



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:20 PM UTC

PDB ID : 8BDF / pdb_00008bdf
Title : Tubulin-taxane-2a complex
Authors : Prota, A.E.; Lucena-Agell, D.; Ma, Y.; Estevez-Gallego, J.; Li, S.; Bargsten, K.; Altmann, K.H.; Gaillard, N.; Kamimura, S.; Muehlethaler, T.; Gago, F.; Oliva, M.A.; Steinmetz, M.O.; Fang, W.S.; Diaz, J.F.
Deposited on : 2022-10-19
Resolution : 1.95 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

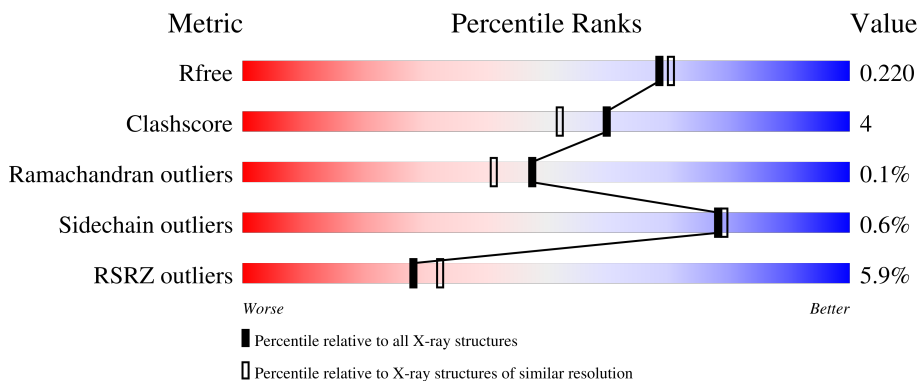
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.



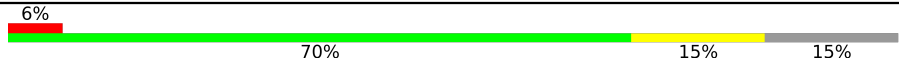

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	451	 4% 90% 8%
1	C	451	 4% 88% 9%
2	B	445	 5% 84% 12%
2	D	445	 7% 82% 13%

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Mol	Chain	Length	Quality of chain
3	E	143	 6% 70% 15% 15%
4	F	384	 9% 75% 8% 17%

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 18392 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
			Total	C	N	O	S			
1	A	441	Total	C	N	O	S	0	0	0
			3446	2179	585	660	22			
1	C	440	Total	C	N	O	S	0	2	0
			3447	2181	585	659	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	Total	C	N	O	S	0	0	0
			3359	2110	575	647	27			
2	D	426	Total	C	N	O	S	0	1	0
			3354	2104	574	649	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

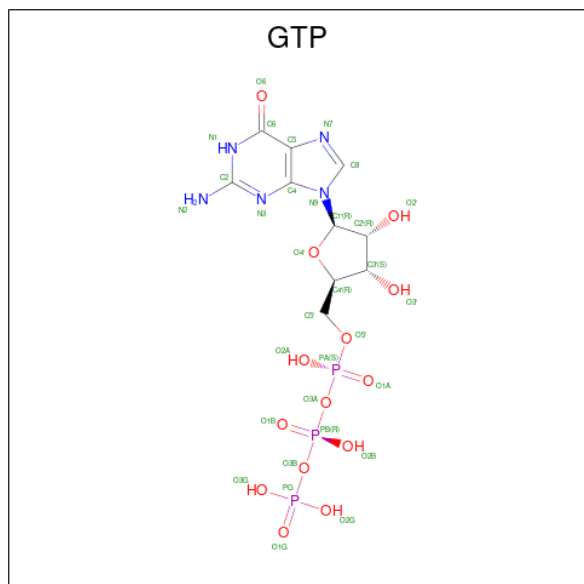
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	319	Total	C	N	O	S	0	0	0
			2614	1687	441	472	14			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 6 is MAGNESIUM ION (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		
6	D	1	Total	Mg	0	0
			1	1		

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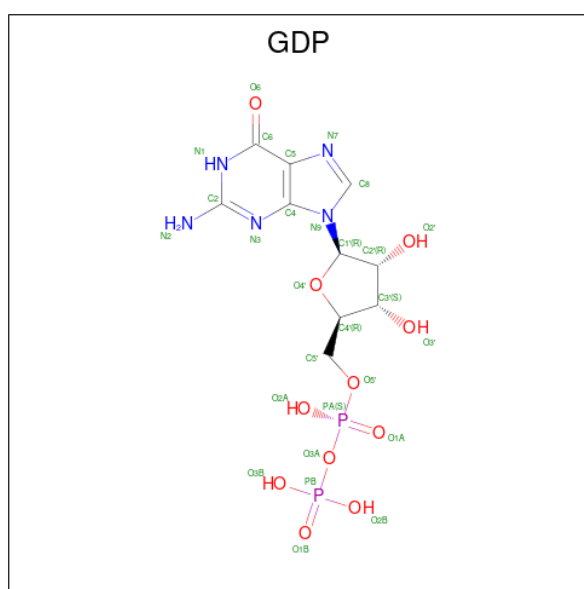
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- 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		

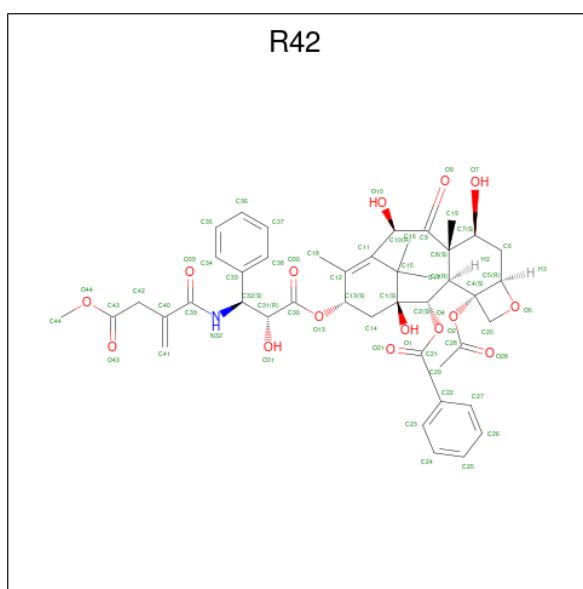
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





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

- Molecule 10 is [(1 {S},2 {S},3 {R},4 {S},7 {R},9 {S},10 {S},12 {R},15 {S})-4-acetyloxy-15-[(2 {R},3 {S})-3-[(4-methoxy-2-methylidene-4-oxidanylidene-butanoyl)amino]-2-oxidanyl-3-phenyl-propanoyl]oxy-10,14,16,16-tetramethyl-1,9,12-tris(oxidanyl)-11-oxidanylidene-6-oxatetracyclo[11.3.1.0^{3,10}.0^{4,7}]heptadec-13-en-2-yl] benzoate (CCD ID: R42) (formula: C₄₄H₅₁NO₁₅) (labeled as "Ligand of Interest" by depositor).



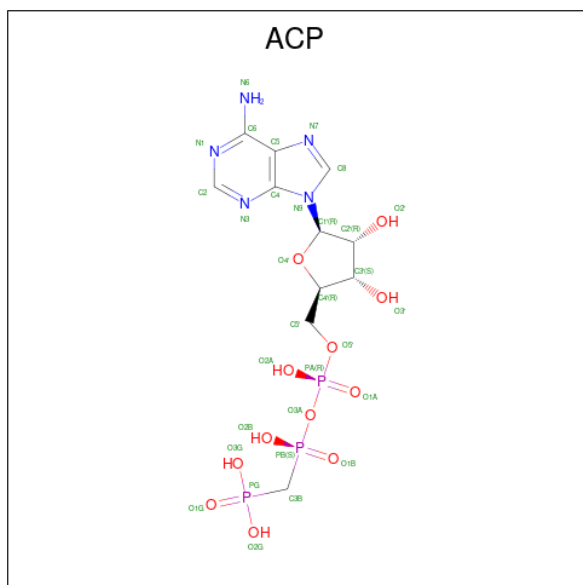
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	60	44	1	15	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
10	D	1	60	44	1	15	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

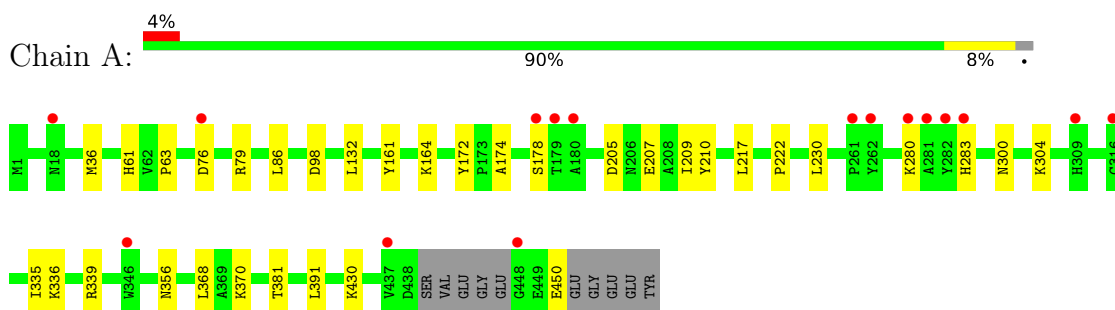
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	169	Total	O	0	0
			169	169		
12	B	156	Total	O	0	0
			156	156		
12	C	316	Total	O	0	0
			316	316		
12	D	122	Total	O	0	0
			122	122		
12	E	47	Total	O	0	0
			47	47		
12	F	73	Total	O	0	0
			73	73		

