



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:35 pm BST

PDB ID : 6JCJ
Title : Structure of crolibulin in complex with tubulin
Authors : Zhang, Z.; Yang, J.
Deposited on : 2019-01-29
Resolution : 2.50 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

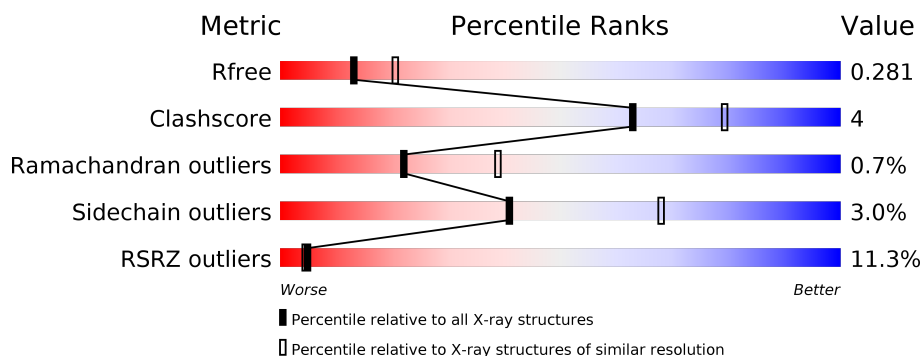
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	450	<div> <div></div> <div>86% 10% .</div> </div>
1	C	450	<div> <div></div> <div>85% 13% .</div> </div>
2	B	445	<div> <div>3%</div> <div>82% 13% . 5%</div> </div>
2	D	445	<div> <div>24%</div> <div>80% 14% . 5%</div> </div>
3	E	143	<div> <div>14%</div> <div>74% 9% . 16%</div> </div>
4	F	384	<div> <div>24%</div> <div>71% 9% . 20%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3441	2179	586	652	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- 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	1	0
			3342	2101	570	644	27			
2	D	421	Total	C	N	O	S	0	1	0
			3306	2079	562	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	2	0
			1004	621	181	196	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	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	309	Total	C	N	O	S	0	3	0
			2553	1645	438	455	15			

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		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

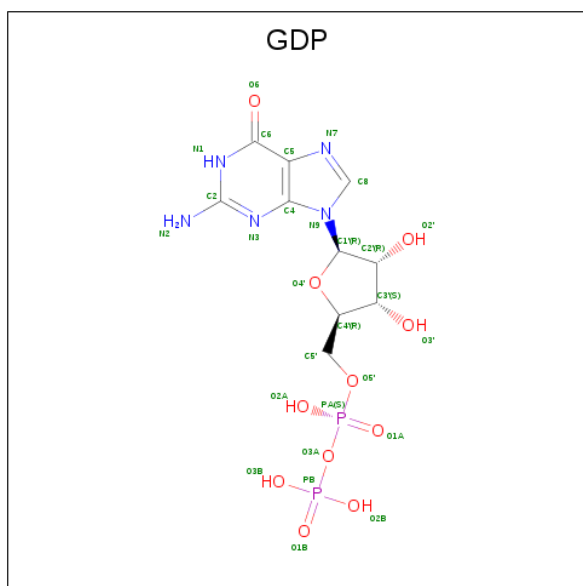
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

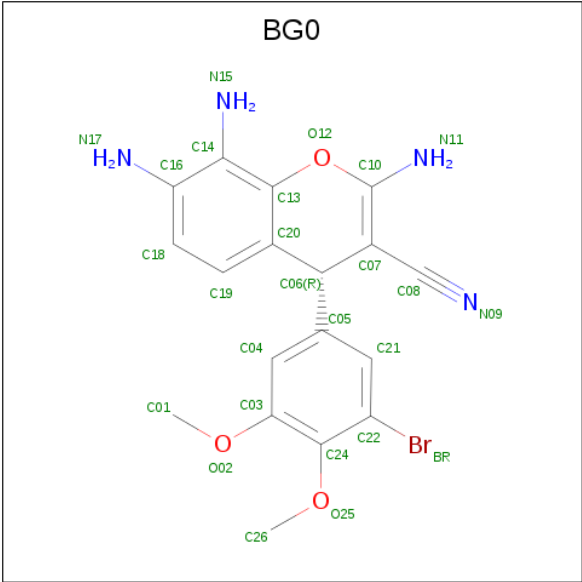
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



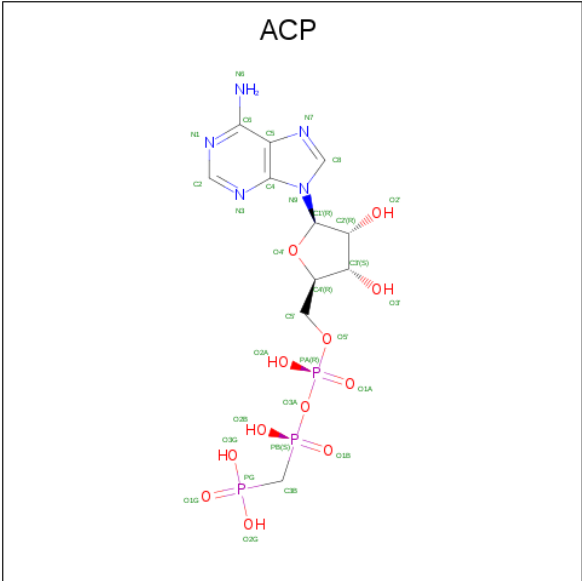
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is (4R)-2,7,8-triamino-4-(3-bromo-4,5-dimethoxyphenyl)-4H-1-benzopyran-3-carbonitrile (three-letter code: BG0) (formula: C₁₈H₁₇BrN₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	Br	C	N	O	0	0
			26	1	18	4	3		
9	D	1	Total	Br	C	N	O	0	0
			26	1	18	4	3		

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



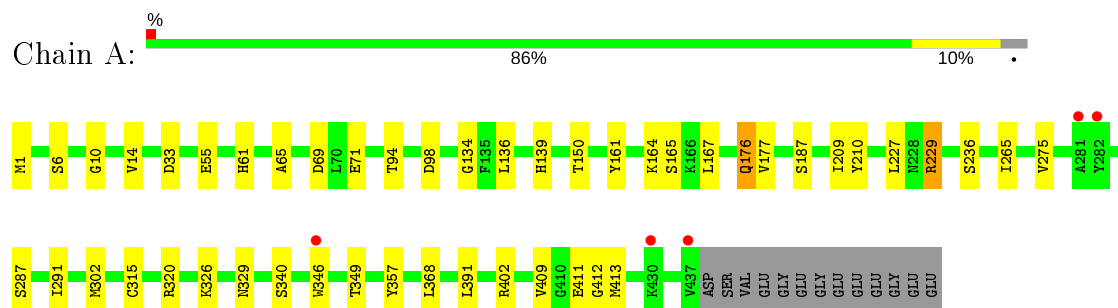
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	16	Total 16	O 16	0	0
11	B	16	Total 16	O 16	0	0
11	C	46	Total 46	O 46	0	0
11	D	4	Total 4	O 4	0	0
11	E	1	Total 1	O 1	0	0

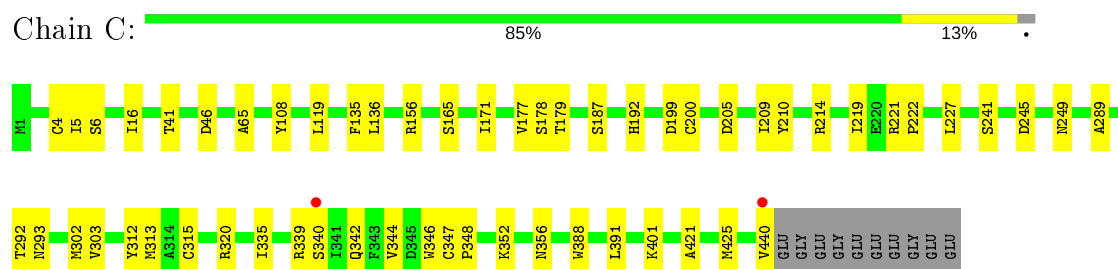
3 Residue-property plots [i](#)

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.

