GLY	3.7
1	C	218	ASP	3.7
4	F	102	PRO	3.7
1	A	416	GLY	3.7
4	F	373	SER	3.7
2	B	143	GLY	3.7
1	A	9	VAL	3.6
1	A	438	ASP	3.6
4	F	194	PRO	3.6
1	A	177	VAL	3.6
4	F	360	PRO	3.6
4	F	252	ASN	3.6
4	F	306	HIS	3.6
2	D	255	LEU	3.6
2	D	372	LYS	3.6
2	D	401	ARG	3.5
2	D	260	VAL	3.5
2	B	438	ALA	3.5
2	D	94	PHE	3.5
2	B	33	THR	3.5
2	D	89	PRO	3.5
4	F	166	ALA	3.5
2	D	33	THR	3.5
2	D	403	ALA	3.5
4	F	31	ARG	3.5
4	F	177	GLY	3.4
1	C	181[A]	VAL	3.4
2	B	142	GLY	3.4
2	B	144	GLY	3.4
4	F	245	ILE	3.4
4	F	125	THR	3.4
4	F	255	ARG	3.4
1	A	283	HIS	3.4
2	B	37	HIS	3.4
4	F	149	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	235	ASP	3.3
2	D	95	GLY	3.3
3	E	28	SER	3.3
2	D	76	ASP	3.3
4	F	256	TYR	3.3
4	F	4	PHE	3.3
4	F	141	GLY	3.3
1	A	163	LYS	3.3
1	A	42	ILE	3.3
2	B	369	ARG	3.3
4	F	188	LYS	3.2
2	D	415	GLU	3.2
4	F	330	ILE	3.2
1	A	201	ALA	3.2
2	D	414	ASP	3.2
4	F	259	GLY	3.2
4	F	228	TYR	3.2
2	B	40	SER	3.2
2	B	284	ARG	3.2
2	D	317	ALA	3.2
2	D	407	TRP	3.2
1	A	340	SER	3.2
4	F	375	PHE	3.2
1	C	4[A]	CYS	3.1
4	F	341	LYS	3.1
2	D	38	GLY	3.1
2	B	339	ASN	3.1
2	D	74	THR	3.1
1	A	218	ASP	3.1
2	D	202	TYR	3.1
2	D	46	LEU	3.1
4	F	230	SER	3.0
4	F	241	THR	3.0
2	D	71	GLU	3.0
4	F	258	GLU	3.0
2	D	219	LEU	3.0
1	A	88	HIS	3.0
4	F	127	GLU	3.0
2	D	1	MET	3.0
4	F	32	LYS	3.0
2	B	80	SER	2.9
4	F	27	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	86	ILE	2.9
4	F	200	ASP	2.9
4	F	23	ALA	2.9
1	A	285	GLN	2.8
2	D	418	PHE	2.8
2	B	9	ALA	2.8
1	A	345	ASP	2.8
4	F	15	ALA	2.8
4	F	343	TYR	2.8
2	B	81	GLY	2.8
3	E	25	LYS	2.8
2	B	250	ALA	2.8
4	F	91	CYS	2.8
4	F	189	PRO	2.8
3	E	44	ASP	2.8
2	D	257	VAL	2.8
3	E	48	GLU	2.8
3	E	138	GLU	2.8
4	F	248	GLU	2.8
1	A	326	LYS	2.8
2	D	97	SER	2.8
2	D	198	THR	2.7
4	F	144	GLY	2.7
1	C	339	ARG	2.7
1	C	180	ALA	2.7
1	A	83	TYR	2.7
2	D	78	VAL	2.7
3	E	7	GLU	2.7
1	A	171	ILE	2.7
4	F	359	PHE	2.7
1	C	201	ALA	2.7
2	B	46	LEU	2.7
4	F	196	HIS	2.6
2	D	90	ASP	2.6
2	D	268	PHE	2.6
3	E	135	LYS	2.6
2	B	127	GLU	2.6
4	F	96	GLU	2.6
4	F	274	ALA	2.6
2	B	74	THR	2.6
2	B	38	GLY	2.6
2	B	36	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	46	SER	2.6
3	E	59	GLU	2.6
2	D	177	VAL	2.6
1	C	238	ILE	2.6
2	D	213	CYS	2.6
2	D	42	LEU	2.6
3	E	24	LEU	2.6
1	A	159	VAL	2.6
2	B	147[A]	SER	2.6
4	F	174	ASP	2.5
1	A	284	GLU	2.5
4	F	192	LEU	2.5
1	A	172	TYR	2.5
1	C	257	THR	2.5
2	D	221	THR	2.5
2	D	252	LEU	2.5
1	C	1	MET	2.5
2	B	414	ASP	2.5
1	C	260	VAL	2.5
1	A	43	GLY	2.5
1	C	337	THR	2.4
2	D	286	LEU	2.4
4	F	342	LEU	2.4
2	B	283	TYR	2.4
4	F	134	ALA	2.4
1	A	196	GLU	2.4
2	B	141	LEU	2.4
3	E	11	LEU	2.4
4	F	324	GLU	2.4
2	D	441	ASP	2.4
4	F	163	SER	2.4
1	C	83	TYR	2.4
1	A	38	SER	2.4
4	F	332	VAL	2.4
2	D	175	PRO	2.4
1	A	141	PHE	2.4
2	B	260	VAL	2.4
1	A	120	ASP	2.4
4	F	232	ASN	2.4
2	D	406	HIS	2.4
1	A	357	TYR	2.4
2	B	34	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	181[A]	VAL	2.4
1	A	329	ASN	2.4
1	A	100	ALA	2.4
4	F	349	GLY	2.4
1	A	332	ILE	2.4
1	C	355	ILE	2.4
1	A	351	PHE	2.3
4	F	193	GLU	2.3
3	E	128	LYS	2.3
1	A	10	GLY	2.3
2	B	248	LEU	2.3
2	D	96	GLN	2.3
2	D	242	LEU	2.3
4	F	348	GLN	2.3
4	F	146	VAL	2.3
1	A	44	GLY	2.3
2	D	378	ILE	2.3
1	A	359	PRO	2.3
4	F	190	LEU	2.3
3	E	140	LYS	2.3
2	D	212	ILE	2.3
1	C	252	LEU	2.3
4	F	195	GLY	2.3
2	D	88	ARG	2.3
2	D	256	ALA	2.3
1	A	173	PRO	2.3
2	B	246	GLY	2.3
4	F	10	ASN	2.3
3	E	47	LEU	2.2
1	C	82	THR	2.2
1	C	250	VAL	2.2
4	F	6	VAL	2.2
2	D	60	LYS	2.2
1	A	231	ILE	2.2
1	C	284	GLU	2.2
1	A	182	VAL	2.2
2	B	88	ARG	2.2
2	D	93	VAL	2.2
1	A	279	GLU	2.2
1	C	178	SER	2.2
2	B	181	VAL	2.2
2	D	39	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	293	GLN	2.2
2	D	439	THR	2.2
4	F	376	ILE	2.2
4	F	206	LEU	2.2
1	A	434	GLU	2.2
2	D	238	VAL	2.2
4	F	197	ARG	2.2
4	F	226	GLU	2.2
2	D	215	ARG	2.2
1	A	224	TYR	2.1
2	D	267	PHE	2.1
1	A	143	GLY	2.1
1	C	134	GLY	2.1
1	C	48	SER	2.1
2	D	165	ILE	2.1
2	B	101	ASN	2.1
1	C	282	TYR	2.1
4	F	44	ARG	2.1
2	D	170	SER	2.1
2	B	180	THR	2.1
2	D	72	PRO	2.1
3	E	45	PRO	2.1
4	F	229	ASN	2.1
1	A	167	LEU	2.1
1	C	318	LEU	2.1
1	C	378	LEU	2.1
1	C	13	GLY	2.1
1	A	140	SER	2.1
2	D	178	SER	2.1
2	D	416	MET	2.1
4	F	320	MET	2.1
1	A	270	ALA	2.1
2	B	317	ALA	2.1
2	D	245	PRO	2.1
2	B	12	CYS	2.1
4	F	340	GLN	2.1
1	C	81	GLY	2.1
1	C	259	LEU	2.1
2	D	80	SER	2.1
2	D	397	ALA	2.1
1	A	13	GLY	2.1
1	C	241	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	49	ILE	2.1
2	D	405	LEU	2.1
4	F	257	GLU	2.1
1	C	5	ILE	2.0
2	B	255	LEU	2.0
2	D	384	ILE	2.0
2	B	416	MET	2.0
4	F	262	MET	2.0
2	B	372	LYS	2.0
1	C	244	PHE	2.0
2	B	224	TYR	2.0
2	D	201	THR	2.0
3	E	121	GLU	2.0
1	A	430	LYS	2.0
2	B	55	GLU	2.0
1	A	41	THR	2.0
1	A	269	LEU	2.0
2	D	241	CYS	2.0
4	F	75	ALA	2.0
4	F	337	ALA	2.0
2	B	85	GLN	2.0
4	F	351	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NW6	D	504	21/21	0.77	0.37	39,48,60,62	32

