Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2022 – 10:19 AM EST

PDB ID	:	5SBC
Title	:	Tubulin-maytansinoid-5a-complex
Authors	:	Marzullo, P.; Boiarska, Z.; Perez-Pena, H.; Abel, A.-C.; Alvarez-Bernad, B.; Lucena-Agell, D.; Vasile, F.; Sironi, M.; Steinmetz, M.O.; Prota, A.E.; Diaz, J.F.; Pieraccini, S.; Passarella, D.
Deposited on	:	2021-07-20
Resolution	:	2.32 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 following versions of software and data (see references (i)) were used in the production of this report:

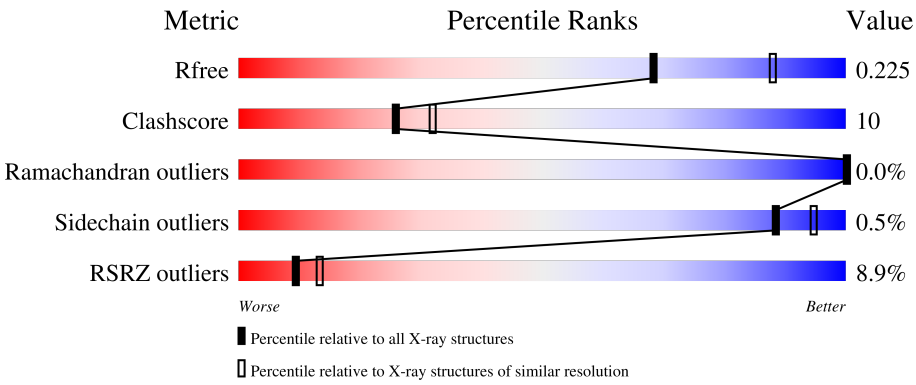
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	5%, 77%, 20%, •
1	C	451	%, 79%, 18%, •
2	B	445	4%, 71%, 24%, 5%
2	D	445	7%, 71%, 25%, •
3	E	143	8%, 73%, 12%, 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	28% 66% 23% 11%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 18401 atoms, of which 13 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	438	3436	2173	584	655	24	0	2	0
1	C	440	3476	2199	591	663	23	0	6	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	3345	2102	572	644	27	0	1	0
2	D	426	3343	2098	570	648	27	0	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	1000	617	181	197	5	0	0	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

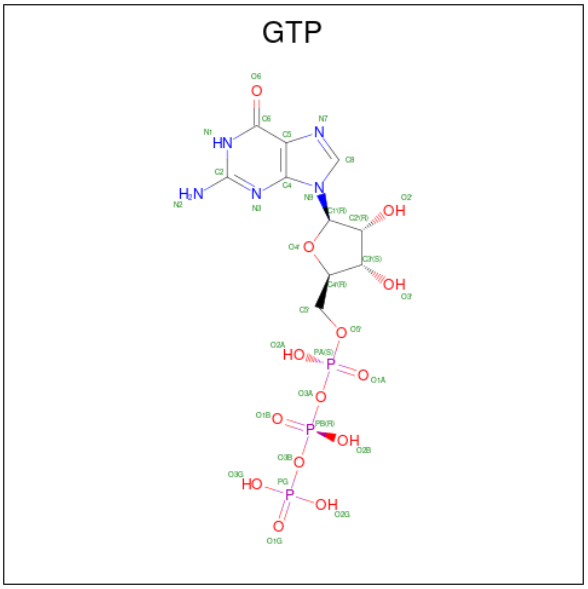
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	341	2806	1801	480	510	15	0	2	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
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

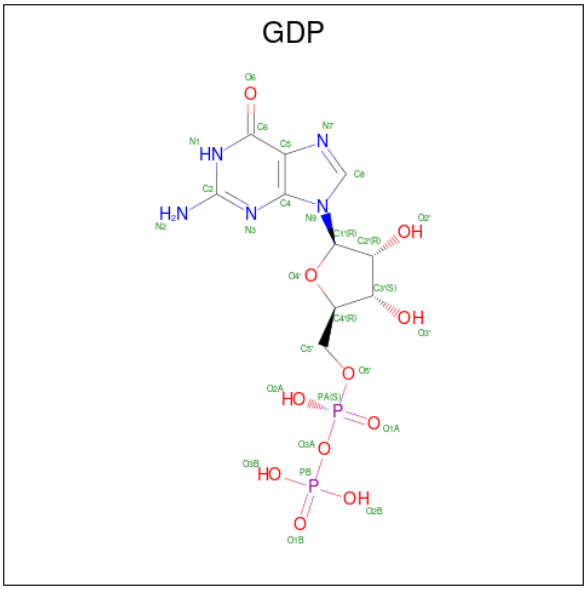
Continued from previous page...

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

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

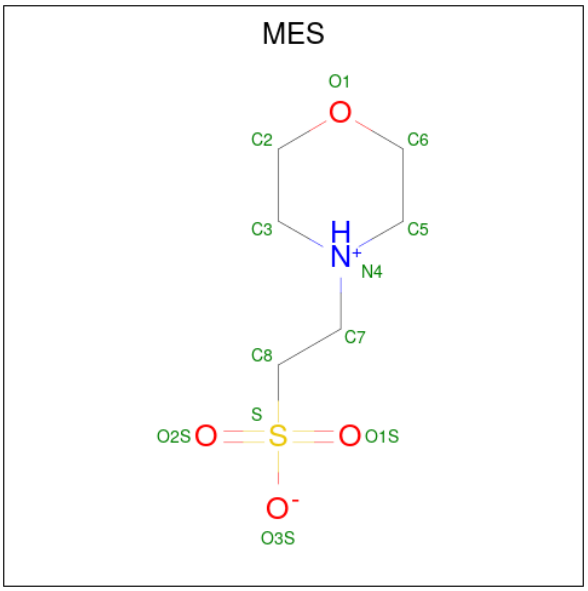
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	B	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0
			Total	Ca		
7	E	1	1	1	0	0

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



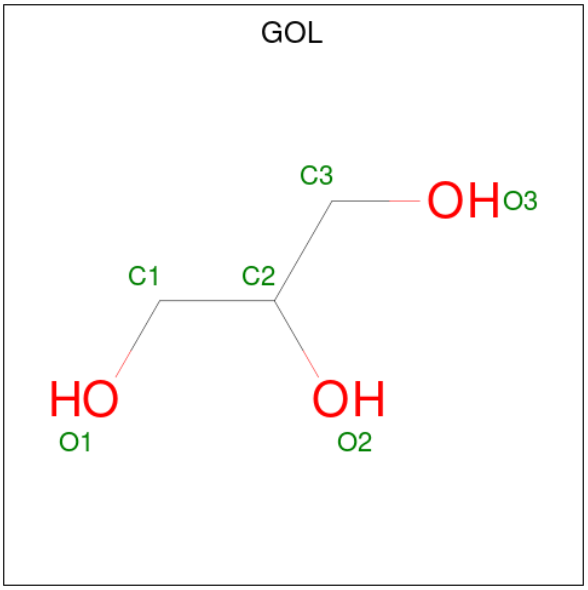
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
8	D	1	28	10	5	11	2	0	0

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



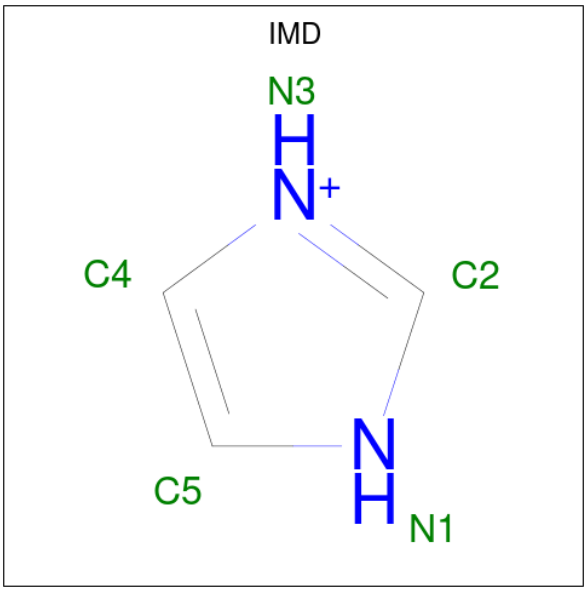
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



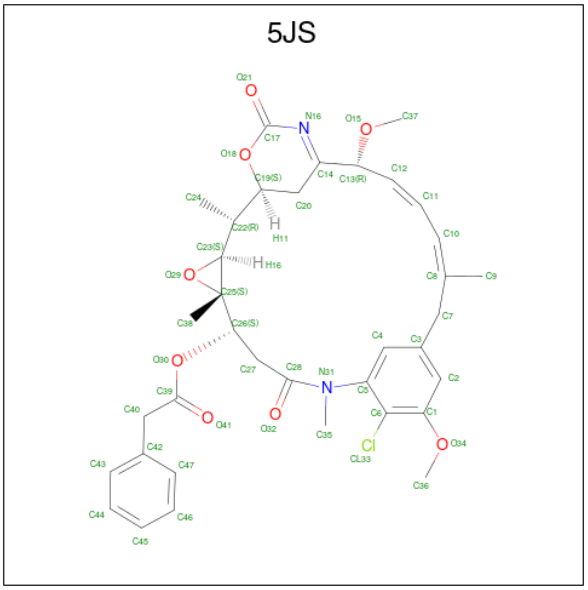
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
10	B	1	14	3	8	3	0	0

- Molecule 11 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



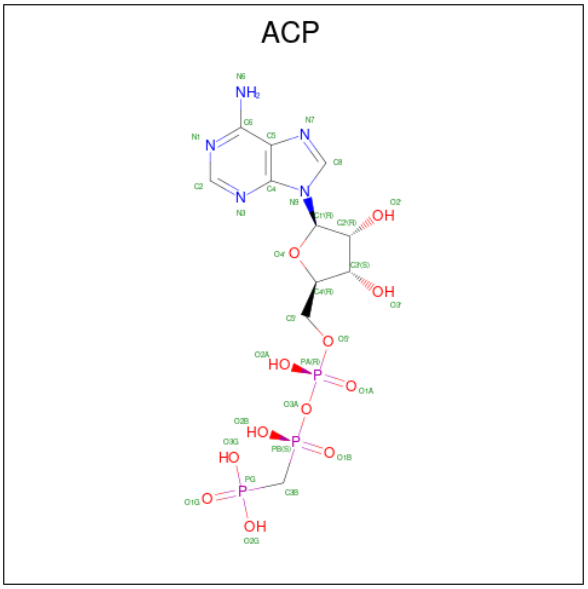
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
11	C	1	10	3	5	2	0	0

- Molecule 12 is (1S,2R,3S,5S,6S,16E,18E,20R)-11-chloro-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16,18,21-hexaen-6-yl phenylacetate (three-letter code: 5JS) (formula: $C_{36}H_{41}ClN_2O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
12	D	1	47	36	1	2	8	0	0

- Molecule 13 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		
13	F	1	31	11	5	12	3	0	0

- Molecule 14 is water.

