



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:55 PM UTC

PDB ID : 6JCJ / pdb_00006jcj
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

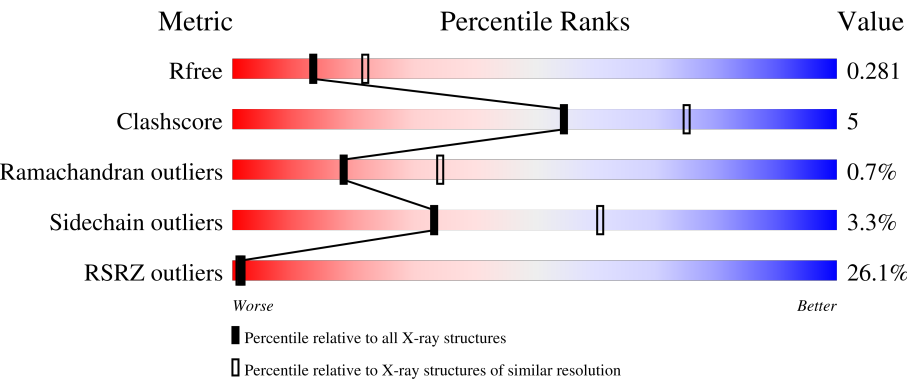
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	8% 86% 11% • •
1	C	450	4% 84% 14% •
2	B	445	8% 81% 13% • 5%
2	D	445	57% 78% 15% • 5%
3	E	143	40% 73% 11% 16%

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Mol	Chain	Length	Quality of chain
4	F	384	42% 70% 10% 20%

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

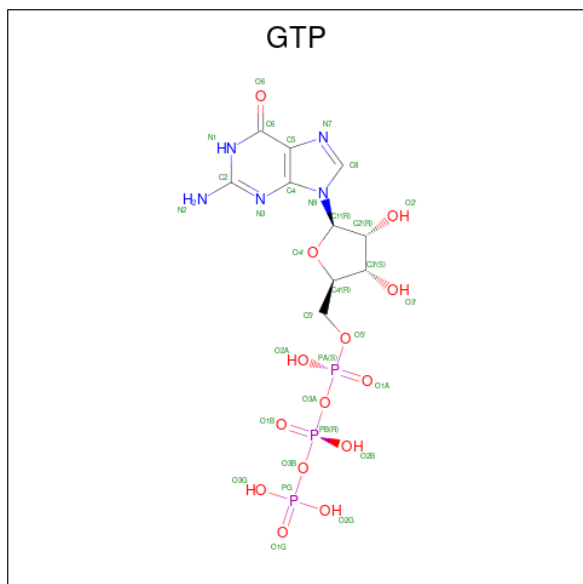
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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 (CCD ID: 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		

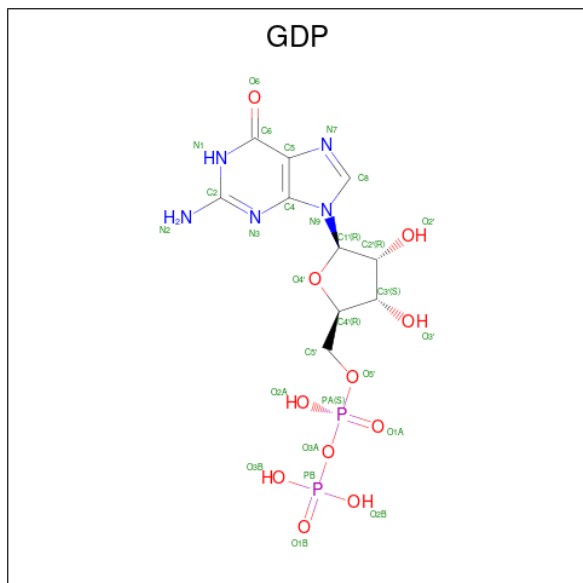
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

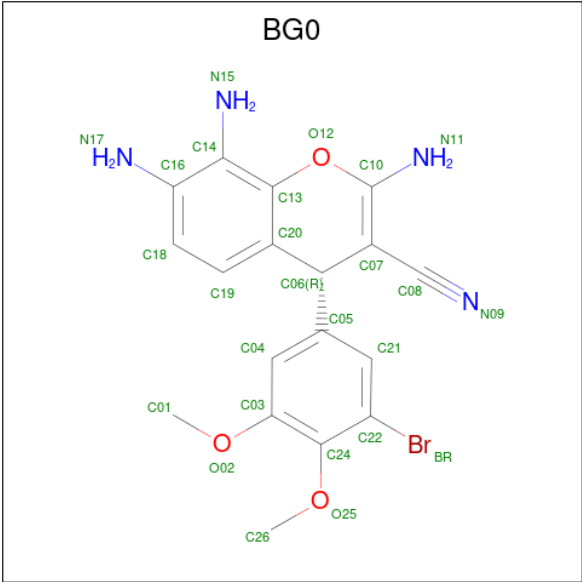
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: 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		

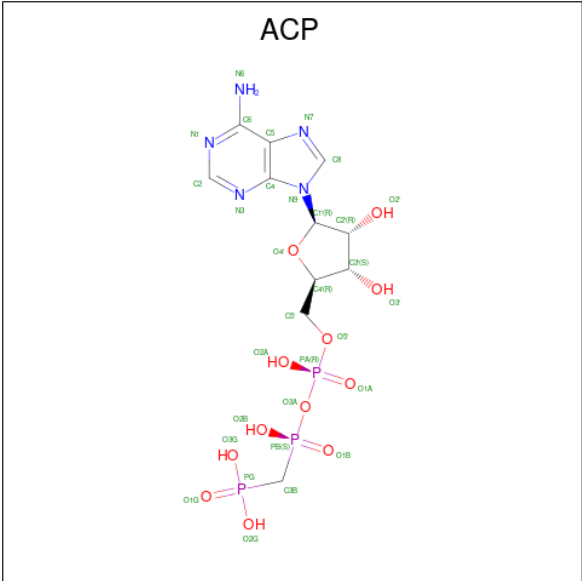
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





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 (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

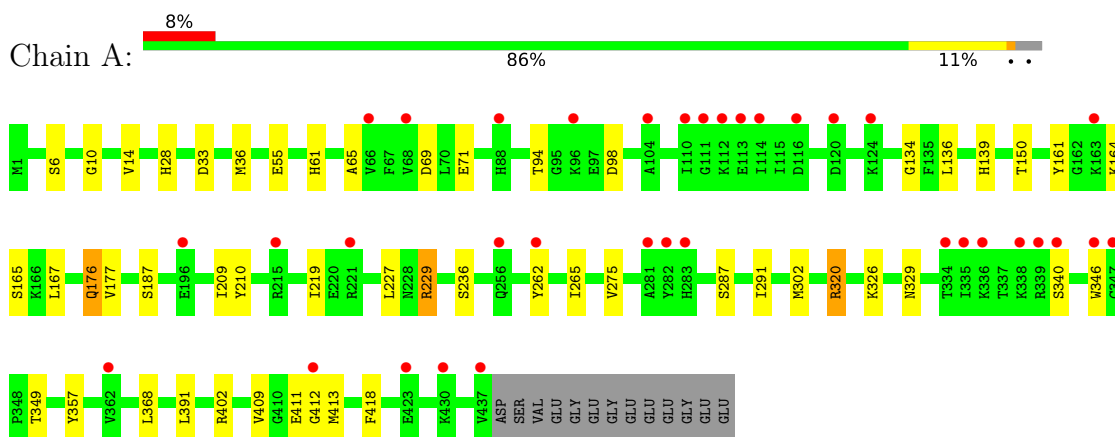


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

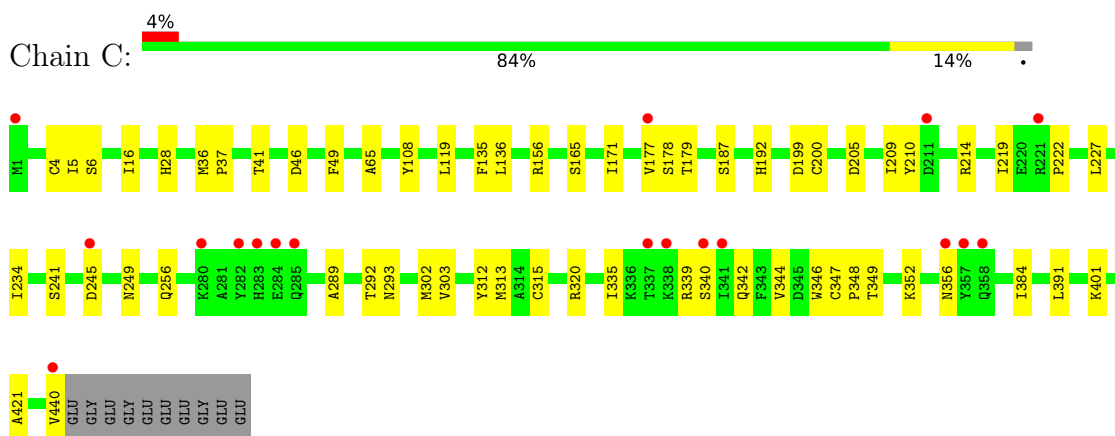
- Molecule 11 is water.

