



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:09 am BST

PDB ID : 6FII
Title : Tubulin-Spongistatin complex
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Deposited on : 2018-01-18
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

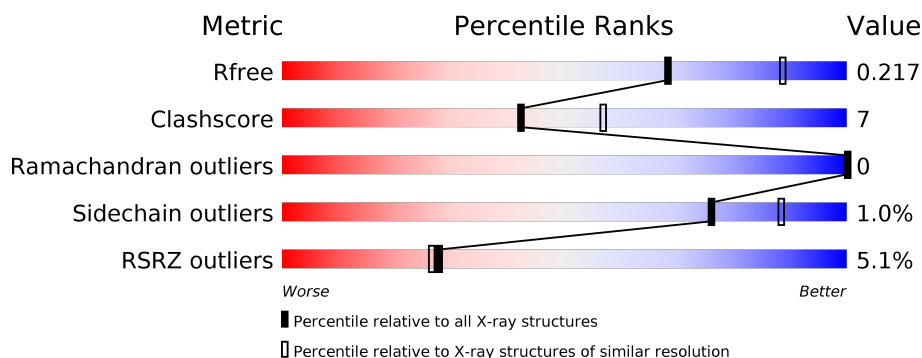
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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 $\leq 5\%$. 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 83%, yellow 14%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 83% 14% • </div> </div>
1	C	451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 85%, yellow 12%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 85% 12% • </div> </div>
2	B	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 81%, yellow 14%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 14% 5% </div> </div>
2	D	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 75%, yellow 20%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 75% 20% 5% </div> </div>
3	E	143	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, green 75%, yellow 10%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 75% 10% • 14% </div> </div>
4	F	384	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 20%, green 76%, yellow 15%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 20% 76% 15% 9% </div> </div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18343 atoms, of which 131 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3339	2099	569	644	27			
2	D	423	Total	C	N	O	S	0	0	0
			3321	2087	564	643	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

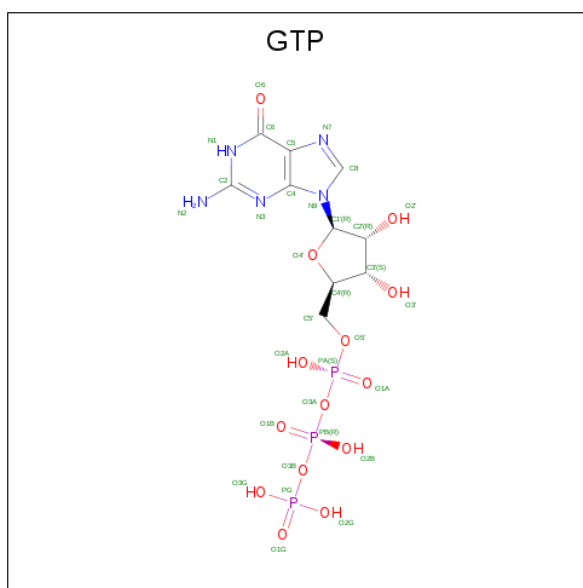
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	0	0
			2846	1824	486	522	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

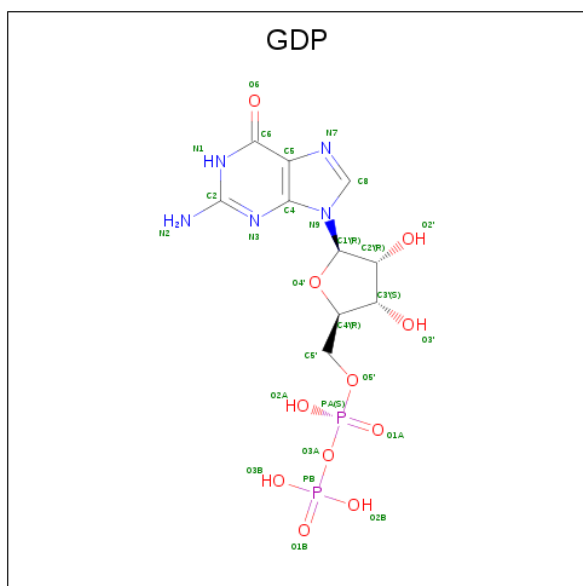
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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



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

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



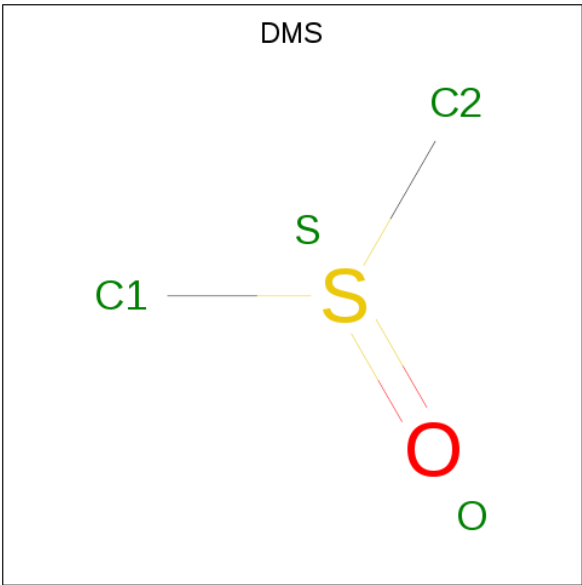
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



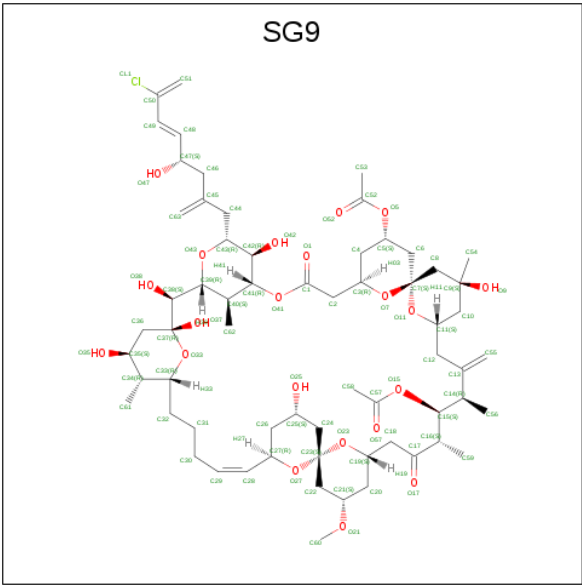
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			14	3	8	3		
10	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 11 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



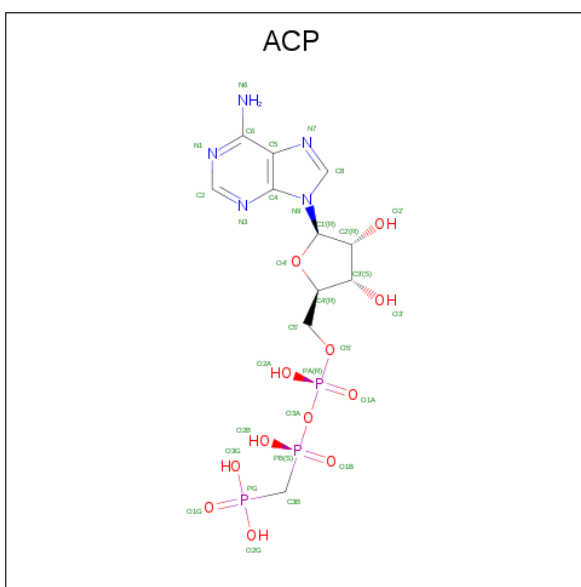
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
11	C	1	10	2	6	1	1	0	0

- Molecule 12 is Spongistatin-1 (three-letter code: SG9) (formula: $C_{63}H_{95}ClO_{21}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	H	O		
12	D	1	180	63	1	95	21	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	
13	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

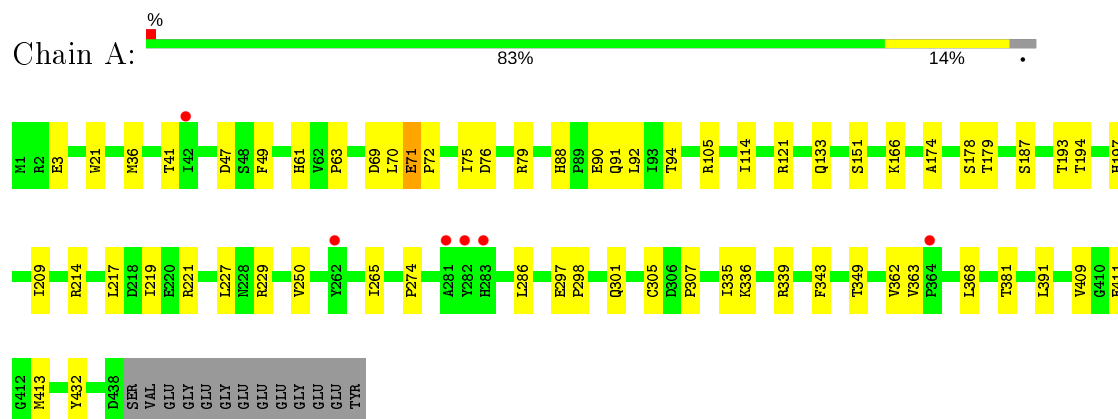
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	110	Total O 110 110	0	0
14	B	103	Total O 103 103	0	0
14	C	212	Total O 212 212	0	0
14	D	68	Total O 68 68	0	0
14	E	29	Total O 29 29	0	0
14	F	37	Total O 37 37	0	0