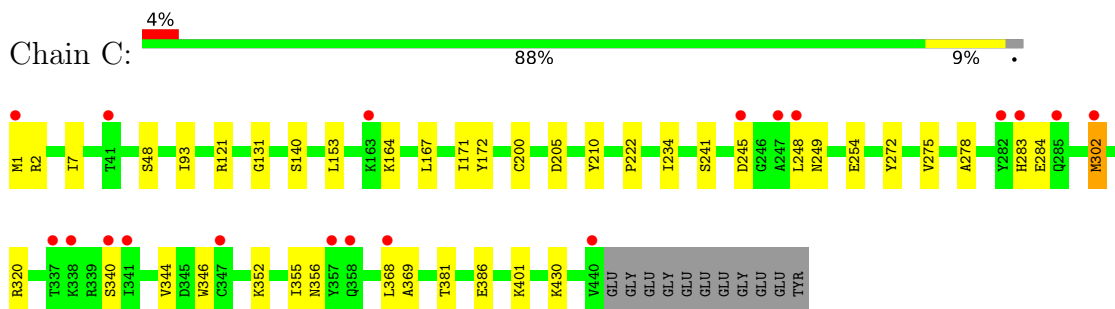
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

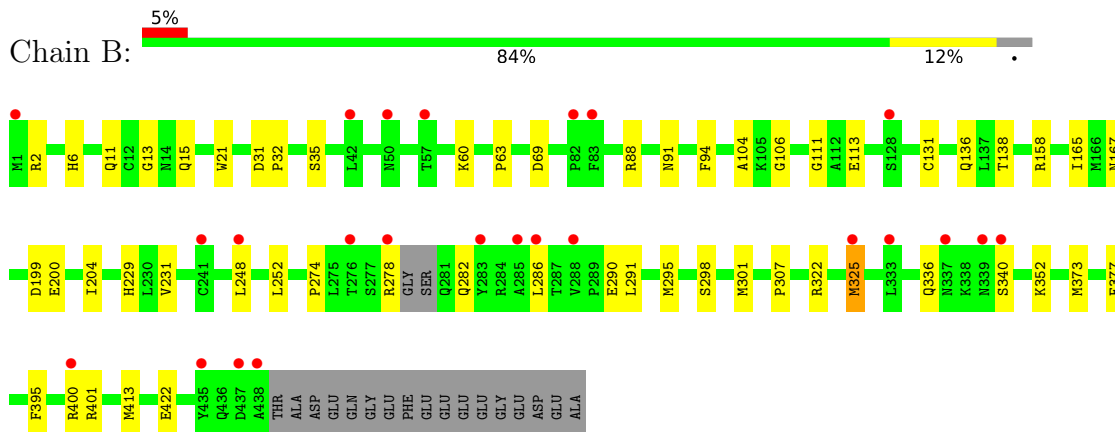
- Molecule 1: Tubulin alpha-1B chain



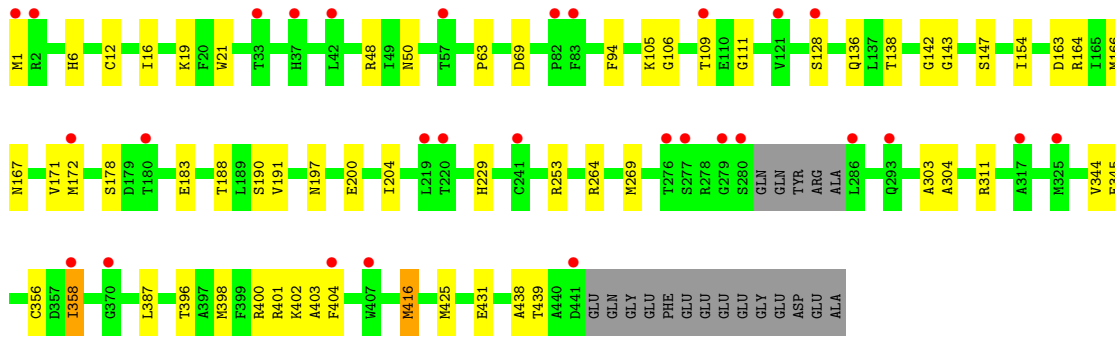
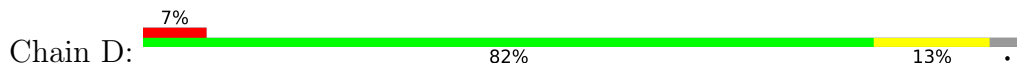
- Molecule 1: Tubulin alpha-1B chain



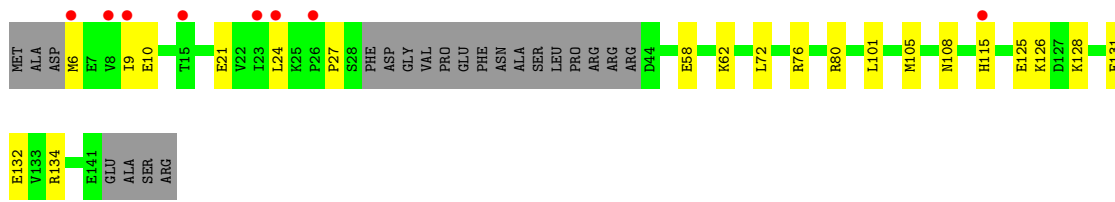
- Molecule 2: Tubulin beta-2B chain



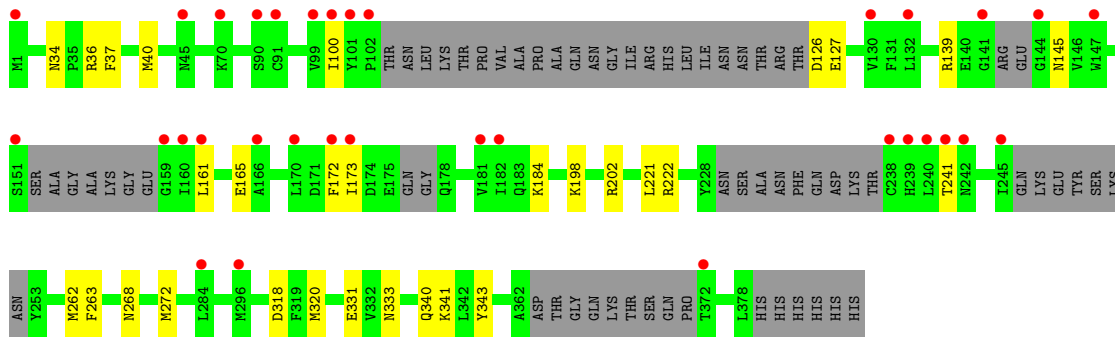
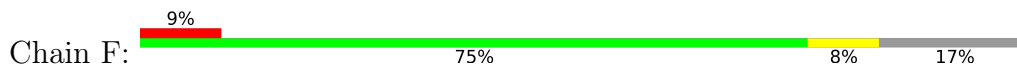
- Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin beta-2B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.84Å 157.89Å 179.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 1.95 49.28 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.28-1.95) 100.0 (49.28-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.95Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.189 , 0.216 0.192 , 0.220	Depositor DCC
R_{free} test set	10797 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtrriage
Anisotropy	0.151	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18392	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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, MG, CA, MES, R42, 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	0.14	0/3523	0.37	0/4780
1	C	0.16	0/3528	0.39	0/4790
2	B	0.14	0/3433	0.36	0/4648
2	D	0.13	0/3427	0.34	0/4640
3	E	0.11	0/1008	0.27	0/1337
4	F	0.10	0/2670	0.31	0/3603
All	All	0.14	0/17589	0.35	0/23798