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

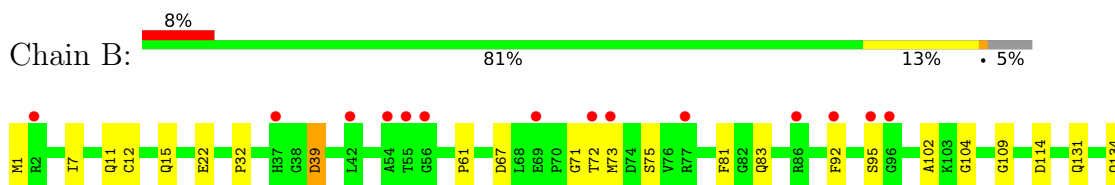
- Molecule 1: Tubulin alpha-1B chain

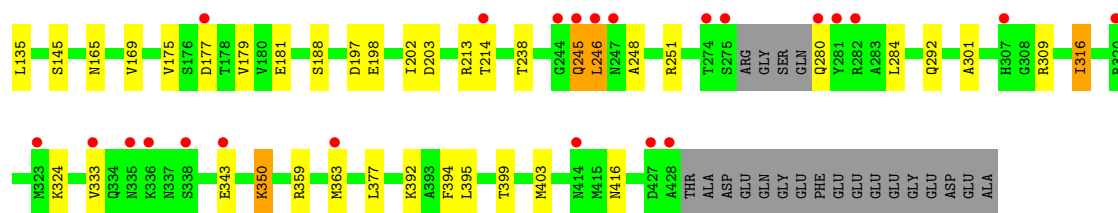


- Molecule 1: Tubulin alpha-1B chain

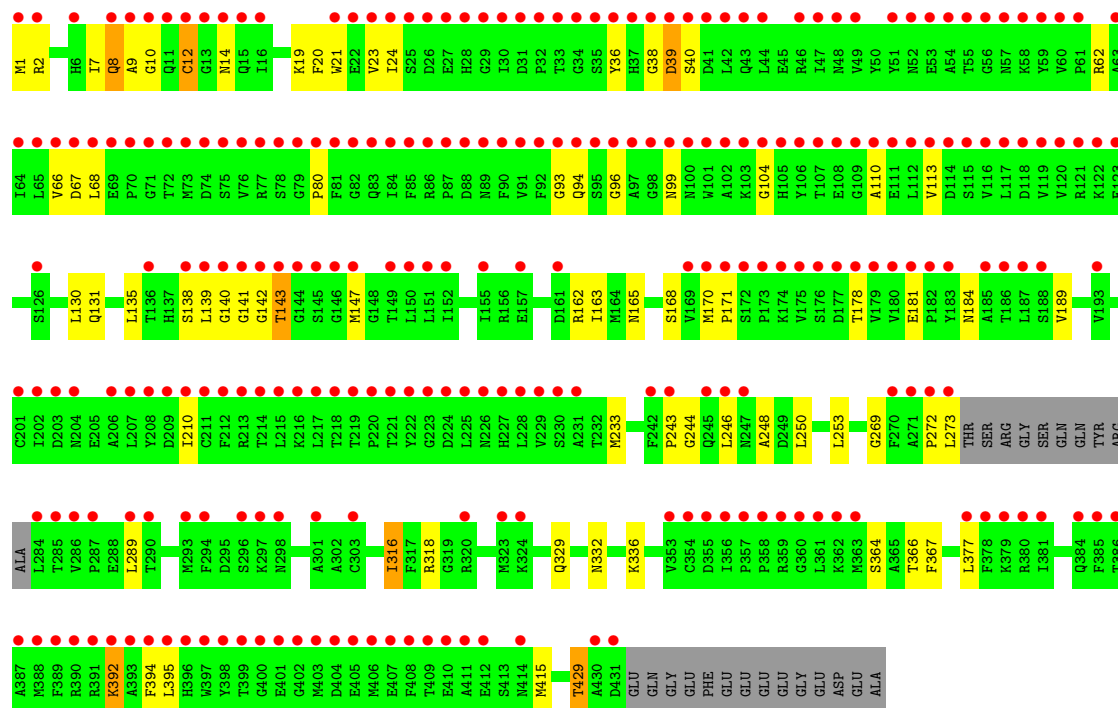
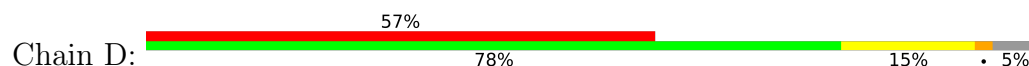


- Molecule 2: Tubulin beta-2B chain

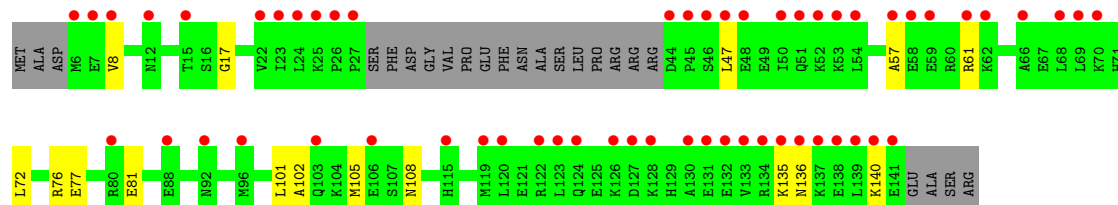




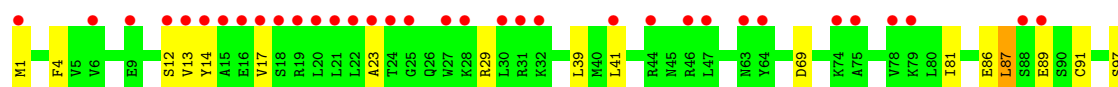
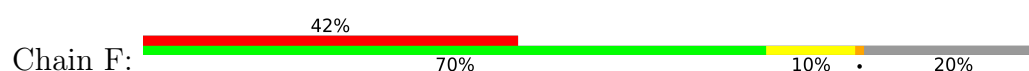
• Molecule 2: Tubulin beta-2B chain



• 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 48.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.42-2.50) 99.1 (48.42-2.50)	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 (4.87%)	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)	0.31 , 34.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BG0, GDP, CA, ACP, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.01	0/3525	1.44	1/4784 (0.0%)
1	C	1.00	0/3572	1.42	1/4850 (0.0%)
2	B	1.00	0/3416	1.41	2/4626 (0.0%)
2	D	1.03	0/3379	1.48	2/4577 (0.0%)
3	E	1.02	0/1018	1.61	4/1350 (0.3%)
4	F	1.05	0/2618	1.36	0/3537
All	All	1.02	0/17528	1.44	10/23724 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	TYR	CB-CA-C	6.04	115.88	110.44
2	B	399	THR	CB-CA-C	5.37	119.98	110.85
2	B	416	ASN	CB-CA-C	5.36	119.68	110.79
2	D	12	CYS	CA-C-N	5.23	125.75	119.94
2	D	12	CYS	C-N-CA	5.23	125.75	119.94
3	E	81	GLU	CA-C-N	5.18	127.08	120.56
3	E	81	GLU	C-N-CA	5.18	127.08	120.56
3	E	102	ALA	CA-C-N	5.08	127.04	120.44
3	E	102	ALA	C-N-CA	5.08	127.04	120.44
1	C	349	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3441	0	3362	37	0
1	C	3482	0	3384	27	0
2	B	3342	0	3216	31	0
2	D	3306	0	3181	43	0
3	E	1004	0	1028	11	0
4	F	2553	0	2519	21	0
5	A	32	0	12	0	0
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	4	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	162	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 5.

All (162) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ASN:ND2	11:D:601:HOH:O	2.21	0.74
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:HG2	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:HD12	1:A:368[B]:LEU:N	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
3:E:135:LYS:C	3:E:136:ASN:HD22	2.06	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
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
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:19:LYS:O	2:D:23:VAL:HG23	2.06	0.55
2:D:139:LEU:HD11	2:D:168:SER:HB3	1.88	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
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:HD12	1:A:368[B]:LEU:H	1.74	0.52
2:D:1:MET:HE3	2:D:131:GLN:CB	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:HE3	2:D:131:GLN:HB2	1.93	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:289:ALA:O	1:C:293[B]:ASN:CG	2.55	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:C:36:MET:HE1	1:C:49:PHE:CE2	2.47	0.50
4:F:320:MET:HE2	10:F:401:ACP:H2	1.94	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:33:ASP:OD1	1:A:33:ASP:C	2.55	0.49
4:F:320:MET:HE2	10:F:401:ACP:C2	2.42	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
2:B:248:ALA:HA	9:B:503:BG0:N09	2.28	0.49
1:C:108:TYR:CD2	3:E:108:ASN:CG	2.91	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.48
4:F:4:PHE:HA	4:F:39:LEU:O	2.14	0.48
4:F:277:THR:HG21	4:F:282:SER:HB3	1.95	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:197:ASP:C	2:B:198:GLU:HG3	2.39	0.48
2:B:145:SER:HG	2:B:188:SER:HG	1.62	0.47
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:A:413:MET:HE2	1:A:418:PHE:CE1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:HD23	2:B:246:LEU:HA	1.75	0.44
3:E:47:LEU:HD12	3:E:47:LEU:O	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:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.44
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.44
2:B:203:ASP:CB	2:B:301:ALA:HA	2.48	0.44
1:A:98:ASP:OD1	1:A:98:ASP:C	2.61	0.43
1:C:401:LYS:NZ	2:D:429:THR:O	2.31	0.43
2:D:272:PRO:HD3	2:D:289:LEU:HD21	1.99	0.43
2:B:39:ASP:N	2:B:39:ASP:OD1	2.51	0.43
2:D:67:ASP:HA	2:D:143:THR:HG21	2.00	0.43
2:D:170:MET:HE3	2:D:171:PRO:HD2	2.01	0.43
2:D:36:TYR:OH	2:D:40:SER:O	2.35	0.43
1:A:28:HIS:O	1:A:36:MET:HE3	2.18	0.43
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.55	0.43
1:C:28:HIS:O	1:C:36:MET:HE3	2.18	0.43
2:B:73:MET:SD	2:B:92:PHE:HB3	2.59	0.43
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.48	0.43
1:C:119:LEU:HD12	1:C:156:ARG:NH2	2.34	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:4:PHE:CZ	4:F:29:ARG:HB2	2.55	0.42
4:F:189:PRO:HG3	4:F:198:LYS:HE2	2.01	0.42
2:D:20:PHE:HB2	2:D:233:MET:HE2	2.01	0.42
2:D:269:GLY:O	2:D:367:PHE:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.54	0.42
1:A:329:ASN:ND2	3:E:8:VAL:HG21	2.34	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:A:357:TYR:CD2	3:E:17:GLY:HA2	2.55	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
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
2:D:38:GLY:C	2:D:39:ASP:OD1	2.63	0.41
2:D:170:MET:HE2	2:D:377:LEU:HD21	2.01	0.41
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
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: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
2:D:246:LEU:CD2	2:D:248:ALA:HB2	2.51	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
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:B:377:LEU:HD23	2:B:377:LEU:C	2.46	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
4:F:208:ASP:OD1	4:F:208:ASP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	43	63
1	C	446/450 (99%)	435 (98%)	10 (2%)	1 (0%)	43	63
2	B	421/445 (95%)	400 (95%)	18 (4%)	3 (1%)	18	34
2	D	417/445 (94%)	372 (89%)	37 (9%)	8 (2%)	6	11
3	E	118/143 (82%)	116 (98%)	1 (1%)	1 (1%)	16	31
4	F	300/384 (78%)	276 (92%)	23 (8%)	1 (0%)	36	55
All	All	2141/2317 (92%)	2016 (94%)	110 (5%)	15 (1%)	18	34

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
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%)	363 (98%)	9 (2%)	43	70
1	C	379/378 (100%)	366 (97%)	13 (3%)	32	60
2	B	366/383 (96%)	347 (95%)	19 (5%)	21	42
2	D	362/383 (94%)	353 (98%)	9 (2%)	42	69
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	87
4	F	281/342 (82%)	270 (96%)	11 (4%)	28	55
All	All	1870/1991 (94%)	1808 (97%)	62 (3%)	33	61

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	177	VAL
1	A	219	ILE
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	320	ARG
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	175	VAL
2	B	214	THR
2	B	245	GLN
2	B	246	LEU
2	B	251	ARG
2	B	280	GLN