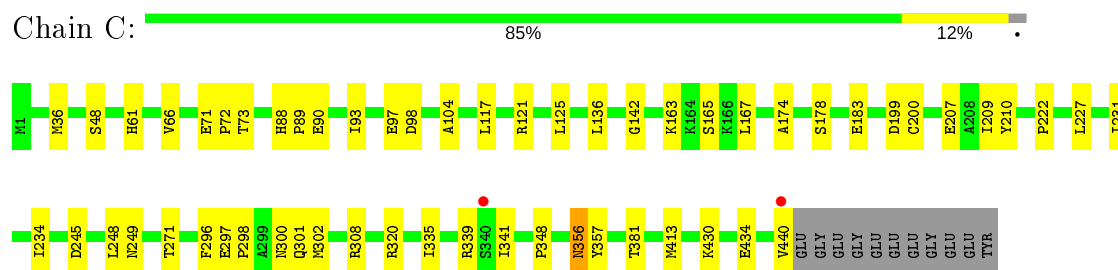
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

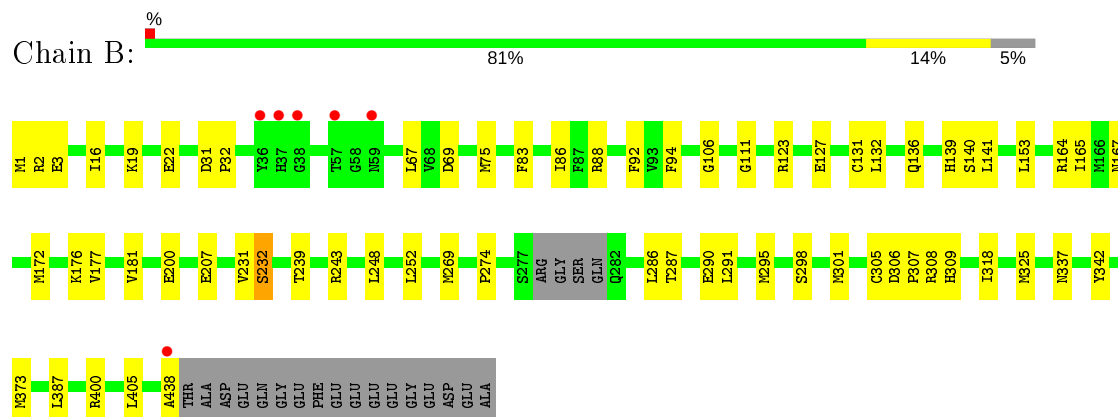
- Molecule 1: Tubulin alpha-1B chain



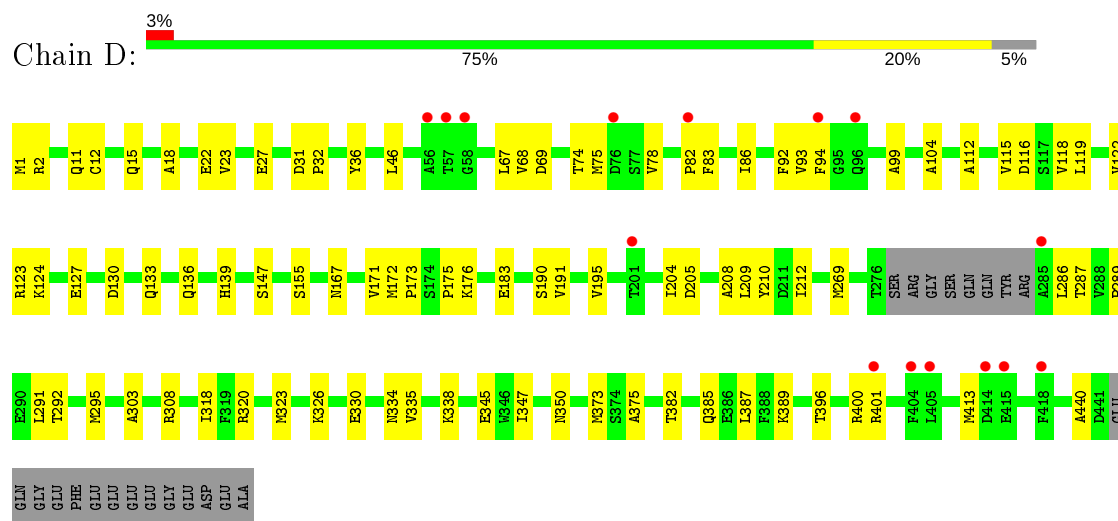
- Molecule 1: Tubulin alpha-1B chain



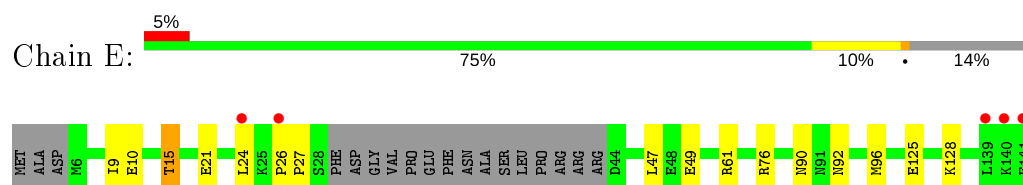
- Molecule 2: Tubulin beta-2B chain



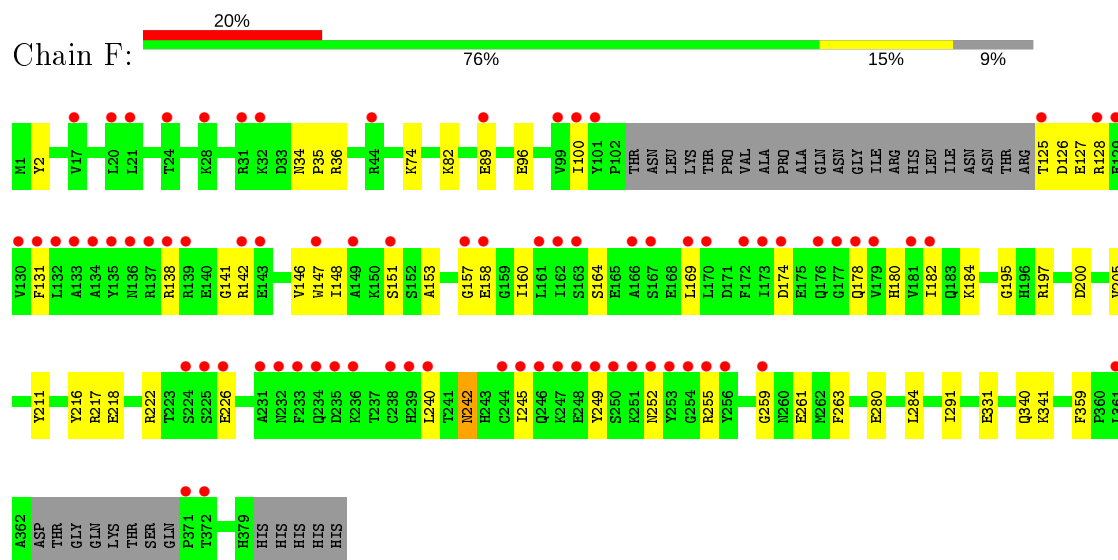
- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.67Å 159.92Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.17 – 2.40 50.17 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.17-2.40) 96.7 (50.17-2.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_2875: ???)	Depositor
R, R_{free}	0.168 , 0.216 0.169 , 0.217	Depositor DCC
R_{free} test set	5768 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18343	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SG9, GOL, MG, CA, GDP, GTP, DMS, MES, ACP

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	0.29	0/3502	0.46	0/4754
1	C	0.32	0/3515	0.50	0/4772
2	B	0.31	0/3413	0.47	0/4622
2	D	0.27	0/3394	0.45	0/4598
3	E	0.27	0/1022	0.39	0/1356
4	F	0.26	0/2911	0.44	0/3932
All	All	0.29	0/17757	0.46	0/24034

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	3424	0	3335	39	0
1	C	3437	0	3348	41	0
2	B	3339	0	3220	50	0
2	D	3321	0	3201	55	0
3	E	1014	0	1029	12	0
4	F	2846	0	2817	48	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
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	1	0
9	B	12	0	12	0	0
10	B	12	16	16	2	0
11	C	4	6	6	0	0
12	D	85	95	0	3	0
13	F	31	14	14	1	0
14	A	110	0	0	2	0
14	B	103	0	0	4	0
14	C	212	0	0	0	0
14	D	68	0	0	2	0
14	E	29	0	0	0	0
14	F	37	0	0	1	0
All	All	18212	131	17046	239	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 7.