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	284	GLU	Peptide

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	3446	0	3348	21	0
1	C	3447	0	3360	25	1
2	B	3359	0	3241	33	1
2	D	3354	0	3234	38	0
3	E	1000	0	1018	12	0
4	F	2614	0	2597	22	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	12	2	0
10	B	60	0	0	1	0
10	D	60	0	0	1	0
11	F	31	0	14	4	0
12	A	169	0	0	3	0
12	B	156	0	0	1	0
12	C	316	0	0	4	0
12	D	122	0	0	3	0
12	E	47	0	0	3	0
12	F	73	0	0	1	0
All	All	18392	0	16872	147	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.68	0.75
1:A:370:LYS:NZ	12:A:601:HOH:O	2.20	0.72
1:C:241:SER:HA	1:C:249:ASN:HD21	1.53	0.72
2:D:416:MET:HA	2:D:416:MET:HE2	1.73	0.70
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.76	0.68
3:E:10:GLU:OE2	12:E:201:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ILE:HD11	4:F:173:ILE:HD13	1.76	0.67
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.67
2:D:188:THR:HA	2:D:425:MET:HE1	1.79	0.66
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.29	0.64
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.79	0.63
1:C:340:SER:O	12:C:601:HOH:O	2.14	0.63
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.80	0.62
2:D:19:LYS:NZ	12:D:606:HOH:O	2.32	0.62
2:B:325:MET:H	2:B:325:MET:HE3	1.64	0.62
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.82	0.61
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.64	0.61
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.82	0.61
2:D:438:ALA:O	12:D:601:HOH:O	2.16	0.60
1:C:1:MET:O	12:C:602:HOH:O	2.16	0.60
2:B:158:ARG:CZ	9:B:503:MES:H21	2.32	0.59
2:B:199:ASP:OD2	9:B:503:MES:H52	2.04	0.58
1:C:234:ILE:HG12	1:C:302:MET:HE3	1.86	0.57
2:B:278:ARG:HH21	2:B:282:GLN:HE22	1.53	0.55
3:E:80:ARG:NH1	12:E:205:HOH:O	2.39	0.55
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.40	0.55
1:A:280:LYS:HB2	1:A:283:HIS:NE2	2.20	0.55
4:F:139:ARG:HB2	4:F:145:ASN:HD21	1.72	0.55
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.89	0.54
2:D:396:THR:O	2:D:400:ARG:HB2	2.07	0.54
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
2:D:147:SER:HG	2:D:190:SER:HG	1.52	0.53
2:D:229:HIS:NE2	10:D:503:R42:O39	2.34	0.53
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.90	0.53
1:C:2:ARG:HB2	1:C:2:ARG:HH11	1.73	0.52
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.28	0.52
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.92	0.52
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.91	0.52
2:D:1:MET:HE1	2:D:48:ARG:HG2	1.91	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.74	0.51
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.92	0.51
2:D:311[B]:ARG:HH21	2:D:344:VAL:HA	1.75	0.51
2:D:401:ARG:HG3	2:D:403:ALA:HB2	1.92	0.51
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.93	0.50
2:D:142:GLY:O	2:D:183:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:36:ARG:NH1	12:F:504:HOH:O	2.43	0.50
1:C:320:ARG:HA	1:C:356:ASN:O	2.12	0.50
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.30	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.49
1:A:280:LYS:HB2	1:A:283:HIS:CE1	2.47	0.49
2:B:291:LEU:HD12	2:B:373:MET:HE2	1.94	0.49
1:C:386:GLU:OE2	12:C:603:HOH:O	2.20	0.49
3:E:131:GLU:HG3	3:E:134:ARG:HH21	1.77	0.49
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.48
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.95	0.48
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.48
4:F:320:MET:HB3	4:F:320:MET:HE2	1.83	0.47
4:F:139:ARG:HB2	4:F:145:ASN:ND2	2.29	0.47
3:E:108:ASN:ND2	12:E:206:HOH:O	2.44	0.47
2:B:295:MET:CG	2:B:377:PHE:HB2	2.45	0.47
2:D:128:SER:O	2:D:128:SER:OG	2.29	0.47
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.96	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
2:B:422:GLU:HG3	12:B:615:HOH:O	2.15	0.47
2:B:69:ASP:O	2:B:94:PHE:HA	2.15	0.47
1:C:48:SER:OG	1:C:245:ASP:HB2	2.15	0.47
2:D:197:ASN:HD21	3:E:126:LYS:HE2	1.80	0.47
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.51	0.46
2:D:311[B]:ARG:NH2	2:D:345:GLU:OE2	2.45	0.46
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.98	0.46
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.96	0.46
4:F:222:ARG:NH1	11:F:401:ACP:O2G	2.49	0.46
2:B:11:GLN:O	2:B:15:GLN:HG3	2.15	0.46
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.51	0.46
2:D:106:GLY:O	2:D:111:GLY:HA3	2.15	0.46
2:B:2:ARG:NH1	2:B:131:CYS:SG	2.88	0.46
4:F:145:ASN:HA	4:F:184:LYS:HE2	1.97	0.46
2:D:147:SER:OG	2:D:190:SER:OG	2.24	0.45
2:B:298:SER:HA	2:B:301:MET:HE2	1.98	0.45
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.16	0.45
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.81	0.45
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.45
4:F:161:LEU:HD12	4:F:172:PHE:CG	2.52	0.45
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.45
3:E:125:GLU:O	3:E:128:LYS:HG3	2.17	0.45
1:C:272:TYR:N	1:C:302:MET:HE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ASP:O	2:D:253:ARG:NH2	2.50	0.45
2:D:178:SER:OG	2:D:183:GLU:OE2	2.27	0.45
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.98	0.45
3:E:101:LEU:O	3:E:105:MET:HG2	2.17	0.44
1:C:430:LYS:HE2	1:C:430:LYS:HB3	1.75	0.44
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.99	0.44
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.00	0.44
2:D:356:CYS:SG	2:D:358:ILE:HG23	2.58	0.44
2:D:398:MET:HE3	2:D:404:PHE:CD1	2.53	0.44
1:A:132:LEU:O	1:A:164:LYS:NZ	2.50	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.44
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.52	0.44
1:A:430:LYS:HB3	1:A:430:LYS:HE2	1.55	0.44
2:D:191:VAL:HB	2:D:425:MET:HE2	2.00	0.44
1:A:300:ASN:ND2	12:A:610:HOH:O	2.50	0.44
12:C:623:HOH:O	3:E:115:HIS:HE1	2.01	0.44
1:A:450:GLU:OE1	4:F:333:ASN:HB3	2.18	0.43
2:B:274:PRO:HB3	2:B:286:LEU:HD22	2.01	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.84	0.43
1:A:207:GLU:OE2	1:A:304:LYS:HE2	2.19	0.43
1:A:174:ALA:O	1:A:178:SER:HB3	2.19	0.43
1:A:356:ASN:ND2	12:A:608:HOH:O	2.47	0.43
2:B:340:SER:HB3	4:F:34:ASN:HD21	1.84	0.43
2:D:402:LYS:O	2:D:402:LYS:HD2	2.19	0.43
2:D:16:ILE:HD11	2:D:138:THR:HB	2.01	0.42
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.42
2:B:229:HIS:HB3	10:B:504:R42:C25	2.49	0.42
2:B:301:MET:HE1	2:B:307:PRO:HD3	2.00	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.02	0.42
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.20	0.42
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.42
2:B:104:ALA:HB2	2:B:413:MET:SD	2.59	0.42
4:F:161:LEU:HA	4:F:161:LEU:HD23	1.80	0.42
4:F:318:ASP:OD2	11:F:401:ACP:O3G	2.37	0.42
3:E:9:ILE:HG12	3:E:21:GLU:HB3	2.01	0.42
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.02	0.41
1:C:302:MET:N	1:C:302:MET:SD	2.93	0.41
2:B:322:ARG:HD3	2:B:322:ARG:HA	1.87	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.54	0.41
2:B:88:ARG:HD2	2:B:91:ASN:OD1	2.19	0.41
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.03	0.41
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.02	0.41
1:C:401:LYS:NZ	2:D:439:THR:O	2.37	0.41
2:B:35:SER:OG	2:B:60:LYS:NZ	2.54	0.41
4:F:202:ARG:HB2	4:F:222:ARG:NH2	2.36	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
2:D:171:VAL:HA	2:D:204:ILE:O	2.21	0.41
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.21	0.41
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.03	0.41
2:B:13:GLY:HA2	2:B:138:THR:HG22	2.03	0.40
4:F:126:ASP:OD1	4:F:127:GLU:N	2.55	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	2.21	0.40
4:F:263:PHE:CE2	4:F:341:LYS:HE2	2.56	0.40
2:D:164:ARG:NH1	12:D:607:HOH:O	2.55	0.40
2:D:105:LYS:HA	2:D:109:THR:OG1	2.22	0.40
4:F:268:ASN:O	4:F:272:MET:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLU:OE2	1:C:283:HIS:NE2[4_555]	2.19	0.01

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	437/451 (97%)	431 (99%)	6 (1%)	0	100 100
1	C	440/451 (98%)	430 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	422/445 (95%)	415 (98%)	7 (2%)	0	100	100
2	D	423/445 (95%)	415 (98%)	7 (2%)	1 (0%)	43	36
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	14	6
4	F	303/384 (79%)	296 (98%)	7 (2%)	0	100	100
All	All	2142/2319 (92%)	2102 (98%)	38 (2%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27	PRO
2	D	304	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/379 (98%)	369 (100%)	2 (0%)	81	82
1	C	373/379 (98%)	371 (100%)	2 (0%)	81	82
2	B	369/383 (96%)	367 (100%)	2 (0%)	81	82
2	D	369/383 (96%)	366 (99%)	3 (1%)	73	74
3	E	109/127 (86%)	108 (99%)	1 (1%)	70	70
4	F	287/342 (84%)	286 (100%)	1 (0%)	86	87
All	All	1878/1993 (94%)	1867 (99%)	11 (1%)	78	79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	LYS
1	A	381	THR
2	B	325	MET
2	B	336	GLN
1	C	302	MET

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Mol	Chain	Res	Type
1	C	381	THR
2	D	50	ASN
2	D	358	ILE
2	D	416	MET
3	E	132	GLU
4	F	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	300	ASN
1	A	356	ASN
2	B	50	ASN
2	B	167	ASN
2	B	192	HIS
2	B	349	ASN
2	B	424	ASN
2	B	434	GLN
1	C	11	GLN
1	C	249	ASN
2	D	50	ASN
2	D	59	ASN
2	D	101	ASN
2	D	167	ASN
2	D	197	ASN
2	D	331	GLN
2	D	426	ASN
3	E	12	ASN
3	E	84	GLN
3	E	108	ASN
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	D	501	6	29,30,30	1.16	3 (10%)	45,47,47	1.70	6 (13%)
10	R42	B	504	-	65,65,65	0.92	4 (6%)	99,101,101	2.01	24 (24%)
5	GTP	A	501	6	33,34,34	0.97	3 (9%)	50,54,54	1.51	8 (16%)
5	GTP	C	501	6	33,34,34	0.94	2 (6%)	50,54,54	1.51	9 (18%)
11	ACP	F	401	6	31,33,33	1.66	8 (25%)	47,52,52	1.83	10 (21%)
10	R42	D	503	-	65,65,65	0.92	3 (4%)	99,101,101	1.86	24 (24%)
9	MES	B	503	-	12,12,12	2.27	1 (8%)	15,16,16	1.80	3 (20%)
8	GDP	B	501	6	29,30,30	1.15	3 (10%)	45,47,47	1.69	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	6	-	3/16/32/32	0/3/3/3
10	R42	B	504	-	-	5/43/129/129	0/6/6/6
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	6	-	5/19/38/38	0/3/3/3
10	R42	D	503	-	-	8/43/129/129	0/6/6/6
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.64	1.66	1.77
11	F	401	ACP	C5-C4	4.78	1.47	1.39
10	D	503	R42	O39-C39	3.45	1.30	1.23
10	B	504	R42	O39-C39	3.43	1.30	1.23
8	D	501	GDP	C5-C4	3.12	1.47	1.38
8	B	501	GDP	C5-C4	2.97	1.46	1.38
11	F	401	ACP	PG-O3G	2.93	1.61	1.55
11	F	401	ACP	PG-O2G	2.91	1.61	1.55
11	F	401	ACP	C5-C6	2.71	1.48	1.41
11	F	401	ACP	PB-O3A	2.60	1.61	1.58
5	C	501	GTP	PA-O3A	2.44	1.62	1.59
5	A	501	GTP	PA-O3A	2.41	1.62	1.59
8	B	501	GDP	C6-N1	-2.38	1.34	1.38
11	F	401	ACP	C8-N7	2.35	1.36	1.31
8	D	501	GDP	C6-N1	-2.33	1.34	1.38
11	F	401	ACP	C5-N7	-2.22	1.35	1.39
8	B	501	GDP	C5-N7	-2.12	1.34	1.39
5	A	501	GTP	C2-N3	2.11	1.38	1.33
5	A	501	GTP	PB-O3B	2.09	1.61	1.59
10	B	504	R42	C22-C21	-2.09	1.45	1.50
10	B	504	R42	O13-C13	-2.08	1.42	1.45
10	B	504	R42	C4-C3	2.08	1.59	1.54
5	C	501	GTP	C2-N3	2.08	1.38	1.33
11	F	401	ACP	PB-O2B	2.07	1.61	1.56
10	D	503	R42	C22-C21	-2.07	1.45	1.50
10	D	503	R42	C4-C3	2.06	1.59	1.54
8	D	501	GDP	C5-N7	-2.01	1.35	1.39