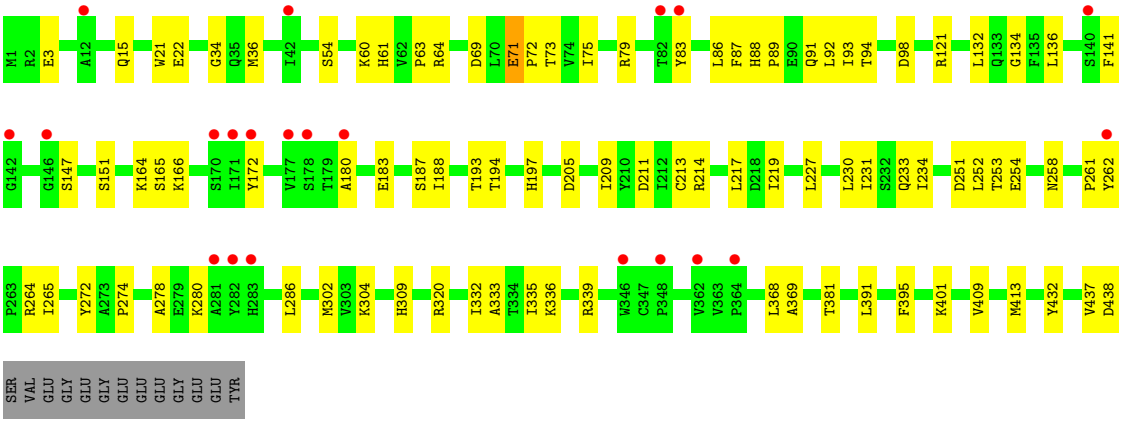
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	147	147	147	0	0
14	B	169	Total 169	O 169	0	0
14	C	289	Total 289	O 289	0	0
14	D	79	Total 79	O 79	0	0
14	E	26	Total 26	O 26	0	0
14	F	42	Total 42	O 42	0	0

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.

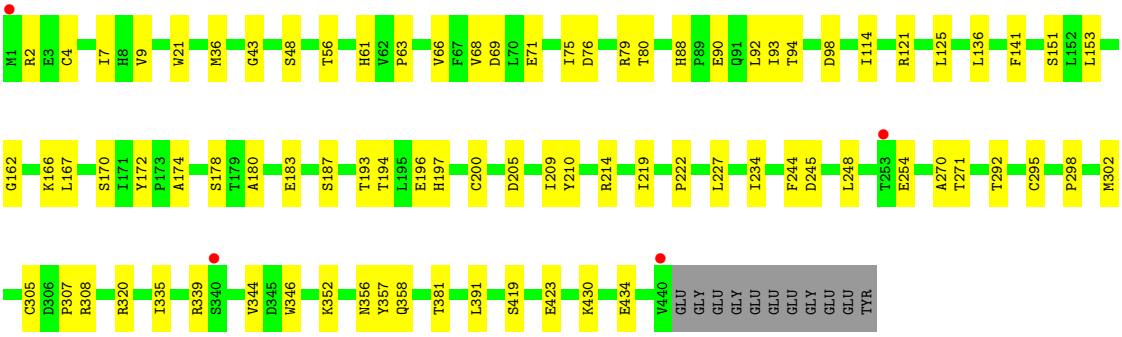
• Molecule 1: Tubulin alpha-1B chain

Chain A:



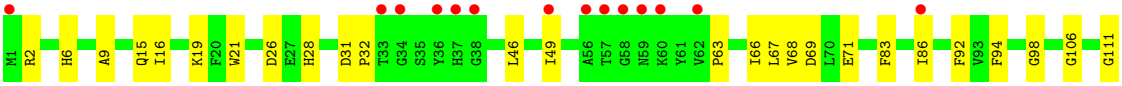
• Molecule 1: Tubulin alpha-1B chain

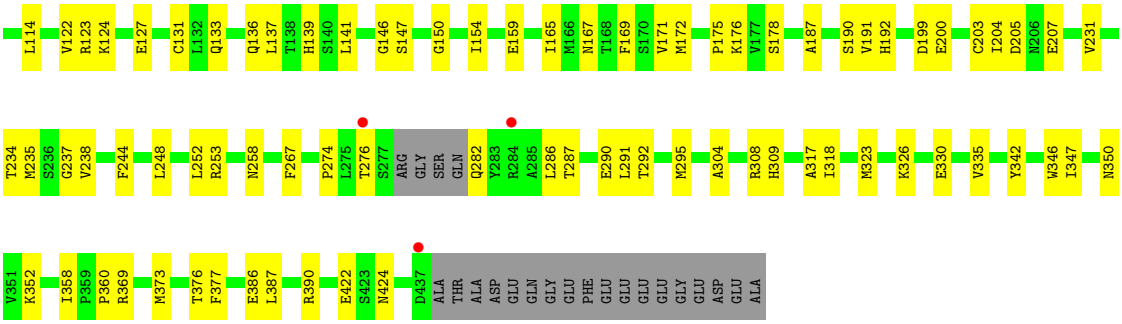
Chain C:



• Molecule 2: Tubulin beta-2B chain

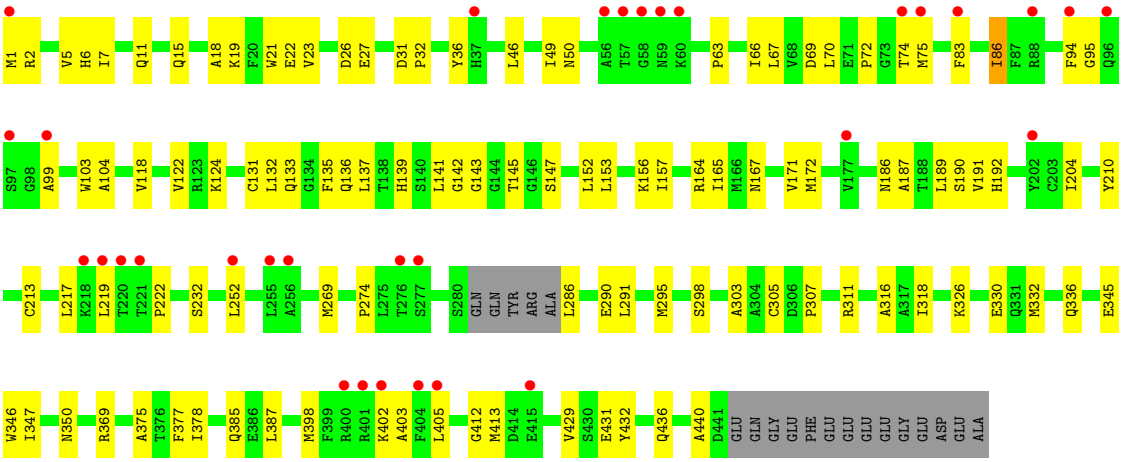
Chain B:





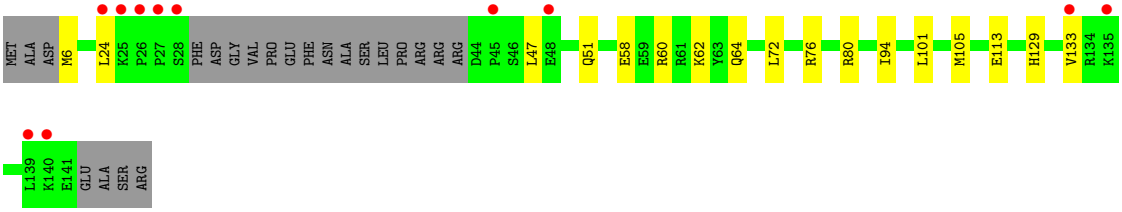
- Molecule 2: Tubulin beta-2B chain

Chain D:



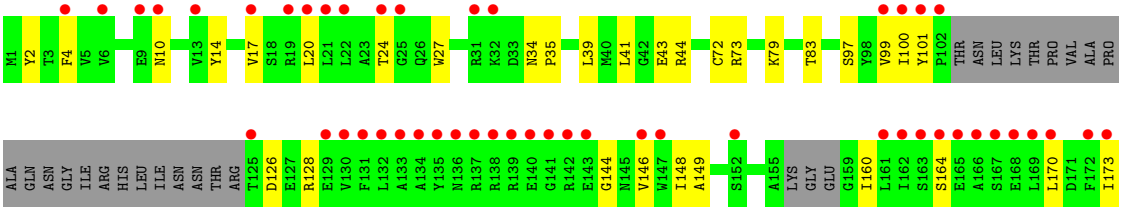
- Molecule 3: Stathmin-4

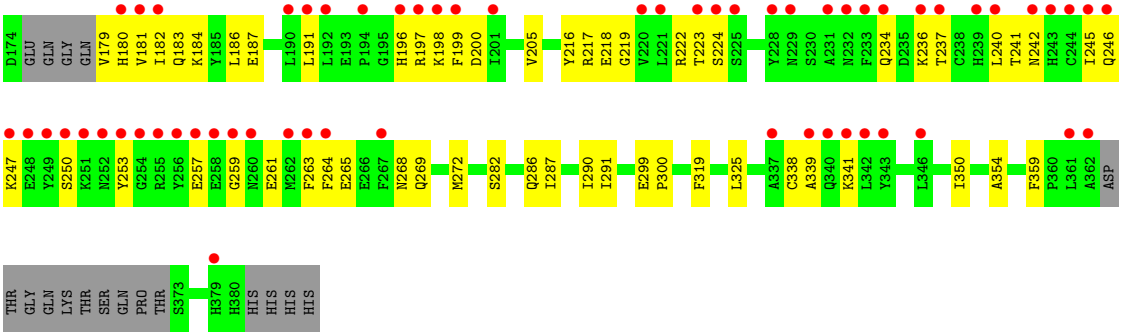
Chain E:



- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:




D174 GLU GLN GLY GLN V179 H180 V181 I182 Q183 K184 Y185 L186 E187 L190 L191 L192 E193 P194 G195 H196 R197 K198 F199 D200 I201 V205 Y216 R217 E218 G219 V220 L221 R222 T223 S224 S225 Y228 N229 S230 A231 N232 F233 Q234 D235 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 E265 E266 F267 N268 Q269 M272 S282 Q286 I287 I290 I291 E299 P300 F319 L325 A337 C338 A339 Q340 K341 L342 Y343 L346 I350 A354 F359 P360 L361 A362 ASP
THR GLY GLN LYS THR SER GLN PRO THR S373 H379 H380 HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.91Å 157.91Å 181.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.32 48.02 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.02-2.32) 100.0 (48.02-2.32)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.186 , 0.228 0.183 , 0.225	Depositor DCC
R_{free} test set	6548 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18401	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: IMD, MG, GTP, ACP, CA, 5JS, MES, GDP, GOL

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	0/3514	0.46	0/4770
1	C	0.24	0/3564	0.45	0/4840
2	B	0.24	0/3419	0.46	0/4629
2	D	0.24	0/3416	0.45	0/4626
3	E	0.23	0/1008	0.41	0/1337
4	F	0.24	0/2869	0.45	0/3873
All	All	0.24	0/17790	0.45	0/24075

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	3436	0	3343	68	0
1	C	3476	0	3384	58	0
2	B	3345	0	3227	80	0
2	D	3343	0	3222	85	0
3	E	1000	0	1018	18	0
4	F	2806	0	2775	61	0
5	A	32	0	12	2	0

Continued on next page...

Continued from previous page...