All (239) 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)
1:C:97:GLU:HG3	2:D:1:MET:HG3	1.59	0.83
14:A:642:HOH:O	3:E:15:THR:HG22	1.82	0.80
13:F:401:ACP:H5'1	13:F:401:ACP:H8	1.63	0.79
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.64	0.79
2:D:323:MET:HB3	2:D:373:MET:HE2	1.68	0.75
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.68	0.73
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.75	0.69
2:D:82:PRO:O	2:D:83:PHE:HB2	1.91	0.69
2:D:83:PHE:O	2:D:86:ILE:HG22	1.93	0.68
4:F:263:PHE:CE2	4:F:341:LYS:HE2	2.30	0.67
2:D:123:ARG:O	2:D:127:GLU:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.78	0.65
2:D:323:MET:HB3	2:D:373:MET:CE	2.26	0.65
2:D:173:PRO:HB3	2:D:183:GLU:OE1	1.97	0.65
1:A:166:LYS:HE2	1:A:197:HIS:O	1.96	0.65
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.79	0.65
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.34	0.63
4:F:126:ASP:OD1	4:F:127:GLU:N	2.32	0.63
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.81	0.62
2:B:136:GLN:HA	2:B:167:ASN:O	2.00	0.61
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.82	0.61
4:F:158:GLU:HA	4:F:158:GLU:OE1	2.00	0.61
1:A:229:ARG:HH12	1:A:363:VAL:HG11	1.66	0.61
1:A:229:ARG:NH1	1:A:363:VAL:HG11	2.16	0.61
2:B:176:LYS:HD2	14:B:622:HOH:O	2.01	0.60
2:B:83:PHE:O	2:B:86:ILE:HG22	2.01	0.60
2:D:191:VAL:O	2:D:195:VAL:HG23	2.01	0.60
2:D:99:ALA:HB3	14:D:606:HOH:O	2.02	0.60
1:A:411:GLU:O	3:E:61:ARG:HD3	2.02	0.59
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.38	0.59
2:B:19:LYS:HB3	2:B:232:SER:OG	2.03	0.59
2:B:132:LEU:HB3	2:B:164:ARG:NH1	2.17	0.58
4:F:153:ALA:HB3	4:F:178:GLN:OE1	2.04	0.58
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.84	0.58
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.04	0.58
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.87	0.57
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.87	0.57
1:A:174:ALA:O	1:A:178:SER:HB3	2.05	0.57
1:C:71:GLU:OE2	1:C:73:THR:HB	2.04	0.57
2:D:326:LYS:O	2:D:330:GLU:HG3	2.05	0.57
2:D:286:LEU:HD23	2:D:291:LEU:HG	1.87	0.56
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.56
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.06	0.56
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.71	0.56
2:D:176:LYS:HD3	2:D:210:TYR:CD2	2.41	0.56
2:D:318:ILE:N	2:D:318:ILE:HD12	2.21	0.55
2:D:147:SER:HB2	2:D:190:SER:OG	2.06	0.55
3:E:47:LEU:HD12	3:E:47:LEU:O	2.07	0.55
4:F:157:GLY:CA	4:F:245:ILE:HD11	2.37	0.55
2:D:1:MET:HB3	2:D:133:GLN:HG2	1.88	0.55
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.88	0.55
2:D:205:ASP:O	2:D:209:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:OE2	1:C:73:THR:CB	2.55	0.54
2:D:136:GLN:HA	2:D:167:ASN:O	2.06	0.54
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.43	0.54
2:D:308:ARG:NH1	14:D:604:HOH:O	2.41	0.54
2:B:1:MET:N	2:B:131:CYS:SG	2.69	0.54
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.90	0.54
2:B:176:LYS:HE3	2:B:207:GLU:OE2	2.08	0.54
2:D:208:ALA:O	2:D:212:ILE:HG13	2.08	0.54
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.43	0.53
2:B:2:ARG:HG3	2:B:3:GLU:N	2.22	0.53
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.44	0.53
2:D:2:ARG:HD2	2:D:130:ASP:HB3	1.91	0.53
1:A:297:GLU:OE1	1:A:297:GLU:HA	2.09	0.53
4:F:96:GLU:CB	4:F:184:LYS:HE3	2.37	0.53
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.90	0.53
2:D:396:THR:O	2:D:400:ARG:HG2	2.09	0.53
1:A:3:GLU:O	1:A:133:GLN:HG2	2.09	0.53
1:A:71:GLU:HG2	1:A:72:PRO:N	2.23	0.52
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.09	0.52
2:B:88:ARG:HD2	14:B:642:HOH:O	2.10	0.52
4:F:245:ILE:HG23	4:F:249:TYR:HD2	1.74	0.52
1:C:227:LEU:O	1:C:231:ILE:HG13	2.09	0.52
1:C:320:ARG:HA	1:C:356:ASN:O	2.10	0.52
12:D:502:SG9:O17	12:D:502:SG9:O25	2.28	0.52
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.45	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.45	0.52
4:F:263:PHE:CD2	4:F:341:LYS:HE2	2.44	0.52
2:D:118:VAL:O	2:D:122:VAL:HG23	2.10	0.51
3:E:26:PRO:HB2	3:E:27:PRO:HD2	1.91	0.51
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.45	0.51
2:D:112:ALA:O	2:D:115:VAL:HG12	2.11	0.51
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.45	0.51
1:A:179:THR:HA	2:B:248:LEU:HD12	1.92	0.51
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.46	0.50
1:C:142:GLY:CA	1:C:183:GLU:HG2	2.41	0.50
2:D:124:LYS:C	2:D:124:LYS:HD3	2.32	0.50
1:A:214:ARG:HG2	1:A:219:ILE:O	2.11	0.50
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.12	0.50
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.92	0.50
1:C:234:ILE:HD13	1:C:302:MET:SD	2.52	0.50
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.39	0.49
4:F:151:SER:HB3	4:F:180:HIS:NE2	2.27	0.49
1:C:178:SER:HB2	1:C:183:GLU:OE1	2.12	0.49
4:F:89:GLU:O	4:F:89:GLU:HG2	2.13	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.49
2:B:132:LEU:HD23	2:B:164:ARG:HH11	1.78	0.49
2:B:141:LEU:HD12	2:B:172:MET:SD	2.52	0.49
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.95	0.48
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.94	0.48
2:B:177:VAL:HG13	10:B:504:GOL:H32	1.95	0.48
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.44	0.48
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.14	0.48
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.96	0.48
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.48
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.96	0.48
1:A:91:GLN:C	1:A:92:LEU:HD23	2.34	0.48
3:E:125:GLU:HA	3:E:125:GLU:OE1	2.13	0.48
2:D:75:MET:SD	2:D:94:PHE:HB3	2.54	0.48
2:B:298:SER:HA	2:B:301:MET:HG3	1.96	0.47
1:A:221:ARG:HG3	2:B:325:MET:HG2	1.97	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.44	0.47
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.43	0.47
1:A:305:CYS:O	1:A:307:PRO:HD3	2.14	0.47
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.96	0.47
1:C:296:PHE:CE2	1:C:341:ILE:HD11	2.50	0.47
3:E:92:ASN:O	3:E:96:MET:HG2	2.14	0.47
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.39	0.47
4:F:138:ARG:HH21	4:F:184:LYS:NZ	2.12	0.47
1:A:70:LEU:CD2	1:A:114:ILE:HD12	2.44	0.47
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.48	0.47
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.48	0.47
2:B:239:THR:O	2:B:243:ARG:HG3	2.15	0.47
1:C:165:SER:HA	1:C:199:ASP:OD2	2.14	0.47
4:F:280:GLU:HB2	14:F:515:HOH:O	2.14	0.47
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.50	0.47
4:F:240:LEU:HD12	4:F:245:ILE:CD1	2.45	0.47
2:D:18:ALA:O	2:D:22:GLU:HG3	2.15	0.46
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.97	0.46
4:F:96:GLU:HB2	4:F:184:LYS:HE3	1.97	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.97	0.46
2:B:69:ASP:O	2:B:94:PHE:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:HG3	3:E:90:ASN:OD1	2.16	0.46
4:F:126:ASP:OD1	4:F:128:ARG:N	2.48	0.46
4:F:157:GLY:HA2	4:F:245:ILE:HD11	1.96	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.46
2:B:295:MET:HE3	2:B:295:MET:HB2	1.76	0.46
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.98	0.46
2:D:320:ARG:O	2:D:373:MET:HA	2.16	0.46
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.97	0.46
2:B:305:CYS:O	2:B:307:PRO:HD3	2.16	0.46
1:A:362:VAL:HG22	14:A:613:HOH:O	2.15	0.45
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.49	0.45
4:F:96:GLU:HB3	4:F:184:LYS:HE3	1.97	0.45
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.51	0.45
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.97	0.45
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.45
2:B:318:ILE:N	2:B:318:ILE:HD12	2.31	0.45
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.45
4:F:259:GLY:O	4:F:261:GLU:HG3	2.17	0.45
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.51	0.45
1:A:70:LEU:HD22	1:A:114:ILE:HD12	1.98	0.45
4:F:126:ASP:OD1	4:F:128:ARG:HG3	2.16	0.45
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.98	0.45
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.98	0.45
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.47	0.45
2:D:295:MET:SD	2:D:375:ALA:HB1	2.57	0.45
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.45
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.44
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.00	0.44
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.99	0.44
2:D:400:ARG:HH12	2:D:401:ARG:HE	1.65	0.44
2:D:67:LEU:CD2	2:D:78:VAL:HG11	2.47	0.44
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.82	0.44
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.51	0.44
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.32	0.44
4:F:226:GLU:HA	4:F:226:GLU:OE1	2.17	0.44
2:B:123:ARG:O	2:B:127:GLU:HG3	2.18	0.44
2:B:132:LEU:HB3	2:B:164:ARG:HH11	1.82	0.44
4:F:125:THR:HB	4:F:126:ASP:H	1.66	0.44
1:C:104:ALA:HB2	1:C:413:MET:SD	2.58	0.43
2:B:298:SER:HA	2:B:301:MET:CG	2.48	0.43
2:D:69:ASP:O	2:D:94:PHE:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:ALA:O	10:B:505:GOL:O2	2.36	0.43
1:C:142:GLY:HA3	1:C:183:GLU:HG2	1.98	0.43
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.49	0.43
1:C:248:LEU:HD11	1:C:357:TYR:OH	2.18	0.43
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.54	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
2:D:175:PRO:HG3	12:D:502:SG9:CL1	2.56	0.43
14:B:601:HOH:O	3:E:76:ARG:HG3	2.19	0.43
4:F:157:GLY:HA3	4:F:245:ILE:HD11	2.00	0.43
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.01	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.43
1:C:440:VAL:HG12	1:C:440:VAL:O	2.19	0.43
3:E:9:ILE:CG2	3:E:21:GLU:HB3	2.48	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.19	0.42
2:D:175:PRO:HD3	12:D:502:SG9:CL1	2.56	0.42
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.01	0.42
2:B:2:ARG:HG3	2:B:3:GLU:CD	2.39	0.42
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.00	0.42
4:F:141:GLY:O	4:F:142:ARG:HB2	2.20	0.42
2:B:2:ARG:HG3	2:B:3:GLU:H	1.85	0.42
1:C:298:PRO:HA	1:C:301:GLN:OE1	2.19	0.42
1:C:209:ILE:HD11	1:C:302:MET:SD	2.59	0.42
2:D:23:VAL:O	2:D:27:GLU:HG3	2.20	0.42
2:B:153:LEU:HD23	2:B:153:LEU:HA	1.93	0.42
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.20	0.42
2:D:116:ASP:HA	2:D:119:LEU:HD12	2.02	0.42
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.42
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.55	0.41
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.50	0.41
2:B:400:ARG:HD2	14:B:659:HOH:O	2.21	0.41
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.02	0.41
2:D:385:GLN:OE1	2:D:389:LYS:HE3	2.19	0.41
3:E:9:ILE:HG13	3:E:10:GLU:HG3	2.02	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.41
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.56	0.41
2:B:140:SER:OG	8:B:501:GDP:H5'	2.21	0.41
2:B:269:MET:HE3	2:B:269:MET:HB3	1.93	0.41
1:C:48:SER:OG	1:C:245:ASP:HB2	2.20	0.41
2:D:308:ARG:HG2	2:D:308:ARG:HH11	1.85	0.41
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.81	0.41
1:A:194:THR:HG22	1:A:194:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.36	0.41
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.02	0.41
3:E:49:GLU:HA	3:E:49:GLU:OE1	2.21	0.41
1:A:90:GLU:O	1:A:121:ARG:HD2	2.21	0.41
1:A:151:SER:HB2	1:A:193:THR:OG1	2.21	0.41
1:A:47:ASP:HB2	1:A:49:PHE:CE1	2.55	0.41
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.51	0.41
2:D:68:VAL:HA	2:D:93:VAL:O	2.21	0.41
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.35	0.41
2:D:11:GLN:HA	2:D:74:THR:HG21	2.04	0.41
2:B:2:ARG:HG3	2:B:3:GLU:OE1	2.20	0.40
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.36	0.40
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.56	0.40
4:F:252:ASN:O	4:F:255:ARG:HB2	2.21	0.40
1:C:88:HIS:ND1	1:C:89:PRO:HD2	2.36	0.40
4:F:242:ASN:N	4:F:242:ASN:OD1	2.54	0.40
1:C:271:THR:HG23	1:C:300:ASN:O	2.21	0.40
4:F:340:GLN:HA	4:F:340:GLN:OE1	2.22	0.40
4:F:82:LYS:O	4:F:89:GLU:HB2	2.21	0.40
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.21	0.40
2:B:405:LEU:HA	2:B:405:LEU:HD23	1.91	0.40
1:C:121:ARG:HA	1:C:121:ARG:HD3	1.92	0.40
2:D:382:THR:O	2:D:385:GLN:HG2	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	436/451 (97%)	425 (98%)	11 (2%)	0	100	100
1	C	438/451 (97%)	431 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	420/445 (94%)	412 (98%)	8 (2%)	0	100	100
2	D	419/445 (94%)	405 (97%)	14 (3%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	343/384 (89%)	328 (96%)	15 (4%)	0	100	100
All	All	2175/2319 (94%)	2118 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	369/379 (97%)	364 (99%)	5 (1%)	67	82
1	C	371/379 (98%)	368 (99%)	3 (1%)	81	91
2	B	367/383 (96%)	363 (99%)	4 (1%)	73	87
2	D	365/383 (95%)	362 (99%)	3 (1%)	81	91
3	E	110/127 (87%)	108 (98%)	2 (2%)	59	76
4	F	311/342 (91%)	309 (99%)	2 (1%)	86	94
All	All	1893/1993 (95%)	1874 (99%)	19 (1%)	76	88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	71	GLU
1	A	105	ARG
1	A	250	VAL
1	A	381	THR
2	B	139	HIS
2	B	200	GLU
2	B	232	SER
2	B	373	MET