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	R42	C40-C39-N32	6.78	126.88	117.63
10	D	503	R42	O4-C28-C29	6.51	121.70	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	R42	O4-C28-C29	6.47	121.63	110.67
8	D	501	GDP	C5-C4-N3	-5.82	119.12	128.39
11	F	401	ACP	C5-C4-N3	-5.77	118.78	126.72
10	B	504	R42	C2-O2-C21	5.73	128.26	117.80
8	B	501	GDP	C5-C4-N3	-5.70	119.32	128.39
10	D	503	R42	C2-O2-C21	5.69	128.19	117.80
9	B	503	MES	C5-N4-C3	5.14	119.92	108.84
10	D	503	R42	C31-C32-N32	5.05	121.71	109.27
8	D	501	GDP	C2-N3-C4	4.89	120.72	112.30
8	B	501	GDP	C2-N3-C4	4.86	120.67	112.30
5	C	501	GTP	C5-C4-N3	-4.68	120.94	128.39
11	F	401	ACP	N3-C4-N9	4.63	135.04	127.17
5	A	501	GTP	C5-C4-N3	-4.63	121.03	128.39
5	A	501	GTP	C2-N3-C4	4.44	119.95	112.30
5	C	501	GTP	C2-N3-C4	4.41	119.89	112.30
8	B	501	GDP	N9-C4-N3	4.40	134.75	125.95
8	D	501	GDP	N9-C4-N3	4.34	134.64	125.95
10	B	504	R42	O39-C39-C40	-4.29	114.67	120.95
10	B	504	R42	C17-C15-C16	-3.88	95.27	106.29
10	B	504	R42	C31-C32-N32	3.85	118.74	109.27
10	D	503	R42	O4-C28-O28	-3.79	117.00	123.61
10	B	504	R42	O4-C28-O28	-3.76	117.05	123.61
10	B	504	R42	C18-C12-C11	-3.75	120.86	125.32
10	D	503	R42	C8-C9-C10	3.75	128.27	122.69
10	D	503	R42	C17-C15-C16	-3.72	95.73	106.29
10	D	503	R42	C40-C39-N32	3.65	122.61	117.63
10	D	503	R42	C18-C12-C11	-3.65	120.98	125.32
11	F	401	ACP	C2-N3-C4	3.63	120.71	111.83
10	B	504	R42	C8-C9-C10	3.61	128.06	122.69
11	F	401	ACP	PB-O3A-PA	-3.60	120.61	132.37
11	F	401	ACP	C4-C5-N7	-3.43	106.66	110.58
10	B	504	R42	C33-C32-N32	3.42	118.66	112.07
8	D	501	GDP	C6-C5-N7	3.33	136.35	130.29
8	B	501	GDP	C6-C5-N7	3.17	136.06	130.29
11	F	401	ACP	N3-C2-N1	-3.16	123.80	128.58
10	B	504	R42	C10-C11-C12	-3.11	115.94	120.65
10	D	503	R42	O10-C10-C11	-3.10	106.48	111.48
10	B	504	R42	O10-C10-C9	3.08	114.63	109.51
10	B	504	R42	O44-C43-C42	3.06	117.47	111.28
10	D	503	R42	O10-C10-C9	3.01	114.53	109.51
10	D	503	R42	O13-C30-C31	3.01	115.90	111.13
10	B	504	R42	C4-C3-C2	2.99	117.46	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	R42	C4-O4-C28	2.99	126.74	119.17
5	C	501	GTP	N9-C4-N3	2.99	131.93	125.95
10	B	504	R42	O10-C10-C11	-2.99	106.66	111.48
10	B	504	R42	C20-O5-C5	2.90	94.65	91.42
10	D	503	R42	C4-O4-C28	2.90	126.52	119.17
10	D	503	R42	C4-C3-C2	2.89	117.26	111.70
5	A	501	GTP	N9-C4-N3	2.85	131.65	125.95
5	C	501	GTP	N9-C8-N7	-2.80	108.20	113.40
10	D	503	R42	O44-C43-C42	2.77	116.87	111.28
10	D	503	R42	C20-O5-C5	2.74	94.47	91.42
5	A	501	GTP	N9-C8-N7	-2.74	108.33	113.40
10	D	503	R42	O39-C39-C40	-2.72	116.97	120.95
5	A	501	GTP	C2-N1-C6	-2.69	120.24	125.11
5	C	501	GTP	C2-N1-C6	-2.69	120.24	125.11
10	D	503	R42	C33-C32-C31	2.68	118.13	111.46
11	F	401	ACP	C4-N9-C8	2.68	108.55	105.74
10	B	504	R42	O39-C39-N32	-2.63	118.45	123.09
10	D	503	R42	C10-C11-C12	-2.58	116.75	120.65
5	C	501	GTP	C8-N7-C5	2.54	108.78	104.26
8	B	501	GDP	O6-C6-C5	-2.52	119.88	126.53
8	D	501	GDP	C4-C5-N7	-2.52	106.68	110.67
11	F	401	ACP	C5-N7-C8	2.47	107.33	103.45
5	A	501	GTP	C5-C6-N1	2.47	119.54	113.25
5	A	501	GTP	C8-N7-C5	2.40	108.54	104.26
11	F	401	ACP	C3'-C2'-C1'	2.37	105.94	101.46
5	C	501	GTP	C5-C6-N1	2.36	119.25	113.25
5	C	501	GTP	O6-C6-C5	-2.35	120.34	126.53
10	B	504	R42	O13-C30-C31	2.34	114.83	111.13
10	D	503	R42	C1-C2-C3	-2.33	114.70	118.19
10	B	504	R42	C1-C2-C3	-2.28	114.78	118.19
5	C	501	GTP	O2A-PA-O3A	2.27	113.42	107.27
10	D	503	R42	O1-C1-C2	2.24	110.40	105.54
5	A	501	GTP	O6-C6-C5	-2.23	120.64	126.53
10	B	504	R42	O9-C9-C10	-2.21	114.85	117.37
10	B	504	R42	O5-C20-C4	-2.19	89.54	91.94
9	B	503	MES	C7-N4-C5	2.19	117.07	111.24
10	D	503	R42	O13-C30-O30	-2.18	120.02	123.95
8	D	501	GDP	O6-C6-C5	-2.17	120.80	126.53
8	B	501	GDP	C4-C5-N7	-2.17	107.23	110.67
10	D	503	R42	O9-C9-C10	-2.15	114.92	117.37
10	B	504	R42	O1-C1-C2	2.13	110.17	105.54
10	D	503	R42	C17-C15-C1	2.12	115.61	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	R42	C17-C15-C1	2.07	115.50	111.13
10	D	503	R42	O5-C20-C4	-2.06	89.69	91.94
11	F	401	ACP	C6-C5-N7	2.05	136.04	132.09
9	B	503	MES	O3S-S-C8	2.03	109.98	106.00
8	B	501	GDP	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
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	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
10	B	504	R42	C42-C43-O44-C44
10	B	504	R42	O43-C43-O44-C44
10	D	503	R42	C42-C43-O44-C44
11	F	401	ACP	C3'-C4'-C5'-O5'
10	D	503	R42	O43-C43-O44-C44
10	D	503	R42	O31-C31-C32-N32
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
10	D	503	R42	C39-C40-C42-C43
10	D	503	R42	C31-C32-N32-C39
10	D	503	R42	C41-C40-C42-C43
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
10	D	503	R42	C30-C31-C32-N32