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
7	E	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	12	3	0
10	B	6	8	8	0	0
11	C	5	5	5	0	0
12	D	47	0	0	0	0
13	F	31	0	14	2	0
14	A	147	0	0	4	0
14	B	169	0	0	9	0
14	C	289	0	0	4	0
14	D	79	0	0	4	0
14	E	26	0	0	2	0
14	F	42	0	0	2	0
All	All	18388	13	17056	363	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 10.

All (363) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.40	0.84
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.61	0.82
3:E:6:MET:HE2	3:E:24:LEU:HD21	1.61	0.81
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.01	0.79
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.65	0.78
1:C:339:ARG:O	14:C:601:HOH:O	2.01	0.78
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.67	0.75
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.68	0.75
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.69	0.74
3:E:6:MET:HG2	3:E:24:LEU:HD23	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:O	2:B:86:ILE:HG22	1.89	0.73
3:E:113:GLU:OE1	14:E:301:HOH:O	2.07	0.73
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.72	0.72
2:D:11:GLN:HA	2:D:74:THR:HG21	1.71	0.72
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.20	0.71
1:A:336:LYS:HG2	3:E:24:LEU:HD13	1.72	0.70
2:D:83:PHE:HD2	2:D:86:ILE:HD12	1.55	0.70
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.75	0.68
2:D:32:PRO:O	2:D:86:ILE:HG13	1.93	0.68
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.76	0.67
2:B:424:ASN:HB3	14:B:601:HOH:O	1.94	0.67
2:D:136:GLN:HA	2:D:167:ASN:O	1.93	0.67
2:B:136:GLN:HA	2:B:167:ASN:O	1.94	0.66
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.96	0.66
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.77	0.66
2:D:147:SER:HB2	2:D:190:SER:OG	1.95	0.65
2:B:276:THR:HG21	2:B:282:GLN:HA	1.78	0.65
2:D:145:THR:N	8:D:501:GDP:O2B	2.28	0.65
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.78	0.65
4:F:237:THR:O	4:F:246:GLN:NE2	2.26	0.65
1:A:309:HIS:HB3	14:A:722:HOH:O	1.97	0.64
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.28	0.64
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.80	0.64
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.79	0.63
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.13	0.63
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.79	0.63
2:B:253[A]:ARG:NH1	9:B:504:MES:O3S	2.31	0.63
2:D:143:GLY:HA3	8:D:501:GDP:O3A	1.98	0.63
2:D:75:MET:SD	2:D:94:PHE:HB3	2.39	0.63
1:A:333:ALA:N	3:E:6:MET:HE1	2.14	0.63
3:E:80:ARG:NH1	14:E:302:HOH:O	2.32	0.63
1:C:76:ASP:O	1:C:80:THR:HG22	1.99	0.62
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.40	0.62
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.81	0.62
1:A:214:ARG:HG2	1:A:219:ILE:O	2.00	0.62
2:B:192:HIS:ND1	14:B:601:HOH:O	2.31	0.62
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.82	0.61
1:C:320:ARG:HA	1:C:356:ASN:O	2.00	0.61
2:D:31:ASP:O	2:D:86:ILE:HD11	2.00	0.61
1:A:83:TYR:HB3	1:A:86:LEU:HD12	1.82	0.61
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.83	0.61
2:D:431:GLU:OE1	14:D:602:HOH:O	2.17	0.60
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.82	0.60
4:F:149:ALA:HB2	4:F:182:ILE:HG12	1.83	0.60
1:C:271:THR:HG21	1:C:295:CYS:O	2.01	0.60
1:C:48:SER:OG	1:C:245:ASP:HB2	2.02	0.60
4:F:79:LYS:O	4:F:83:THR:OG1	2.15	0.59
4:F:241:THR:OG1	13:F:401:ACP:O3'	2.19	0.59
1:C:167:LEU:HD13	14:C:823:HOH:O	2.03	0.59
2:D:171:VAL:HA	2:D:204:ILE:O	2.02	0.59
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.83	0.59
2:D:332:MET:O	2:D:336:GLN:HG3	2.03	0.59
2:D:11:GLN:O	2:D:15:GLN:HG2	2.03	0.58
1:C:209:ILE:HD11	1:C:302:MET:CE	2.33	0.58
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.38	0.58
2:D:2:ARG:NH2	14:D:604:HOH:O	2.36	0.58
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.85	0.58
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.39	0.58
3:E:6:MET:HG2	3:E:24:LEU:CD2	2.33	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.03	0.58
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.86	0.58
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.04	0.58
1:A:166:LYS:HE2	1:A:197:HIS:O	2.04	0.58
2:D:210:TYR:CD2	2:D:222:PRO:HG2	2.39	0.57
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.87	0.57
2:B:141:LEU:HD12	2:B:172:MET:SD	2.44	0.57
4:F:20:LEU:O	4:F:24:THR:HG23	2.04	0.57
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.39	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.40	0.56
2:B:390:ARG:NE	14:B:603:HOH:O	2.38	0.56
1:C:270:ALA:O	1:C:302:MET:HG2	2.04	0.56
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.87	0.56
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.20	0.56
4:F:259:GLY:O	4:F:261:GLU:HG3	2.05	0.56
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.40	0.56
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.87	0.56
2:B:71:GLU:HB3	14:B:648:HOH:O	2.05	0.56
2:B:187:ALA:O	2:B:191:VAL:HG23	2.05	0.56
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ASP:OD1	9:B:504:MES:H62	2.05	0.56
2:B:422:GLU:HG3	14:B:604:HOH:O	2.05	0.56
2:D:295:MET:CG	2:D:377:PHE:HB2	2.35	0.56
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.87	0.56
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.87	0.56
2:D:152:LEU:O	2:D:156:LYS:HG2	2.04	0.56
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.45	0.56
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.87	0.56
4:F:149:ALA:O	4:F:160:ILE:HG23	2.06	0.56
1:C:335:ILE:HG23	1:C:339:ARG:CG	2.36	0.55
2:B:28:HIS:HB3	2:B:49:ILE:HD13	1.88	0.55
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.41	0.55
1:C:180:ALA:O	1:C:183:GLU:HG3	2.07	0.55
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.06	0.55
3:E:72:LEU:O	3:E:76:ARG:HG2	2.06	0.55
2:B:323:MET:HE1	2:B:373:MET:HB2	1.89	0.54
2:B:123:ARG:O	2:B:127:GLU:HG3	2.07	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.41	0.54
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.88	0.54
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.90	0.54
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.88	0.54
2:B:326:LYS:O	2:B:330:GLU:HG3	2.08	0.53
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.89	0.53
4:F:128:ARG:NH1	4:F:170:LEU:HD13	2.23	0.53
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.44	0.53
2:D:398:MET:HE3	2:D:403:ALA:HB3	1.91	0.53
4:F:240:LEU:HD23	4:F:245:ILE:CD1	2.39	0.53
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.43	0.53
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.91	0.52
2:B:234:THR:O	2:B:238:VAL:HG13	2.09	0.52
1:A:69:ASP:O	1:A:94:THR:HA	2.09	0.52
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.91	0.52
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.45	0.52
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.90	0.52
4:F:198:LYS:HG2	4:F:199:PHE:H	1.74	0.52
4:F:265:GLU:O	14:F:501:HOH:O	2.19	0.52
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.45	0.52
1:C:151:SER:HB2	1:C:193:THR:CG2	2.40	0.52
2:D:19:LYS:O	2:D:23:VAL:HG23	2.10	0.52
3:E:101:LEU:O	3:E:105:MET:HG2	2.09	0.52
2:D:1:MET:HA	2:D:1:MET:HE2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:HA	2:D:147:SER:HB3	1.91	0.51
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.92	0.51
2:B:323:MET:HB3	2:B:373:MET:CE	2.40	0.51
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.45	0.51
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.09	0.51
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.46	0.51
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.46	0.51
2:B:124:LYS:HD3	2:B:124:LYS:C	2.32	0.51
1:C:419:SER:O	1:C:423:GLU:HG3	2.11	0.51
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.11	0.50
2:B:323:MET:HB3	2:B:373:MET:HE2	1.93	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
14:B:721:HOH:O	1:C:2:ARG:HD2	2.11	0.50
4:F:197:ARG:HB2	4:F:224:SER:O	2.11	0.50
3:E:60:ARG:O	3:E:64:GLN:HG3	2.11	0.50
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.11	0.50
1:C:88[A]:HIS:CE1	1:C:90:GLU:HG3	2.47	0.50
2:D:1:MET:O	2:D:131:CYS:HB3	2.11	0.50
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.46	0.50
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.92	0.50
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.28	0.50
3:E:129:HIS:O	3:E:133:VAL:HG23	2.11	0.50
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.93	0.49
1:A:332:ILE:HG22	3:E:6:MET:HE2	1.93	0.49
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.26	0.49
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.94	0.49
1:A:187:SER:CB	1:A:391:LEU:HD21	2.42	0.49
2:D:274:PRO:HB3	2:D:286:LEU:CD2	2.42	0.49
1:A:264:ARG:NH1	14:A:601:HOH:O	2.29	0.49
1:A:227:LEU:O	1:A:231:ILE:HG13	2.12	0.49
2:B:295:MET:CG	2:B:377:PHE:HB2	2.42	0.49
4:F:268:ASN:HB3	14:F:501:HOH:O	2.12	0.49
1:A:234:ILE:HD12	1:A:272:TYR:HB2	1.95	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.49
4:F:100:ILE:HG23	4:F:128:ARG:HG3	1.94	0.49
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.94	0.49
2:B:147:SER:HG	2:B:190:SER:HG	1.59	0.49
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.94	0.49
2:D:63:PRO:CD	2:D:86:ILE:HG23	2.42	0.49
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.48	0.49
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.49
2:B:19:LYS:HE3	14:B:725:HOH:O	2.12	0.49
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.95	0.48
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.94	0.48
2:D:345:GLU:CG	2:D:440:ALA:HB2	2.43	0.48
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.43	0.48