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Mol	Chain	Res	Type
1	C	297	GLU
1	C	356	ASN
1	C	381	THR
2	D	15	GLN
2	D	139	HIS
2	D	155	SER
3	E	15	THR
3	E	128	LYS
4	F	211	TYR
4	F	242	ASN

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

Mol	Chain	Res	Type
1	A	88	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	D	501	7	24,30,30	1.20	2 (8%)	31,47,47	1.92	7 (22%)
10	GOL	B	504	-	5,5,5	0.65	0	5,5,5	0.84	0
5	GTP	A	501	7	26,34,34	0.96	1 (3%)	33,54,54	1.70	8 (24%)
5	GTP	C	501	7	26,34,34	0.97	1 (3%)	33,54,54	1.67	6 (18%)
13	ACP	F	401	7	27,33,33	1.75	4 (14%)	32,52,52	1.51	4 (12%)
10	GOL	B	505	-	5,5,5	1.21	0	5,5,5	1.01	0
11	DMS	C	504	-	3,3,3	0.62	0	3,3,3	0.49	0
12	SG9	D	502	-	88,91,91	0.90	0	103,136,136	1.82	22 (21%)
8	GDP	B	501	7	24,30,30	1.16	2 (8%)	31,47,47	2.03	8 (25%)
9	MES	B	502	-	12,12,12	2.10	1 (8%)	14,16,16	1.82	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	7	-	3/12/32/32	0/3/3/3
10	GOL	B	504	-	-	0/4/4/4	-
5	GTP	A	501	7	-	6/18/38/38	0/3/3/3
5	GTP	C	501	7	-	5/18/38/38	0/3/3/3
13	ACP	F	401	7	-	2/15/38/38	0/3/3/3
10	GOL	B	505	-	-	2/4/4/4	-
12	SG9	D	502	-	-	20/71/169/169	-
8	GDP	B	501	7	-	1/12/32/32	0/3/3/3
9	MES	B	502	-	-	0/6/14/14	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.02	1.67	1.77
13	F	401	ACP	PG-O1G	4.92	1.60	1.50
8	D	501	GDP	C6-C5	4.30	1.48	1.41
13	F	401	ACP	PG-O2G	-3.89	1.46	1.54
8	B	501	GDP	C6-C5	3.73	1.47	1.41
13	F	401	ACP	C2'-C1'	-3.55	1.48	1.53
5	C	501	GTP	C6-N1	3.24	1.38	1.33
5	A	501	GTP	C6-N1	2.84	1.38	1.33
13	F	401	ACP	PG-O3G	2.66	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C5-C4	2.37	1.47	1.40
8	B	501	GDP	C5-C4	2.26	1.46	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	502	SG9	C15-O15-C57	5.88	126.82	117.72
5	C	501	GTP	N3-C2-N1	-5.38	120.05	127.22
5	A	501	GTP	N3-C2-N1	-5.31	120.14	127.22
8	D	501	GDP	C2-N3-C4	4.86	120.90	115.36
8	B	501	GDP	C2-N3-C4	4.81	120.85	115.36
12	D	502	SG9	C4-C3-C2	-4.78	107.89	113.56
12	D	502	SG9	C25-C26-C27	4.62	113.81	110.58
12	D	502	SG9	C54-C9-C10	-4.55	107.10	111.34
8	B	501	GDP	C6-N1-C2	4.23	122.64	115.93
8	D	501	GDP	C6-N1-C2	4.16	122.54	115.93
12	D	502	SG9	C37-O33-C33	4.11	119.84	114.61
8	D	501	GDP	C5-C6-N1	-4.03	117.91	123.43
5	A	501	GTP	C2-N3-C4	4.03	119.96	115.36
9	B	502	MES	C5-N4-C3	3.97	117.76	108.83
8	B	501	GDP	C5-C6-N1	-3.95	118.02	123.43
12	D	502	SG9	O43-C43-C42	-3.92	102.58	109.69
8	D	501	GDP	C6-C5-C4	-3.91	117.07	120.80
8	B	501	GDP	C6-C5-C4	-3.90	117.08	120.80
13	F	401	ACP	C3'-C2'-C1'	3.88	106.82	100.98
13	F	401	ACP	N3-C2-N1	-3.85	122.66	128.68
12	D	502	SG9	C41-O41-C1	3.82	123.89	117.53
13	F	401	ACP	PA-O3A-PB	-3.79	120.56	132.56
5	C	501	GTP	C2-N3-C4	3.75	119.64	115.36
8	B	501	GDP	N3-C2-N1	-3.64	122.36	127.22
12	D	502	SG9	O41-C1-C2	3.60	118.08	111.46
12	D	502	SG9	C44-C43-C42	-3.48	110.12	113.01
12	D	502	SG9	O43-C39-C40	3.48	115.55	109.46
12	D	502	SG9	C5-O5-C52	3.40	124.23	117.90
8	D	501	GDP	N3-C2-N1	-3.40	122.69	127.22
12	D	502	SG9	O43-C39-C38	-3.22	100.23	107.56
9	B	502	MES	O1S-S-C8	3.21	110.78	106.92
5	C	501	GTP	C5-C6-N1	-3.08	119.22	123.43
12	D	502	SG9	O7-C3-C2	3.04	108.68	105.78
8	D	501	GDP	C4-C5-N7	-2.93	106.34	109.40
12	D	502	SG9	C23-O23-C19	2.91	119.91	114.49
12	D	502	SG9	O15-C57-C58	2.90	116.42	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	502	MES	O3S-S-C8	2.90	110.46	105.77
12	D	502	SG9	O43-C43-C44	2.83	114.14	106.76
5	C	501	GTP	C6-N1-C2	2.82	120.42	115.93
12	D	502	SG9	C26-C25-C24	2.76	115.02	111.05
5	A	501	GTP	C5-C6-N1	-2.73	119.70	123.43
5	C	501	GTP	PB-O3B-PG	-2.67	123.68	132.83
12	D	502	SG9	O5-C52-C53	2.64	115.95	111.09
5	A	501	GTP	C6-N1-C2	2.60	120.05	115.93
8	B	501	GDP	O2B-PB-O3A	2.59	113.31	104.64
8	B	501	GDP	C4-C5-N7	-2.53	106.77	109.40
8	D	501	GDP	PA-O3A-PB	-2.52	124.18	132.83
12	D	502	SG9	C39-O43-C43	2.47	119.47	113.63
8	B	501	GDP	PA-O3A-PB	-2.38	124.67	132.83
12	D	502	SG9	C7-O11-C11	2.36	118.88	114.49
5	A	501	GTP	PA-O3A-PB	-2.33	124.84	132.83
12	D	502	SG9	O37-C37-C38	-2.32	105.95	110.49
5	A	501	GTP	PB-O3B-PG	-2.30	124.94	132.83
5	A	501	GTP	O2G-PG-O3B	2.18	111.93	104.64
5	C	501	GTP	PA-O3A-PB	-2.16	125.42	132.83
5	A	501	GTP	C6-C5-C4	-2.14	118.76	120.80
9	B	502	MES	C7-N4-C5	2.12	116.65	111.23
12	D	502	SG9	C19-C20-C21	-2.08	104.36	110.78
13	F	401	ACP	N6-C6-N1	2.08	122.88	118.57