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Mol	Chain	Res	Type
2	B	316	ILE
2	B	324	LYS
2	B	333	VAL
2	B	350	LYS
2	B	359	ARG
2	B	363	MET
1	C	37	PRO
1	C	41	THR
1	C	46	ASP
1	C	177	VAL
1	C	178	SER
1	C	179	THR
1	C	234	ILE
1	C	245	ASP
1	C	256	GLN
1	C	340	SER
1	C	342	GLN
1	C	384	ILE
1	C	440	VAL
2	D	2	ARG
2	D	8	GLN
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
4	F	1	MET
4	F	12	SER
4	F	69	ASP
4	F	86	GLU
4	F	87	LEU
4	F	89	GLU
4	F	91	CYS
4	F	165	GLU
4	F	200	ASP
4	F	331	GLU
4	F	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	101	ASN
1	A	329	ASN
1	A	393	HIS
2	B	8	GLN
2	B	11	GLN
2	B	37	HIS
2	B	83	GLN
2	B	94	GLN
2	B	245	GLN
2	B	292	GLN
2	B	307	HIS
2	B	329	GLN
2	B	334	GLN
1	C	101	ASN
1	C	249	ASN
1	C	283	HIS
1	C	342	GLN
1	C	356	ASN
1	C	393	HIS
2	D	48	ASN
2	D	329	GLN
2	D	347	ASN
2	D	375	GLN
3	E	90	ASN
3	E	136	ASN
4	F	38	ASN
4	F	145	ASN
4	F	180	HIS
4	F	196	HIS
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 oligosaccharides 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
5	GTP	C	501	6	33,34,34	0.56	0	50,54,54	0.62	1 (2%)
5	GTP	D	501	-	33,34,34	0.48	0	50,54,54	0.77	1 (2%)
9	BG0	D	502	-	27,28,28	4.11	10 (37%)	34,41,41	3.52	15 (44%)
10	ACP	F	401	-	31,33,33	1.86	10 (32%)	47,52,52	1.99	12 (25%)
5	GTP	A	501	6	33,34,34	0.73	1 (3%)	50,54,54	0.63	0
9	BG0	B	503	-	27,28,28	4.05	10 (37%)	34,41,41	3.08	13 (38%)
8	GDP	B	501	6	29,30,30	1.61	5 (17%)	45,47,47	1.76	6 (13%)

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
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
5	GTP	D	501	-	-	7/22/38/38	0/3/3/3
9	BG0	D	502	-	-	2/8/26/26	0/3/3/3
10	ACP	F	401	-	-	7/19/38/38	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
9	BG0	B	503	-	-	1/8/26/26	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	502	BG0	C07-C10	14.78	1.48	1.35
9	B	503	BG0	C07-C10	14.74	1.48	1.35
9	D	502	BG0	C10-N11	9.79	1.45	1.33
9	B	503	BG0	C10-N11	9.23	1.44	1.33
9	D	502	BG0	C08-C07	8.28	1.52	1.42
9	B	503	BG0	C08-C07	7.28	1.50	1.42
8	B	501	GDP	PA-O3A	4.76	1.64	1.59
10	F	401	ACP	C5-C4	4.60	1.47	1.39
9	B	503	BG0	C06-C07	-4.44	1.49	1.52
10	F	401	ACP	PA-O3A	3.87	1.63	1.59
10	F	401	ACP	PB-O3A	3.84	1.62	1.58
9	D	502	BG0	C06-C07	-3.65	1.49	1.52
9	B	503	BG0	O12-C13	3.54	1.43	1.38
9	D	502	BG0	O02-C03	3.47	1.42	1.37
9	B	503	BG0	BR-C22	3.38	1.97	1.89
8	B	501	GDP	PB-O1B	3.20	1.60	1.50
9	D	502	BG0	BR-C22	3.19	1.97	1.89
10	F	401	ACP	PG-O3G	2.99	1.61	1.55
10	F	401	ACP	C5-C6	2.97	1.49	1.41
8	B	501	GDP	C5-C4	2.81	1.46	1.38
8	B	501	GDP	C6-N1	-2.78	1.33	1.38
9	D	502	BG0	O12-C13	2.76	1.42	1.38
9	B	503	BG0	O12-C10	2.75	1.39	1.36
10	F	401	ACP	C5-N7	-2.71	1.34	1.39
10	F	401	ACP	PG-O2G	2.56	1.60	1.55
9	D	502	BG0	O12-C10	2.51	1.39	1.36
9	B	503	BG0	O02-C03	2.47	1.41	1.37
5	A	501	GTP	PA-O3A	2.45	1.62	1.59
9	D	502	BG0	C14-N15	2.40	1.45	1.37
10	F	401	ACP	C8-N7	2.38	1.36	1.31
8	B	501	GDP	C5-N7	-2.35	1.34	1.39
9	B	503	BG0	C14-N15	2.30	1.44	1.37
9	B	503	BG0	C16-N17	2.20	1.45	1.38
10	F	401	ACP	C4-N9	-2.18	1.33	1.37
9	D	502	BG0	C16-N17	2.18	1.45	1.38
10	F	401	ACP	PB-O2B	2.01	1.61	1.56

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	BG0	C07-C10-N11	-12.57	116.86	127.89
9	B	503	BG0	C07-C10-N11	-11.58	117.73	127.89
9	D	502	BG0	O12-C10-C07	-9.94	117.01	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	BG0	O12-C10-C07	-8.20	117.95	122.33
10	F	401	ACP	C5-C4-N3	-5.72	118.84	126.72
8	B	501	GDP	C5-C4-N3	-5.70	119.32	128.39
8	B	501	GDP	C2-N3-C4	5.08	121.05	112.30
9	D	502	BG0	C06-C07-C10	-4.76	120.90	123.48
10	F	401	ACP	C4-C5-N7	-4.63	105.29	110.58
8	B	501	GDP	N9-C4-N3	4.55	135.06	125.95
9	B	503	BG0	O12-C10-N11	4.37	113.33	110.24
9	D	502	BG0	C05-C06-C07	-4.37	106.39	111.38
9	D	502	BG0	C06-C07-C08	4.02	123.01	118.25
9	B	503	BG0	C06-C07-C10	-4.00	121.32	123.48
10	F	401	ACP	N3-C4-N9	3.89	133.78	127.17
9	B	503	BG0	C05-C06-C07	-3.71	107.14	111.38
10	F	401	ACP	C2-N3-C4	3.68	120.81	111.83
9	D	502	BG0	O12-C10-N11	3.51	112.72	110.24
9	B	503	BG0	C21-C05-C06	-3.39	115.43	120.54
10	F	401	ACP	N3-C2-N1	-3.35	123.51	128.58
10	F	401	ACP	O4'-C1'-N9	3.32	114.47	108.09
10	F	401	ACP	C5-N7-C8	3.31	108.66	103.45
9	D	502	BG0	C13-O12-C10	-3.24	116.67	118.61
9	B	503	BG0	C20-C06-C07	3.18	113.73	108.39
9	D	502	BG0	C21-C05-C06	-3.17	115.77	120.54
8	B	501	GDP	C6-C5-N7	3.17	136.06	130.29
9	D	502	BG0	C01-O02-C03	3.05	121.99	117.51
10	F	401	ACP	C3'-C2'-C1'	2.85	106.86	101.46
9	D	502	BG0	C20-C06-C07	2.83	113.14	108.39
9	B	503	BG0	C21-C22-C24	-2.77	117.75	122.59
8	B	501	GDP	O6-C6-C5	-2.74	119.29	126.53
10	F	401	ACP	C2'-C1'-N9	-2.71	106.58	113.30
9	D	502	BG0	BR-C22-C24	2.67	122.33	118.50
10	F	401	ACP	C6-C5-N7	2.62	137.15	132.09
9	D	502	BG0	C14-C13-C20	2.60	122.97	120.44
10	F	401	ACP	N9-C8-N7	-2.47	110.43	113.94
10	F	401	ACP	C4-N9-C8	2.38	108.24	105.74
9	D	502	BG0	C04-C03-C24	-2.31	117.65	120.22
5	C	501	GTP	O2A-PA-O3A	2.25	113.37	107.27
9	B	503	BG0	BR-C22-C24	2.22	121.67	118.50
9	B	503	BG0	C01-O02-C03	2.21	120.75	117.51
8	B	501	GDP	C5-C6-N1	2.21	118.87	113.25
9	B	503	BG0	C06-C07-C08	2.18	120.82	118.25
9	B	503	BG0	C04-C05-C06	2.12	123.73	120.54
9	D	502	BG0	C21-C05-C04	2.09	120.95	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	BG0	C21-C22-C24	-2.07	118.98	122.59
5	D	501	GTP	O2B-PB-O1B	2.05	121.97	112.44
9	B	503	BG0	C21-C05-C04	2.01	120.84	118.09

There are no chirality outliers.

All (31) torsion outliers are listed below:

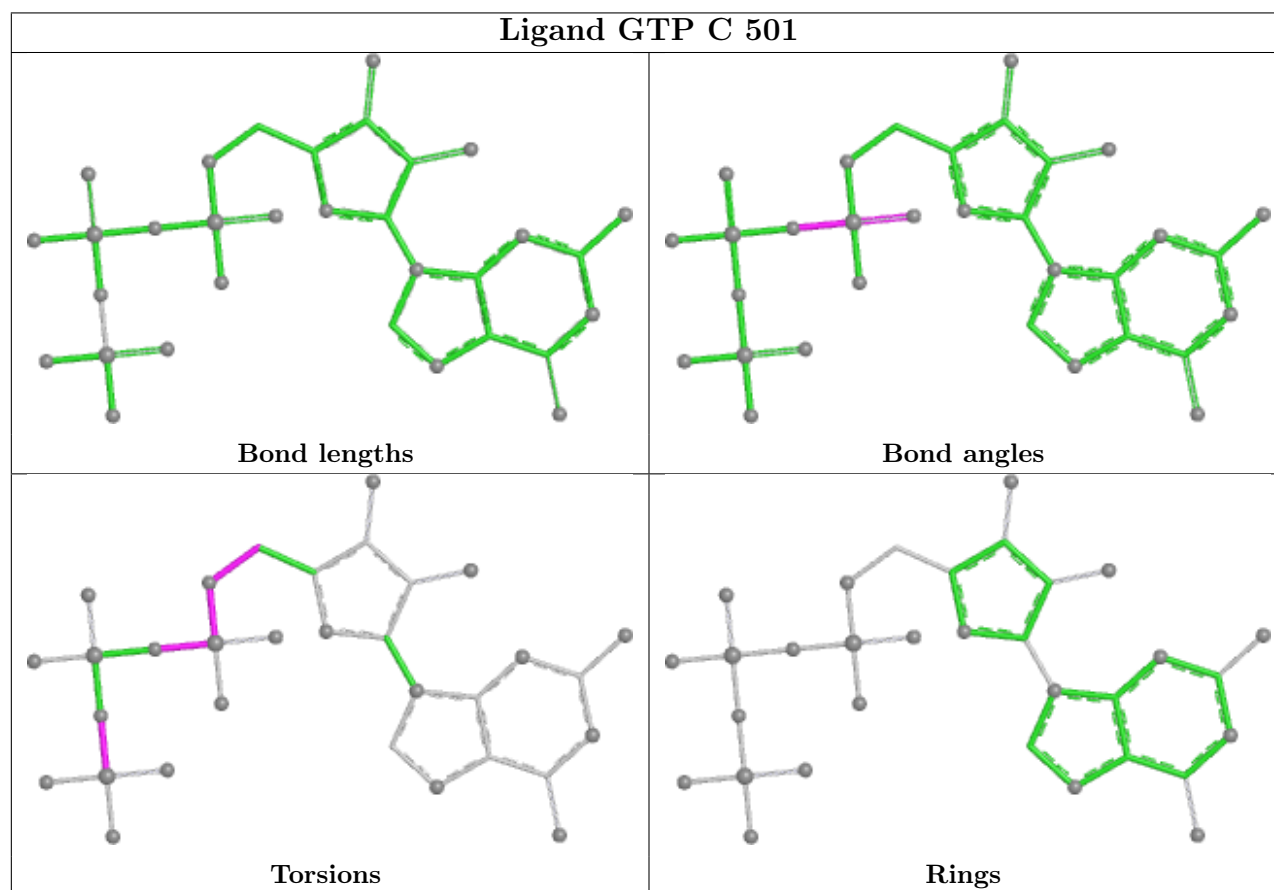
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501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