2:B:231:VAL:O	2:B:235:MET:HG3	2.12	0.48
4:F:43:GLU:OE1	4:F:43:GLU:N	2.33	0.48
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.49	0.48
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.48
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.45	0.48
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.49	0.48
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.49	0.48
1:A:180:ALA:O	1:A:183:GLU:HG3	2.14	0.48
4:F:286:GLN:O	4:F:290:ILE:HG13	2.14	0.48
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.95	0.47
1:C:196:GLU:HG2	14:C:684:HOH:O	2.13	0.47
4:F:101:TYR:N	4:F:126:ASP:OD1	2.42	0.47
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.44	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.47
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.95	0.47
1:A:409:VAL:HA	1:A:413:MET:O	2.14	0.47
2:B:248:LEU:CD2	2:B:352:LYS:HB3	2.44	0.47
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.49	0.47
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.95	0.47
4:F:10:ASN:HB2	4:F:44:ARG:NH2	2.21	0.47
4:F:246:GLN:O	4:F:250:SER:HB3	2.14	0.47
2:B:15:GLN:O	2:B:19:LYS:HG2	2.14	0.47
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.50	0.47
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.50	0.47
2:B:304:ALA:N	14:B:612:HOH:O	2.48	0.47
1:C:88[A]:HIS:HE1	1:C:90:GLU:HG3	1.80	0.47
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.97	0.47
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.50	0.47
4:F:191:LEU:HA	4:F:197:ARG:O	2.15	0.47
2:D:23:VAL:O	2:D:27:GLU:HG3	2.15	0.47
2:D:311:ARG:NH1	2:D:436:GLN:O	2.48	0.47
1:A:71:GLU:HG2	1:A:72:PRO:N	2.30	0.46
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.50	0.46
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.96	0.46
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HB	1:A:94:THR:CG2	2.46	0.46
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.46
1:A:251:ASP:OD1	1:A:253:THR:HB	2.15	0.46
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.16	0.46
4:F:149:ALA:CB	4:F:182:ILE:HG12	2.44	0.46
2:B:71:GLU:HG3	2:B:98:GLY:HA2	1.97	0.46
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.97	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.46
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.51	0.46
1:A:134:GLY:HA3	1:A:165:SER:O	2.16	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.46
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.98	0.46
1:C:9:VAL:HG22	1:C:68[B]:VAL:CG2	2.46	0.46
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.98	0.46
2:D:2:ARG:HB3	2:D:133:GLN:HG3	1.97	0.46
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.97	0.46
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.97	0.46
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.97	0.46
2:D:7:ILE:O	2:D:137:LEU:HA	2.15	0.46
2:D:295:MET:SD	2:D:375:ALA:HB1	2.56	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.51	0.45
1:A:79:ARG:HG2	1:A:92:LEU:CD1	2.46	0.45
2:D:18:ALA:O	2:D:22:GLU:HG3	2.15	0.45
1:A:54:SER:O	1:A:61:HIS:HA	2.16	0.45
1:A:209:ILE:HD11	1:A:302:MET:SD	2.56	0.45
2:D:7:ILE:O	2:D:137:LEU:HD12	2.17	0.45
2:D:412:GLY:C	3:E:133:VAL:HG13	2.37	0.45
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.98	0.45
2:D:143:GLY:O	2:D:147:SER:OG	2.25	0.45
2:B:46:LEU:HA	2:B:49:ILE:HB	1.99	0.45
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.32	0.45
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.97	0.45
2:D:213:CYS:HB3	2:D:219:LEU:HD12	1.98	0.45
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.99	0.45
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.52	0.45
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.99	0.45
2:D:46:LEU:HA	2:D:49:ILE:HB	1.99	0.45
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.99	0.45
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.47	0.45
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.52	0.45
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:VAL:O	2:D:122:VAL:HG23	2.17	0.44
4:F:72:CYS:O	4:F:73:ARG:HD2	2.17	0.44
2:D:432:TYR:OH	14:D:601:HOH:O	2.12	0.44
2:D:104:ALA:HB2	2:D:413:MET:SD	2.58	0.44
2:D:387:LEU:HD23	2:D:387:LEU:C	2.38	0.44
4:F:217:ARG:HG3	4:F:218:GLU:N	2.33	0.44
2:D:72:PRO:HD3	2:D:95:GLY:O	2.17	0.44
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.50	0.44
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.53	0.44
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.00	0.44
1:A:136:LEU:HD21	1:A:252:LEU:HD21	1.99	0.43
1:C:43:GLY:HA2	1:C:56:THR:O	2.18	0.43
2:D:69:ASP:O	2:D:94:PHE:HA	2.19	0.43
2:D:142:GLY:O	2:D:186:ASN:ND2	2.49	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.19	0.43
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.48	0.43
2:D:153:LEU:O	2:D:157:ILE:HG13	2.19	0.43
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.00	0.43
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.01	0.43
1:A:75:ILE:HB	1:A:94:THR:HG21	2.00	0.43
2:B:317:ALA:C	2:B:318:ILE:HD12	2.39	0.43
1:C:66:VAL:HG12	1:C:68[B]:VAL:HG13	2.01	0.43
2:B:67:LEU:N	2:B:67:LEU:HD12	2.34	0.43
3:E:47:LEU:HD11	3:E:51:GLN:HE21	1.83	0.43
4:F:199:PHE:HB3	4:F:223:THR:HG22	2.01	0.43
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.43
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.84	0.43
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.18	0.43
2:D:1:MET:HA	2:D:1:MET:CE	2.48	0.43
4:F:247:LYS:HE3	4:F:253:TYR:CE2	2.53	0.43
1:A:320:ARG:HD2	14:A:671:HOH:O	2.19	0.42
2:D:132:LEU:O	2:D:164:ARG:NH1	2.51	0.42
2:D:274:PRO:HB3	2:D:286:LEU:HD22	2.00	0.42
2:D:303:ALA:O	2:D:305:CYS:N	2.52	0.42
1:A:88:HIS:HB2	1:A:89:PRO:HD2	2.01	0.42
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.59	0.42
1:C:48:SER:HB2	14:C:712:HOH:O	2.18	0.42
1:C:75:ILE:HD12	1:C:94:THR:HG22	2.02	0.42
4:F:338:CYS:SG	4:F:339:ALA:N	2.92	0.42
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.49	0.42
1:A:132:LEU:O	1:A:164:LYS:NZ	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:HB2	1:A:193:THR:OG1	2.20	0.42
2:D:187:ALA:O	2:D:191:VAL:HG23	2.20	0.42
4:F:144:GLY:O	4:F:184:LYS:HE2	2.20	0.42
4:F:350:ILE:O	4:F:354:ALA:HB3	2.19	0.42
4:F:99:VAL:HG22	4:F:181:VAL:HG12	2.00	0.42
2:B:2:ARG:HA	2:B:131:CYS:O	2.20	0.42
1:A:437:VAL:HG12	1:A:438:ASP:N	2.34	0.42
1:C:194:THR:O	1:C:194:THR:HG22	2.19	0.42
4:F:242:ASN:ND2	13:F:401:ACP:H3B1	2.35	0.42
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.01	0.42
1:A:280:LYS:HE2	1:A:280:LYS:HB3	1.88	0.41
2:B:295:MET:HG3	2:B:377:PHE:HB2	2.02	0.41
2:D:1:MET:HG3	2:D:50:ASN:HD22	1.84	0.41
1:C:166:LYS:HE2	1:C:197:HIS:O	2.20	0.41
2:D:124:LYS:C	2:D:124:LYS:HD3	2.40	0.41
2:D:298:SER:HB3	2:D:307:PRO:HD2	2.02	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.94	0.41
2:B:235:MET:HB3	2:B:235:MET:HE2	1.92	0.41
1:C:305:CYS:O	1:C:307:PRO:HD3	2.20	0.41
2:D:295:MET:HG2	2:D:377:PHE:HB2	2.00	0.41
4:F:97:SER:HA	4:F:183:GLN:HA	2.02	0.41
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.55	0.41
1:C:234:ILE:HD12	1:C:234:ILE:N	2.35	0.41
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.84	0.41
3:E:6:MET:CE	3:E:24:LEU:HD21	2.41	0.41
4:F:4:PHE:HA	4:F:39:LEU:O	2.20	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.20	0.41
9:B:504:MES:H82	9:B:504:MES:H51	1.85	0.41
1:C:234:ILE:HG12	1:C:302:MET:SD	2.61	0.41
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.90	0.41
2:D:291:LEU:HG	2:D:375:ALA:HB2	2.03	0.41
4:F:14:TYR:HA	4:F:17:VAL:HB	2.03	0.41
1:A:194:THR:O	1:A:194:THR:HG22	2.21	0.41
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.45	0.41
4:F:269:GLN:HA	4:F:272:MET:HE2	2.03	0.41
1:A:87:PHE:HA	1:A:91:GLN:OE1	2.21	0.41
1:A:213:CYS:O	1:A:217:LEU:HB2	2.21	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.41
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.21	0.41
2:B:114:LEU:O	2:B:114:LEU:HG	2.20	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ALA:O	1:C:178:SER:HB3	2.20	0.41
2:D:326:LYS:O	2:D:330:GLU:HG3	2.21	0.41
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.21	0.41
1:C:69:ASP:O	1:C:94:THR:HA	2.21	0.41
2:D:142:GLY:N	14:D:605:HOH:O	2.44	0.41
2:B:175:PRO:HA	2:B:178:SER:HB2	2.03	0.40
2:B:199:ASP:C	2:B:200:GLU:HG3	2.41	0.40
2:B:318:ILE:HD12	2:B:318:ILE:N	2.36	0.40
1:C:151:SER:HB2	1:C:193:THR:HG21	2.03	0.40
2:D:63:PRO:HD3	2:D:86:ILE:HG23	2.02	0.40
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.49	0.40
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.51	0.40
4:F:184:LYS:NZ	4:F:187:GLU:HG3	2.36	0.40
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.56	0.40
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.45	0.40
2:B:360:PRO:HG3	14:B:707:HOH:O	2.21	0.40
1:A:75:ILE:CG2	1:A:92:LEU:HB3	2.51	0.40
1:A:261:PRO:HD2	14:A:650:HOH:O	2.21	0.40
1:C:79:ARG:HG2	1:C:92:LEU:HD12	2.04	0.40
1:C:214:ARG:HG2	1:C:219:ILE:O	2.22	0.40
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.21	0.40
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.57	0.40
2:D:66:ILE:CD1	2:D:122:VAL:HG22	2.51	0.40
2:B:9:ALA:HA	2:B:68:VAL:O	2.21	0.40
2:B:146:GLY:O	2:B:150:GLY:HA3	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	438/451 (97%)	424 (97%)	14 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	444/451 (98%)	434 (98%)	10 (2%)	0	100	100
2	B	420/445 (94%)	411 (98%)	9 (2%)	0	100	100
2	D	422/445 (95%)	416 (99%)	6 (1%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	333/384 (87%)	326 (98%)	6 (2%)	1 (0%)	41	50
All	All	2174/2319 (94%)	2128 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	186	LEU