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O1A
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
13	F	401	ACP	C5'-O5'-PA-O1A
12	D	502	SG9	C12-C13-C14-C15
12	D	502	SG9	C55-C13-C14-C15
12	D	502	SG9	O37-C37-C38-C39
12	D	502	SG9	C44-C45-C46-C47
12	D	502	SG9	C63-C45-C46-C47
12	D	502	SG9	C58-C57-O15-C15
12	D	502	SG9	O57-C57-O15-C15

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Mol	Chain	Res	Type	Atoms
10	B	505	GOL	O1-C1-C2-C3
12	D	502	SG9	C56-C14-C15-O15
12	D	502	SG9	C16-C15-O15-C57
5	C	501	GTP	PB-O3B-PG-O2G
8	D	501	GDP	C5'-O5'-PA-O3A
10	B	505	GOL	O1-C1-C2-O2
8	D	501	GDP	C5'-O5'-PA-O2A
12	D	502	SG9	C17-C18-C19-O23
12	D	502	SG9	O33-C37-C38-O38
8	B	501	GDP	C4'-C5'-O5'-PA
12	D	502	SG9	C37-C38-C39-C40
5	C	501	GTP	PB-O3A-PA-O2A
12	D	502	SG9	C36-C37-C38-O38
12	D	502	SG9	O33-C37-C38-C39
5	A	501	GTP	PB-O3B-PG-O3G
12	D	502	SG9	O15-C15-C16-C59
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
12	D	502	SG9	C36-C37-C38-C39
12	D	502	SG9	O37-C37-C38-O38
5	A	501	GTP	PB-O3A-PA-O2A
12	D	502	SG9	C55-C13-C14-C56
13	F	401	ACP	O4'-C4'-C5'-O5'
12	D	502	SG9	C56-C14-C15-C16
12	D	502	SG9	C12-C13-C14-C56

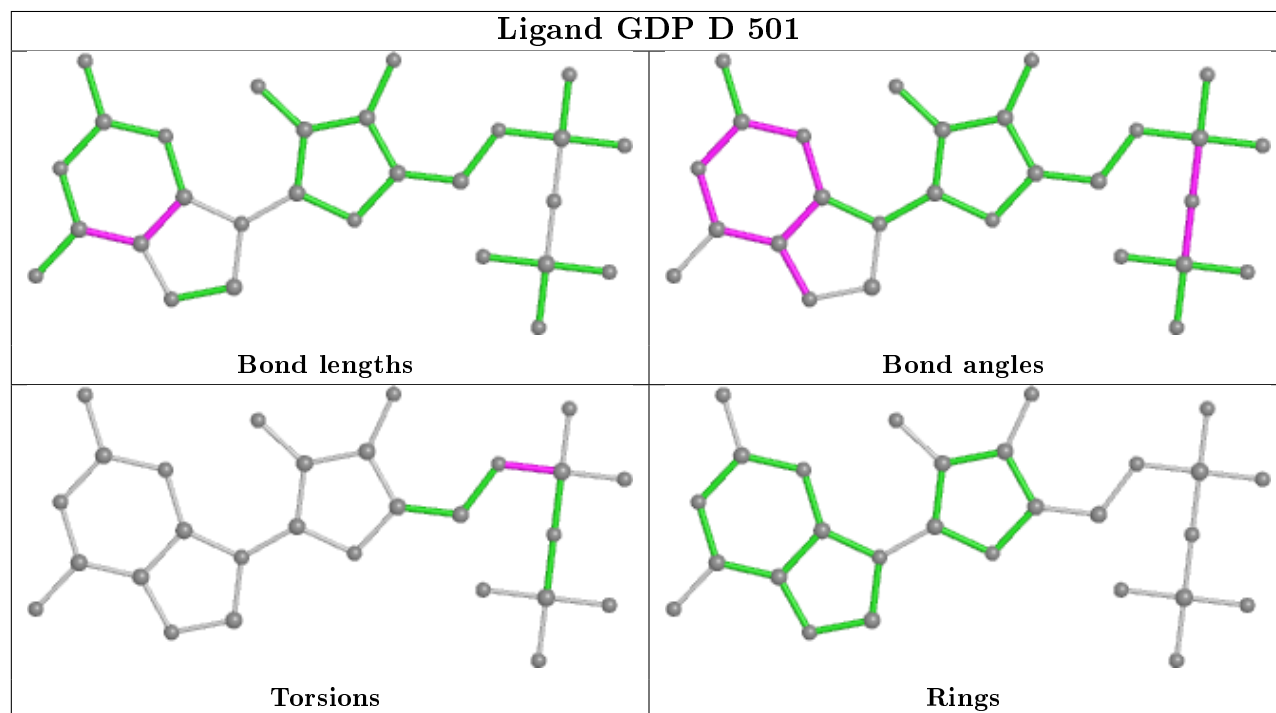
There are no ring outliers.

6 monomers are involved in 8 short contacts:

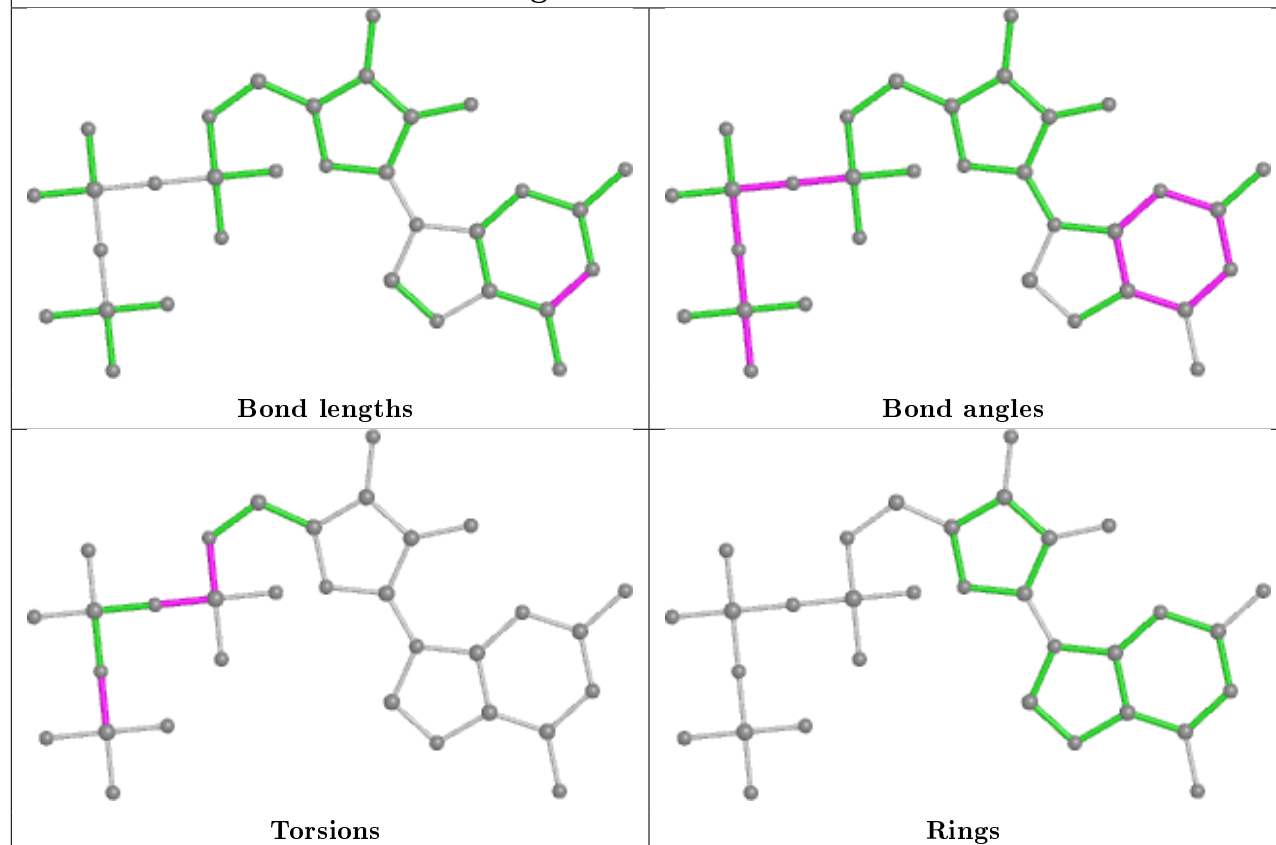
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
10	B	504	GOL	1	0
13	F	401	ACP	1	0
10	B	505	GOL	1	0
12	D	502	SG9	3	0
8	B	501	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