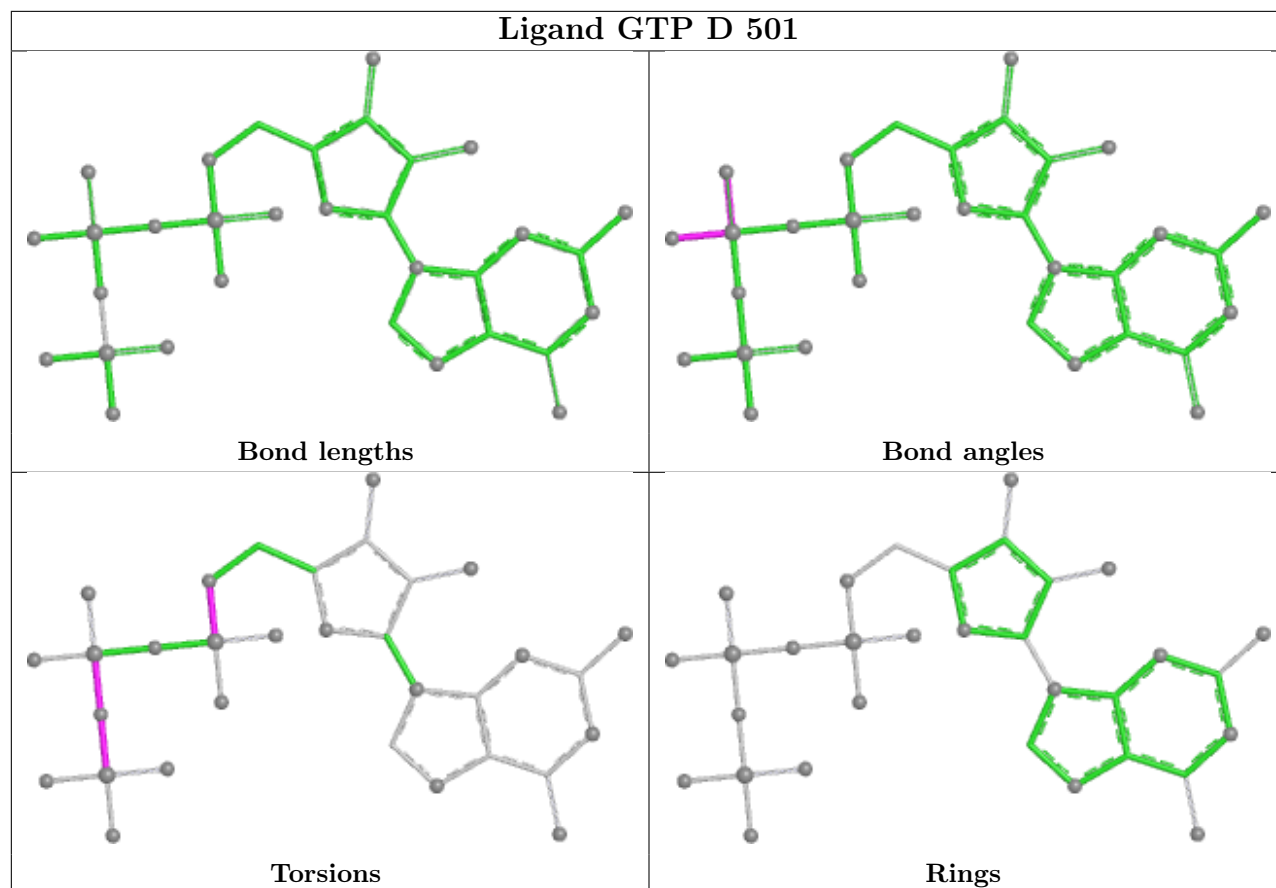
There are no ring outliers.

4 monomers are involved in 11 short contacts:

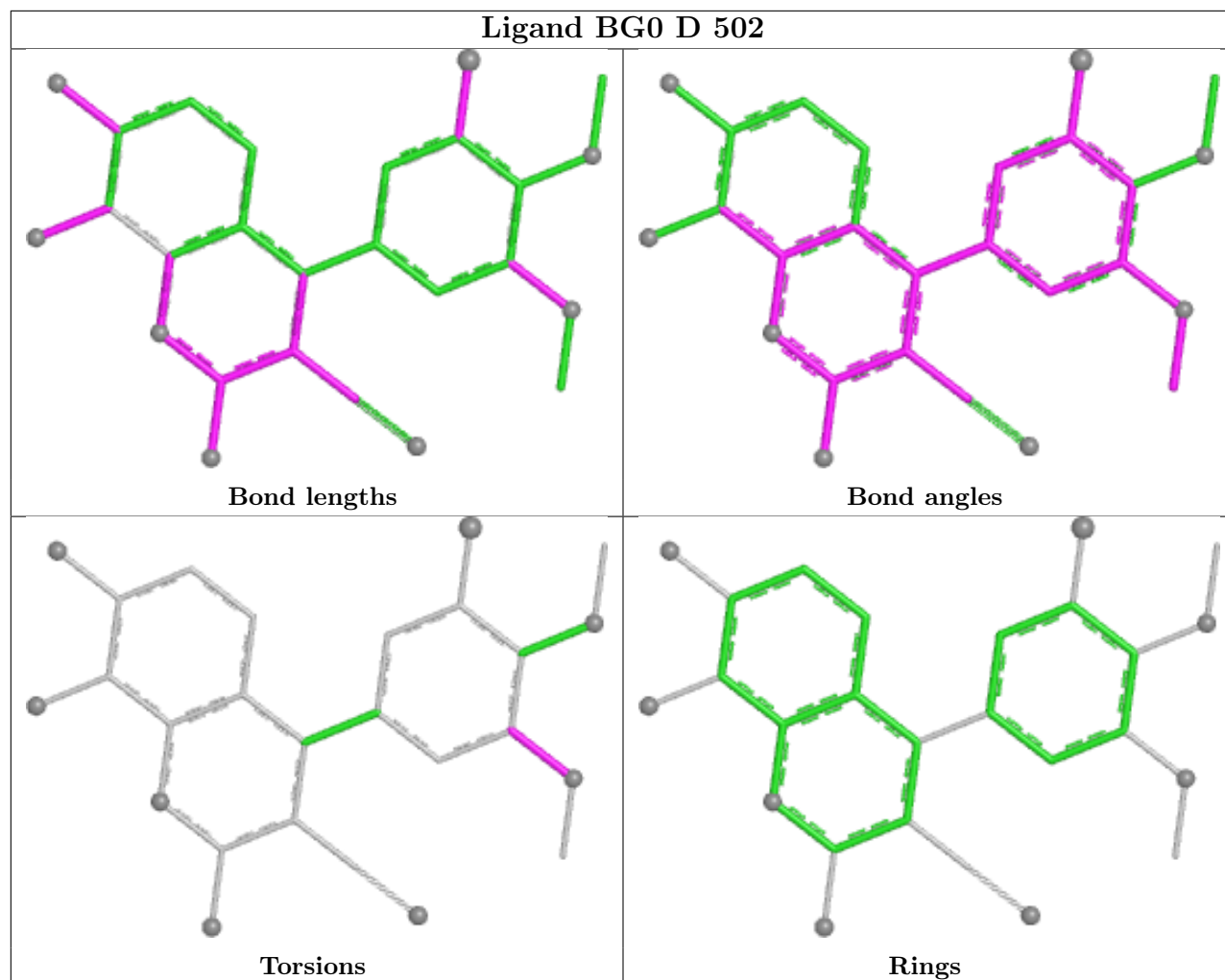
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	GTP	3	0
9	D	502	BG0	1	0
10	F	401	ACP	4	0
9	B	503	BG0	3	0

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.