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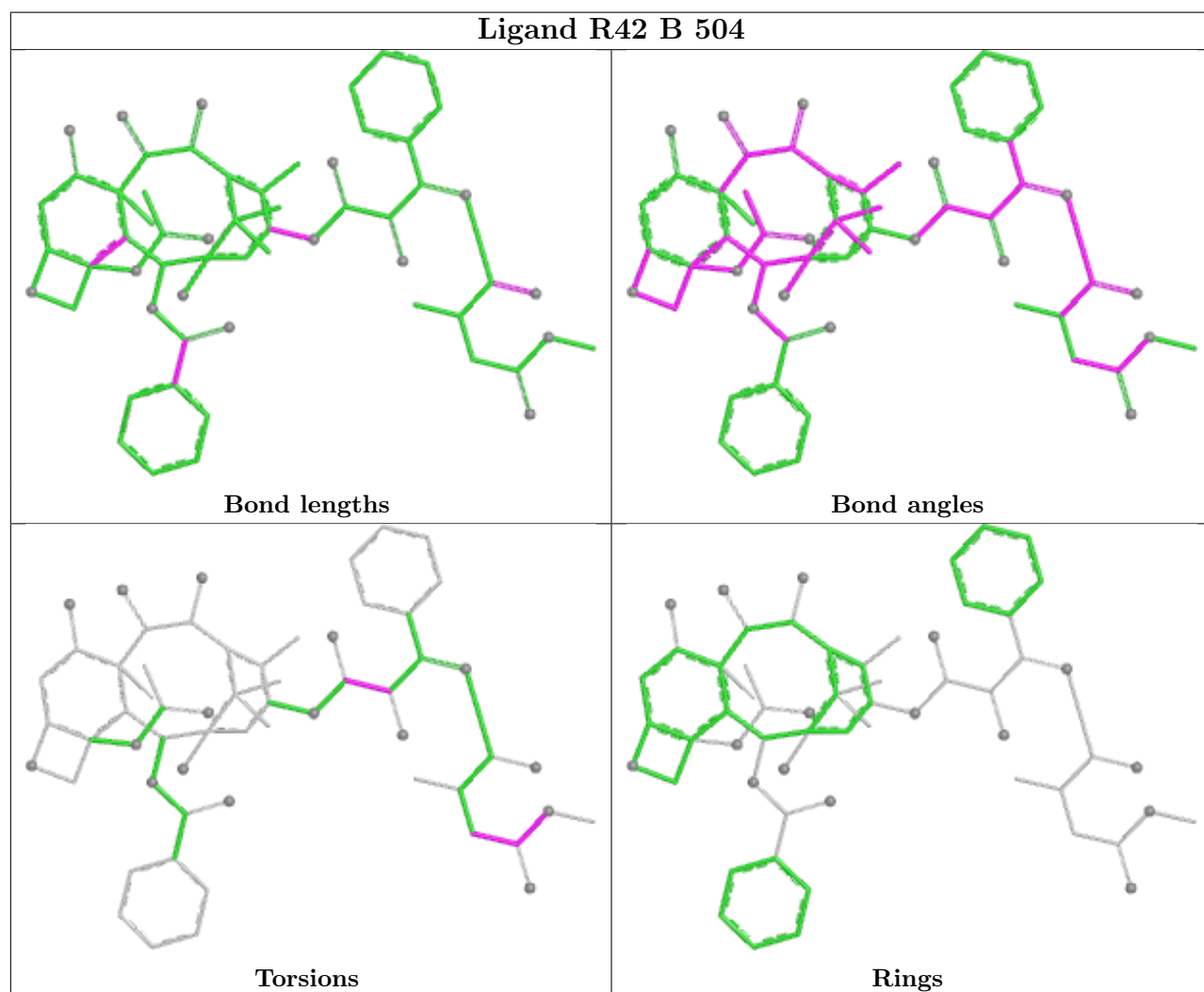
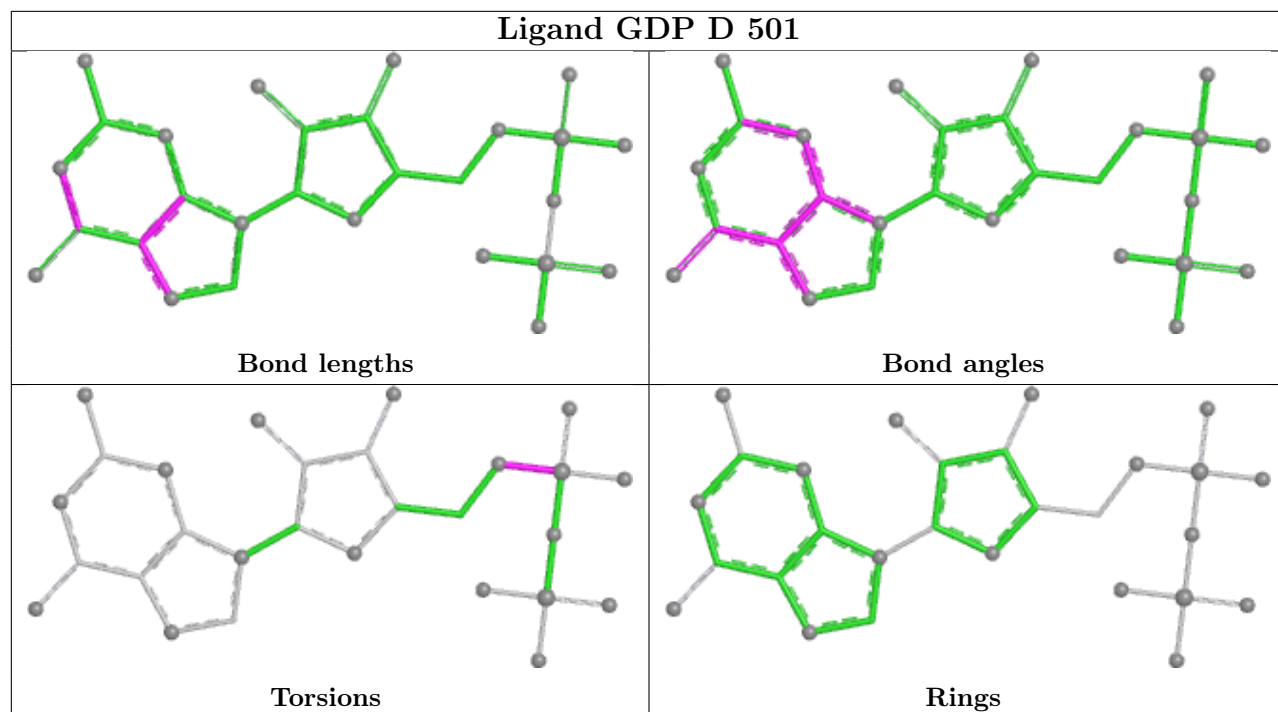
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A
10	B	504	R42	C40-C42-C43-O44
10	D	503	R42	C40-C42-C43-O44
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	504	R42	O13-C30-C31-O31
10	B	504	R42	O30-C30-C31-O31

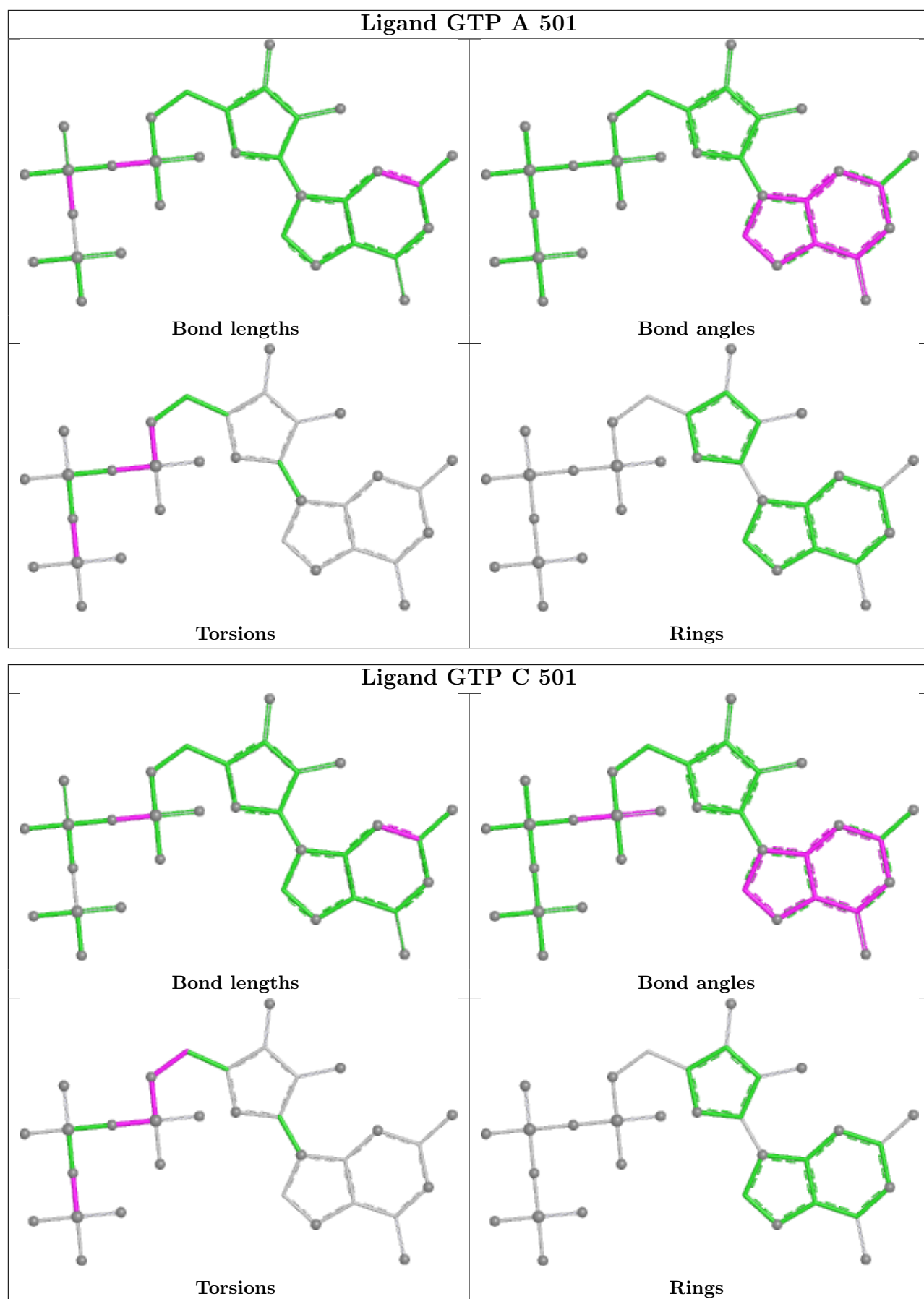
There are no ring outliers.