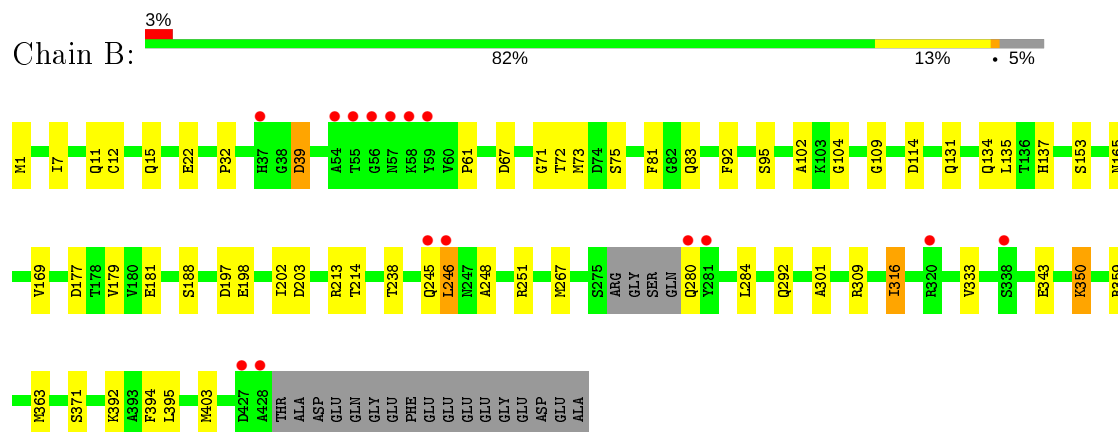
- Molecule 1: Tubulin alpha-1B chain



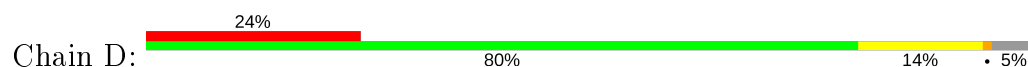
- Molecule 1: Tubulin alpha-1B chain

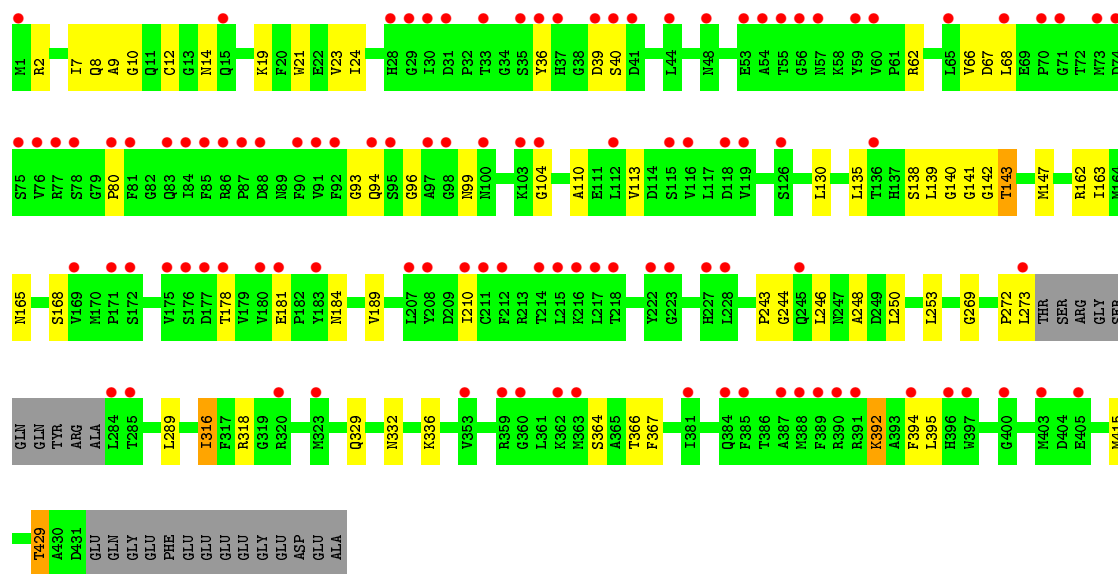


- Molecule 2: Tubulin beta-2B chain

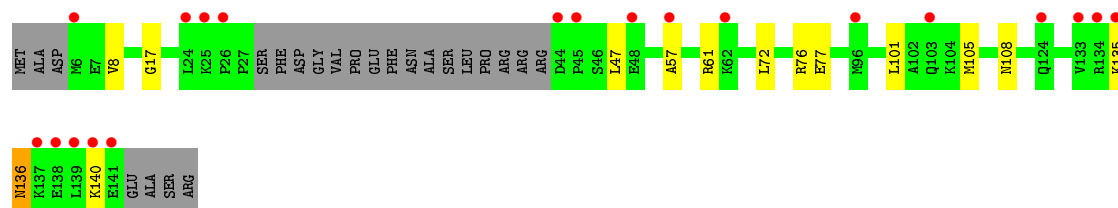
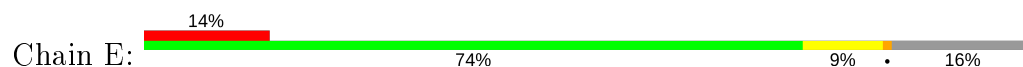


- Molecule 2: Tubulin beta-2B chain

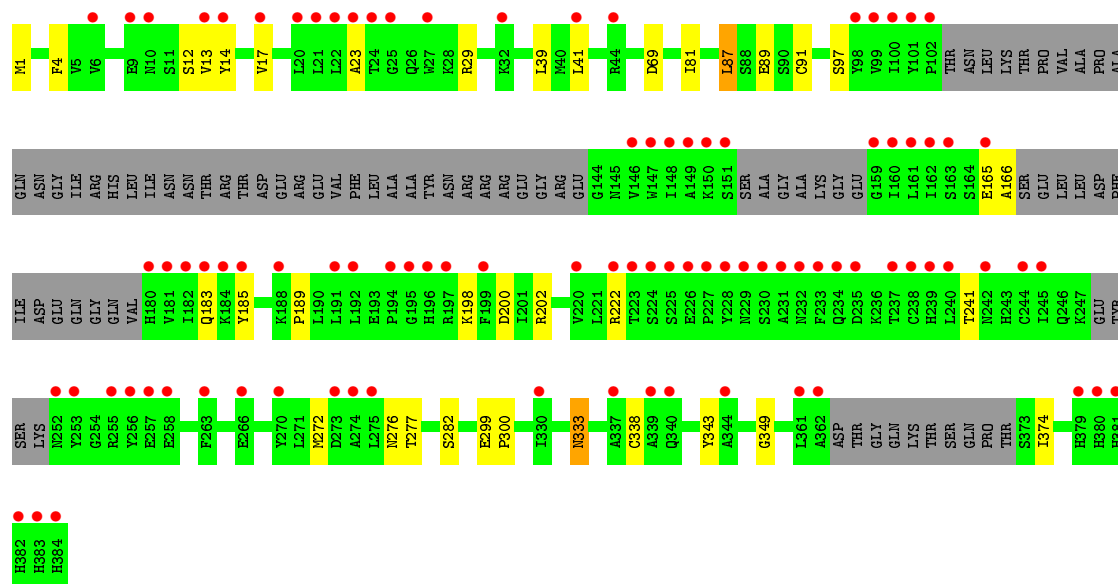




• Molecule 3: Stathmin-4



• 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	105.54Å 157.33Å 184.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 2.50 48.37 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.42-2.50) 97.8 (48.37-2.48)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.241 , 0.282 0.242 , 0.281	Depositor DCC
R_{free} test set	5334 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17423	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: GDP, GTP, MG, CA, BG0, 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	0.66	0/3525	0.80	0/4784
1	C	0.66	0/3572	0.82	0/4850
2	B	0.66	0/3416	0.78	0/4626
2	D	0.68	0/3379	0.77	0/4577
3	E	0.68	0/1018	0.79	0/1350
4	F	0.68	0/2618	0.75	0/3537
All	All	0.67	0/17528	0.79	0/23724

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	3441	0	3362	34	0
1	C	3482	0	3384	26	0
2	B	3342	0	3216	30	0
2	D	3306	0	3181	37	0
3	E	1004	0	1028	11	0
4	F	2553	0	2519	18	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
5	D	32	0	12	3	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	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	26	0	0	3	0
9	D	26	0	0	1	0
10	F	31	0	14	2	0
11	A	16	0	0	1	0
11	B	16	0	0	0	0
11	C	46	0	0	0	0
11	D	4	0	0	1	0
11	E	1	0	0	0	0
All	All	17423	0	16752	148	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 4.