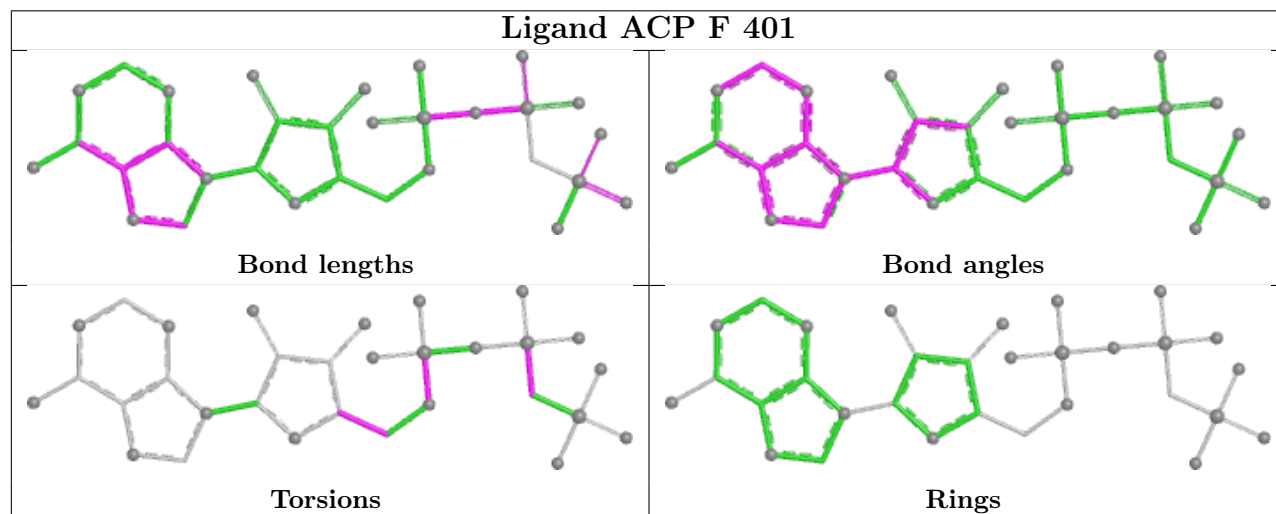


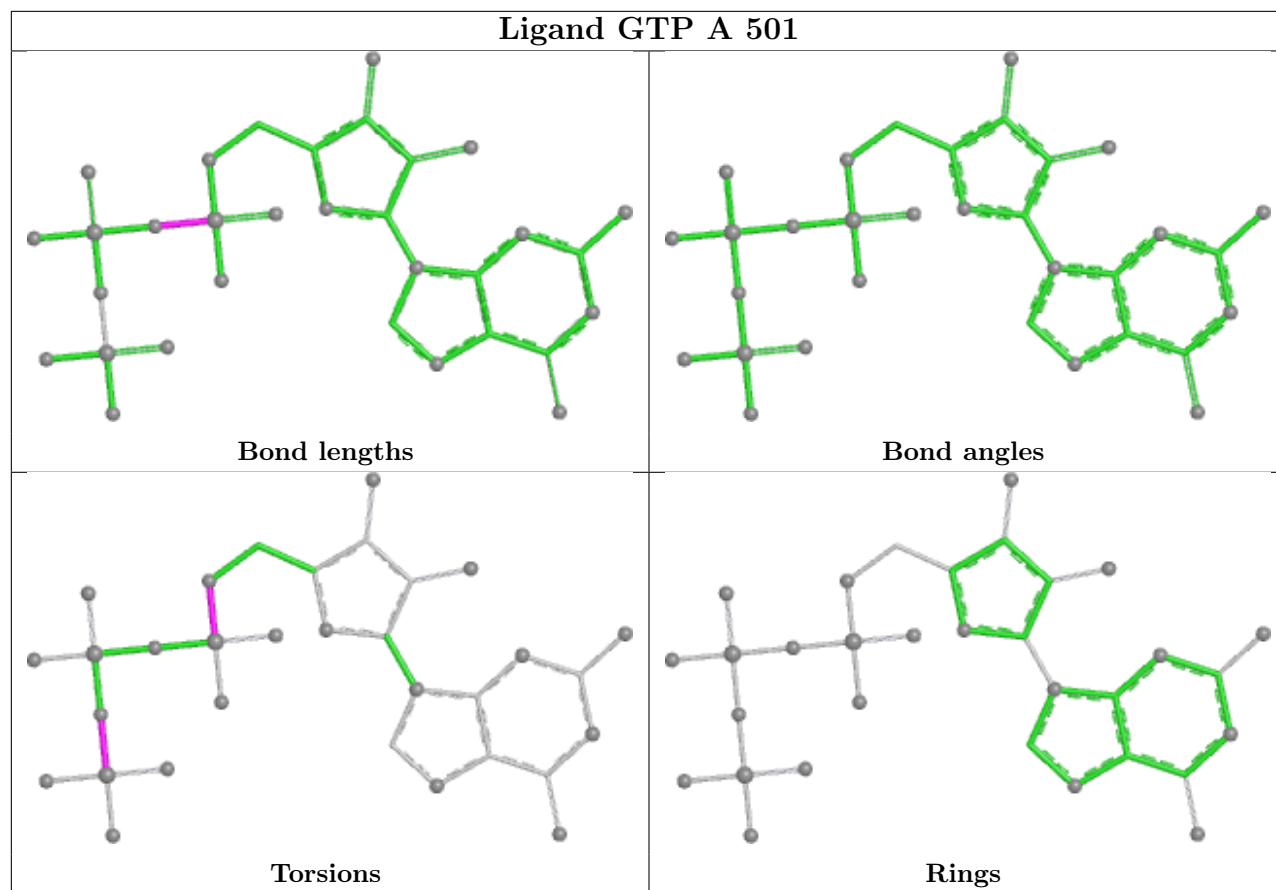


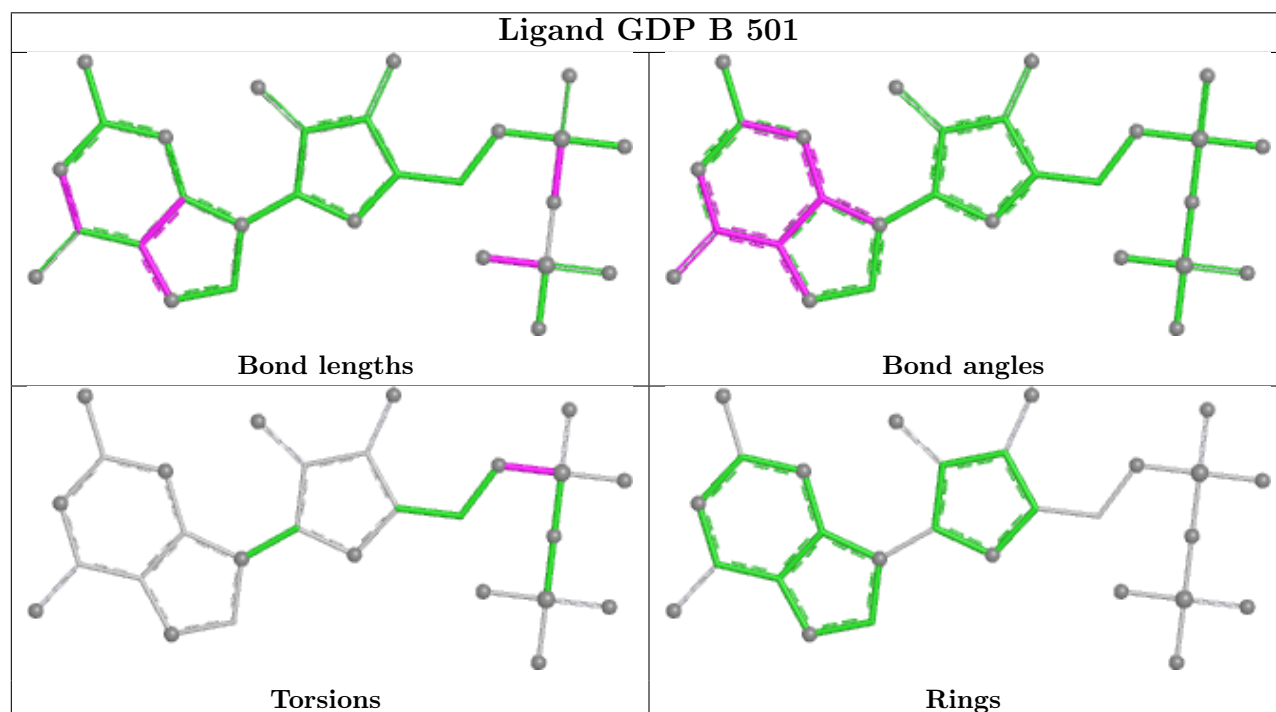
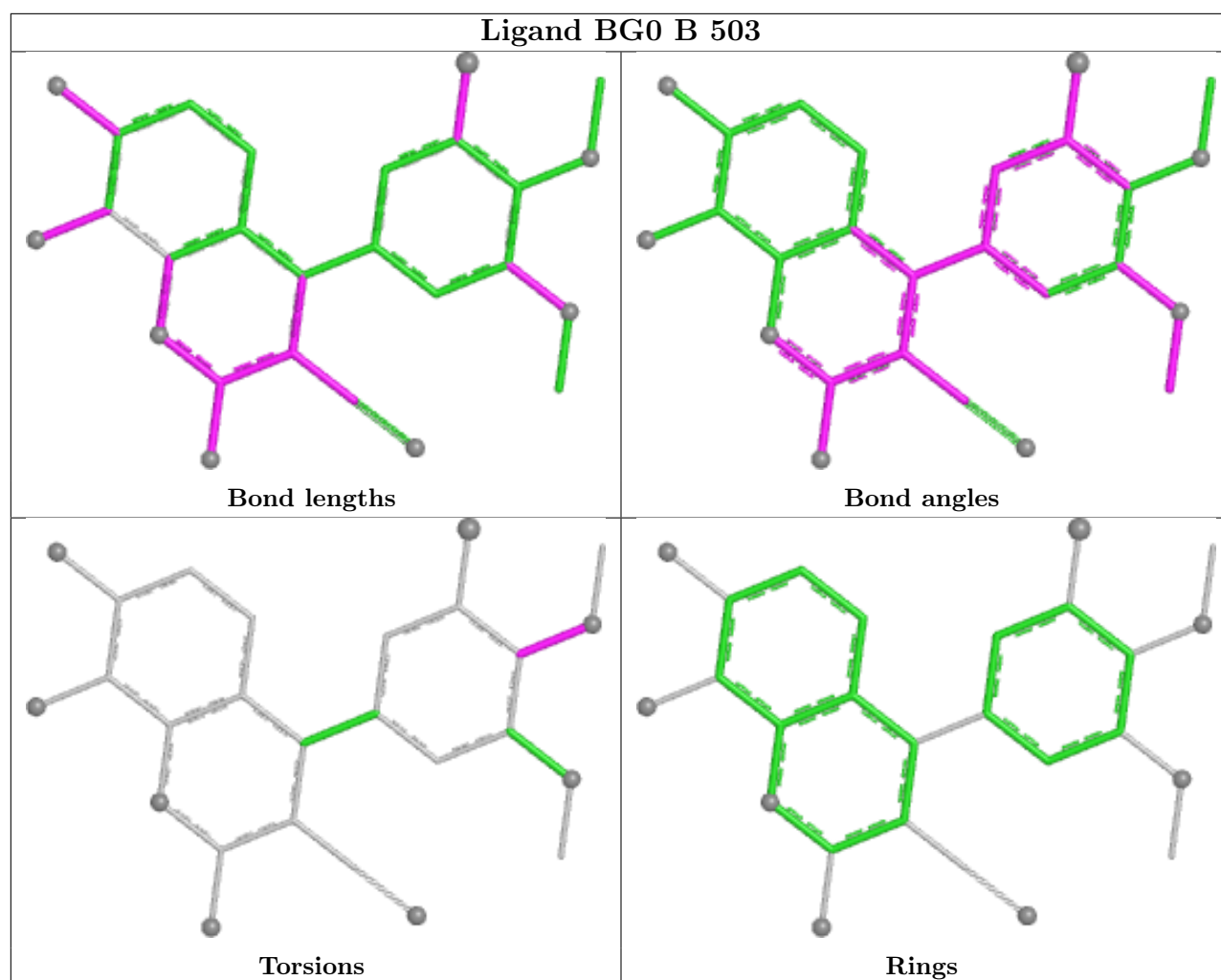
Ligand BG0 D 502



Ligand ACP F 401







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	437/450 (97%)	0.55	35 (8%)	18 16	12, 34, 66, 96	4 (0%)
1	C	440/450 (97%)	0.05	18 (4%)	41 37	8, 24, 52, 71	9 (2%)
2	B	424/445 (95%)	0.52	37 (8%)	16 14	12, 32, 66, 103	2 (0%)
2	D	421/445 (94%)	2.66	254 (60%)	0 0	22, 69, 126, 167	4 (0%)
3	E	120/143 (83%)	2.06	57 (47%)	0 0	25, 55, 124, 131	2 (1%)
4	F	309/384 (80%)	2.37	160 (51%)	0 0	14, 67, 131, 167	3 (0%)
All	All	2151/2317 (92%)	1.20	561 (26%)	1 1	8, 40, 110, 167	24 (1%)