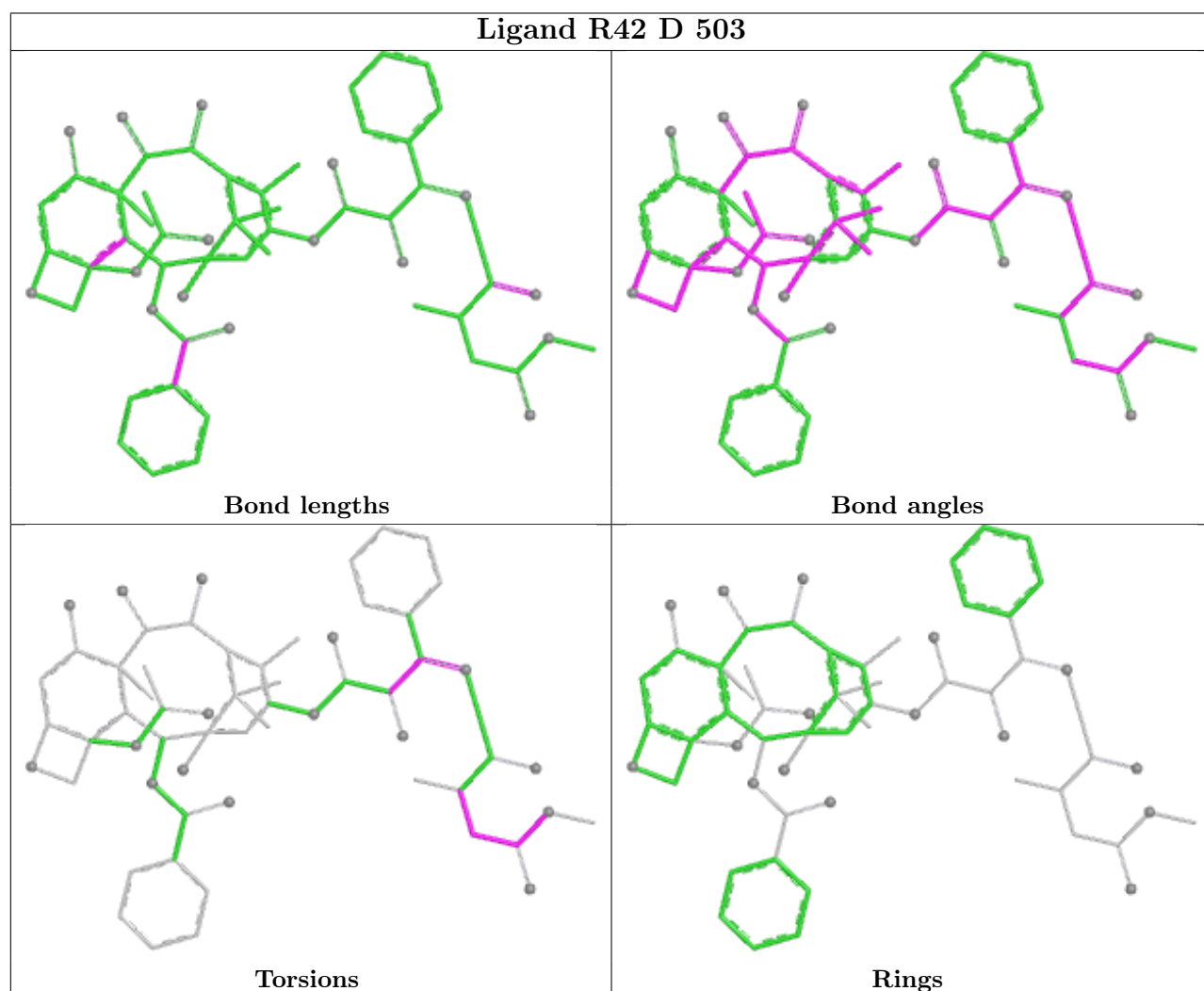
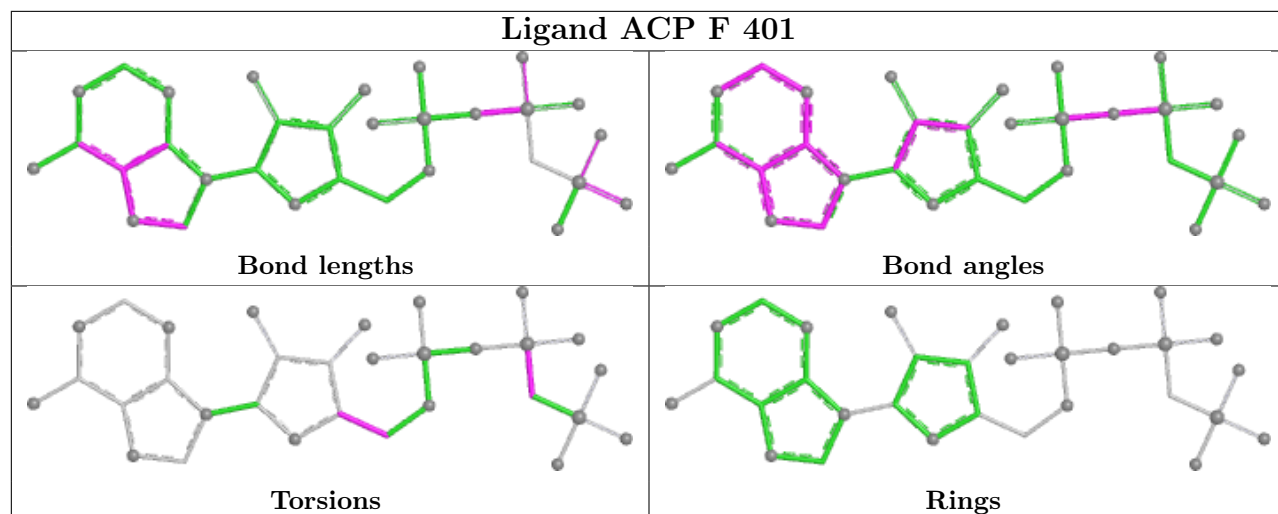
6 monomers are involved in 11 short contacts:

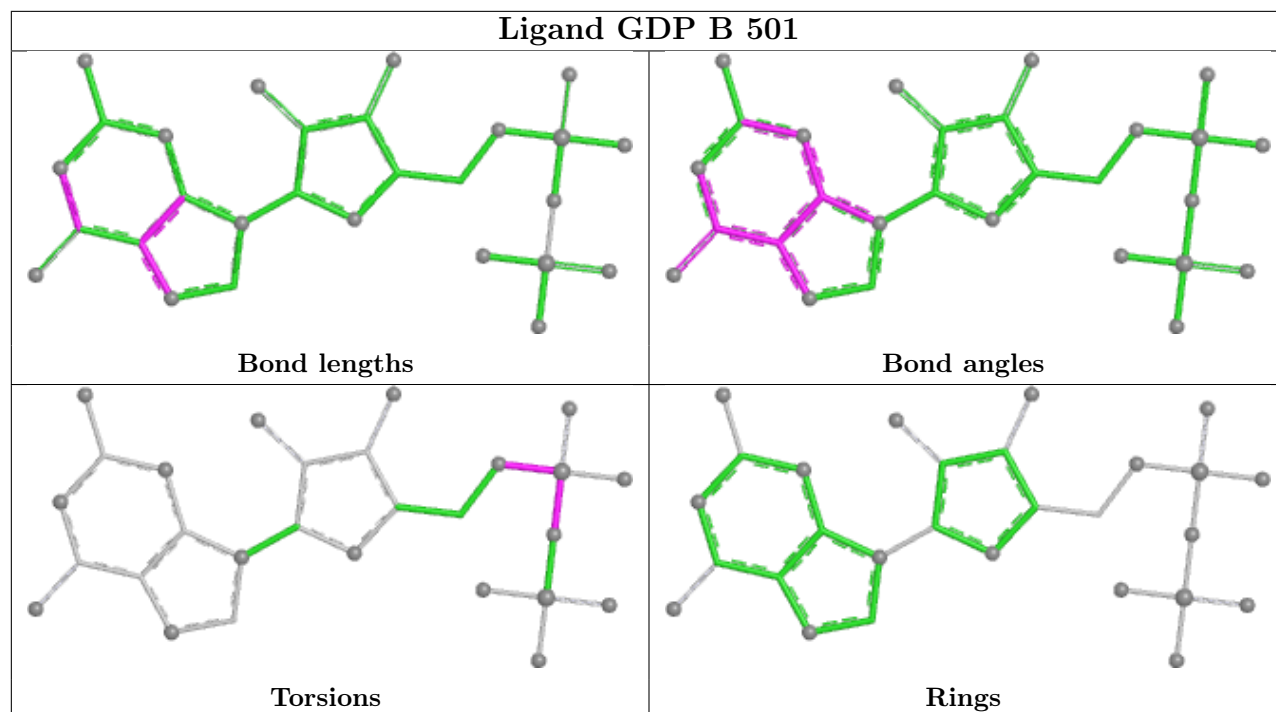
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
10	B	504	R42	1	0
5	A	501	GTP	1	0
11	F	401	ACP	4	0
10	D	503	R42	1	0
9	B	503	MES	2	0

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.