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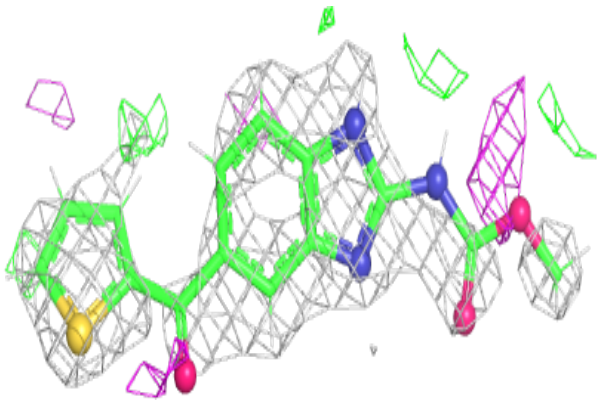
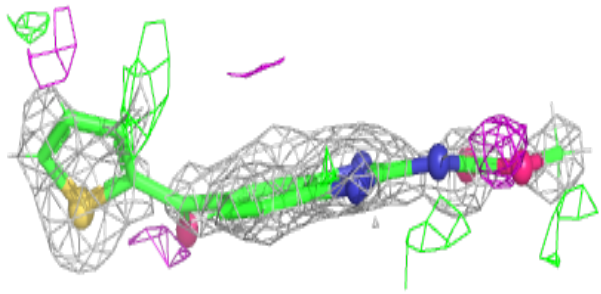
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MES	D	503	12/12	0.79	0.31	47,53,57,60	12
10	ACP	F	401	31/31	0.85	0.16	61,73,90,95	0
6	MG	D	502	1/1	0.91	0.10	52,52,52,52	0
9	NW6	B	504	21/21	0.93	0.14	30,36,41,46	0
6	MG	F	402	1/1	0.94	0.09	57,57,57,57	0
7	GDP	D	501	28/28	0.94	0.13	38,45,51,54	0
6	MG	C	502	1/1	0.94	0.11	26,26,26,26	0
6	MG	A	502	1/1	0.95	0.13	27,27,27,27	0
8	MES	B	503	12/12	0.95	0.15	34,39,48,49	0
5	GTP	A	501	32/32	0.96	0.18	23,29,34,34	0
5	GTP	C	501	32/32	0.96	0.18	19,25,29,30	0
7	GDP	B	501	28/28	0.96	0.18	23,29,31,32	0
6	MG	B	502	1/1	0.98	0.18	18,18,18,18	0