All (561) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	215	LEU	9.9
2	D	180	VAL	9.2
2	D	211	CYS	9.0
4	F	161	LEU	7.9
4	F	233	PHE	7.8
4	F	383	HIS	7.7
4	F	100	ILE	7.5
2	D	181	GLU	7.4
2	D	217	LEU	7.3
2	D	284	LEU	7.2
4	F	384	HIS	7.1
2	D	175	VAL	7.1
3	E	139	LEU	7.0
2	D	273	LEU	6.8
2	D	30	ILE	6.7
2	D	394	PHE	6.7
2	D	210	ILE	6.6
4	F	149	ALA	6.6
2	D	397	TRP	6.4

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Mol	Chain	Res	Type	RSRZ
2	D	362	LYS	6.4
4	F	182	ILE	6.3
4	F	166	ALA	6.3
2	D	92	PHE	6.3
2	D	214	THR	6.3
2	D	218	THR	6.3
2	D	80	PRO	6.2
4	F	245	ILE	6.2
4	F	186	LEU	6.1
4	F	381	HIS	6.1
2	D	389	PHE	6.1
2	D	212	PHE	6.1
2	B	245	GLN	6.0
2	D	112	LEU	6.0
2	D	84	ILE	6.0
2	D	395	LEU	6.0
4	F	194	PRO	6.0
4	F	160	ILE	6.0
2	D	384	GLN	6.0
2	D	44	LEU	5.9
2	D	228	LEU	5.9
4	F	242	ASN	5.9
4	F	147	TRP	5.9
2	D	73	MET	5.8
3	E	12[A]	ASN	5.8
2	D	70	PRO	5.7
2	D	171	PRO	5.7
2	D	98	GLY	5.7
2	D	222	TYR	5.7
4	F	263	PHE	5.6
2	D	179	VAL	5.6
4	F	382	HIS	5.6
3	E	6	MET	5.5
2	D	387	ALA	5.5
2	D	396	HIS	5.5
2	D	208	TYR	5.5
4	F	101	TYR	5.5
4	F	159	GLY	5.5
2	D	91	VAL	5.5
4	F	99	VAL	5.5
4	F	220	VAL	5.5
4	F	240	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	281	TYR	5.5
2	D	72	THR	5.5
2	D	85	PHE	5.5
2	D	55	THR	5.4
4	F	146	VAL	5.4
2	D	323	MET	5.4
2	D	68	LEU	5.3
4	F	231	ALA	5.3
2	D	285	THR	5.3
4	F	148	ILE	5.3
2	D	207	LEU	5.2
4	F	191	LEU	5.2
2	D	385	PHE	5.2
2	D	87	PRO	5.2
4	F	227	PRO	5.2
2	D	54	ALA	5.2
2	D	361	LEU	5.2
2	D	97	ALA	5.1
4	F	181	VAL	5.1
4	F	21	LEU	5.1
4	F	237	THR	5.0
2	D	356	ILE	5.0
3	E	44	ASP	5.0
2	D	75	SER	5.0
3	E	135	LYS	5.0
4	F	150	LYS	5.0
2	D	65	LEU	5.0
2	B	280	GLN	5.0
2	D	15	GLN	5.0
2	D	36	TYR	5.0
2	D	101	TRP	4.9
4	F	184	LYS	4.9
1	A	437	VAL	4.9
4	F	102	PRO	4.9
2	D	90	PHE	4.9
2	D	76	VAL	4.9
2	D	227	HIS	4.8
3	E	45	PRO	4.8
4	F	222	ARG	4.8
2	D	71	GLY	4.7
4	F	162	ILE	4.7
4	F	197	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	353	VAL	4.7
2	D	100	ASN	4.7
2	D	388	MET	4.7
4	F	259	GLY	4.7
4	F	380	HIS	4.7
4	F	199	PHE	4.7
4	F	253	TYR	4.6
4	F	225	SER	4.6
4	F	337	ALA	4.6
2	D	183	TYR	4.6
2	D	178	THR	4.6
2	D	358	PRO	4.6
3	E	137	LYS	4.6
2	D	399	THR	4.6
2	D	220	PRO	4.5
2	D	1	MET	4.5
2	D	223	GLY	4.5
4	F	238	CYS	4.5
2	D	24	ILE	4.5
4	F	339	ALA	4.5
2	D	219	THR	4.4
4	F	241	THR	4.4
2	D	381	ILE	4.4
2	D	37	HIS	4.4
4	F	247	LYS	4.4
2	D	221	THR	4.4
1	C	280	LYS	4.4
3	E	53	LYS	4.4
2	D	81	PHE	4.4
2	D	99	ASN	4.4
4	F	144	GLY	4.4
4	F	228	TYR	4.4
2	D	116	VAL	4.4
2	D	169	VAL	4.4
1	A	346	TRP	4.3
2	D	136	THR	4.3
4	F	192	LEU	4.3
2	D	245	GLN	4.3
3	E	57	ALA	4.3
2	D	115	SER	4.3
2	D	359	ARG	4.3
2	D	23	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	182	PRO	4.2
3	E	134	ARG	4.2
2	D	102	ALA	4.2
2	D	103	LYS	4.2
4	F	223	THR	4.2
4	F	32	LYS	4.2
4	F	221	LEU	4.2
2	D	216	LYS	4.2
2	D	363	MET	4.2
2	D	172	SER	4.1
2	D	74	ASP	4.1
2	D	16	ILE	4.1
4	F	330	ILE	4.1
2	D	170	MET	4.1
2	D	400	GLY	4.1
4	F	151	SER	4.1
1	C	440	VAL	4.1
2	D	13	GLY	4.0
2	D	42	LEU	4.0
2	D	119	VAL	4.0
2	D	66	VAL	4.0
4	F	195	GLY	4.0
4	F	254	GLY	4.0
4	F	379	HIS	4.0
4	F	13	VAL	4.0
4	F	17	VAL	4.0
2	D	46	ARG	4.0
4	F	188	LYS	4.0
2	D	12	CYS	4.0
2	D	360	GLY	4.0
3	E	23	ILE	4.0
2	D	150	LEU	3.9
4	F	234	GLN	3.9
1	A	282	TYR	3.9
3	E	24	LEU	3.9
4	F	362	ALA	3.8
2	D	226	ASN	3.8
2	D	224	ASP	3.8
2	D	94	GLN	3.8
2	B	54	ALA	3.8
2	D	393	ALA	3.8
4	F	185	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	10	GLY	3.8
2	D	64	ILE	3.8
4	F	189	PRO	3.8
4	F	239	HIS	3.8
3	E	140	LYS	3.8
2	D	151	LEU	3.8
2	D	225	LEU	3.8
3	E	133	VAL	3.7
2	D	110	ALA	3.7
4	F	257	GLU	3.7
3	E	103	GLN	3.7
3	E	124	GLN	3.7
2	D	31	ASP	3.7
2	D	59	TYR	3.7
2	D	69	GLU	3.7
4	F	252	ASN	3.7
2	D	173	PRO	3.7
2	D	60	VAL	3.6
4	F	224	SER	3.6
2	D	104	GLY	3.6
2	D	355	ASP	3.6
2	D	105	HIS	3.6
4	F	321	VAL	3.6
4	F	198	LYS	3.6
2	D	11	GLN	3.6
4	F	244	CYS	3.6
4	F	196	HIS	3.6
2	D	174	LYS	3.6
2	D	139	LEU	3.6
4	F	98	TYR	3.6
1	A	336	LYS	3.6
4	F	236	LYS	3.6
4	F	230	SER	3.6
4	F	193	GLU	3.5
2	D	28	HIS	3.5
4	F	243	HIS	3.5
2	D	403	MET	3.5
2	D	409	THR	3.5
2	D	398	TYR	3.5
2	D	33	THR	3.5
3	E	51	GLN	3.5
2	B	246	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	20	LEU	3.5
4	F	190	LEU	3.5
2	B	247	ASN	3.4
2	D	14	ASN	3.4
2	D	401	GLU	3.4
2	D	34	GLY	3.4
2	D	206	ALA	3.4
4	F	14	TYR	3.4
2	B	333	VAL	3.4
1	A	196	GLU	3.4
2	D	390	ARG	3.4
3	E	96	MET	3.4
4	F	145	ASN	3.4
2	D	386	THR	3.4
4	F	18	SER	3.4
2	D	106	TYR	3.4
2	D	391	ARG	3.4
4	F	16	GLU	3.4
2	D	118	ASP	3.4
2	D	89	ASN	3.4
2	D	29	GLY	3.4
2	D	202	ILE	3.4
2	D	32	PRO	3.3
2	D	272	PRO	3.3
4	F	19	ARG	3.3
3	E	130	ALA	3.3
3	E	25	LYS	3.3
4	F	201	ILE	3.3
3	E	127	ASP	3.3
4	F	256	TYR	3.3
3	E	138	GLU	3.3
2	D	9	ALA	3.3
2	D	392	LYS	3.3
1	C	221	ARG	3.3
3	E	54	LEU	3.3
2	B	323	MET	3.3
4	F	262	MET	3.3
4	F	320	MET	3.3
2	D	185	ALA	3.3
1	C	282	TYR	3.2
2	D	213	ARG	3.2
2	D	405	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	1	MET	3.2
2	D	78	SER	3.2
2	D	412	GLU	3.2
1	A	281	ALA	3.2
2	D	431	ASP	3.2
1	C	283	HIS	3.2
2	D	377	LEU	3.2
1	A	262	TYR	3.2
2	D	58	LYS	3.2
2	D	82	GLY	3.2
2	D	88	ASP	3.2
3	E	131	GLU	3.2
4	F	28	LYS	3.2
2	D	79	GLY	3.2
2	D	109	GLY	3.2
2	B	55	THR	3.2
2	B	320	ARG	3.1
2	B	338	SER	3.1
2	B	56	GLY	3.1
2	D	140	GLY	3.1
2	D	243	PRO	3.1
4	F	22	LEU	3.1
4	F	346	LEU	3.1
2	D	320	ARG	3.1
1	A	96	LYS	3.1
2	D	177	ASP	3.1
2	D	77	ARG	3.1
2	D	22	GLU	3.1
2	D	247	ASN	3.1
3	E	122	ARG	3.1
2	D	297	LYS	3.0
4	F	341	LYS	3.0
4	F	272	MET	3.0
2	D	303	CYS	3.0
2	D	203	ASP	3.0
2	D	8	GLN	3.0
2	D	270	PHE	3.0
1	A	339	ARG	3.0
2	D	229	VAL	3.0
1	A	88	HIS	3.0
2	D	51	TYR	3.0
2	D	35	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	204	ASN	3.0
3	E	50	ILE	3.0
2	D	26	ASP	3.0
2	D	67	ASP	3.0
2	D	113	VAL	2.9
2	D	231	ALA	2.9
2	D	271	ALA	2.9
4	F	180	HIS	2.9
4	F	204	TRP	2.9
4	F	30	LEU	2.9
4	F	275	LEU	2.9
1	C	211[A]	ASP	2.9
4	F	273	ASP	2.9
2	D	145[A]	SER	2.9
2	D	83	GLN	2.9
2	D	144	GLY	2.9
3	E	22	VAL	2.9
3	E	48	GLU	2.9
1	A	112	LYS	2.9
3	E	61	ARG	2.9
4	F	344	ALA	2.9
2	B	86	ARG	2.9
2	D	107	THR	2.9
2	D	406	MET	2.9
4	F	246	GLN	2.9
2	D	53	GLU	2.9
2	D	141	GLY	2.9
2	D	48	ASN	2.8
2	D	86	ARG	2.8
4	F	163	SER	2.8
1	A	163	LYS	2.8
2	D	246	LEU	2.8
2	B	177	ASP	2.8
2	D	147	MET	2.8
4	F	226	GLU	2.8
4	F	270	TYR	2.8
3	E	52	LYS	2.8
3	E	62	LYS	2.8
2	B	214	THR	2.8
1	A	113	GLU	2.8
2	D	2	ARG	2.8
3	E	115	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	138	SER	2.8
3	E	15	THR	2.8
2	D	289	LEU	2.8
2	D	121	ARG	2.8
2	D	47	ILE	2.8
2	D	176	SER	2.8
4	F	229	ASN	2.8
4	F	9	GLU	2.8
2	D	242	PHE	2.8
3	E	126	LYS	2.7
2	B	282	ARG	2.7
2	D	61	PRO	2.7
2	D	143	THR	2.7
2	D	290	THR	2.7
2	D	157	GLU	2.7
1	A	116	ASP	2.7
1	A	114	ILE	2.7
4	F	232	ASN	2.7
2	B	275	SER	2.7
2	D	230	SER	2.7
2	D	296	SER	2.7
4	F	271	LEU	2.7
4	F	31	ARG	2.7
2	D	410	GLU	2.7
1	A	111	GLY	2.7
2	B	96	GLY	2.7
2	D	142	GLY	2.7
2	D	117	LEU	2.7
3	E	46	SER	2.7
4	F	332	VAL	2.7
2	B	428	ALA	2.7
4	F	15	ALA	2.7
4	F	324[A]	GLU	2.7
4	F	264	PHE	2.6
1	C	1	MET	2.6
2	B	363	MET	2.6
2	B	42	LEU	2.6
3	E	8	VAL	2.6
3	E	7	GLU	2.6
1	C	337	THR	2.6
2	D	430	ALA	2.6
2	D	38	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	41	ASP	2.6
2	D	93	GLY	2.6
2	D	408	PHE	2.6
4	F	317	PHE	2.6
2	B	73	MET	2.6
2	D	414	ASN	2.6
3	E	120	LEU	2.6
3	E	141	GLU	2.6
1	A	338	LYS	2.6
2	D	404	ASP	2.6
1	C	177	VAL	2.6
4	F	6	VAL	2.6
4	F	266	GLU	2.6
4	F	331	GLU	2.6
2	B	414	ASN	2.6
1	A	283	HIS	2.6
4	F	64	TYR	2.6
2	D	402	GLY	2.5
1	C	285	GLN	2.5
1	C	338	LYS	2.5
2	D	324	LYS	2.5
2	D	379	LYS	2.5
4	F	23	ALA	2.5
3	E	26	PRO	2.5
4	F	27	TRP	2.5
4	F	283	ILE	2.5
4	F	183	GLN	2.5
4	F	75	ALA	2.5
2	D	126	SER	2.5
2	D	186	THR	2.5
4	F	373	SER	2.5
1	A	110	ILE	2.5
2	D	108	GLU	2.5
4	F	361	LEU	2.5
4	F	260	ASN	2.5
4	F	44	ARG	2.5
3	E	59	GLU	2.5
4	F	89	GLU	2.5
3	E	69	LEU	2.5
4	F	41	LEU	2.5
4	F	255	ARG	2.5
2	D	96	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	200	ASP	2.4
3	E	68	LEU	2.4
4	F	342	LEU	2.4
2	B	2	ARG	2.4
2	B	335	ASN	2.4
2	B	274	THR	2.4
2	D	95	SER	2.4
4	F	164	SER	2.4
3	E	128	LYS	2.4
2	D	155	ILE	2.4
2	D	294	PHE	2.4
2	D	111	GLU	2.4
4	F	219	GLY	2.4
1	A	68	VAL	2.4
2	D	293	MET	2.4
2	D	357	PRO	2.4
4	F	165	GLU	2.4
2	D	146	GLY	2.4
2	B	343	GLU	2.4
4	F	12	SER	2.3
4	F	203	SER	2.3
2	B	307	HIS	2.3
2	D	6	HIS	2.3
2	D	209	ASP	2.3
4	F	306	HIS	2.3
1	C	340	SER	2.3
1	C	245	ASP	2.3
2	D	122	LYS	2.3
2	D	378	PHE	2.3
1	A	66	VAL	2.3
4	F	46	ARG	2.3
2	B	95	SER	2.3
2	D	188	SER	2.3
4	F	340	GLN	2.3
2	D	120	VAL	2.3
2	D	63	ALA	2.3
2	D	149	THR	2.3
2	B	37	HIS	2.3
2	D	43	GLN	2.3
2	D	25	SER	2.3
3	E	123	LEU	2.3
4	F	74	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	58	GLU	2.3
2	D	354	CYS	2.3
2	D	411	ALA	2.2
3	E	66	ALA	2.2
4	F	343	TYR	2.3
4	F	24	THR	2.2
4	F	47	LEU	2.2
4	F	88	SER	2.2
2	D	286	VAL	2.2
4	F	63	ASN	2.2
4	F	338	CYS	2.2
2	B	244	GLY	2.2
2	B	336	LYS	2.2
1	A	340	SER	2.2
1	A	334	THR	2.2
4	F	25	GLY	2.2
1	A	335	ILE	2.2
2	D	40	SER	2.2
1	A	120	ASP	2.2
1	C	284	GLU	2.2
1	A	215	ARG	2.2
2	D	21	TRP	2.2
2	B	92	PHE	2.2
2	B	72	THR	2.2
4	F	277	THR	2.2
3	E	80	ARG	2.2
4	F	202	ARG	2.2
1	C	356	ASN	2.1
1	C	358	GLN	2.1
1	C	341	ILE	2.1
2	D	152	ILE	2.1
1	A	221	ARG	2.1
1	A	423	GLU	2.1
2	B	77	ARG	2.1
2	D	123	GLU	2.1
3	E	88	GLU	2.1
2	D	114	ASP	2.1
1	A	430	LYS	2.1
2	D	287	PRO	2.1
3	E	70	LYS	2.1
3	E	136	ASN	2.1
3	E	47	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	132	GLU	2.1
4	F	258	GLU	2.1
2	D	201	CYS	2.1
4	F	282	SER	2.1
1	A	104	ALA	2.1
3	E	92	ASN	2.1
2	D	27	GLU	2.1
2	D	407	GLU	2.1
4	F	374	ILE	2.1
1	A	124	LYS	2.1
1	A	347	CYS	2.1
4	F	78	VAL	2.1
2	D	57	ASN	2.1
2	D	187	LEU	2.1
1	A	412	GLY	2.1
2	D	56	GLY	2.1
4	F	217	ARG	2.1
4	F	79	LYS	2.1
2	D	161	ASP	2.1
3	E	27	PRO	2.1
2	D	193	VAL	2.0
2	D	380	ARG	2.0
2	D	52	ASN	2.0
3	E	106	GLU	2.0
4	F	261	GLU	2.0
1	C	357	TYR	2.0
2	B	427	ASP	2.0
1	A	256	GLN	2.0
1	A	362	VAL	2.0
2	D	49	VAL	2.0
4	F	327	VAL	2.0
2	D	301	ALA	2.0
2	B	69	GLU	2.0
4	F	187	GLU	2.0
2	D	298	ASN	2.0
2	D	39	ASP	2.0
3	E	119	MET	2.0
4	F	336	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