All (148) 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:A:229[A]:ARG:CG	1:A:229[A]:ARG:HH11	1.83	0.90
2:B:238:THR:HG21	2:B:316:ILE:HD11	1.57	0.87
1:A:209:ILE:HD11	1:A:302:MET:SD	2.20	0.81
1:A:176:GLN:HB2	11:A:609:HOH:O	1.87	0.74
2:D:165:ASN:ND2	11:D:601:HOH:O	2.21	0.74
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.55	0.71
2:B:177:ASP:O	1:C:352:LYS:NZ	2.22	0.70
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:HG3	1.56	0.68
1:C:241:SER:HA	1:C:249:ASN:HD21	1.59	0.68
2:D:316:ILE:HG23	2:D:366:THR:HB	1.77	0.67
1:A:368[B]:LEU:N	1:A:368[B]:LEU:HD12	2.11	0.66
2:D:142:GLY:N	5:D:501:GTP:O2B	2.29	0.65
4:F:202:ARG:NH2	10:F:401:ACP:O2G	2.30	0.65
1:A:411:GLU:O	3:E:61:ARG:NH1	2.29	0.65
1:C:313:MET:O	1:C:347[B]:CYS:SG	2.54	0.63
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.82	0.62
2:D:141:GLY:O	2:D:184:ASN:ND2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:ASN:HD21	2:D:336:LYS:HE3	1.65	0.60
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.86	0.58
2:D:332:ASN:ND2	2:D:336:LYS:HE3	2.18	0.58
3:E:135:LYS:C	3:E:136:ASN:HD22	2.06	0.58
2:D:110:ALA:O	2:D:113:VAL:HG12	2.03	0.57
1:A:409:VAL:HA	1:A:413:MET:O	2.05	0.57
2:D:248:ALA:HA	9:D:502:BG0:N09	2.21	0.56
2:D:246:LEU:HD21	2:D:248:ALA:HB2	1.88	0.56
2:B:104:GLY:O	2:B:109:GLY:HA3	2.05	0.55
1:A:69:ASP:O	1:A:94:THR:HA	2.07	0.55
2:D:139:LEU:HD11	2:D:168:SER:HB3	1.88	0.55
2:D:19:LYS:O	2:D:23:VAL:HG23	2.06	0.55
2:B:169:VAL:HA	2:B:202:ILE:O	2.06	0.55
2:B:134:GLN:HA	2:B:165:ASN:O	2.07	0.55
2:B:67:ASP:O	2:B:92:PHE:HA	2.06	0.55
1:C:209:ILE:HD11	1:C:302:MET:SD	2.47	0.54
2:B:177:ASP:HB2	2:B:181:GLU:OE2	2.08	0.54
3:E:101:LEU:O	3:E:105[A]:MET:HG2	2.08	0.54
2:D:7:ILE:O	2:D:135:LEU:HD12	2.07	0.53
2:B:309:ARG:NH2	2:B:343:GLU:OE1	2.41	0.53
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.91	0.53
1:C:401:LYS:NZ	2:D:429:THR:O	2.31	0.53
3:E:135:LYS:O	3:E:136:ASN:ND2	2.40	0.53
1:A:209:ILE:CD1	1:A:302:MET:SD	2.95	0.53
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.43	0.52
1:A:368[B]:LEU:H	1:A:368[B]:LEU:HD12	1.74	0.52
2:B:11:GLN:HA	2:B:72:THR:HG21	1.92	0.51
2:B:7:ILE:O	2:B:135:LEU:HA	2.09	0.51
4:F:333:ASN:ND2	10:F:401:ACP:O2G	2.44	0.51
9:B:503:BG0:BR	9:B:503:BG0:C26	3.14	0.50
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.44	0.50
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.50
2:D:10:GLY:O	2:D:14:ASN:ND2	2.42	0.50
1:A:275:VAL:HG13	1:A:368[A]:LEU:HD21	1.92	0.50
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.47	0.50
2:D:329:GLN:O	2:D:332:ASN:HB3	2.12	0.49
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	2.21	0.49
2:B:245:GLN:NE2	2:B:245:GLN:HA	2.27	0.49
1:C:192:HIS:CG	1:C:421:ALA:HA	2.48	0.49
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.78	0.49
1:A:236:SER:OG	1:A:320:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ALA:HA	9:B:503:BG0:N09	2.28	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.48
4:F:277:THR:HG21	4:F:282:SER:HB3	1.95	0.48
4:F:4:PHE:HA	4:F:39:LEU:O	2.14	0.48
2:D:130:LEU:O	2:D:162:ARG:NH1	2.46	0.48
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.48	0.48
2:B:284:LEU:HD21	2:B:292:GLN:HE22	1.79	0.47
2:B:350:LYS:HB3	9:B:503:BG0:C16	2.44	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.47
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.97	0.47
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.44	0.47
2:D:141:GLY:HA3	5:D:501:GTP:O3A	2.14	0.47
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.96	0.47
2:B:392:LYS:HB3	2:B:395:LEU:HD12	1.97	0.47
2:D:104:GLY:O	2:D:147:MET:HA	2.15	0.46
1:C:165:SER:HA	1:C:199:ASP:OD2	2.16	0.46
1:C:293[A]:ASN:OD1	1:C:339:ARG:NE	2.41	0.46
2:B:179:VAL:HG21	2:B:394:PHE:CZ	2.51	0.46
4:F:81:ILE:O	4:F:87:LEU:O	2.33	0.46
2:B:1:MET:SD	2:B:131:GLN:HB3	2.56	0.46
2:D:99:ASN:ND2	2:D:178:THR:HG21	2.31	0.46
1:C:214:ARG:HA	1:C:219:ILE:O	2.16	0.46
4:F:97:SER:OG	4:F:183:GLN:NE2	2.48	0.46
4:F:222:ARG:O	4:F:241:THR:OG1	2.34	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.45
1:C:289:ALA:O	1:C:293[B]:ASN:CG	2.55	0.45
2:D:12:CYS:CB	2:D:138:SER:HB3	2.46	0.45
4:F:338:CYS:O	4:F:343:TYR:CE2	2.70	0.45
1:A:33:ASP:OD1	1:A:33:ASP:C	2.55	0.45
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.45
2:B:102:ALA:HB2	2:B:403:MET:SD	2.56	0.45
2:D:68:LEU:HD23	2:D:93:GLY:HA3	1.98	0.45
2:B:246:LEU:HA	2:B:246:LEU:HD23	1.75	0.44
3:E:47:LEU:O	3:E:47:LEU:HD12	2.17	0.44
1:A:10:GLY:O	1:A:14:VAL:HG23	2.17	0.44
1:A:134:GLY:HA3	1:A:165:SER:O	2.17	0.44
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.44
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.44
2:B:203:ASP:CB	2:B:301:ALA:HA	2.48	0.44
1:C:108:TYR:CD2	3:E:108:ASN:CG	2.91	0.43
2:D:272:PRO:HD3	2:D:289:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ASP:OD1	2:B:39:ASP:N	2.51	0.43
2:D:67:ASP:HA	2:D:143:THR:HG21	2.00	0.43
2:D:36:TYR:OH	2:D:40:SER:O	2.35	0.43
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.55	0.43
2:B:197:ASP:C	2:B:198:GLU:HG3	2.39	0.43
2:B:73:MET:SD	2:B:92:PHE:HB3	2.59	0.43
1:C:119:LEU:HD12	1:C:156:ARG:NH2	2.34	0.43
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.48	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.01	0.43
2:D:8:GLN:HB2	2:D:14:ASN:HA	2.01	0.43
4:F:14:TYR:HA	4:F:17:VAL:HB	2.01	0.43
1:A:346:TRP:CD1	1:A:346:TRP:O	2.72	0.42
1:A:412:GLY:HA3	3:E:57:ALA:O	2.19	0.42
4:F:189:PRO:HG3	4:F:198:LYS:HE2	2.01	0.42
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.55	0.42
2:D:269:GLY:O	2:D:367:PHE:N	2.50	0.42
1:A:329:ASN:ND2	3:E:8:VAL:HG21	2.34	0.42
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.54	0.42
2:D:12:CYS:SG	2:D:138:SER:HB3	2.60	0.42
4:F:165:GLU:O	4:F:166:ALA:HB3	2.20	0.42
1:C:5:ILE:O	1:C:135:PHE:HA	2.20	0.42
2:D:140:GLY:HA3	5:D:501:GTP:H4'	2.02	0.42
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.55	0.42
2:D:9:ALA:HA	2:D:66:VAL:O	2.19	0.42
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.02	0.42
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.02	0.42
2:B:203:ASP:HB3	2:B:301:ALA:HA	2.02	0.42
4:F:272:MET:O	4:F:276:ASN:HA	2.20	0.42
3:E:72:LEU:O	3:E:76:ARG:HG2	2.19	0.41
2:B:238:THR:HB	2:B:316:ILE:HD12	2.03	0.41
1:C:312:TYR:CD1	1:C:315[B]:CYS:SG	3.13	0.41
1:C:388:TRP:CE3	1:C:425:MET:HE1	2.55	0.41
2:B:267:MET:HE3	2:B:371:SER:HB3	2.02	0.41
2:B:238:THR:CG2	2:B:316:ILE:HD11	2.38	0.41
2:D:392:LYS:HB3	2:D:395:LEU:HD12	2.02	0.41
2:D:246:LEU:CD2	2:D:248:ALA:HB2	2.51	0.41
2:B:12:CYS:SG	2:B:169:VAL:HG21	2.61	0.41
2:D:68:LEU:O	2:D:96:GLY:HA2	2.21	0.41
1:C:6:SER:O	1:C:65:ALA:HA	2.21	0.41
2:D:189:VAL:HG11	2:D:415:MET:SD	2.60	0.41
4:F:13:VAL:O	4:F:17:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD13	1:A:167:LEU:HB2	2.03	0.40
1:A:287:SER:O	1:A:291:ILE:HG23	2.21	0.40
4:F:39:LEU:HD21	4:F:41:LEU:HD21	2.04	0.40
1:A:265:ILE:O	1:A:265:ILE:HG22	2.22	0.40
1:A:6:SER:O	1:A:65:ALA:HA	2.22	0.40
2:D:210:ILE:HG23	2:D:273:LEU:HD13	2.04	0.40
1:A:176:GLN:HG2	1:A:210:TYR:CE2	2.56	0.40
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.57	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	439/450 (98%)	417 (95%)	21 (5%)	1 (0%)	47	68
1	C	446/450 (99%)	435 (98%)	10 (2%)	1 (0%)	47	68
2	B	421/445 (95%)	400 (95%)	18 (4%)	3 (1%)	22	39
2	D	417/445 (94%)	372 (89%)	37 (9%)	8 (2%)	8	13
3	E	118/143 (82%)	116 (98%)	1 (1%)	1 (1%)	19	35
4	F	300/384 (78%)	276 (92%)	23 (8%)	1 (0%)	41	61
All	All	2141/2317 (92%)	2016 (94%)	110 (5%)	15 (1%)	22	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	243	PRO
2	D	39	ASP
2	D	244	GLY
1	A	349	THR

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Mol	Chain	Res	Type
2	B	71	GLY
2	D	62	ARG
2	D	143	THR
2	D	392	LYS
2	D	394	PHE
3	E	140	LYS
4	F	23	ALA
2	B	213	ARG
2	B	32	PRO
1	C	200	CYS
2	D	80	PRO

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	372/378 (98%)	362 (97%)	10 (3%)	44	71
1	C	379/378 (100%)	369 (97%)	10 (3%)	46	72
2	B	366/383 (96%)	347 (95%)	19 (5%)	23	44
2	D	362/383 (94%)	354 (98%)	8 (2%)	52	77
3	E	110/127 (87%)	108 (98%)	2 (2%)	59	81
4	F	281/342 (82%)	273 (97%)	8 (3%)	43	70
All	All	1870/1991 (94%)	1813 (97%)	57 (3%)	41	68

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	176	GLN
1	A	177	VAL
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	315[A]	CYS
1	A	315[B]	CYS

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Mol	Chain	Res	Type
1	A	326	LYS
1	A	340	SER
1	A	402	ARG
2	B	15	GLN
2	B	39	ASP
2	B	61	PRO
2	B	75	SER
2	B	83	GLN
2	B	95	SER
2	B	114	ASP
2	B	137	HIS
2	B	153	SER
2	B	188	SER
2	B	214	THR
2	B	246	LEU
2	B	251	ARG
2	B	280	GLN
2	B	316	ILE
2	B	333	VAL
2	B	350	LYS
2	B	359	ARG
2	B	363	MET
1	C	41	THR
1	C	46	ASP
1	C	177	VAL
1	C	178	SER
1	C	179	THR
1	C	221	ARG
1	C	245	ASP
1	C	340	SER
1	C	342	GLN
1	C	440	VAL
2	D	2	ARG
2	D	94	GLN
2	D	181	GLU
2	D	253	LEU
2	D	316	ILE
2	D	318	ARG
2	D	364	SER
2	D	429	THR
3	E	77	GLU
3	E	136	ASN