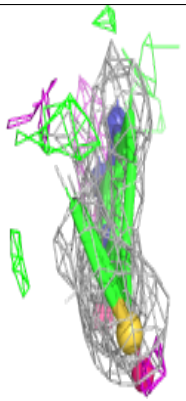
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NW6 D 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

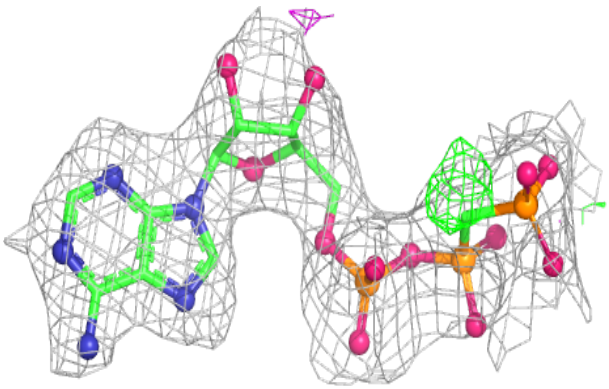


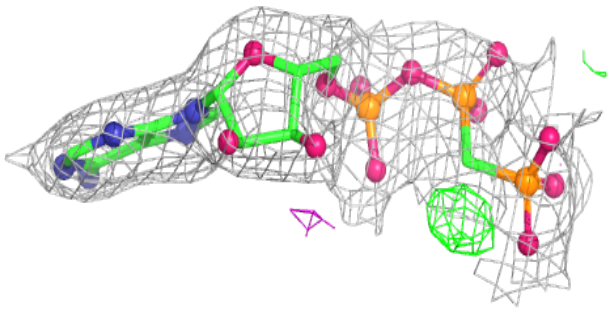


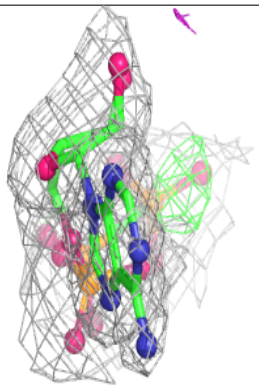


Electron density around ACP F 401:

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

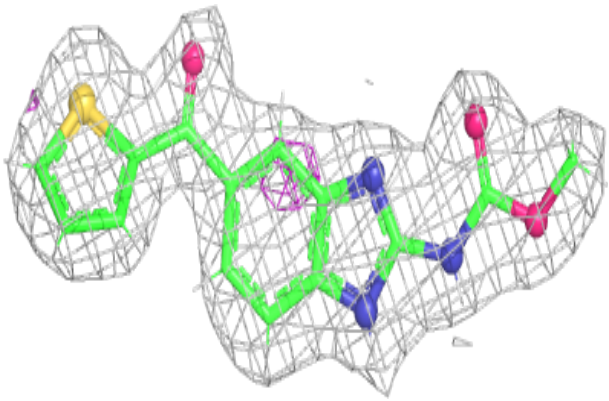


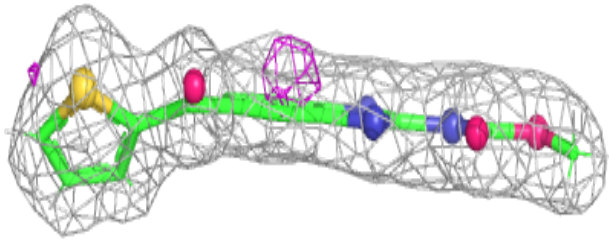




Electron density around NW6 B 504:

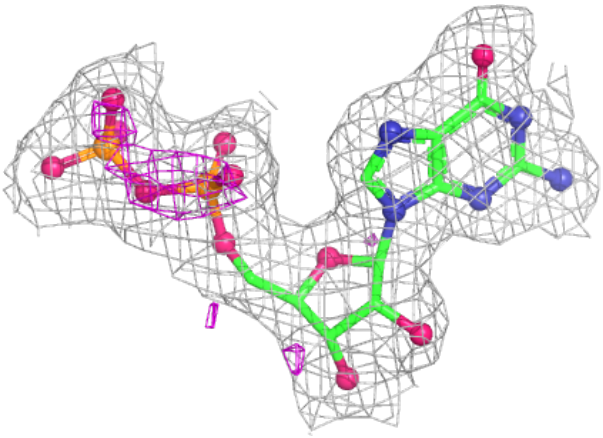
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

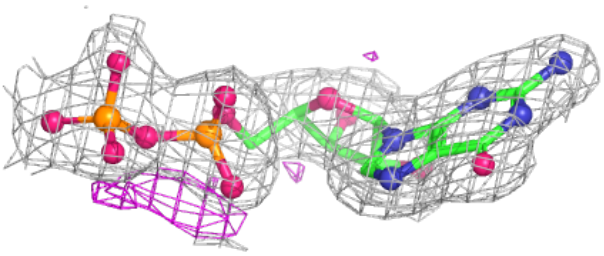


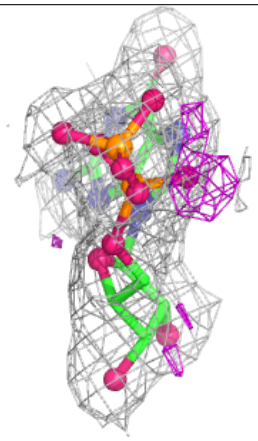


Electron density around GDP D 501:

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

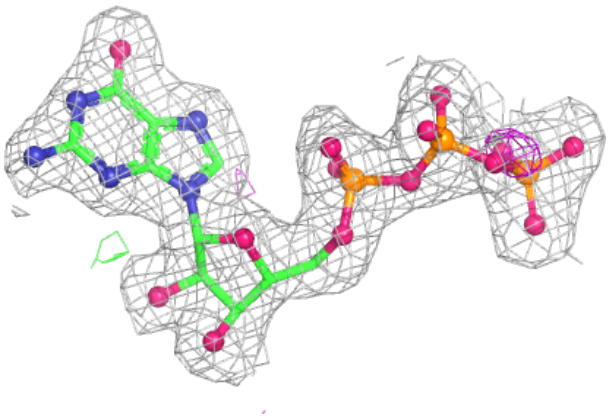


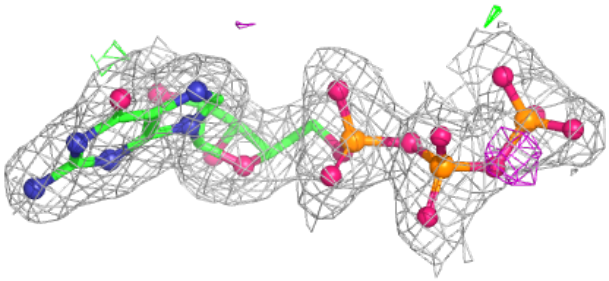


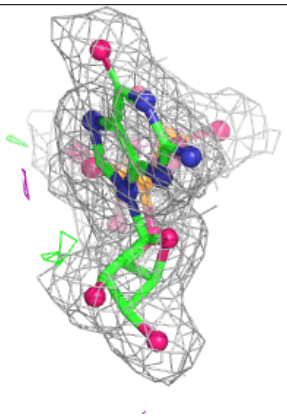


Electron density around GTP A 501:

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

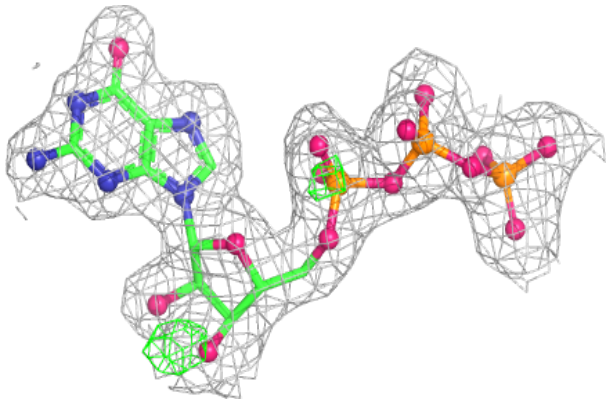


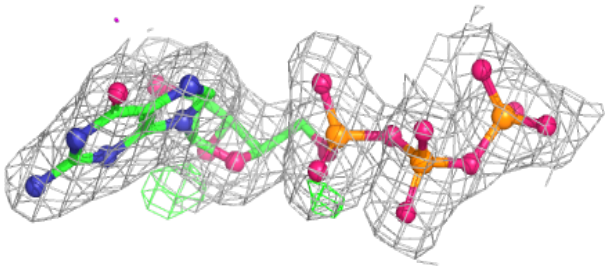


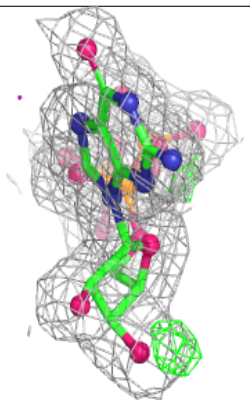


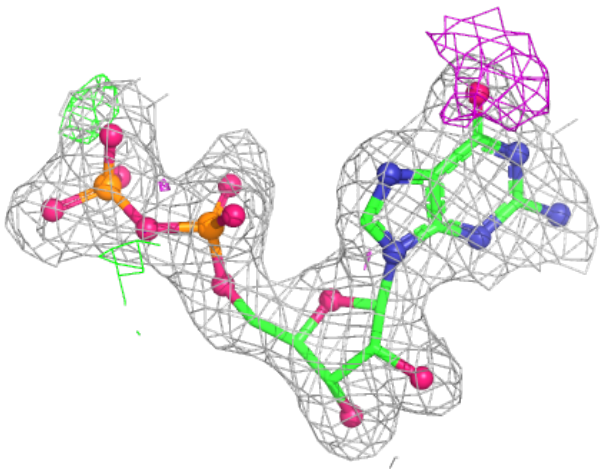
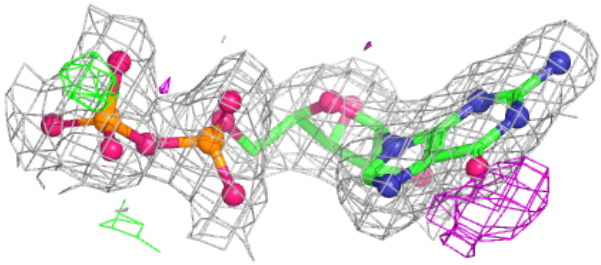
Electron density around GTP C 501:

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







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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.