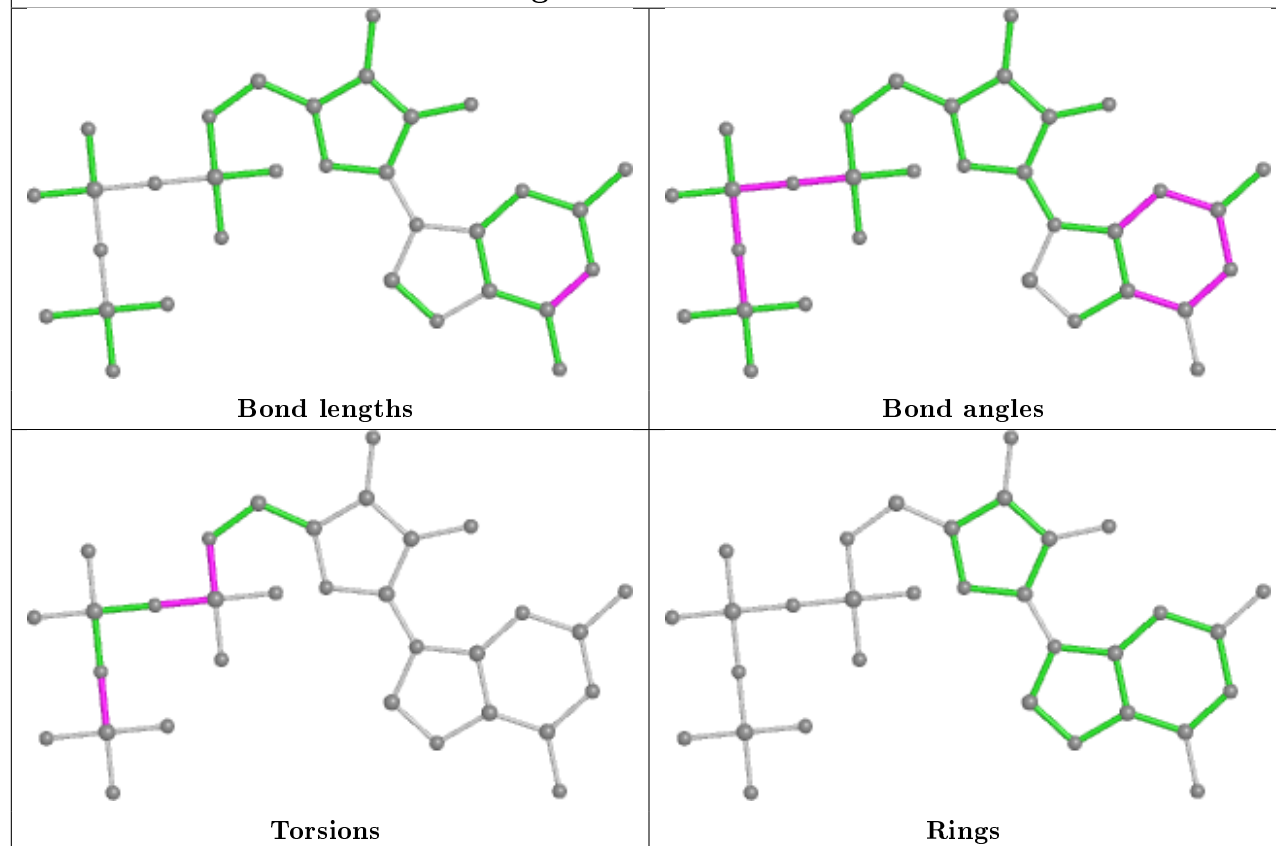
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