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	371/379 (98%)	368 (99%)	3 (1%)	81	90
1	C	377/379 (100%)	375 (100%)	2 (0%)	88	95
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	96
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	90
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	307/342 (90%)	306 (100%)	1 (0%)	92	96
All	All	1900/1993 (95%)	1890 (100%)	10 (0%)	88	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	262	TYR
1	A	381	THR
2	B	139	HIS
1	C	71	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	381	THR
2	D	86	ILE
2	D	139	HIS
2	D	192	HIS
4	F	234	GLN

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 18 ligands modelled in this entry, 9 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	MES	B	504	-	12,12,12	2.23	1 (8%)	14,16,16	1.95	5 (35%)
13	ACP	F	401	6	27,33,33	1.99	7 (25%)	32,52,52	1.33	4 (12%)
11	IMD	C	504	-	3,5,5	0.39	0	4,5,5	0.59	0
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.75	6 (18%)
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.74	6 (18%)

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	1.92	7 (22%)
8	GDP	D	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.96	8 (25%)
12	5JS	D	503	-	50,51,51	2.63	7 (14%)	55,74,74	1.96	14 (25%)
10	GOL	B	505	-	5,5,5	0.84	0	5,5,5	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
13	ACP	F	401	6	-	7/15/38/38	0/3/3/3
11	IMD	C	504	-	-	-	0/1/1/1
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
12	5JS	D	503	-	-	15/48/72/72	0/3/5/5
10	GOL	B	505	-	-	4/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	5JS	C20-C14	-13.29	1.34	1.50
12	D	503	5JS	C14-N16	9.68	1.44	1.28
9	B	504	MES	C8-S	-7.46	1.66	1.77
13	F	401	ACP	PG-O1G	5.43	1.61	1.50
8	B	501	GDP	C5-C6	4.19	1.48	1.41
8	D	501	GDP	C5-C6	4.14	1.48	1.41
13	F	401	ACP	PB-O1B	4.08	1.61	1.51
12	D	503	5JS	C25-C23	3.87	1.52	1.47
12	D	503	5JS	O29-C23	-3.85	1.40	1.45
13	F	401	ACP	PB-O3A	3.47	1.62	1.58
13	F	401	ACP	PB-O2B	-3.45	1.48	1.56
5	A	501	GTP	C6-N1	3.20	1.38	1.33
5	C	501	GTP	C6-N1	3.05	1.38	1.33
13	F	401	ACP	PG-O2G	-2.87	1.48	1.54
12	D	503	5JS	C5-N31	-2.82	1.40	1.44
13	F	401	ACP	PG-O3G	2.76	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	5JS	C17-N16	2.73	1.41	1.34
13	F	401	ACP	C5-C4	2.44	1.47	1.40
8	D	501	GDP	C5-C4	2.40	1.47	1.40
8	B	501	GDP	C5-C4	2.34	1.47	1.40
12	D	503	5JS	C27-C26	2.05	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	503	5JS	C25-O29-C23	6.36	64.62	60.79
5	C	501	GTP	N3-C2-N1	-5.36	120.07	127.22
5	A	501	GTP	N3-C2-N1	-5.27	120.19	127.22
8	D	501	GDP	C2-N3-C4	4.83	120.87	115.36
8	B	501	GDP	C2-N3-C4	4.82	120.86	115.36
12	D	503	5JS	O30-C26-C25	4.80	116.32	105.48
12	D	503	5JS	O29-C25-C23	-4.69	56.23	59.38
12	D	503	5JS	C6-C5-N31	4.20	125.02	120.71
5	A	501	GTP	C2-N3-C4	4.19	120.14	115.36
8	B	501	GDP	C2-N1-C6	4.15	122.52	115.93
8	D	501	GDP	C2-N1-C6	4.12	122.48	115.93
5	C	501	GTP	C2-N3-C4	4.03	119.96	115.36
8	D	501	GDP	C5-C6-N1	-4.02	117.94	123.43
8	B	501	GDP	C4-C5-C6	-4.00	116.98	120.80
8	B	501	GDP	C5-C6-N1	-3.98	117.99	123.43
8	D	501	GDP	C4-C5-C6	-3.89	117.08	120.80
9	B	504	MES	C5-N4-C3	3.78	117.35	108.83
12	D	503	5JS	C19-C20-C14	3.72	122.68	112.00
12	D	503	5JS	C26-O30-C39	3.68	124.86	117.92
13	F	401	ACP	C3'-C2'-C1'	3.59	106.38	100.98
12	D	503	5JS	C20-C14-C13	3.57	126.38	116.61
8	B	501	GDP	N3-C2-N1	-3.43	122.64	127.22
8	D	501	GDP	N3-C2-N1	-3.38	122.72	127.22
5	C	501	GTP	PA-O3A-PB	-3.35	121.34	132.83
9	B	504	MES	O1S-S-C8	3.29	110.88	106.92
5	A	501	GTP	PA-O3A-PB	-3.18	121.90	132.83
13	F	401	ACP	N3-C2-N1	-3.03	123.94	128.68
8	D	501	GDP	PA-O3A-PB	-3.01	122.51	132.83
8	B	501	GDP	PA-O3A-PB	-2.95	122.71	132.83
5	C	501	GTP	C5-C6-N1	-2.94	119.41	123.43
5	A	501	GTP	C5-C6-N1	-2.92	119.43	123.43
12	D	503	5JS	O18-C19-C22	2.87	111.73	105.76
9	B	504	MES	C6-C5-N4	-2.87	105.75	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	501	GTP	PB-O3B-PG	-2.85	123.06	132.83
8	D	501	GDP	C4-C5-N7	-2.71	106.57	109.40
5	A	501	GTP	PB-O3B-PG	-2.70	123.56	132.83
5	C	501	GTP	C2-N1-C6	2.69	120.20	115.93
12	D	503	5JS	C27-C28-N31	-2.66	115.89	118.89
8	B	501	GDP	C4-C5-N7	-2.63	106.66	109.40
5	A	501	GTP	C2-N1-C6	2.56	120.00	115.93
13	F	401	ACP	PB-O3A-PA	-2.53	124.54	132.56
8	D	501	GDP	C3'-C2'-C1'	2.52	104.77	100.98
13	F	401	ACP	C4-C5-N7	-2.49	106.81	109.40
12	D	503	5JS	O30-C39-C40	2.24	115.76	110.99
9	B	504	MES	O3S-S-C8	2.18	109.30	105.77
12	D	503	5JS	C5-C6-CL33	2.18	122.40	120.09
12	D	503	5JS	O34-C1-C6	2.17	118.10	115.53
12	D	503	5JS	O34-C1-C2	-2.14	120.44	124.12
9	B	504	MES	C7-N4-C5	2.14	116.70	111.23
12	D	503	5JS	C4-C5-C6	-2.04	119.94	122.53

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-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
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
10	B	505	GOL	O1-C1-C2-C3
12	D	503	5JS	C11-C12-C13-C14
12	D	503	5JS	C14-C13-O15-C37
12	D	503	5JS	C6-C1-O34-C36
12	D	503	5JS	C20-C19-C22-C24
12	D	503	5JS	O18-C19-C22-C24
12	D	503	5JS	C38-C25-C26-O30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	D	503	5JS	C25-C26-O30-C39
12	D	503	5JS	C40-C39-O30-C26
13	F	401	ACP	PG-C3B-PB-O1B
13	F	401	ACP	PG-C3B-PB-O2B
13	F	401	ACP	PG-C3B-PB-O3A
12	D	503	5JS	O41-C39-O30-C26
13	F	401	ACP	O4'-C4'-C5'-O5'
13	F	401	ACP	C3'-C4'-C5'-O5'
12	D	503	5JS	C2-C1-O34-C36
12	D	503	5JS	C27-C26-O30-C39
10	B	505	GOL	C1-C2-C3-O3
10	B	505	GOL	O2-C2-C3-O3
12	D	503	5JS	O18-C19-C22-C23
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
12	D	503	5JS	O30-C26-C27-C28
10	B	505	GOL	O1-C1-C2-O2
12	D	503	5JS	C20-C19-C22-C23
5	C	501	GTP	C4'-C5'-O5'-PA
13	F	401	ACP	PB-C3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
13	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
12	D	503	5JS	C26-C27-C28-N31

There are no ring outliers.

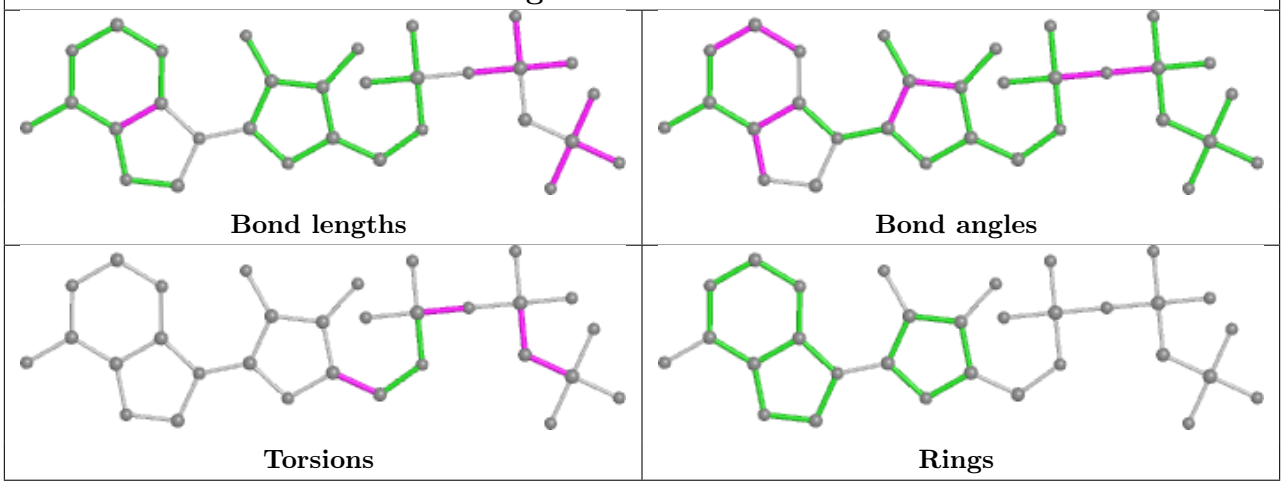
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	MES	3	0
13	F	401	ACP	2	0
5	C	501	GTP	1	0
5	A	501	GTP	2	0
8	D	501	GDP	2	0

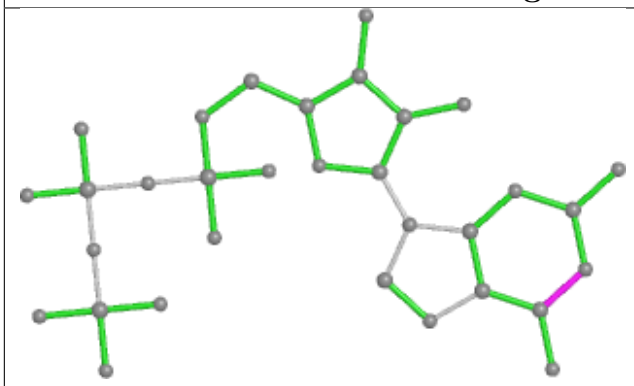
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