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Mol	Chain	Res	Type
4	F	1	MET
4	F	12	SER
4	F	69	ASP
4	F	87	LEU
4	F	89	GLU
4	F	91	CYS
4	F	200	ASP
4	F	333	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	101	ASN
1	A	107	HIS
2	B	83	GLN
2	B	245	GLN
2	B	292	GLN
2	B	307	HIS
2	B	347	ASN
1	C	101	ASN
1	C	249	ASN
1	C	342	GLN
1	C	356	ASN
2	D	8	GLN
2	D	195	ASN
2	D	347	ASN
3	E	136	ASN
4	F	38	ASN
4	F	145	ASN
4	F	252	ASN
4	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	BG0	B	503	-	28,28,28	3.90	10 (35%)	37,41,41	3.09	13 (35%)
5	GTP	A	501	6	26,34,34	1.02	1 (3%)	33,54,54	2.19	4 (12%)
8	GDP	B	501	6	24,30,30	1.32	5 (20%)	31,47,47	1.96	5 (16%)
5	GTP	C	501	6	26,34,34	1.03	1 (3%)	33,54,54	2.12	4 (12%)
5	GTP	D	501	-	26,34,34	1.05	1 (3%)	33,54,54	2.08	4 (12%)
9	BG0	D	502	-	28,28,28	3.97	10 (35%)	37,41,41	3.54	16 (43%)
10	ACP	F	401	-	27,33,33	1.49	6 (22%)	32,52,52	1.59	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BG0	B	503	-	-	1/8/26/26	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
5	GTP	D	501	-	-	7/18/38/38	0/3/3/3
9	BG0	D	502	-	-	2/8/26/26	0/3/3/3
10	ACP	F	401	-	-	7/15/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	502	BG0	C07-C10	14.38	1.48	1.35
9	B	503	BG0	C07-C10	14.34	1.48	1.35
9	D	502	BG0	C10-N11	9.95	1.45	1.33
9	B	503	BG0	C10-N11	9.38	1.44	1.33
9	D	502	BG0	C08-C07	8.07	1.52	1.42
9	B	503	BG0	C08-C07	7.09	1.50	1.42
9	B	503	BG0	C06-C07	-4.38	1.49	1.52
5	D	501	GTP	C6-N1	4.23	1.40	1.33
5	C	501	GTP	C6-N1	3.95	1.39	1.33
10	F	401	ACP	PB-O3A	3.86	1.62	1.58
5	A	501	GTP	C6-N1	3.82	1.39	1.33
9	D	502	BG0	C06-C07	-3.61	1.49	1.52
9	D	502	BG0	O02-C03	3.54	1.42	1.37
9	B	503	BG0	BR-C22	3.32	1.97	1.89
9	B	503	BG0	O12-C13	3.31	1.43	1.38
9	D	502	BG0	BR-C22	3.14	1.97	1.89
8	B	501	GDP	PB-O1B	3.06	1.60	1.50
10	F	401	ACP	PG-O3G	2.94	1.61	1.54
8	B	501	GDP	C6-C5	2.68	1.46	1.41
9	D	502	BG0	O12-C13	2.57	1.42	1.38
8	B	501	GDP	C2'-C1'	-2.53	1.49	1.53
9	B	503	BG0	O02-C03	2.52	1.41	1.37
10	F	401	ACP	PG-O2G	2.52	1.60	1.54
9	B	503	BG0	O12-C10	2.49	1.39	1.36
9	D	502	BG0	C14-N15	2.42	1.45	1.37
10	F	401	ACP	C5-C4	2.41	1.47	1.40
9	B	503	BG0	C14-N15	2.32	1.44	1.37
9	D	502	BG0	O12-C10	2.27	1.39	1.36
9	B	503	BG0	C16-N17	2.21	1.45	1.37
10	F	401	ACP	C2-N3	2.20	1.35	1.32
9	D	502	BG0	C16-N17	2.18	1.45	1.37
10	F	401	ACP	PB-O2B	2.10	1.61	1.56
8	B	501	GDP	O4'-C1'	2.09	1.44	1.41
8	B	501	GDP	C5-C4	2.08	1.46	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	BG0	C07-C10-N11	-12.63	116.86	127.93
9	B	503	BG0	C07-C10-N11	-11.63	117.73	127.93
9	D	502	BG0	O12-C10-C07	-11.37	117.01	122.31
9	B	503	BG0	O12-C10-C07	-9.37	117.95	122.31
5	A	501	GTP	C5-C6-N1	-9.05	111.05	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C5-C6-N1	-8.97	111.16	123.43
5	D	501	GTP	C5-C6-N1	-8.67	111.57	123.43
5	A	501	GTP	C6-N1-C2	6.27	125.89	115.93
5	C	501	GTP	C6-N1-C2	6.15	125.70	115.93
5	D	501	GTP	C6-N1-C2	5.67	124.94	115.93
8	B	501	GDP	C6-C5-C4	-5.10	115.93	120.80
8	B	501	GDP	C2-N3-C4	4.98	121.05	115.36
9	D	502	BG0	C06-C07-C10	-4.97	120.90	123.50
8	B	501	GDP	C6-N1-C2	4.39	122.91	115.93
9	B	503	BG0	O12-C10-N11	4.33	113.33	110.22
9	D	502	BG0	C05-C06-C07	-4.20	106.39	111.38
9	B	503	BG0	C06-C07-C10	-4.18	121.32	123.50
8	B	501	GDP	N3-C2-N1	-3.98	121.91	127.22
9	D	502	BG0	C06-C07-C08	3.98	123.01	118.32
10	F	401	ACP	C4-C5-N7	-3.94	105.29	109.40
10	F	401	ACP	C3'-C2'-C1'	3.91	106.86	100.98
9	B	503	BG0	C05-C06-C07	-3.56	107.14	111.38
9	B	503	BG0	C21-C05-C06	-3.55	115.43	120.56
9	D	502	BG0	O12-C10-N11	3.48	112.72	110.22
8	B	501	GDP	C5-C6-N1	-3.34	118.87	123.43
9	D	502	BG0	C13-O12-C10	-3.33	116.67	118.63
9	D	502	BG0	C21-C05-C06	-3.32	115.77	120.56
10	F	401	ACP	N3-C2-N1	-3.31	123.51	128.68
5	C	501	GTP	N3-C2-N1	-3.16	123.01	127.22
9	B	503	BG0	C20-C06-C07	3.07	113.73	108.17
9	D	502	BG0	C01-O02-C03	2.96	121.99	117.53
9	B	503	BG0	C03-C24-C22	2.95	123.20	119.25
5	A	501	GTP	N3-C2-N1	-2.95	123.29	127.22
9	D	502	BG0	C20-C06-C07	2.75	113.14	108.17
5	A	501	GTP	C2-N3-C4	-2.72	112.25	115.36
5	D	501	GTP	N3-C2-N1	-2.71	123.60	127.22
5	D	501	GTP	C2-N3-C4	-2.67	112.31	115.36
9	D	502	BG0	BR-C22-C24	2.62	122.33	118.51
9	D	502	BG0	C14-C13-C20	2.60	122.97	120.44
9	B	503	BG0	C21-C22-C24	-2.58	117.75	122.54
5	C	501	GTP	C2-N3-C4	-2.46	112.55	115.36
9	D	502	BG0	C13-C14-N15	-2.33	116.50	120.14
9	D	502	BG0	C04-C03-C24	-2.27	117.65	120.22
10	F	401	ACP	C1'-N9-C4	-2.25	122.69	126.64
9	D	502	BG0	C03-C24-C22	2.22	122.22	119.25
9	B	503	BG0	C04-C05-C06	2.19	123.73	120.56
9	B	503	BG0	BR-C22-C24	2.17	121.67	118.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	BG0	C01-O02-C03	2.14	120.75	117.53
9	B	503	BG0	C06-C07-C08	2.12	120.82	118.32
9	D	502	BG0	C21-C05-C04	2.01	120.95	118.08

There are no chirality outliers.

All (31) torsion outliers are listed below:

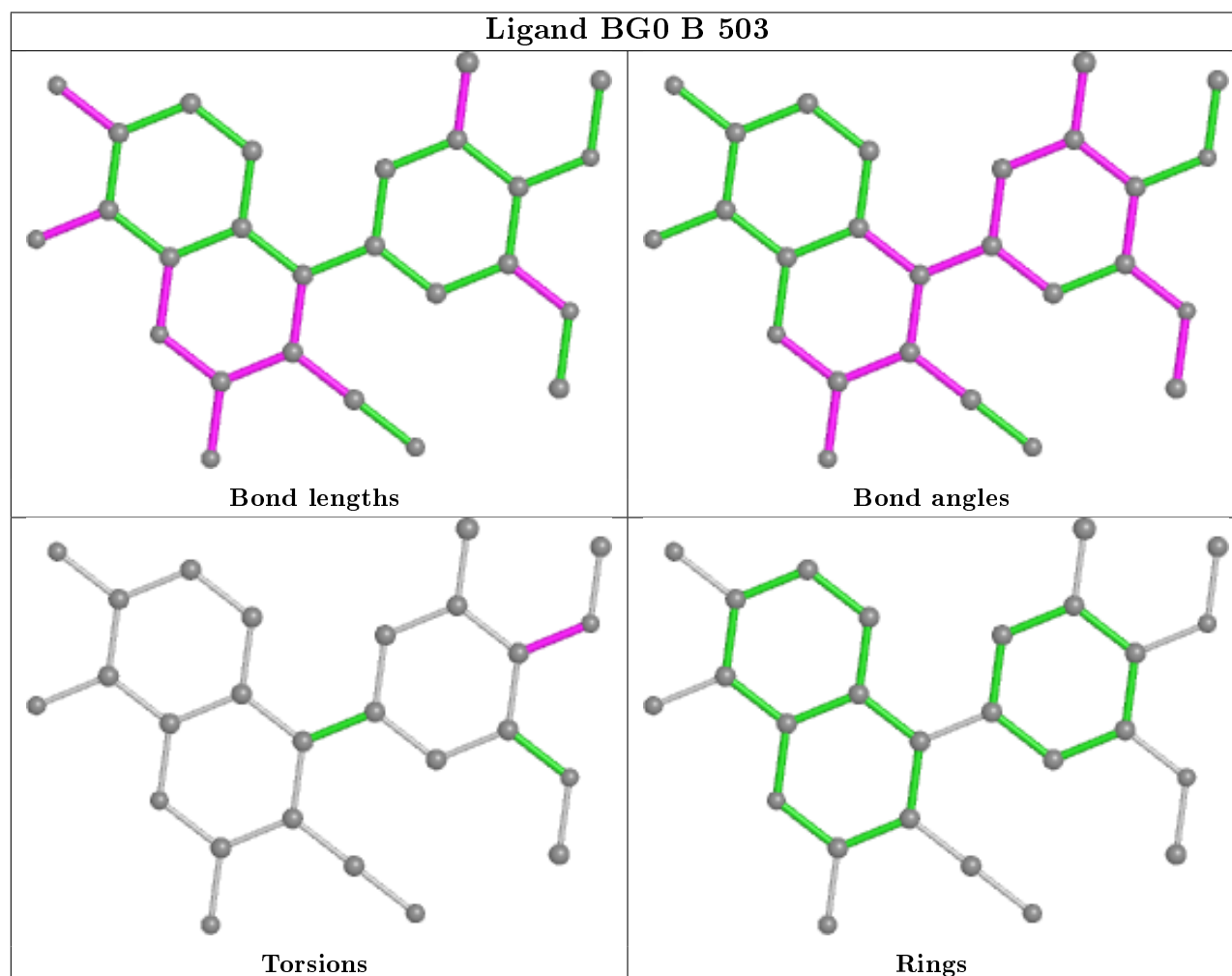
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
10	F	401	ACP	PG-C3B-PB-O1B
10	F	401	ACP	PG-C3B-PB-O3A
10	F	401	ACP	C5'-O5'-PA-O1A
5	D	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
10	F	401	ACP	O4'-C4'-C5'-O5'
10	F	401	ACP	C3'-C4'-C5'-O5'
9	B	503	BG0	C22-C24-O25-C26
8	B	501	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	PG-O3B-PB-O1B
9	D	502	BG0	C24-C03-O02-C01
8	B	501	GDP	C5'-O5'-PA-O2A
10	F	401	ACP	PG-C3B-PB-O2B
5	D	501	GTP	PG-O3B-PB-O2B
5	C	501	GTP	C4'-C5'-O5'-PA
9	D	502	BG0	C04-C03-O02-C01
5	D	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
10	F	401	ACP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G