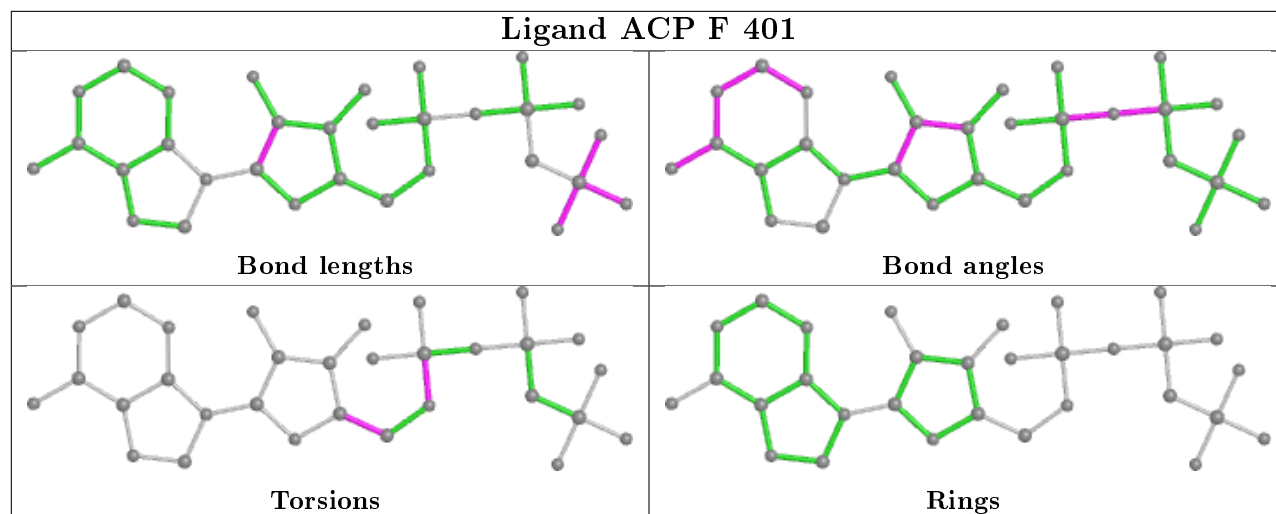
Ligand GTP A 501



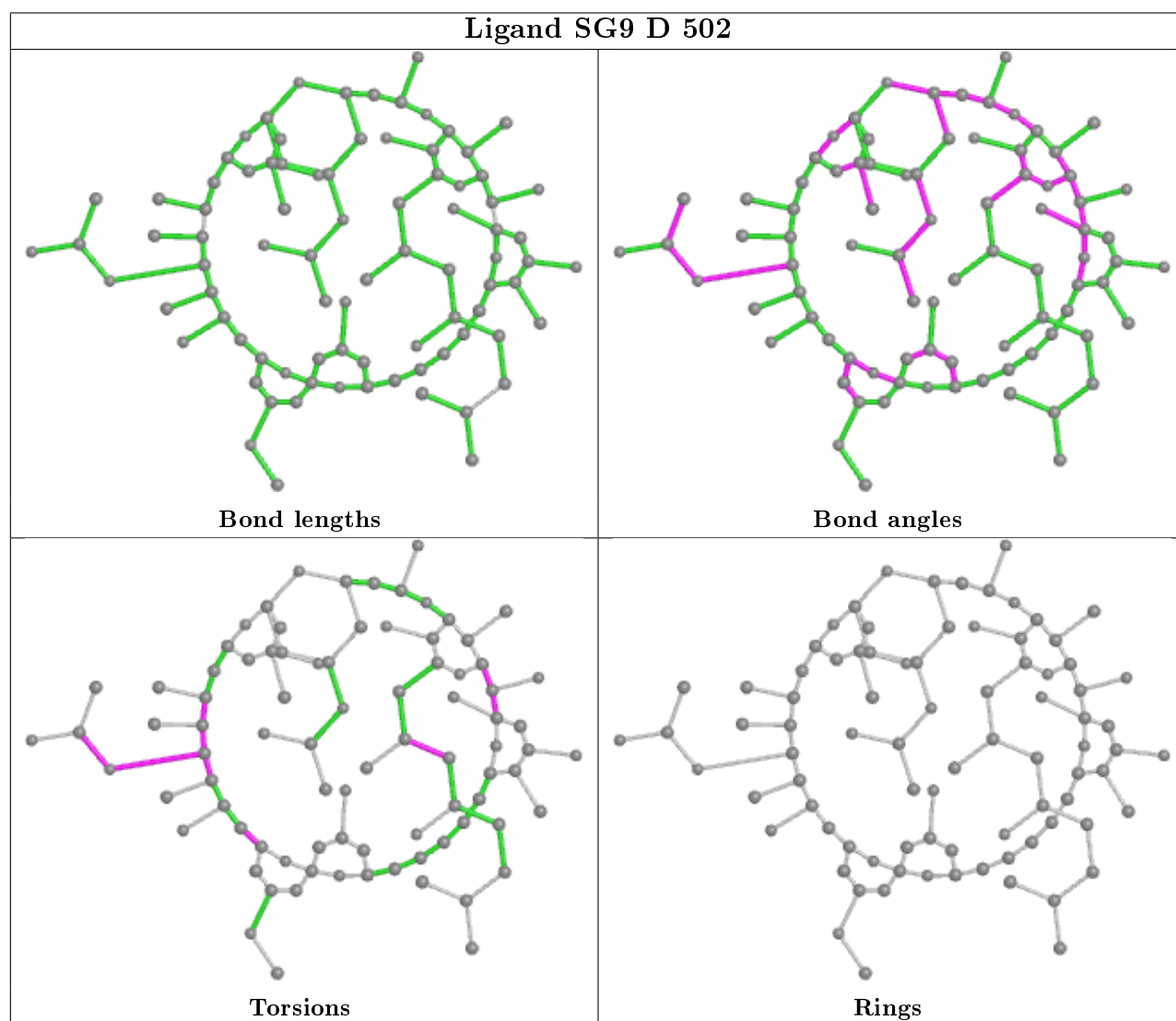
Ligand GTP C 501

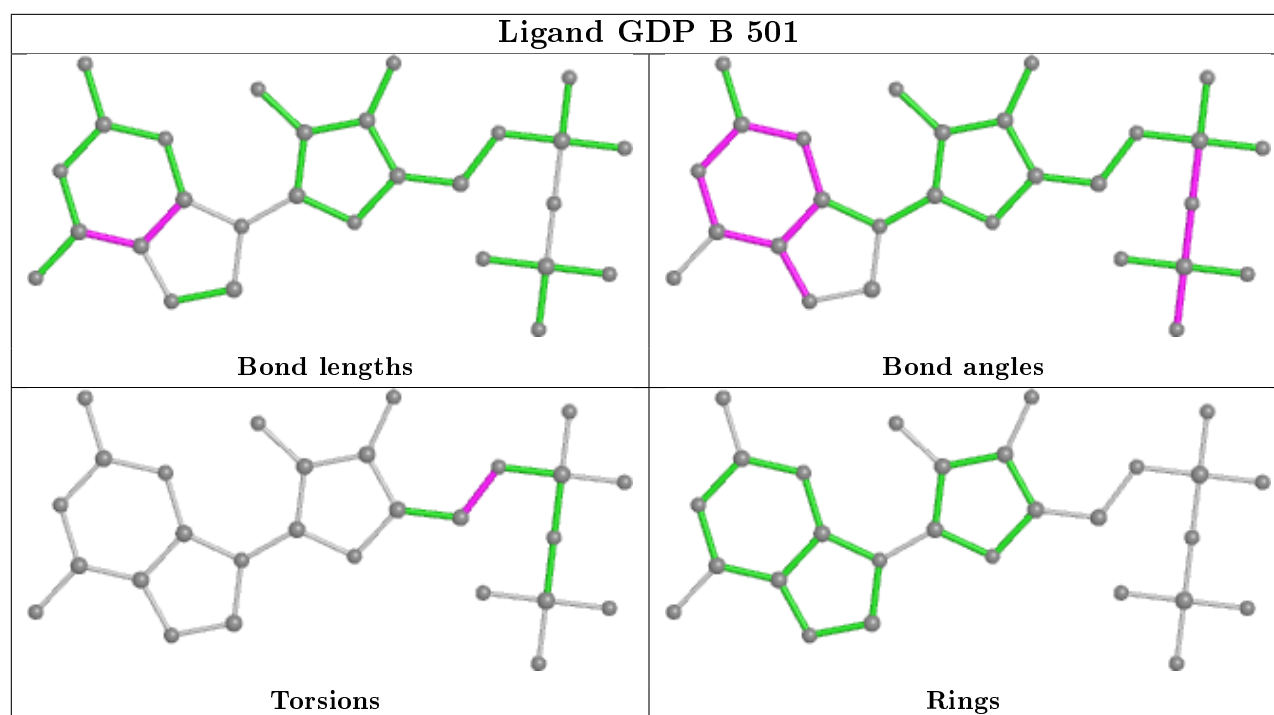


Ligand ACP F 401



Ligand SG9 D 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.17	6 (1%) 75 73	38, 63, 101, 177	0
1	C	440/451 (97%)	-0.43	2 (0%) 91 89	34, 48, 81, 133	0
2	B	424/445 (95%)	-0.27	6 (1%) 75 73	37, 57, 96, 149	0
2	D	423/445 (95%)	0.00	15 (3%) 44 43	43, 72, 113, 146	0
3	E	123/143 (86%)	-0.07	7 (5%) 23 22	45, 79, 127, 149	0
4	F	349/384 (90%)	0.80	77 (22%) 0 0	51, 93, 167, 182	0
All	All	2197/2319 (94%)	-0.05	113 (5%) 28 26	34, 65, 126, 182	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	251	LYS	6.2
4	F	233	PHE	5.9
4	F	173	ILE	5.9
4	F	250	SER	5.7
4	F	249	TYR	5.6
1	A	282	TYR	5.2
2	D	57	THR	4.9
4	F	161	LEU	4.9
2	D	285	ALA	4.6
4	F	177	GLY	4.6
4	F	132	LEU	4.6
4	F	234	GLN	4.5
3	E	143	ALA	4.4
4	F	134	ALA	4.4
4	F	130	VAL	4.4
4	F	169	LEU	4.3
4	F	244	CYS	4.2
4	F	131	PHE	4.2
4	F	133	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	253	TYR	3.9
4	F	231	ALA	3.8
4	F	245	ILE	3.8
4	F	178	GLN	3.8
2	B	59	ASN	3.7
4	F	252	ASN	3.6
4	F	89	GLU	3.6
4	F	232	ASN	3.6
4	F	138	ARG	3.5
4	F	101	TYR	3.5
4	F	100	ILE	3.4
2	D	94	PHE	3.4
4	F	182	ILE	3.4
2	B	57	THR	3.4
4	F	170	LEU	3.3
4	F	17	VAL	3.3
4	F	20	LEU	3.3
4	F	254	GLY	3.3
4	F	125	THR	3.3
4	F	179	VAL	3.3
4	F	157	GLY	3.2
4	F	256	TYR	3.1
4	F	236	LYS	3.1
4	F	181	VAL	3.1
4	F	225	SER	3.1
4	F	259	GLY	3.1
4	F	238	CYS	3.1
4	F	137	ARG	3.0
4	F	21	LEU	3.0
4	F	135	TYR	3.0
4	F	240	LEU	3.0
3	E	26	PRO	3.0
4	F	158	GLU	3.0
4	F	255	ARG	3.0
3	E	142	GLU	2.9
4	F	24	THR	2.8
2	D	56	ALA	2.8
4	F	371	PRO	2.8
4	F	167	SER	2.8
4	F	176	GLN	2.7
1	A	42	ILE	2.7
1	C	340	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	38	GLY	2.7
4	F	149	ALA	2.7
1	A	281	ALA	2.7
4	F	142	ARG	2.6
2	B	37	HIS	2.6
4	F	147	TRP	2.6
4	F	128	ARG	2.6
4	F	143	GLU	2.6
4	F	163	SER	2.6
3	E	139	LEU	2.6
1	A	283	HIS	2.6
4	F	235	ASP	2.6
2	D	82	PRO	2.5
4	F	361	LEU	2.5
4	F	32	LYS	2.5
4	F	166	ALA	2.5
2	D	405	LEU	2.5
4	F	28	LYS	2.5
2	D	415	GLU	2.5
3	E	140	LYS	2.4
4	F	247	LYS	2.4
2	D	401	ARG	2.4
2	D	58	GLY	2.4
4	F	174	ASP	2.4
1	A	262	TYR	2.3
4	F	239	HIS	2.3
4	F	31	ARG	2.3
4	F	136	ASN	2.3
4	F	248	GLU	2.3
4	F	129	GLU	2.3
4	F	224	SER	2.3
4	F	246	GLN	2.3
4	F	162	ILE	2.2
2	D	201	THR	2.2
3	E	24	LEU	2.2
4	F	44	ARG	2.2
2	D	404	PHE	2.2
2	B	438	ALA	2.2
2	D	414	ASP	2.2
2	D	76	ASP	2.2
2	D	96	GLN	2.2
4	F	151	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	440	VAL	2.1
3	E	141	GLU	2.1
4	F	372	THR	2.1
1	A	364	PRO	2.1
4	F	139	ARG	2.1
2	B	36	TYR	2.1
4	F	99	VAL	2.0
4	F	226	GLU	2.0
2	D	418	PHE	2.0
4	F	172	PHE	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 carbohydrates 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	504	6/6	0.72	0.23	75,90,108,108	0
10	GOL	B	505	6/6	0.73	0.22	86,104,124,125	0
7	MG	F	402	1/1	0.83	0.12	161,161,161,161	0
11	DMS	C	504	4/4	0.85	0.49	126,151,157,157	0
7	MG	D	503	1/1	0.87	0.10	80,80,80,80	0
6	CA	A	502	1/1	0.87	0.05	93,93,93,93	0
13	ACP	F	401	31/31	0.89	0.13	90,122,151,181	0
12	SG9	D	502	85/85	0.90	0.27	75,111,140,144	0
6	CA	B	506	1/1	0.95	0.37	107,107,107,107	0
9	MES	B	502	12/12	0.96	0.14	53,70,79,80	0
8	GDP	D	501	28/28	0.97	0.12	60,69,90,94	0
6	CA	C	503	1/1	0.98	0.11	69,69,69,69	0
7	MG	A	503	1/1	0.98	0.17	45,45,45,45	0

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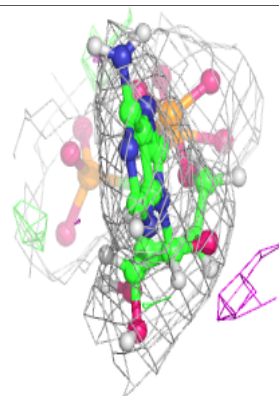
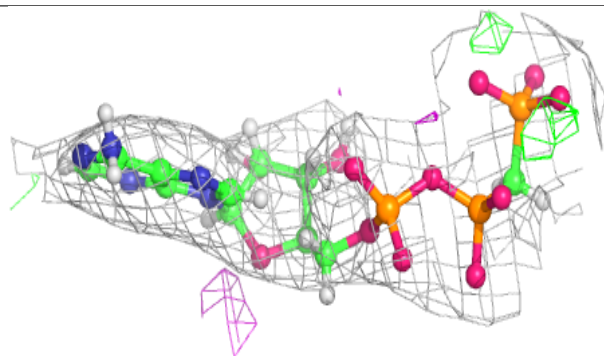
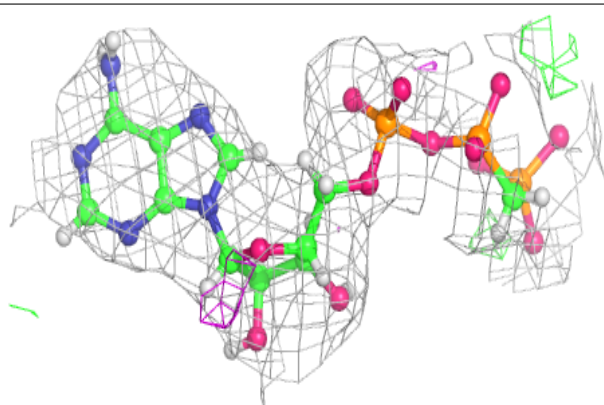
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	B	503	1/1	0.98	0.23	38,38,38,38	0
8	GDP	B	501	28/28	0.98	0.19	34,46,50,50	0
5	GTP	A	501	32/32	0.99	0.20	33,45,51,56	0
7	MG	C	502	1/1	0.99	0.13	40,40,40,40	0
5	GTP	C	501	32/32	0.99	0.15	27,38,47,48	0