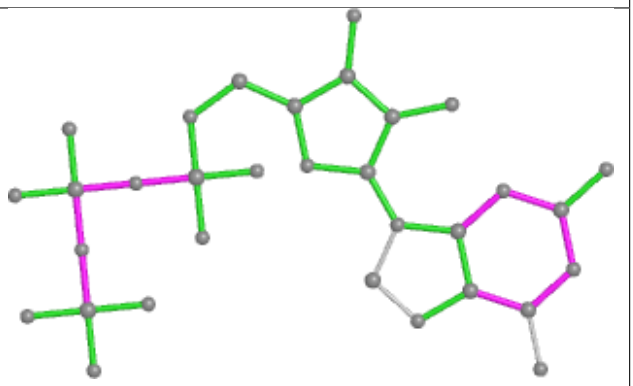
Ligand ACP F 401



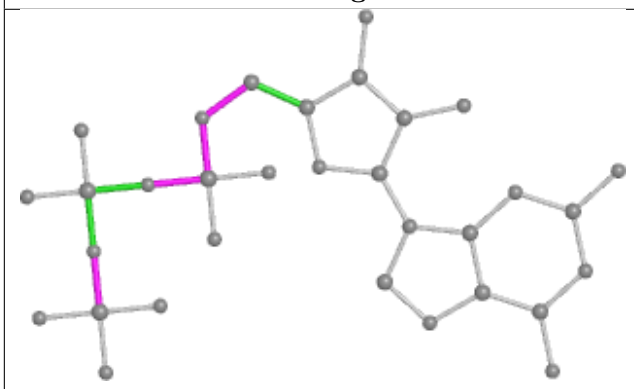
Ligand GTP C 501



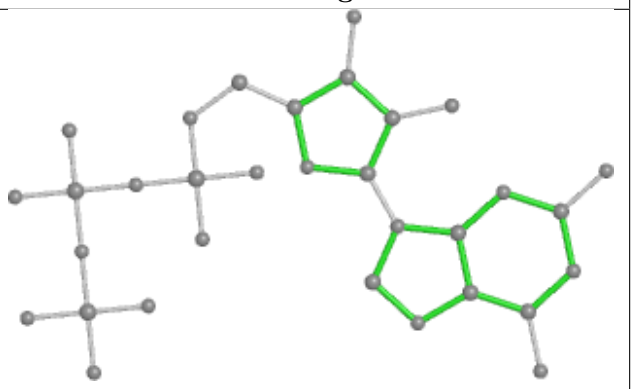
Bond lengths



Bond angles

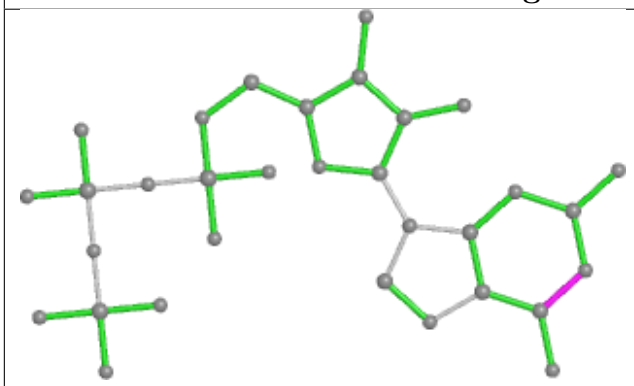


Torsions

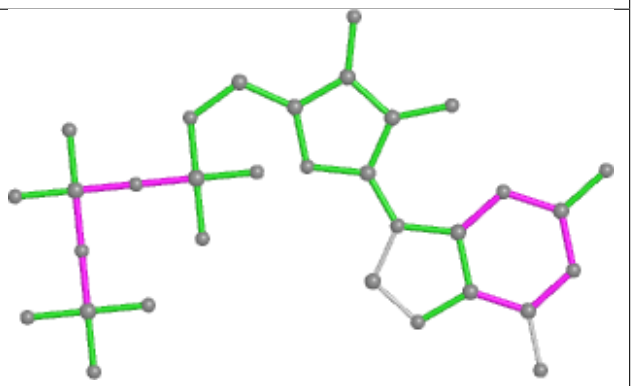


Rings

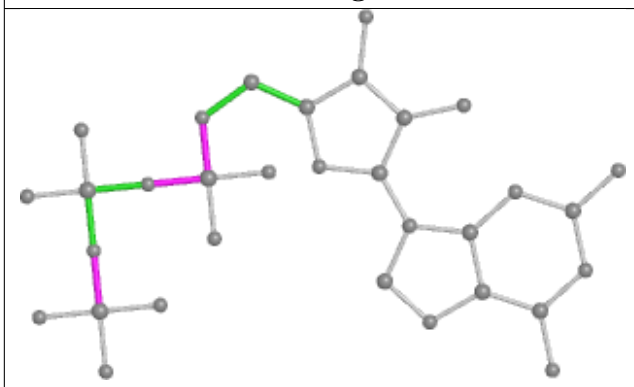
Ligand GTP A 501



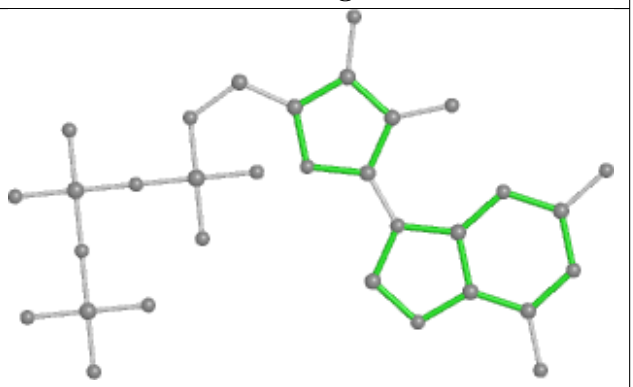
Bond lengths



Bond angles

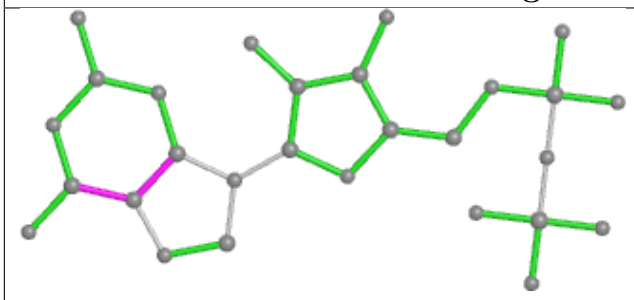


Torsions

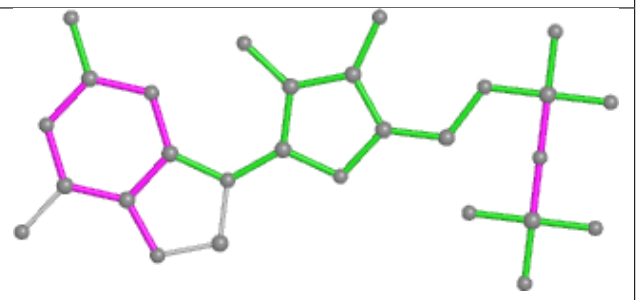


Rings

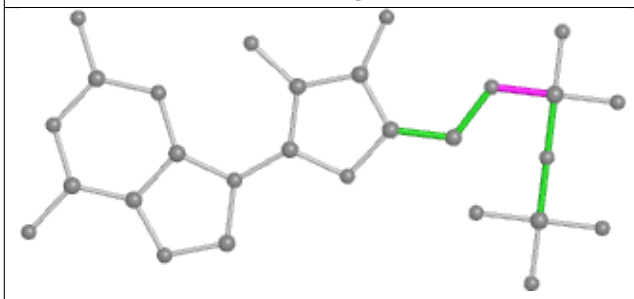
Ligand GDP B 501



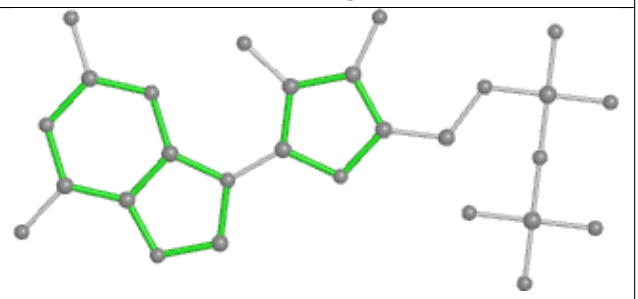
Bond lengths



Bond angles

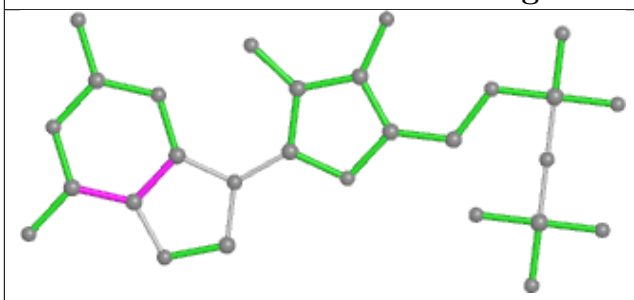


Torsions

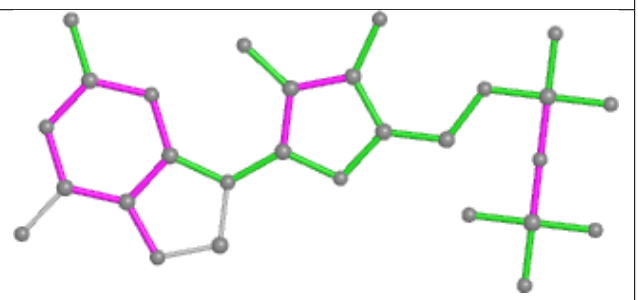


Rings

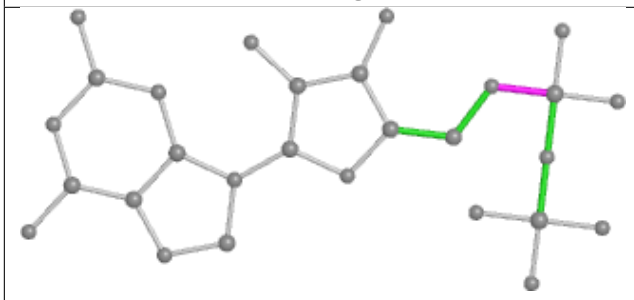
Ligand GDP D 501



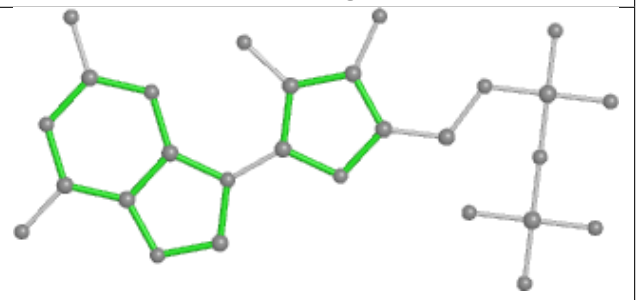
Bond lengths



Bond angles

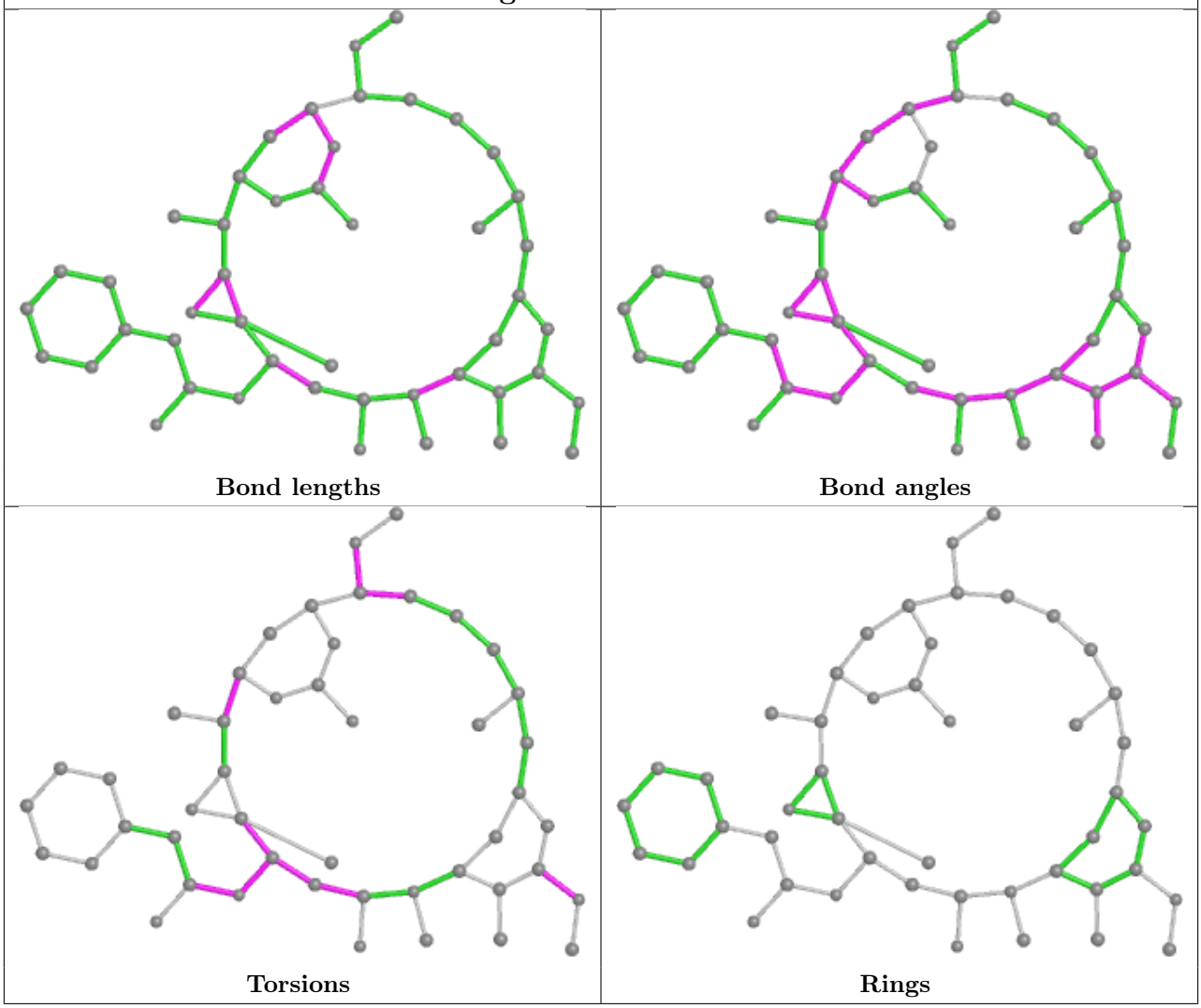


Torsions



Rings

Ligand 5JS D 503



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	438/451 (97%)	0.29	21 (4%) 30 38	42, 59, 93, 155	0
1	C	440/451 (97%)	0.06	4 (0%) 84 88	34, 46, 72, 118	0
2	B	423/445 (95%)	0.23	17 (4%) 38 45	34, 54, 90, 141	0
2	D	426/445 (95%)	0.40	32 (7%) 14 19	45, 71, 109, 139	0
3	E	121/143 (84%)	0.40	11 (9%) 9 12	51, 73, 112, 131	0
4	F	341/384 (88%)	1.40	109 (31%) 0 0	55, 87, 149, 178	0
All	All	2189/2319 (94%)	0.43	194 (8%) 9 13	34, 63, 115, 178	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	8.7
1	A	282	TYR	8.7
4	F	132	LEU	8.3
4	F	251	LYS	8.2
4	F	161	LEU	8.1
4	F	249	TYR	7.3
4	F	244	CYS	7.1
4	F	169	LEU	6.9
4	F	166	ALA	6.6
4	F	131	PHE	6.5
4	F	253	TYR	6.5
3	E	27	PRO	6.4
4	F	232	ASN	6.1
4	F	173	ILE	6.0
4	F	170	LEU	6.0
4	F	233	PHE	5.9
4	F	130	VAL	5.8
4	F	134	ALA	5.8
4	F	250	SER	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	59	ASN	5.8
4	F	135	TYR	5.7
4	F	162	ILE	5.6
2	D	277	SER	5.4
4	F	165	GLU	5.4
4	F	243	HIS	5.2
2	B	57	THR	5.1
2	D	57	THR	4.9
4	F	259	GLY	4.9
4	F	240	LEU	4.8
4	F	133	ALA	4.7
1	A	262	TYR	4.6
4	F	99	VAL	4.6
4	F	231	ALA	4.6
4	F	252	ASN	4.6
3	E	139	LEU	4.6
4	F	138	ARG	4.5
4	F	17	VAL	4.4
3	E	26	PRO	4.4
4	F	142	ARG	4.4
4	F	254	GLY	4.4
4	F	137	ARG	4.3
4	F	245	ILE	4.3
4	F	234	GLN	4.2
4	F	125	THR	4.2
4	F	101	TYR	4.2
4	F	20	LEU	4.1
4	F	100	ILE	4.1
4	F	223	THR	4.1
4	F	192	LEU	4.1
4	F	256	TYR	4.0
4	F	361	LEU	4.0
1	C	440	VAL	4.0
2	B	60	LYS	4.0
1	C	340	SER	4.0
1	A	346	TRP	3.9
4	F	143	GLU	3.8
4	F	194	PRO	3.8
4	F	246	GLN	3.8
2	B	284	ARG	3.7
2	D	1	MET	3.7
4	F	129	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	33	THR	3.6
4	F	248	GLU	3.6
2	B	58	GLY	3.6
4	F	199	PHE	3.5
4	F	32	LYS	3.5
4	F	147	TRP	3.5
2	D	401	ARG	3.5
2	B	37	HIS	3.5
2	D	37	HIS	3.5
2	D	60	LYS	3.5
4	F	163	SER	3.4
4	F	167	SER	3.4
4	F	225	SER	3.4
4	F	236	LYS	3.4