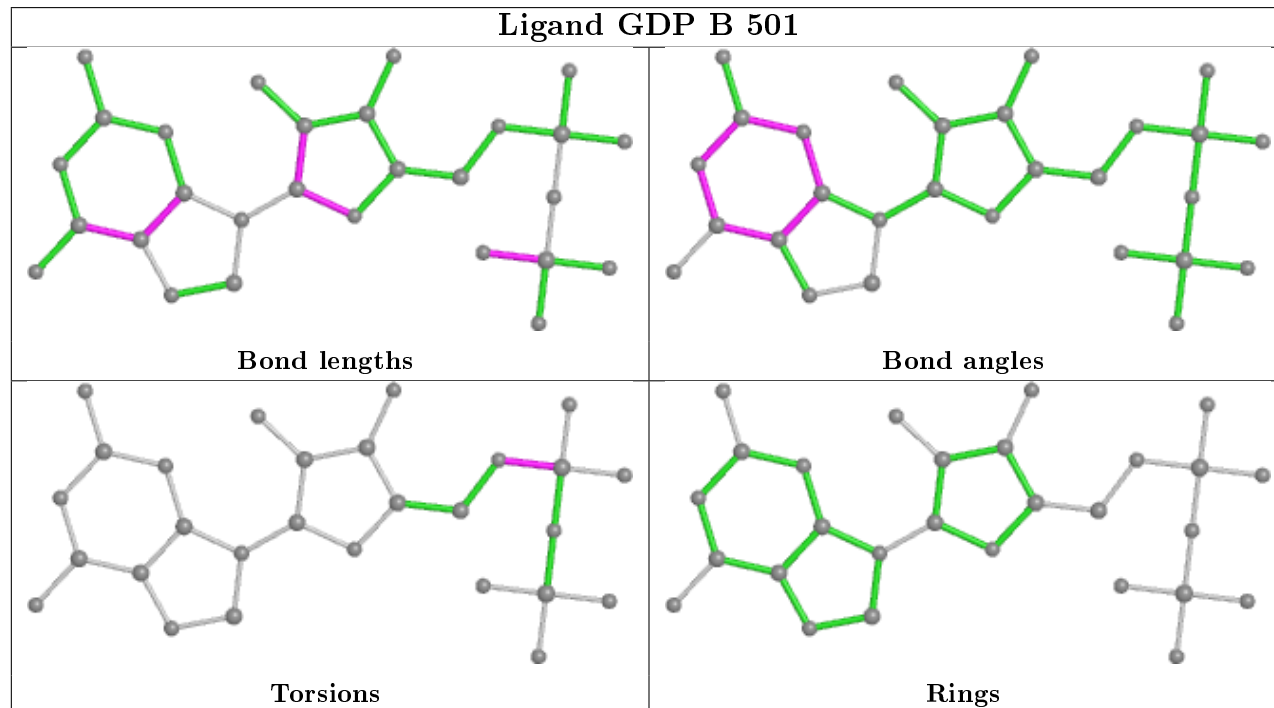
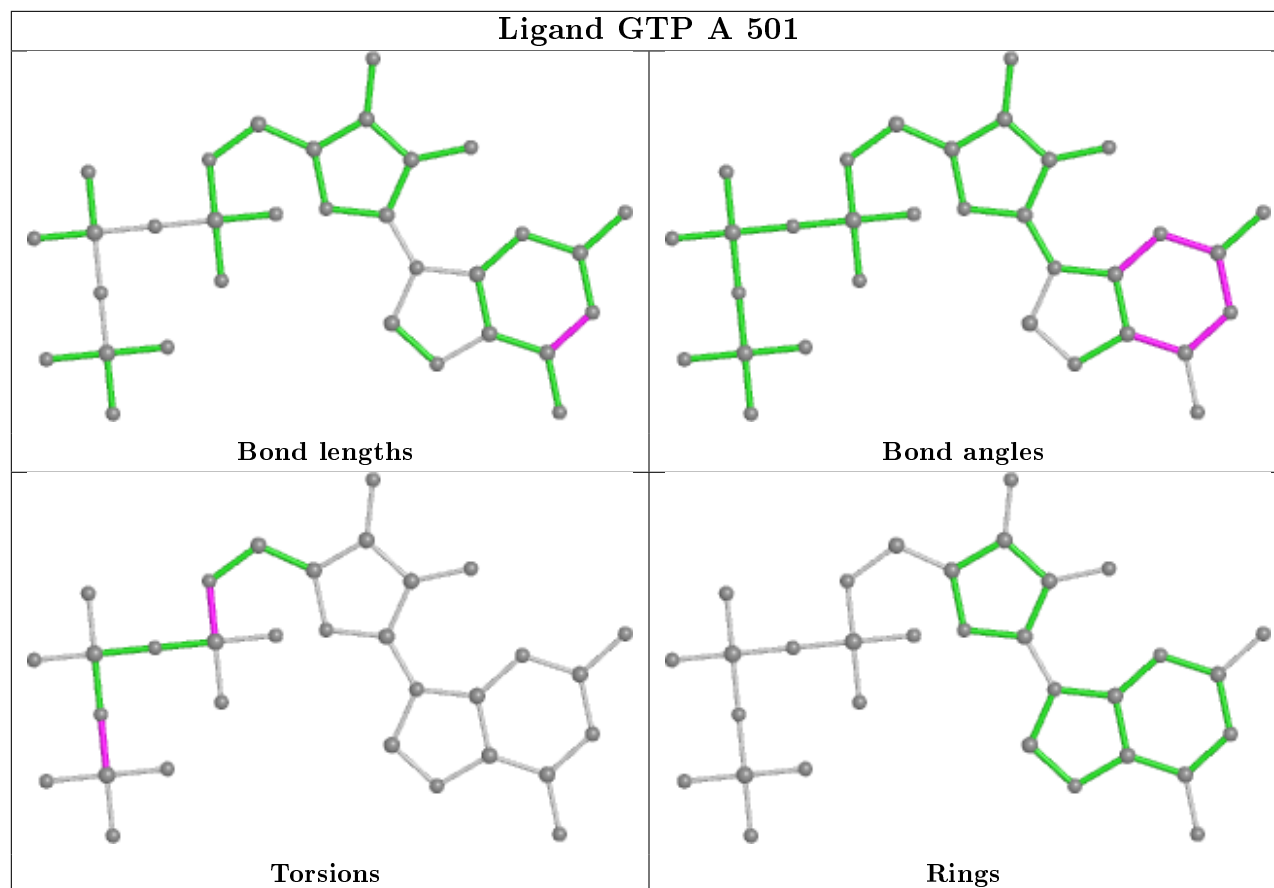
There are no ring outliers.

4 monomers are involved in 9 short contacts:

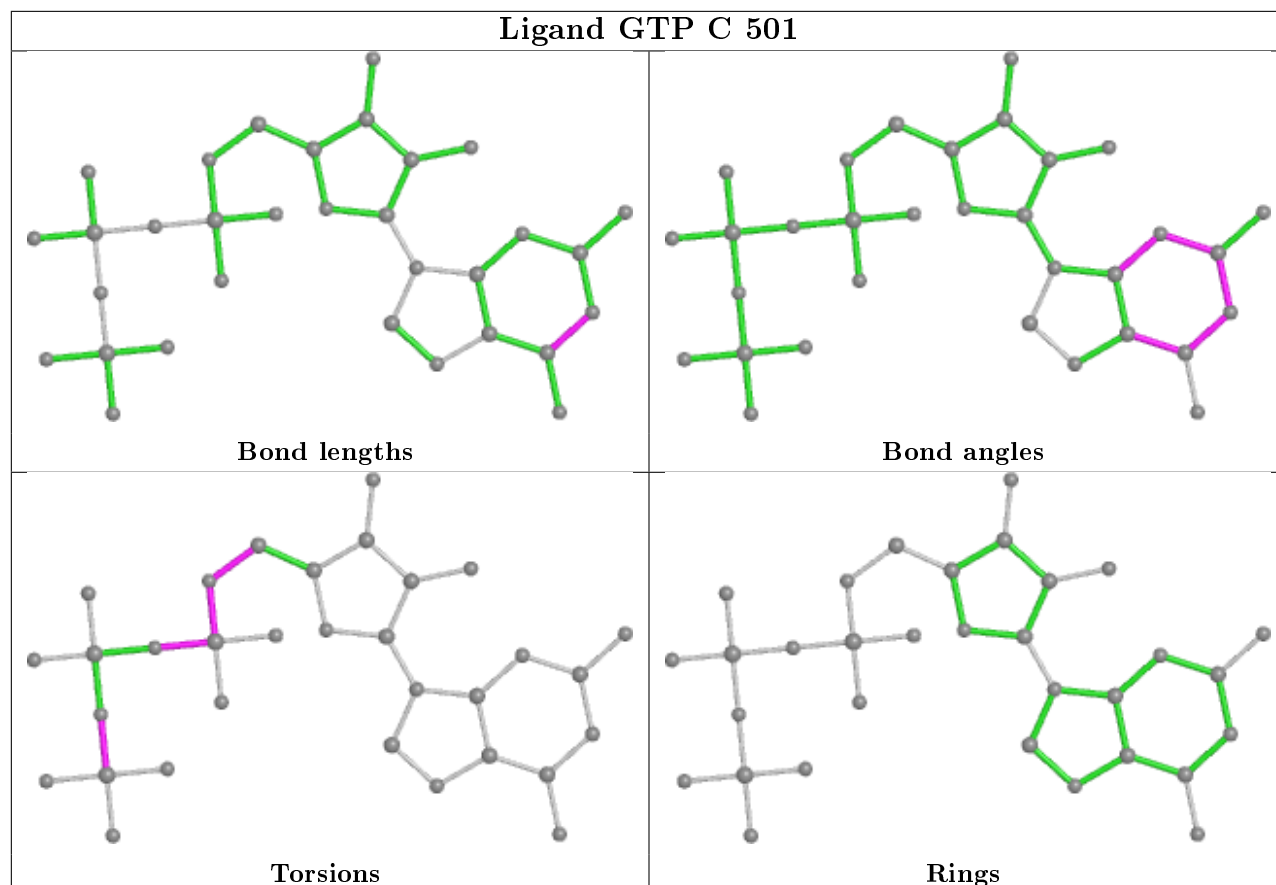
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	BG0	3	0
5	D	501	GTP	3	0
9	D	502	BG0	1	0
10	F	401	ACP	2	0

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 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.