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

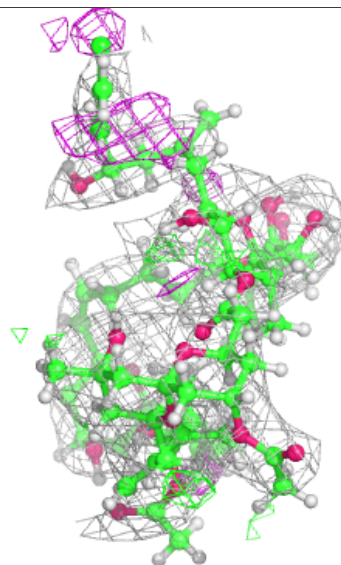
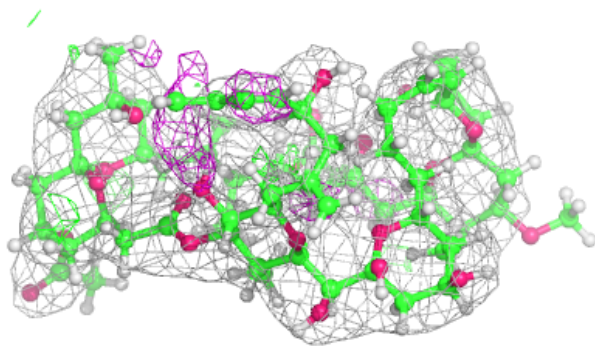
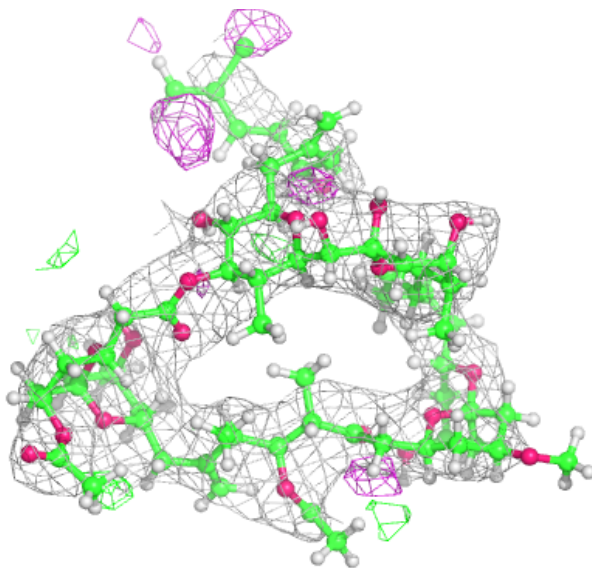
Electron density around ACP F 401:

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



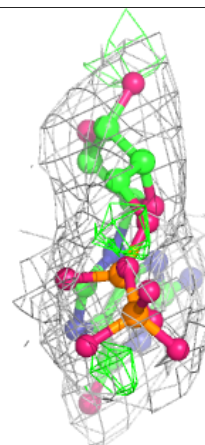
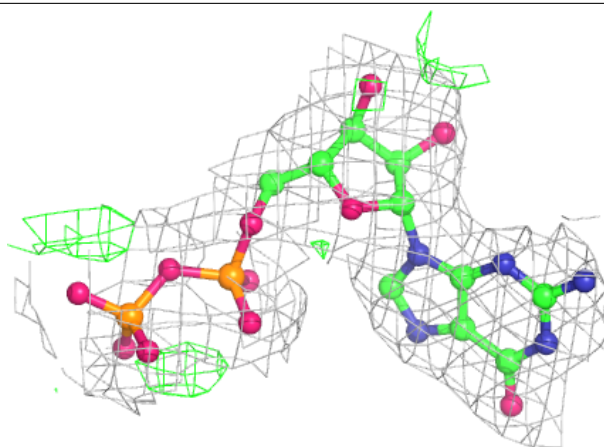
Electron density around SG9 D 502:

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

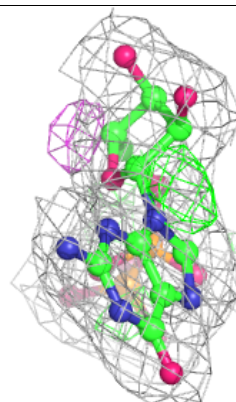
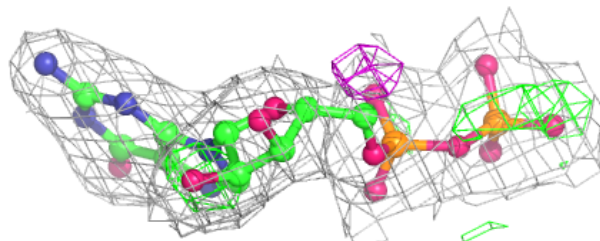
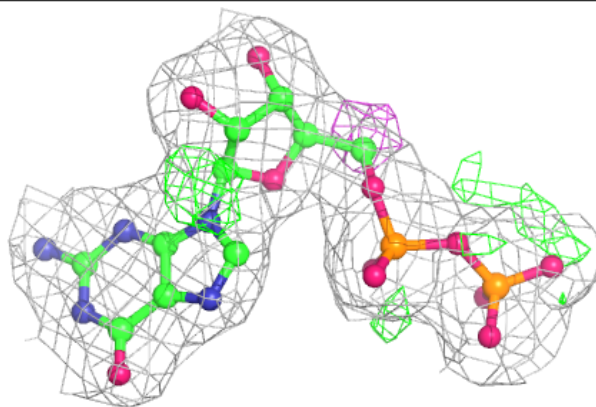


Electron density around GDP D 501:

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

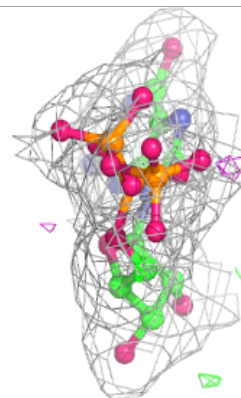
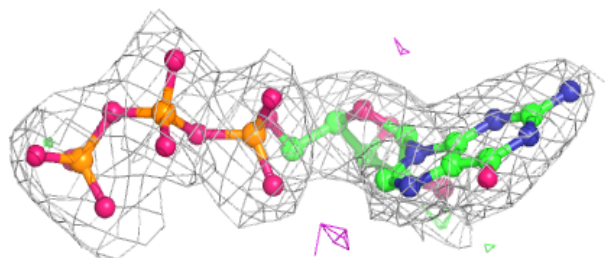
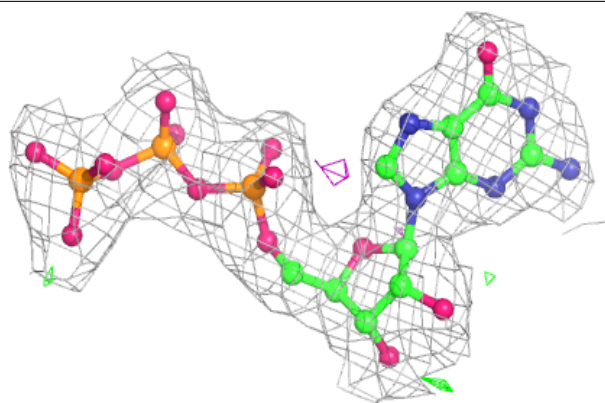
**Electron density around GDP B 501:**

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

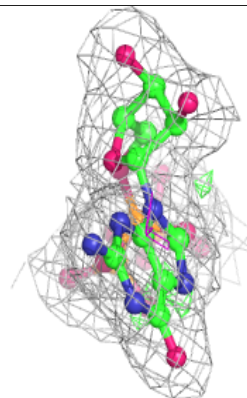
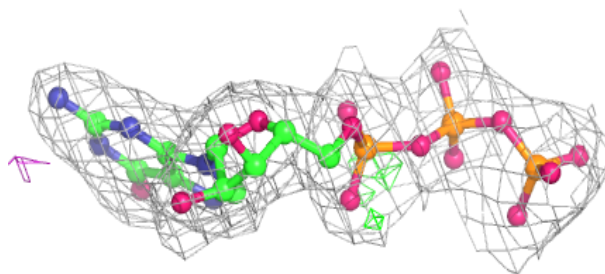
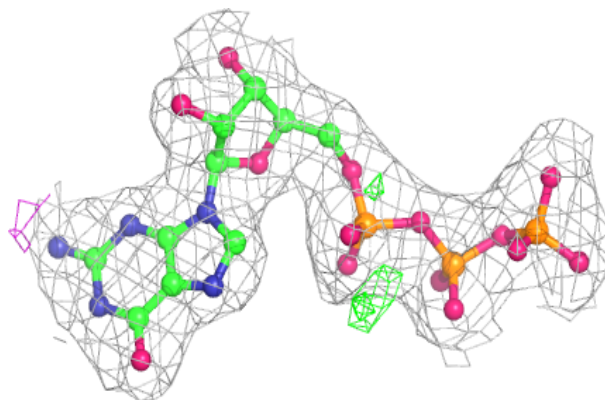


Electron density around GTP A 501:

$2mF_o-DF_c$ (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

There are no such residues in this entry.