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	441/451 (97%)	0.36	16 (3%) 46 53	34, 54, 88, 148	0
1	C	440/451 (97%)	0.10	19 (4%) 40 46	22, 42, 73, 123	2 (0%)
2	B	426/445 (95%)	0.39	24 (5%) 30 35	31, 53, 96, 149	0
2	D	426/445 (95%)	0.54	29 (6%) 23 27	24, 63, 99, 133	1 (0%)
3	E	121/143 (84%)	0.71	8 (6%) 24 28	41, 68, 105, 130	0
4	F	319/384 (83%)	0.81	33 (10%) 12 13	45, 77, 149, 200	0
All	All	2173/2319 (93%)	0.43	129 (5%) 28 32	22, 57, 108, 200	3 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	5.6
1	A	179	THR	5.4
1	A	283	HIS	5.3
4	F	100	ILE	4.8
1	C	41	THR	4.6
2	B	333	LEU	4.2
2	D	286	LEU	4.2
1	C	440	VAL	4.1
4	F	245	ILE	4.1
1	A	262	TYR	3.9
4	F	173	ILE	3.8
4	F	240	LEU	3.7
4	F	99	VAL	3.7
2	B	248	LEU	3.7
2	D	358	ILE	3.7
4	F	241	THR	3.7
2	D	172	MET	3.6
1	C	283	HIS	3.6
1	C	368	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	1	MET	3.5
1	C	340	SER	3.4
2	D	407	TRP	3.4
1	C	357	TYR	3.3
1	C	341	ILE	3.3
1	A	346	TRP	3.3
2	B	325	MET	3.2
1	A	282	TYR	3.2
3	E	8	VAL	3.2
2	D	280	SER	3.2
1	C	1	MET	3.2
2	B	276	THR	3.2
4	F	102	PRO	3.1
2	B	286	LEU	3.1
4	F	161	LEU	3.1
1	C	247	ALA	3.0
4	F	141	GLY	2.9
4	F	182	ILE	2.9
1	C	358	GLN	2.9
4	F	172	PHE	2.9
1	A	309	HIS	2.9
2	D	57	THR	2.9
2	D	276	THR	2.8
1	C	285	GLN	2.8
2	D	241	CYS	2.8
3	E	15	THR	2.8
2	B	435	TYR	2.8
2	D	325	MET	2.8
2	B	283	TYR	2.7
4	F	147	TRP	2.7
1	A	316	CYS	2.7
1	A	178	SER	2.7
1	A	437	VAL	2.6
2	B	340	SER	2.6
4	F	170	LEU	2.6
1	A	448	GLY	2.6
2	B	438	ALA	2.6
2	B	285	ALA	2.6
4	F	372	THR	2.6
1	C	302	MET	2.5
4	F	132	LEU	2.5
3	E	9	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	23	ILE	2.5
2	B	400	ARG	2.5
3	E	26	PRO	2.5
3	E	24	LEU	2.5
2	B	339	ASN	2.5
4	F	242	ASN	2.5
4	F	101	TYR	2.5
2	D	128	SER	2.5
4	F	70	LYS	2.4
4	F	166	ALA	2.4
2	B	337	ASN	2.4
2	D	370	GLY	2.4
4	F	238	CYS	2.4
4	F	296	MET	2.4
2	B	83	PHE	2.4
2	D	404	PHE	2.4
2	D	2	ARG	2.4
2	D	37	HIS	2.4
2	B	128	SER	2.4
2	D	277	SER	2.4
2	B	42	LEU	2.4
1	A	180	ALA	2.3
2	B	57	THR	2.3
3	E	115	HIS	2.3
4	F	159	GLY	2.3
4	F	90	SER	2.3
4	F	181	VAL	2.3
2	D	180	THR	2.3
1	C	338	LYS	2.3
2	D	83	PHE	2.3
4	F	144	GLY	2.3
2	D	279	GLY	2.2
1	C	245	ASP	2.2
2	B	50	ASN	2.2
4	F	239	HIS	2.2
4	F	284	LEU	2.2
2	D	82	PRO	2.2
1	A	76	ASP	2.2
2	B	82	PRO	2.2
1	C	163	LYS	2.2
4	F	45	ASN	2.1
2	D	220	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	347	CYS	2.1
3	E	6	MET	2.1
4	F	1	MET	2.1
1	A	18	ASN	2.1
1	A	281	ALA	2.1
1	C	282	TYR	2.1
2	D	441	ASP	2.1
1	C	337	THR	2.1
4	F	151	SER	2.1
2	B	278	ARG	2.1
2	B	241	CYS	2.1
4	F	91	CYS	2.1
2	D	219	LEU	2.1
2	B	437	ASP	2.1
4	F	160	ILE	2.1
2	B	288	VAL	2.1
1	A	261	PRO	2.1
2	D	293	GLN	2.1
2	D	317	ALA	2.1
2	D	109	THR	2.0
2	D	121	VAL	2.0
1	C	248	LEU	2.0
2	D	42	LEU	2.0
1	A	280	LYS	2.0
2	D	33	THR	2.0
4	F	130	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

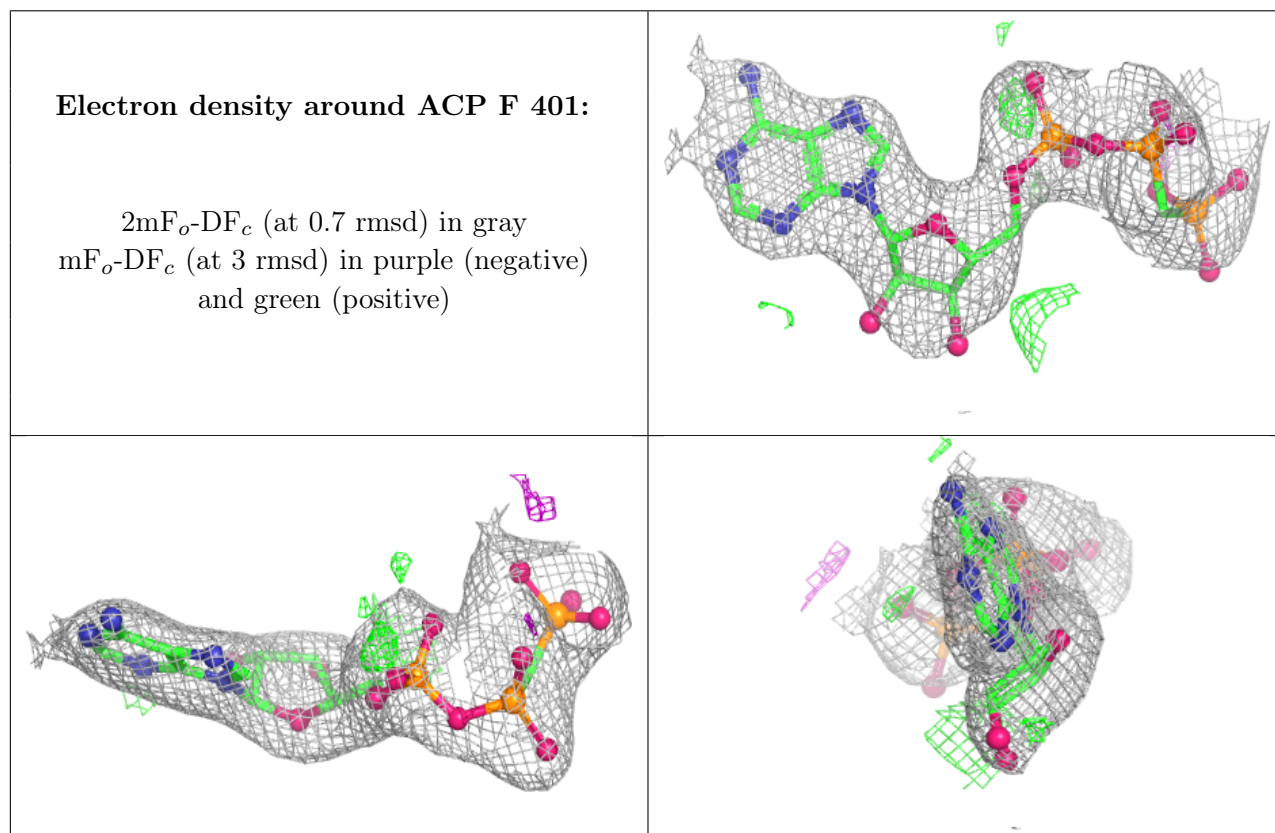
There are no oligosaccharides in this entry.

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.

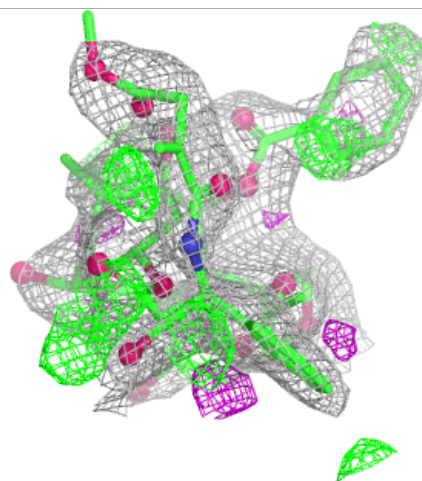
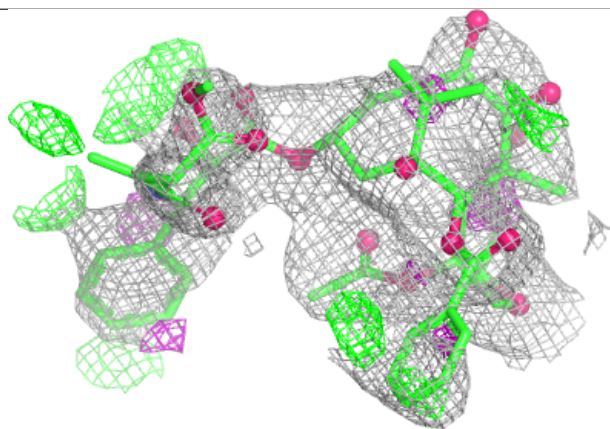
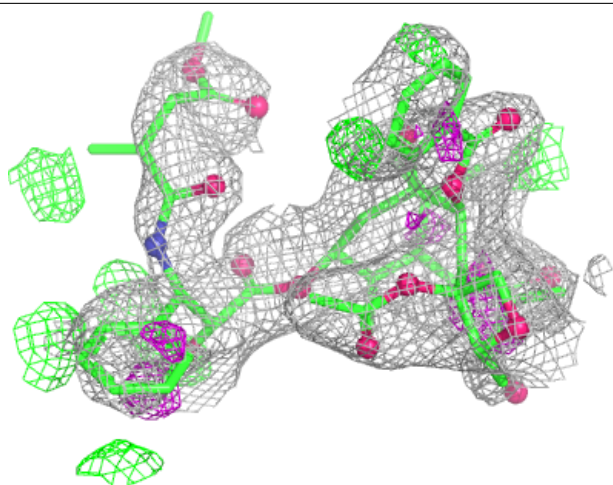
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	A	503	1/1	0.72	0.19	117,117,117,117	0
11	ACP	F	401	31/31	0.81	0.13	80,112,152,153	0
10	R42	B	504	60/60	0.82	0.16	73,115,127,130	0
10	R42	D	503	60/60	0.88	0.13	80,102,120,127	0
6	MG	A	502	1/1	0.88	0.08	40,40,40,40	0
6	MG	F	402	1/1	0.90	0.09	81,81,81,81	0
9	MES	B	503	12/12	0.91	0.12	45,59,67,72	0
8	GDP	D	501	28/28	0.92	0.10	48,58,70,87	0
6	MG	D	502	1/1	0.95	0.08	61,61,61,61	0
5	GTP	A	501	32/32	0.98	0.06	31,37,42,45	0
6	MG	C	502	1/1	0.98	0.05	34,34,34,34	0
8	GDP	B	501	28/28	0.98	0.05	30,36,41,41	0
5	GTP	C	501	32/32	0.98	0.04	27,32,37,37	0
6	MG	B	502	1/1	0.99	0.06	28,28,28,28	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.