4	F	224	SER	3.4
4	F	191	LEU	3.4
2	D	221	THR	3.3
4	F	182	ILE	3.3
2	D	94	PHE	3.3
4	F	31	ARG	3.3
1	A	283	HIS	3.2
4	F	190	LEU	3.2
4	F	172	PHE	3.2
4	F	346	LEU	3.2
1	A	83	TYR	3.2
2	D	177	VAL	3.2
4	F	198	LYS	3.2
4	F	255	ARG	3.2
4	F	196	HIS	3.1
2	B	34	GLY	3.1
3	E	24	LEU	3.1
4	F	164	SER	3.0
4	F	21	LEU	3.0
4	F	13	VAL	3.0
4	F	146	VAL	3.0
2	D	405	LEU	2.9
4	F	24	THR	2.9
4	F	228	TYR	2.9
4	F	242	ASN	2.9
2	B	36	TYR	2.9
2	D	415	GLU	2.8
4	F	263	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	267	PHE	2.8
4	F	181	VAL	2.8
4	F	262	MET	2.8
4	F	260	ASN	2.8
4	F	362	ALA	2.8
2	D	400	ARG	2.8
3	E	25	LYS	2.8
4	F	25	GLY	2.8
4	F	197	ARG	2.8
4	F	239	HIS	2.7
2	D	219	LEU	2.7
4	F	19	ARG	2.7
2	B	38	GLY	2.7
4	F	247	LYS	2.7
4	F	379	HIS	2.7
3	E	48	GLU	2.7
2	B	56	ALA	2.7
4	F	339	ALA	2.7
2	D	404	PHE	2.7
4	F	221	LEU	2.7
4	F	237	THR	2.7
2	D	88	ARG	2.6
1	A	171	ILE	2.6
4	F	258	GLU	2.6
4	F	6	VAL	2.6
4	F	136	ASN	2.6
4	F	264	PHE	2.6
4	F	152	SER	2.6
1	A	364	PRO	2.6
3	E	28	SER	2.5
2	D	83	PHE	2.5
4	F	4	PHE	2.5
4	F	139	ARG	2.5
2	B	62	VAL	2.5
4	F	9	GLU	2.5
2	D	56	ALA	2.5
2	D	96	GLN	2.5
1	A	180	ALA	2.5
2	B	276	THR	2.5
1	C	253	THR	2.4
3	E	140	LYS	2.4
4	F	340	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	257	GLU	2.4
4	F	141	GLY	2.4
3	E	135	LYS	2.4
2	D	202	TYR	2.4
4	F	201	ILE	2.4
2	D	74	THR	2.3
2	D	218	LYS	2.3
1	A	12	ALA	2.3
4	F	337	ALA	2.3
2	D	256	ALA	2.3
2	D	402	LYS	2.3
4	F	168	GLU	2.3
2	B	437	ASP	2.3
2	D	276	THR	2.2
1	C	1	MET	2.2
4	F	10	ASN	2.2
4	F	140	GLU	2.2
1	A	146	GLY	2.2
2	D	220	THR	2.2
4	F	22	LEU	2.2
2	D	97	SER	2.2
4	F	180	HIS	2.2
1	A	142	GLY	2.2
1	A	82	THR	2.2
1	A	172	TYR	2.2
2	D	59	ASN	2.2
2	D	58	GLY	2.2
1	A	362	VAL	2.1
1	A	140	SER	2.1
4	F	229	ASN	2.1
1	A	178	SER	2.1
2	D	252	LEU	2.1
1	A	281	ALA	2.1
4	F	220	VAL	2.1
3	E	45	PRO	2.1
1	A	42	ILE	2.1
4	F	342	LEU	2.1
4	F	343	TYR	2.1
1	A	348	PRO	2.1
4	F	102	PRO	2.1
2	B	86	ILE	2.0
4	F	341	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	170	SER	2.0
3	E	133	VAL	2.0
2	D	99	ALA	2.0
1	A	177	VAL	2.0
2	B	49	ILE	2.0
2	D	255	LEU	2.0
2	D	75	MET	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
10	GOL	B	505	6/6	0.80	0.25	68,90,103,108	0
12	5JS	D	503	47/47	0.84	0.31	79,94,105,112	0
7	CA	E	201	1/1	0.88	0.07	99,99,99,99	0
11	IMD	C	504	5/5	0.92	0.17	60,70,81,84	0
7	CA	B	503	1/1	0.92	0.24	99,99,99,99	0
13	ACP	F	401	31/31	0.92	0.15	85,100,114,124	0
6	MG	D	502	1/1	0.93	0.05	65,65,65,65	0
8	GDP	D	501	28/28	0.95	0.12	57,66,85,101	0
6	MG	F	402	1/1	0.96	0.08	85,85,85,85	0
6	MG	C	502	1/1	0.98	0.17	38,38,38,38	0
8	GDP	B	501	28/28	0.98	0.20	33,39,47,50	0
5	GTP	A	501	32/32	0.98	0.21	32,41,52,58	0
9	MES	B	504	12/12	0.98	0.12	38,50,67,74	0
6	MG	A	502	1/1	0.98	0.18	42,42,42,42	0
7	CA	A	503	1/1	0.98	0.03	75,75,75,75	0
6	MG	B	502	1/1	0.98	0.20	34,34,34,34	0

Continued on next page...