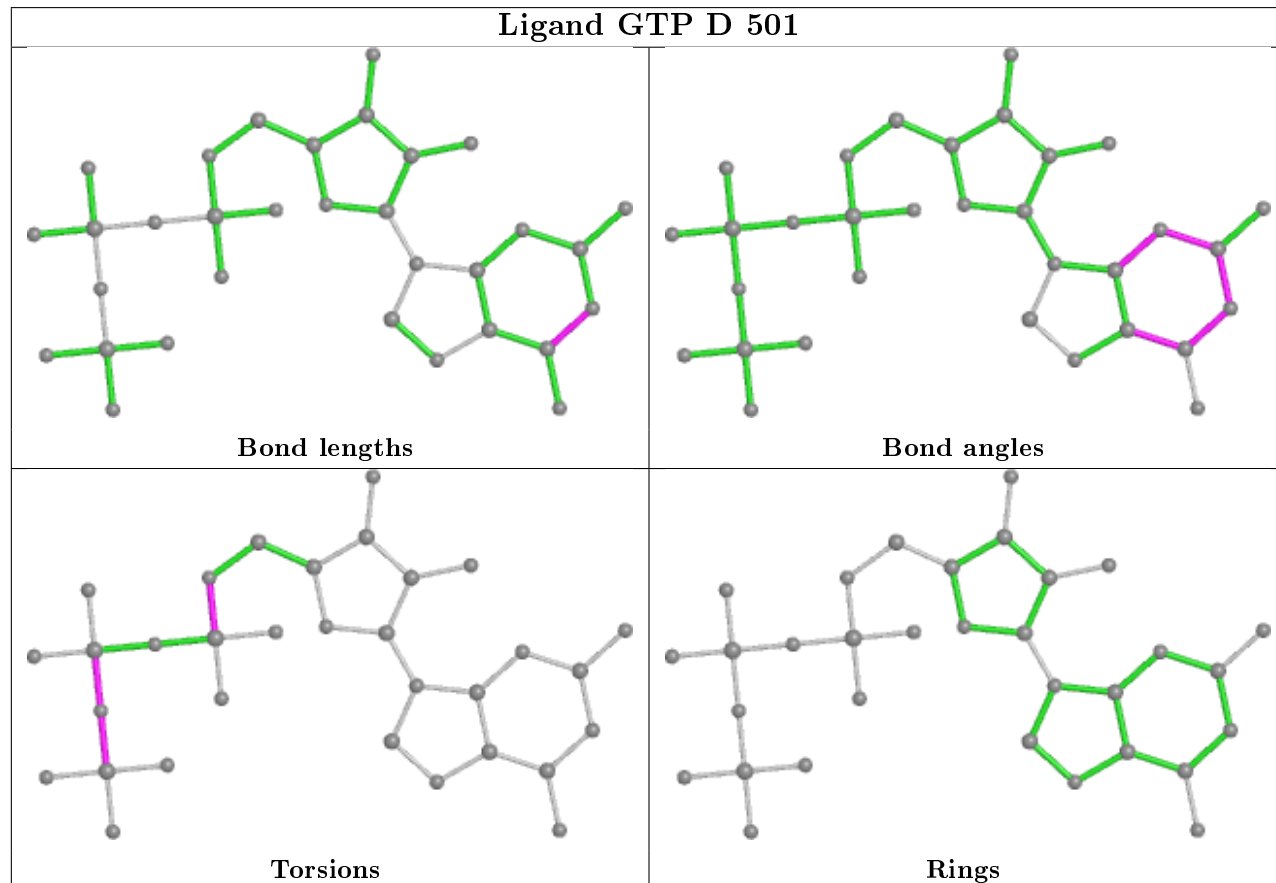


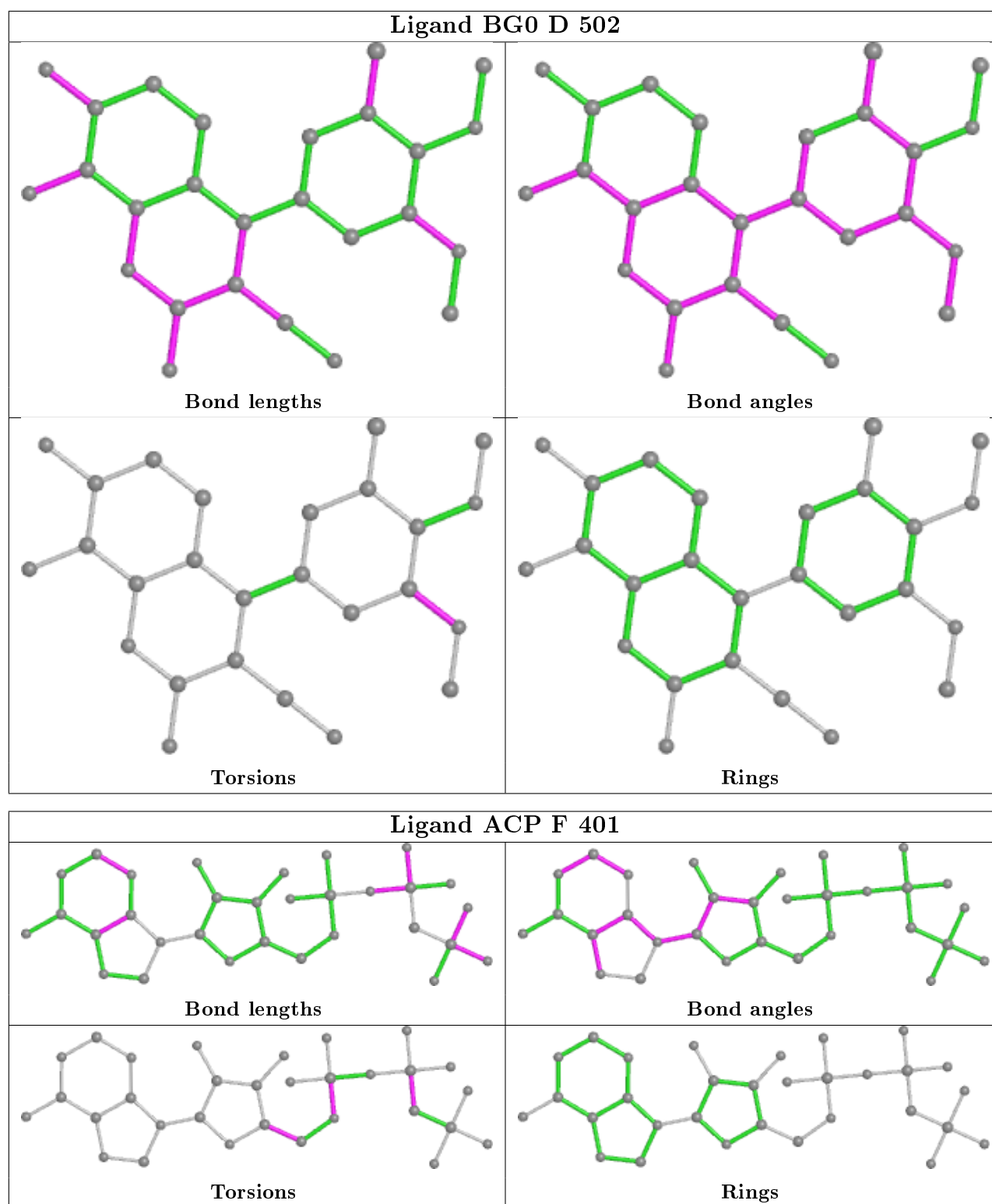


Ligand GTP C 501



Ligand GTP D 501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	437/450 (97%)	0.07	5 (1%) 80 82	16, 34, 66, 96	0
1	C	440/450 (97%)	-0.25	2 (0%) 91 91	8, 25, 52, 71	1 (0%)
2	B	424/445 (95%)	0.04	15 (3%) 44 47	12, 32, 66, 103	1 (0%)
2	D	421/445 (94%)	1.42	106 (25%) 0 0	22, 69, 127, 167	4 (0%)
3	E	120/143 (83%)	0.88	20 (16%) 1 1	25, 55, 124, 131	0
4	F	309/384 (80%)	1.53	94 (30%) 0 0	24, 67, 131, 167	0
All	All	2151/2317 (92%)	0.52	242 (11%) 5 4	8, 41, 110, 167	6 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	215	LEU	15.7
4	F	233	PHE	10.3
2	D	211	CYS	10.2
4	F	383	HIS	8.7
4	F	384	HIS	8.4
2	D	37	HIS	8.4
4	F	159	GLY	8.3
4	F	231	ALA	8.3
4	F	149	ALA	8.2
2	D	394	PHE	8.1
4	F	382	HIS	8.0
4	F	182	ILE	7.8
2	D	84	ILE	7.5
4	F	234	GLN	7.4
2	D	217	LEU	7.2
2	D	396	HIS	7.2
4	F	362	ALA	7.0
4	F	101	TYR	6.9
4	F	194	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
2	D	98	GLY	6.8
4	F	230	SER	6.8
2	D	180	VAL	6.7
2	D	397	TRP	6.3
2	D	83	GLN	6.1
2	B	54	ALA	6.1
4	F	232	ASN	6.0
4	F	181	VAL	6.0
4	F	225	SER	6.0
4	F	191	LEU	5.8
4	F	239	HIS	5.7
4	F	100	ILE	5.6
4	F	245	ILE	5.5
2	D	74	ASP	5.5
2	D	178	THR	5.5
4	F	161	LEU	5.5
2	D	177	ASP	5.5
2	D	30	ILE	5.5
2	D	92	PHE	5.4
2	D	214	THR	5.4
4	F	20	LEU	5.3
2	D	73	MET	5.2
4	F	227	PRO	5.0
2	D	31	ASP	4.9
2	D	284	LEU	4.9
4	F	252	ASN	4.9
4	F	238	CYS	4.9
4	F	147	TRP	4.9
4	F	380	HIS	4.9
4	F	150	LYS	4.9
4	F	381	HIS	4.8
4	F	255	ARG	4.8
2	D	405	GLU	4.7
2	D	175	VAL	4.7
2	D	55	THR	4.7
2	D	216	LYS	4.7
2	D	112	LEU	4.6
2	D	400	GLY	4.5
4	F	99	VAL	4.5
2	D	181	GLU	4.5
4	F	165	GLU	4.5
3	E	138	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	240	LEU	4.4
4	F	256	TYR	4.3
4	F	21	LEU	4.3
2	D	387	ALA	4.3
2	D	78	SER	4.3
2	B	281	TYR	4.3
4	F	223	THR	4.1
2	D	56	GLY	4.1
4	F	160	ILE	4.1
2	D	71	GLY	4.1
2	D	384	GLN	4.1
2	D	29	GLY	4.0
4	F	17	VAL	4.0
2	D	36	TYR	4.0
4	F	253	TYR	4.0
2	D	388	MET	3.9
2	D	80	PRO	3.9
2	D	391	ARG	3.9
4	F	197	ARG	3.9
4	F	162	ILE	3.9
2	D	223	GLY	3.9
4	F	220	VAL	3.9
2	D	44	LEU	3.8
2	B	56	GLY	3.8
3	E	6	MET	3.7
4	F	263	PHE	3.7
4	F	337	ALA	3.7
4	F	242	ASN	3.7
4	F	102	PRO	3.7
3	E	48	GLU	3.6
1	C	440	VAL	3.6
2	D	208	TYR	3.6
2	D	87	PRO	3.5
2	D	53	GLU	3.5
4	F	32	LYS	3.5
2	D	59	TYR	3.5
2	D	212	PHE	3.5
2	B	280	GLN	3.5
2	D	54	ALA	3.5
4	F	244	CYS	3.5
3	E	135	LYS	3.5
2	D	57	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	81	PHE	3.5
2	D	65	LEU	3.4
2	D	77	ARG	3.4
2	D	359	ARG	3.4
2	D	385	PHE	3.4
2	D	285	THR	3.4
4	F	25	GLY	3.3
2	D	1	MET	3.3
4	F	330	ILE	3.2
1	A	346	TRP	3.2
2	D	362	LYS	3.2
2	D	169	VAL	3.2
4	F	13	VAL	3.2
4	F	361	LEU	3.2
4	F	258	GLU	3.2
2	D	183	TYR	3.2
2	B	37	HIS	3.2
4	F	195	GLY	3.2
2	D	320	ARG	3.2
3	E	24	LEU	3.2
4	F	146	VAL	3.2
3	E	45	PRO	3.1
2	D	90	PHE	3.1
2	D	103	LYS	3.1