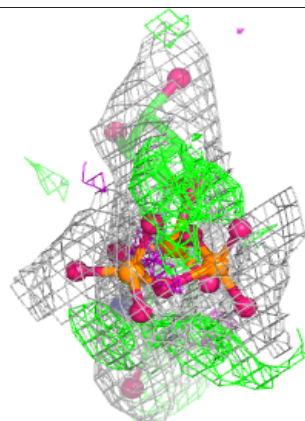
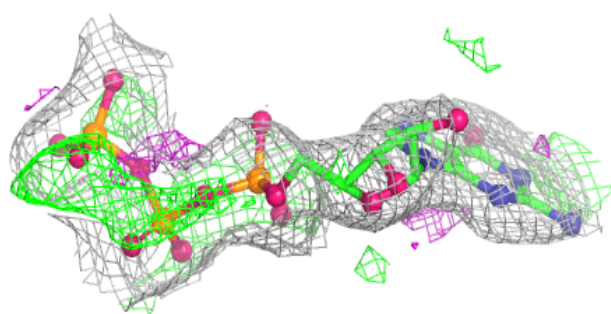
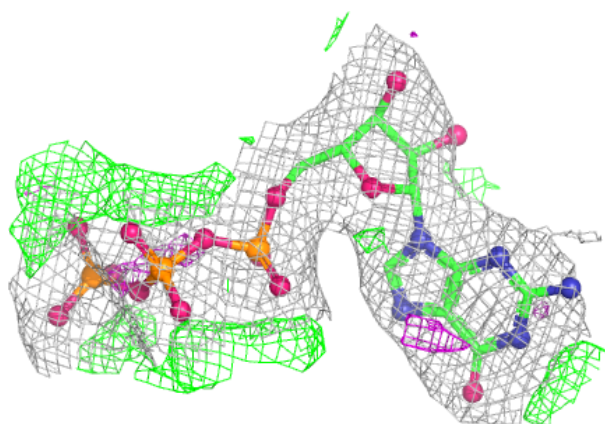
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	D	501	32/32	0.77	0.15	39,49,65,72	0
10	ACP	F	401	31/31	0.78	0.14	62,74,100,104	0
6	MG	B	502	1/1	0.81	0.23	59,59,59,59	0
9	BG0	D	502	26/26	0.94	0.09	26,30,47,64	0
9	BG0	B	503	26/26	0.95	0.09	22,25,36,54	0
7	CA	A	503	1/1	0.96	0.05	54,54,54,54	0
5	GTP	A	501	32/32	0.97	0.06	17,19,20,21	0
7	CA	C	503	1/1	0.97	0.08	37,37,37,37	0
8	GDP	B	501	28/28	0.97	0.06	12,15,16,20	0
6	MG	A	502	1/1	0.98	0.03	23,23,23,23	0
5	GTP	C	501	32/32	0.98	0.05	12,14,15,16	0
6	MG	C	502	1/1	0.99	0.02	16,16,16,16	0