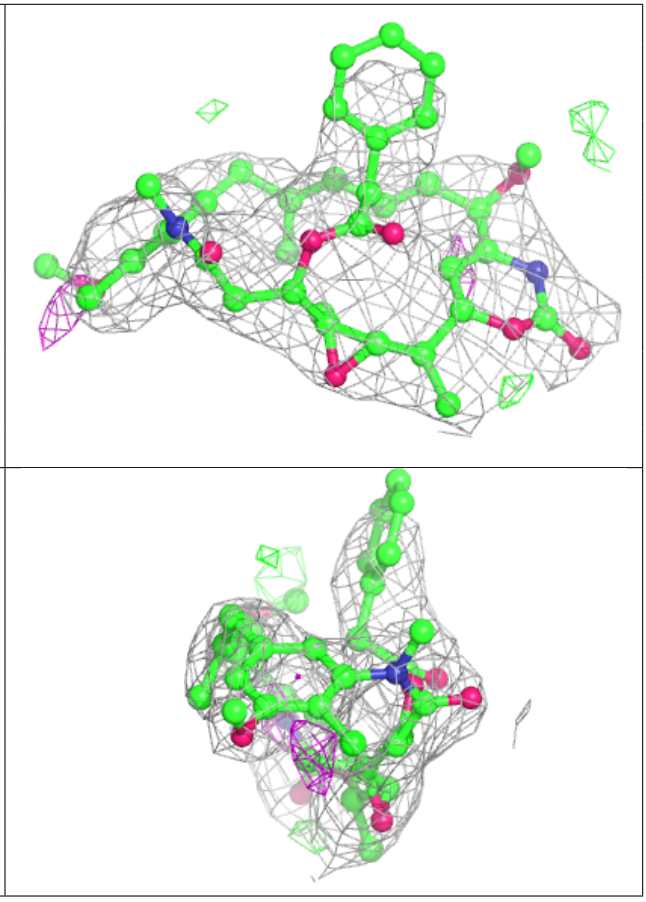
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	C	503	1/1	0.98	0.09	62,62,62,62	0
5	GTP	C	501	32/32	0.99	0.17	33,37,46,49	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.

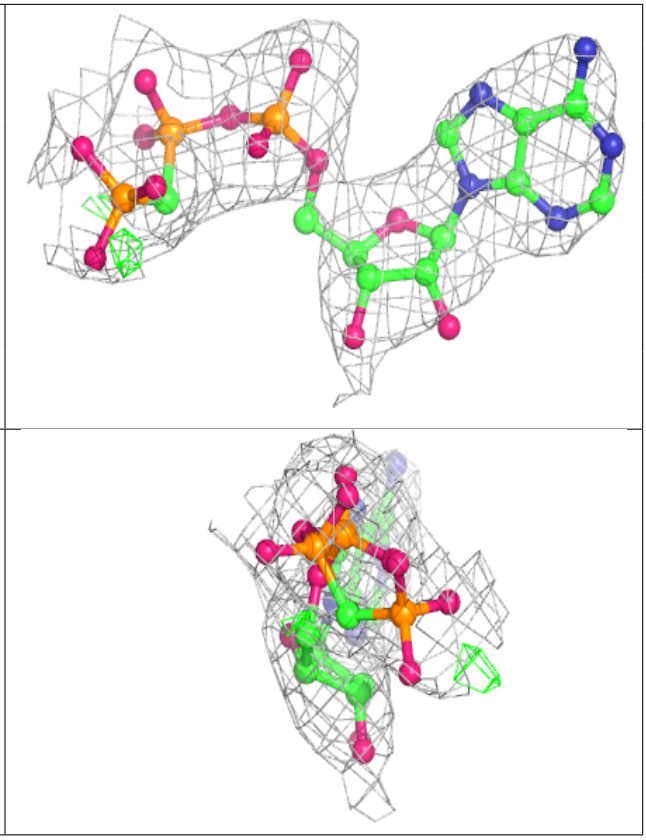
Electron density around 5JS D 503:

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



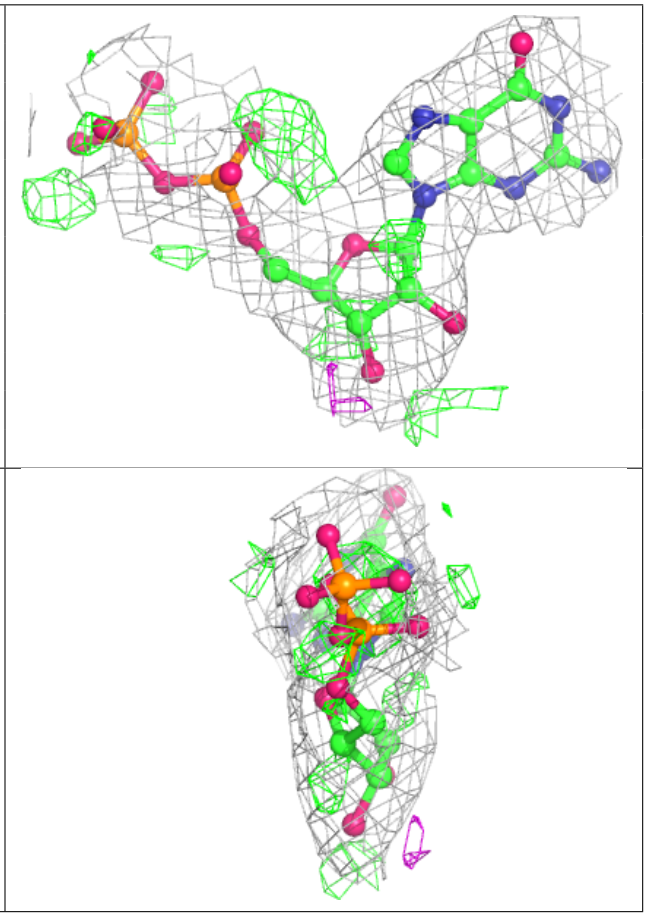
Electron density around ACP F 401:

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



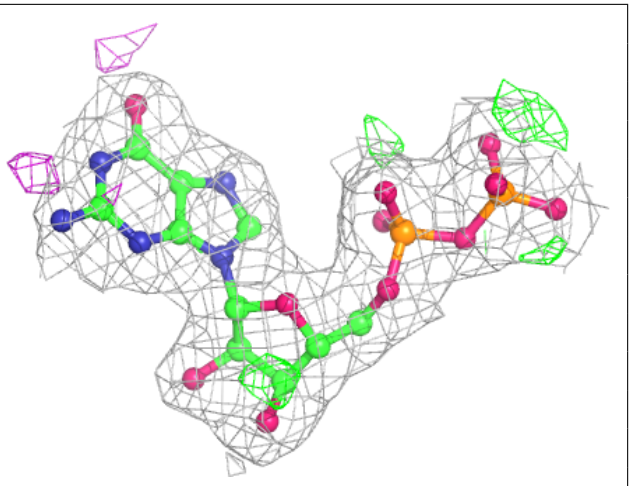
Electron density around GDP D 501:

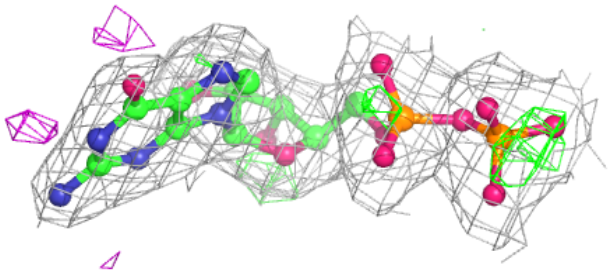
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

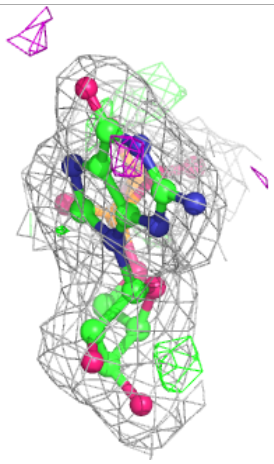


Electron density around GDP B 501:

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

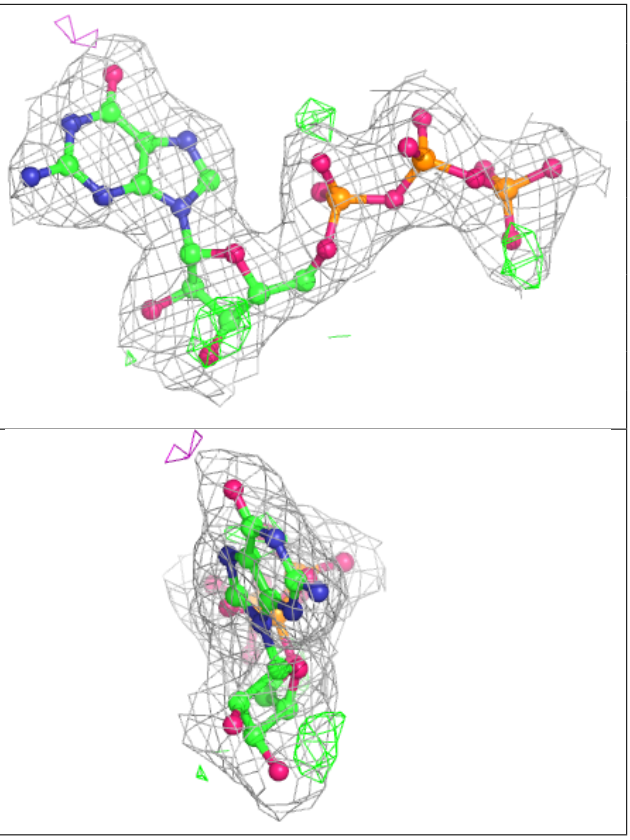


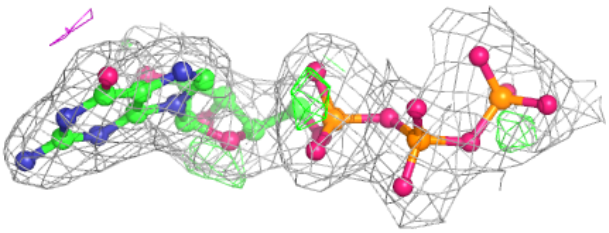




Electron density around GTP A 501:

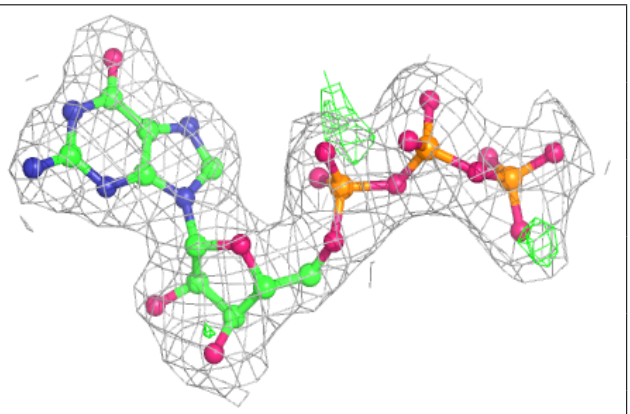
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

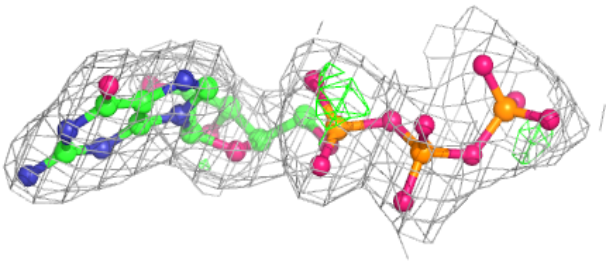


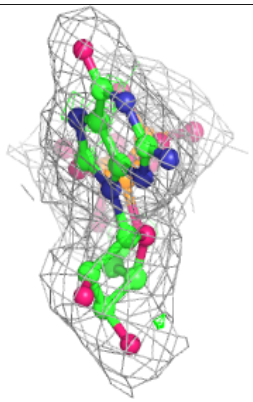


Electron density around GTP C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.