2	D	228	LEU	3.1
2	D	390	ARG	3.1
3	E	124	GLN	3.1
4	F	196	HIS	3.1
2	D	97	ALA	3.0
2	B	245	GLN	3.0
4	F	222	ARG	3.0
4	F	237	THR	3.0
2	D	91	VAL	3.0
2	D	100	ASN	3.0
3	E	44	ASP	3.0
2	D	273	LEU	3.0
4	F	224	SER	3.0
2	D	381	ILE	2.9
2	D	15	GLN	2.9
2	B	59	TYR	2.9
2	D	353	VAL	2.9
4	F	379	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	185	TYR	2.9
2	D	86	ARG	2.9
2	D	40	SER	2.9
3	E	139	LEU	2.9
4	F	23	ALA	2.9
2	D	222	TYR	2.9
2	D	323	MET	2.9
2	D	33	THR	2.9
4	F	24	THR	2.8
3	E	134	ARG	2.8
4	F	151	SER	2.8
1	A	282	TYR	2.8
4	F	226	GLU	2.8
2	D	88	ASP	2.8
2	D	360	GLY	2.8
4	F	183	GLN	2.8
2	B	57	ASN	2.7
3	E	25	LYS	2.7
2	D	389	PHE	2.7
2	D	76	VAL	2.7
4	F	98	TYR	2.7
2	D	75	SER	2.7
2	D	218	THR	2.7
4	F	188	LYS	2.7
4	F	10	ASN	2.7
4	F	41	LEU	2.7
3	E	26	PRO	2.7
2	D	171	PRO	2.7
2	D	104	GLY	2.6
2	D	210	ILE	2.6
3	E	137	LYS	2.6
3	E	133	VAL	2.6
4	F	228	TYR	2.6
4	F	270	TYR	2.6
3	E	57	ALA	2.6
4	F	9	GLU	2.6
4	F	163	SER	2.6
2	D	60	VAL	2.5
4	F	199	PHE	2.5
1	A	281	ALA	2.5
2	B	427	ASP	2.5
4	F	340	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	430	LYS	2.5
2	B	58	LYS	2.5
4	F	180	HIS	2.5
4	F	22	LEU	2.5
3	E	103	GLN	2.5
4	F	257	GLU	2.5
2	D	115	SER	2.5
4	F	148	ILE	2.4
4	F	266	GLU	2.4
2	B	428	ALA	2.4
2	D	28	HIS	2.4
4	F	192	LEU	2.4
2	D	70	PRO	2.4
4	F	235	ASP	2.4
2	D	85	PHE	2.4
4	F	27	TRP	2.4
2	D	207	LEU	2.4
4	F	44	ARG	2.3
4	F	184	LYS	2.3
2	D	126	SER	2.3
2	D	136	THR	2.3
4	F	274	ALA	2.3
4	F	14	TYR	2.3
2	D	119	VAL	2.3
2	D	95	SER	2.3
4	F	339	ALA	2.3
2	B	320	ARG	2.2
3	E	141	GLU	2.2
2	B	246	LEU	2.2
2	B	55	THR	2.2
4	F	229	ASN	2.2
2	D	118	ASP	2.2
2	D	172	SER	2.2
2	D	116	VAL	2.2
4	F	344	ALA	2.2
2	D	41	ASP	2.2
3	E	96	MET	2.2
2	D	39	ASP	2.2
1	C	340	SER	2.2
1	A	437	VAL	2.2
3	E	62	LYS	2.2
2	D	35	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	245	GLN	2.1
2	D	403	MET	2.1
4	F	6	VAL	2.1
2	D	227	HIS	2.1
2	D	48	ASN	2.1
4	F	275	LEU	2.1
2	B	338	SER	2.1
2	D	94	GLN	2.1
2	D	363	MET	2.1
2	D	68	LEU	2.0
2	D	176	SER	2.0
3	E	140	LYS	2.0
4	F	273	ASP	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(\AA^2)	Q<0.9
6	MG	B	502	1/1	0.80	0.34	59,59,59,59	0
10	ACP	F	401	31/31	0.86	0.22	62,74,100,104	0
5	GTP	D	501	32/32	0.87	0.18	39,49,65,72	0
9	BG0	D	502	26/26	0.94	0.13	26,30,47,64	0
7	CA	A	503	1/1	0.94	0.05	54,54,54,54	0
6	MG	A	502	1/1	0.94	0.12	23,23,23,23	0
9	BG0	B	503	26/26	0.95	0.16	22,25,36,54	0
7	CA	C	503	1/1	0.95	0.03	37,37,37,37	0
6	MG	C	502	1/1	0.97	0.11	16,16,16,16	0
5	GTP	A	501	32/32	0.98	0.16	17,19,20,21	0

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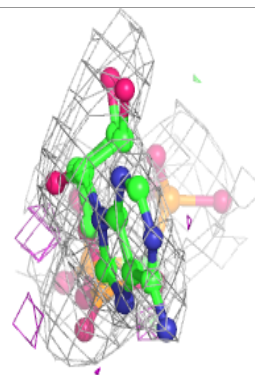
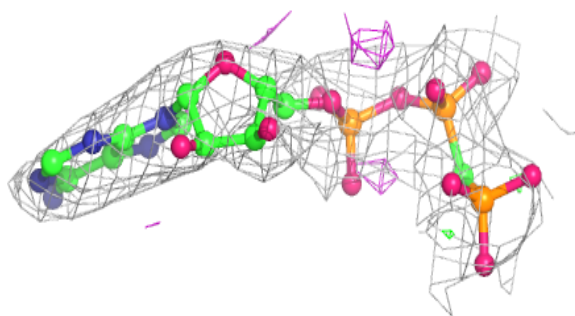
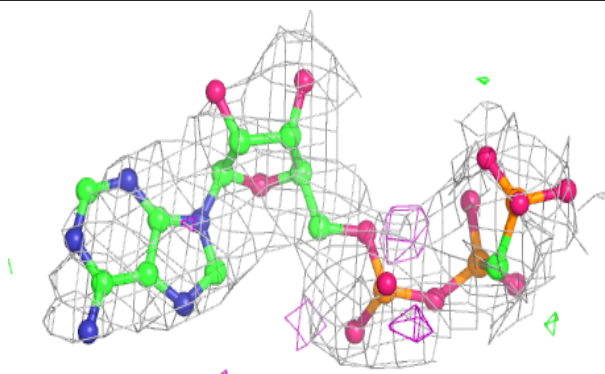
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GDP	B	501	28/28	0.98	0.15	12,15,16,20	0
5	GTP	C	501	32/32	0.99	0.13	12,14,15,16	0

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.