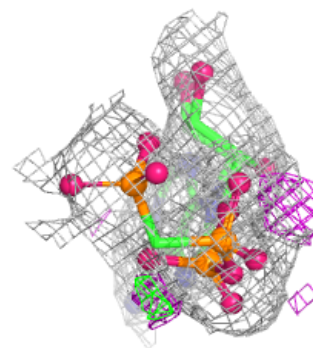
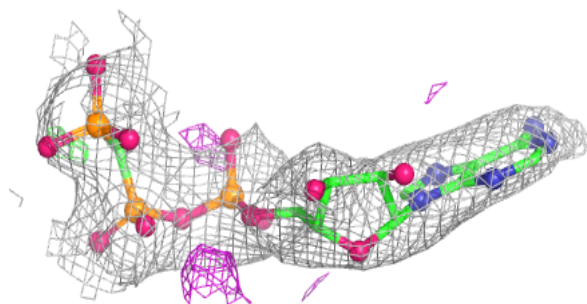
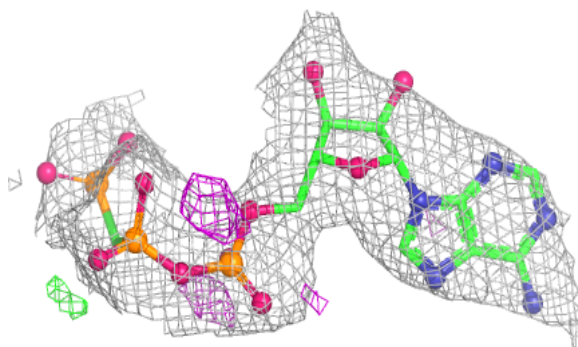
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

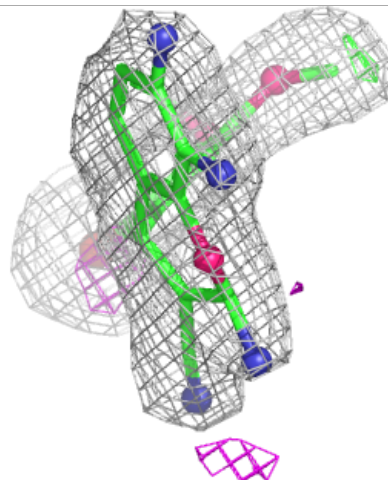
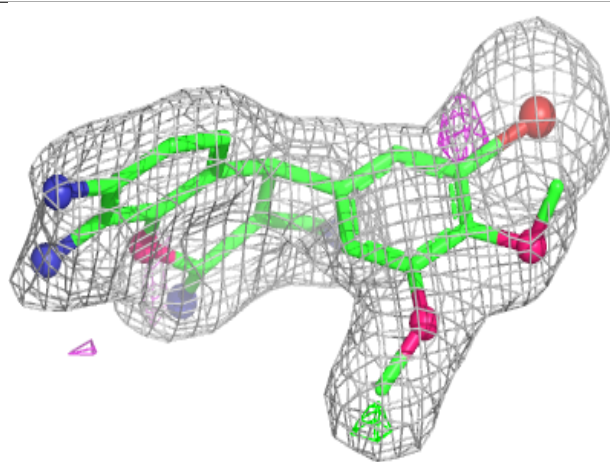
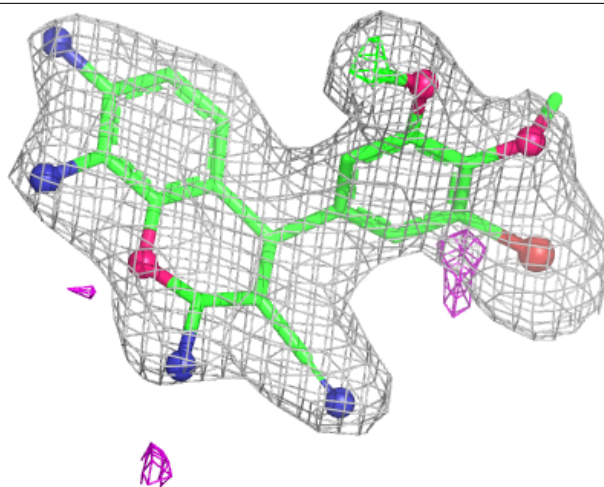
**Electron density around ACP F 401:**

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



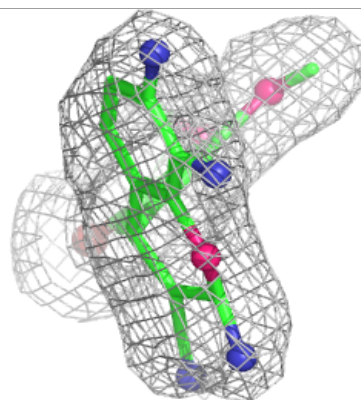
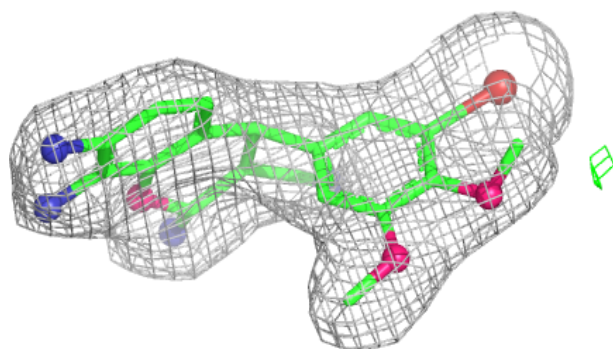
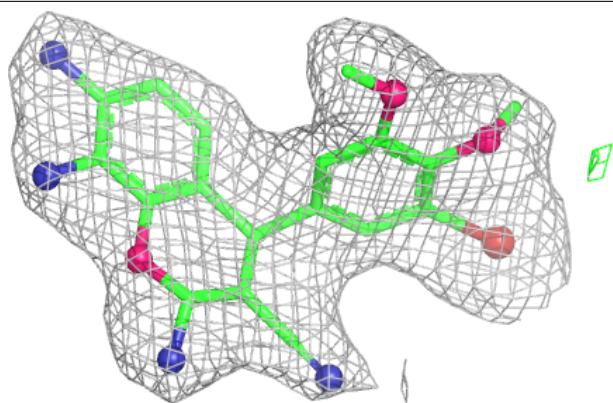
Electron density around BG0 D 502:

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

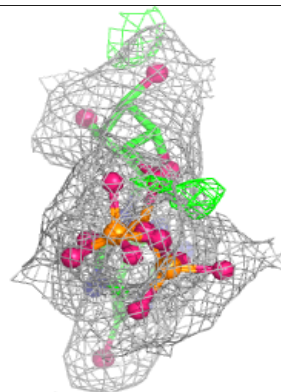
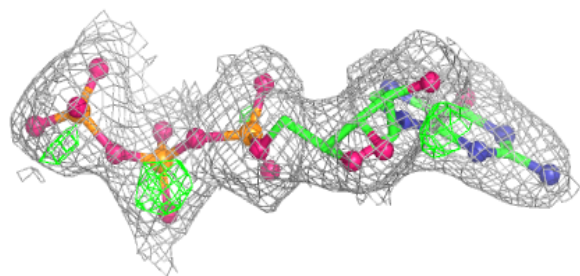
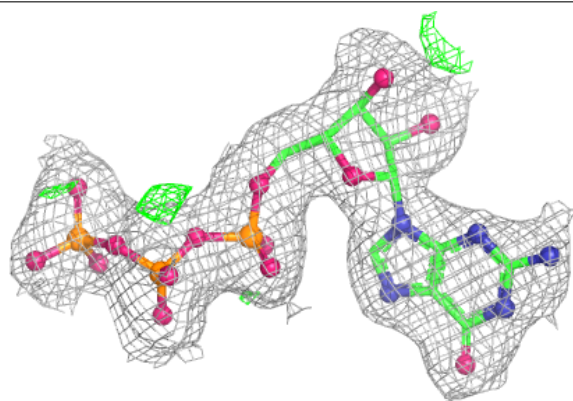


Electron density around BG0 B 503:

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

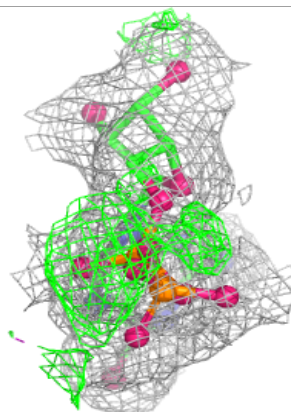
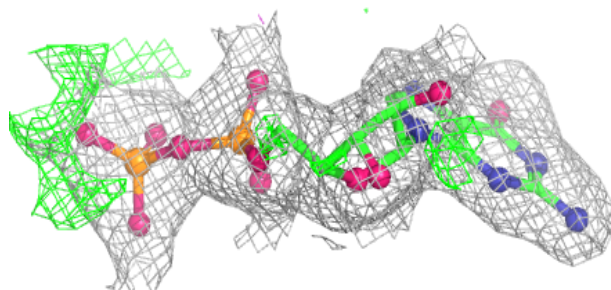
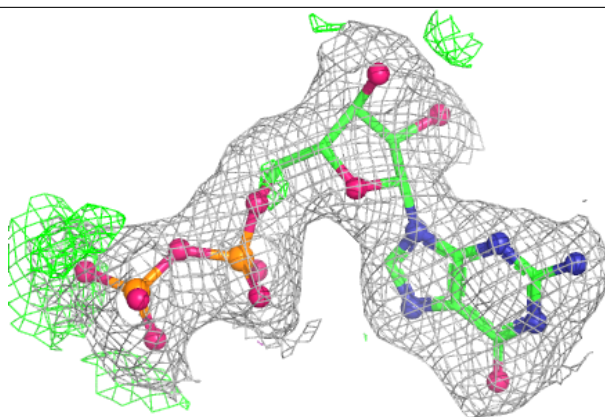
**Electron density around GTP A 501:**

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

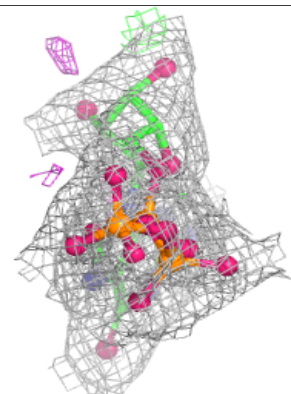
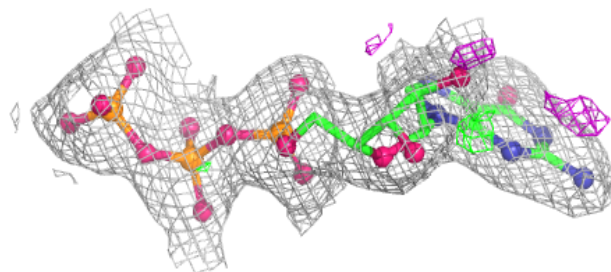
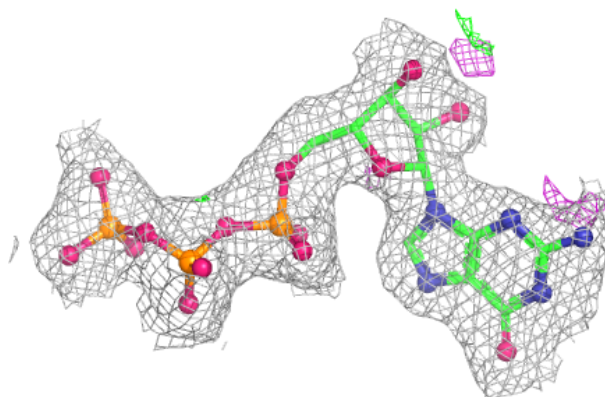


Electron density around GDP B 501:

$2mF_o-DF_c$ (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.