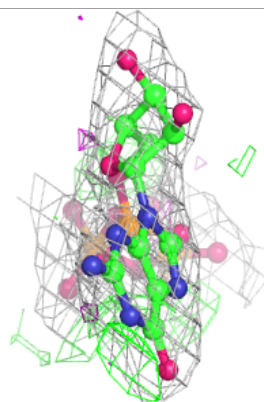
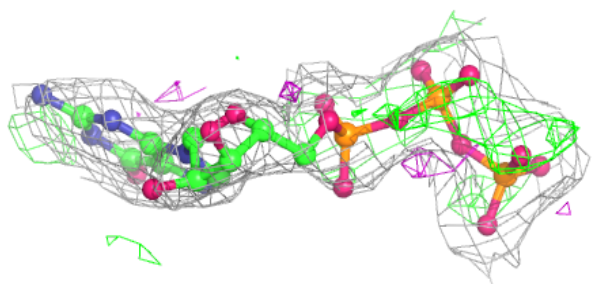
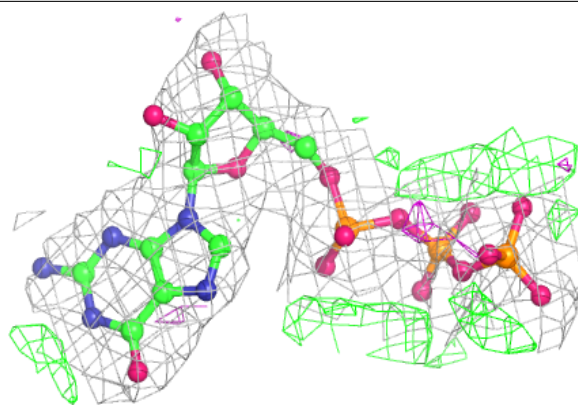
Electron density around ACP F 401:

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



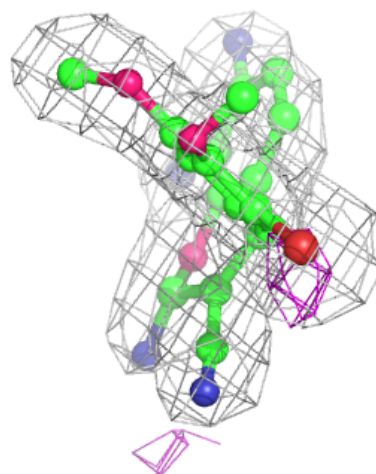
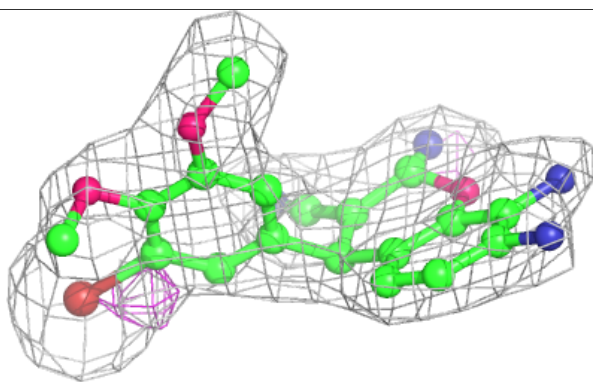
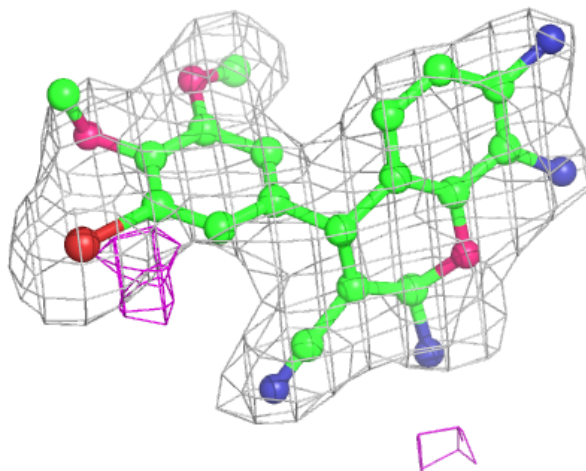
Electron density around GTP D 501:

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



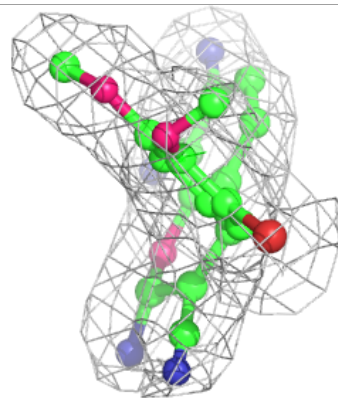
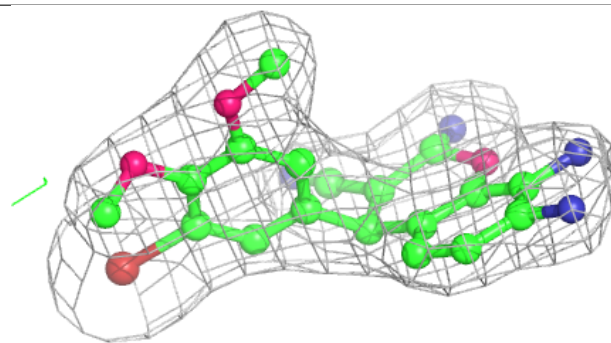
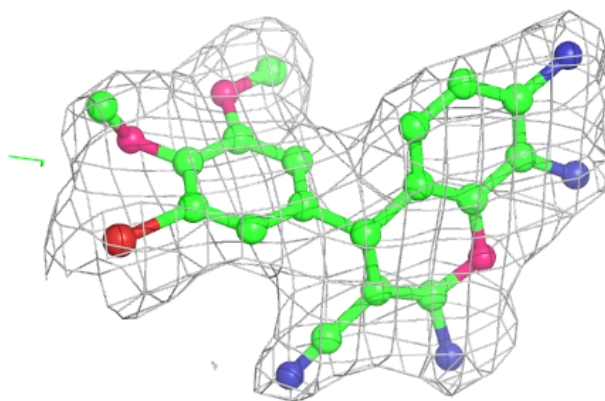
Electron density around BG0 D 502:

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

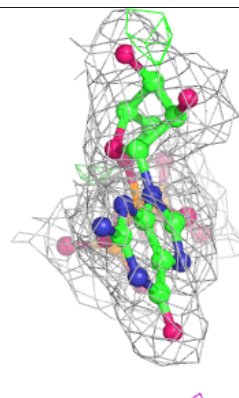
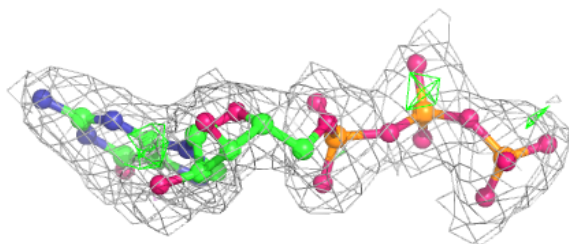
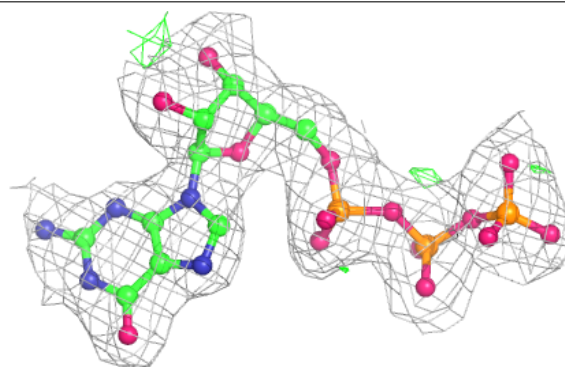


Electron density around BG0 B 503:

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

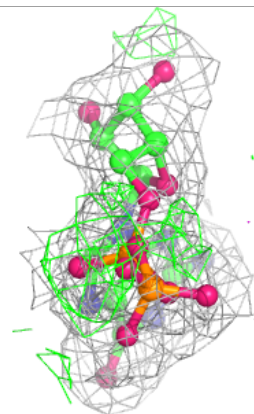
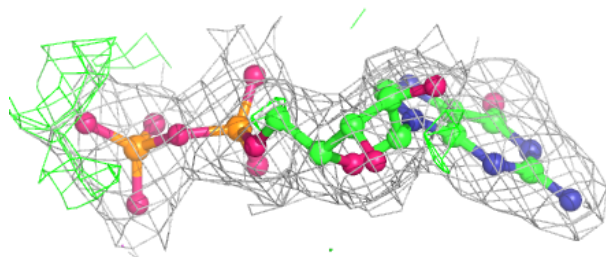
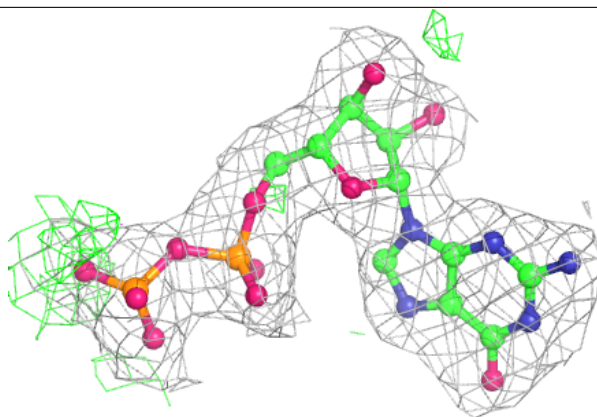
**Electron density around GTP A 501:**

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

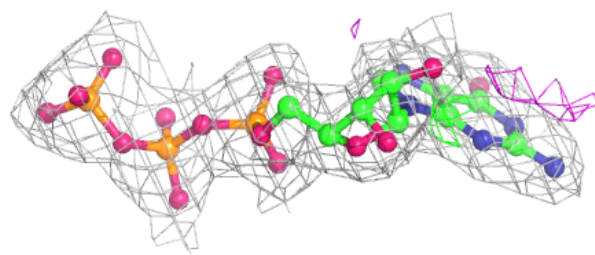
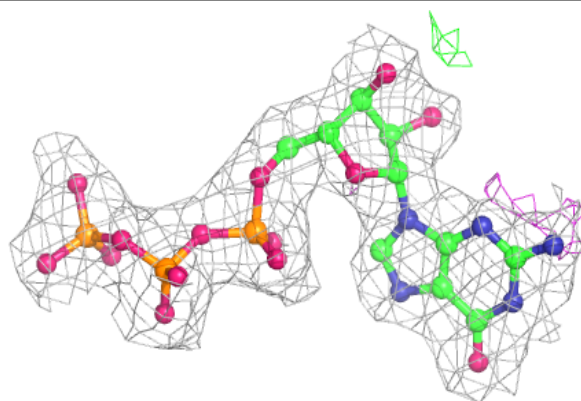


Electron density around GDP B 501:

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

**Electron density around GTP C 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.