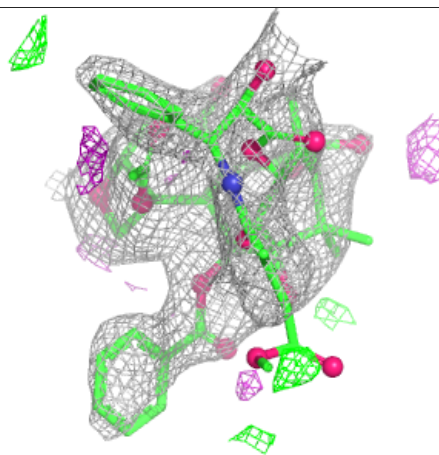
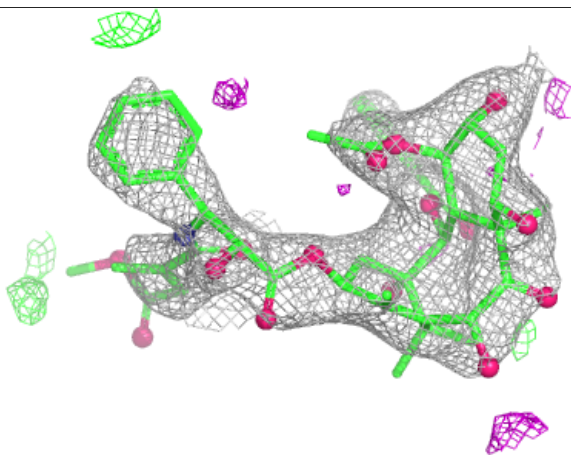
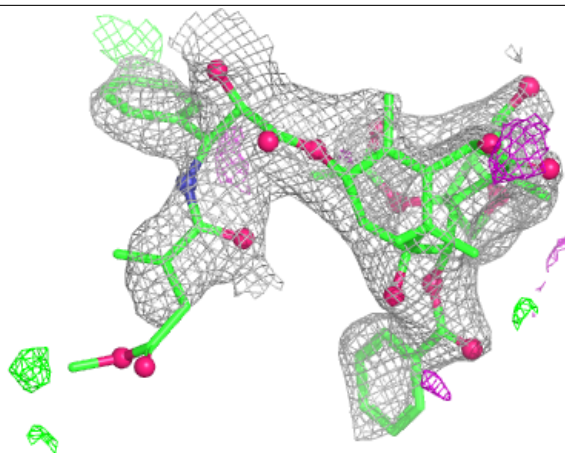
Electron density around R42 B 504:

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



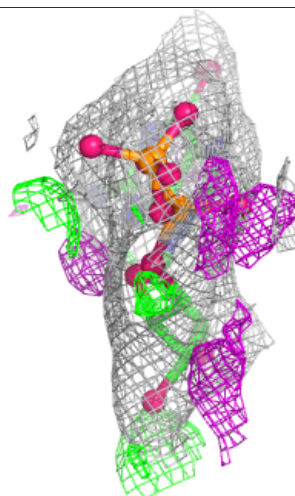
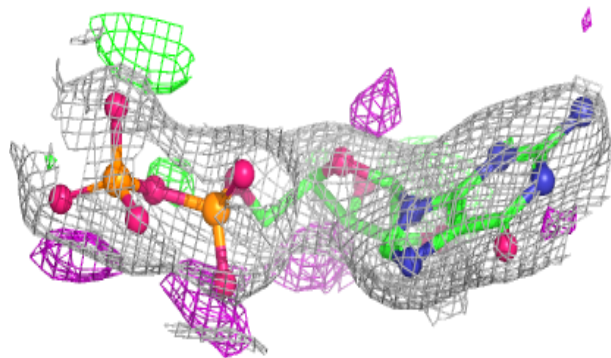
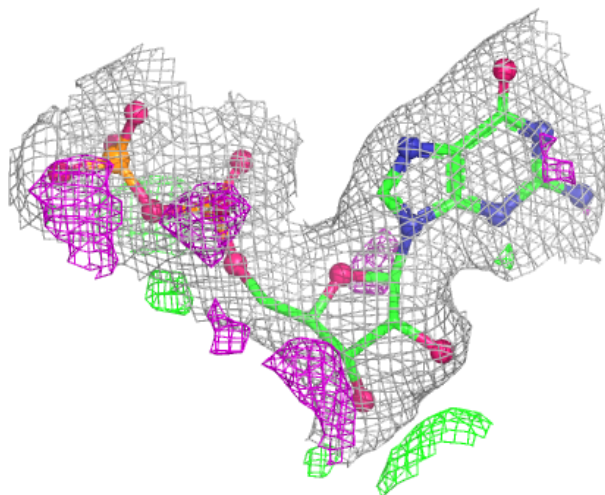
Electron density around R42 D 503:

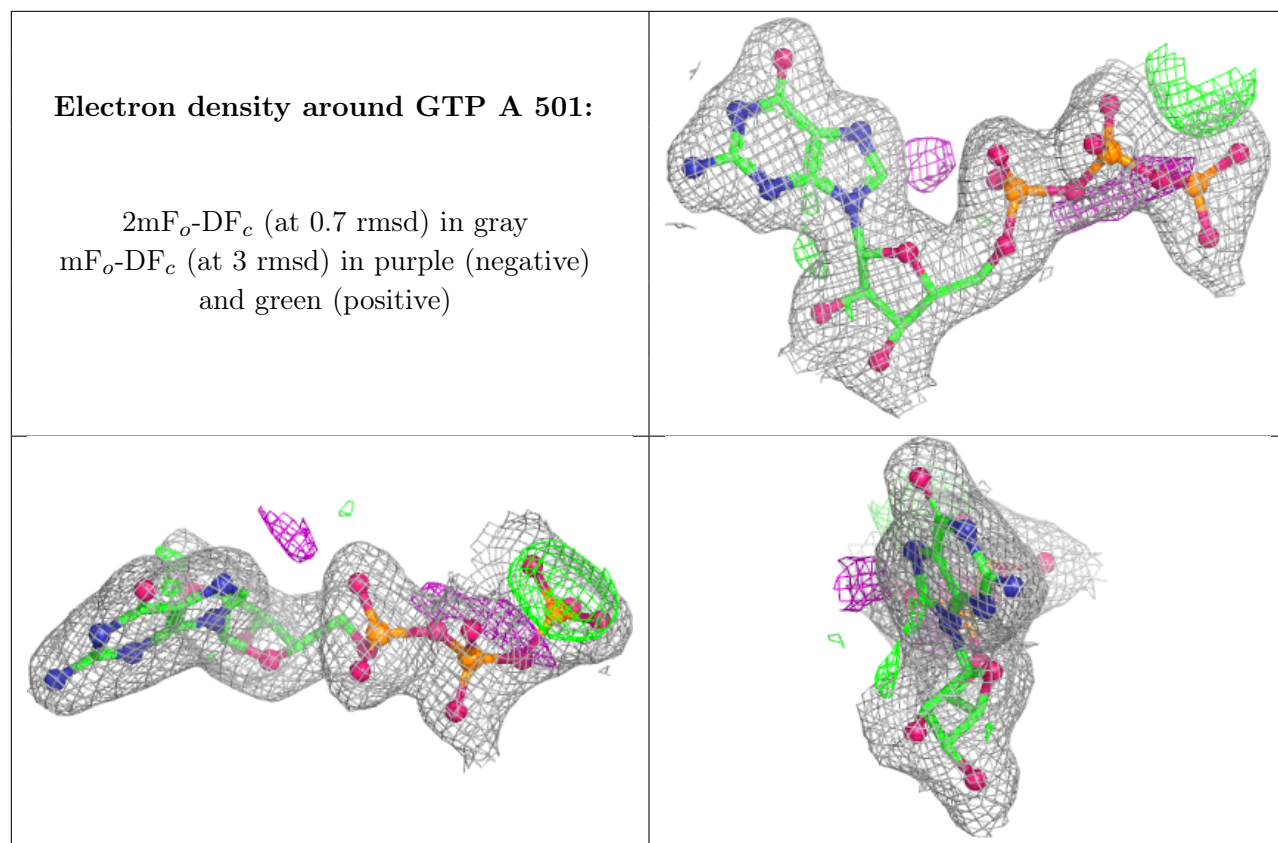
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP D 501:

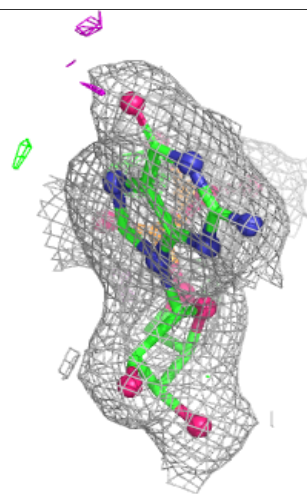
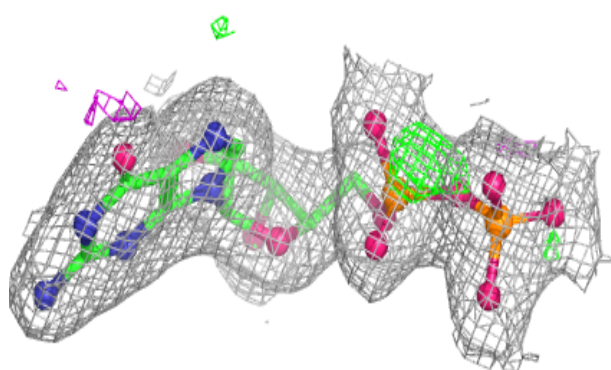
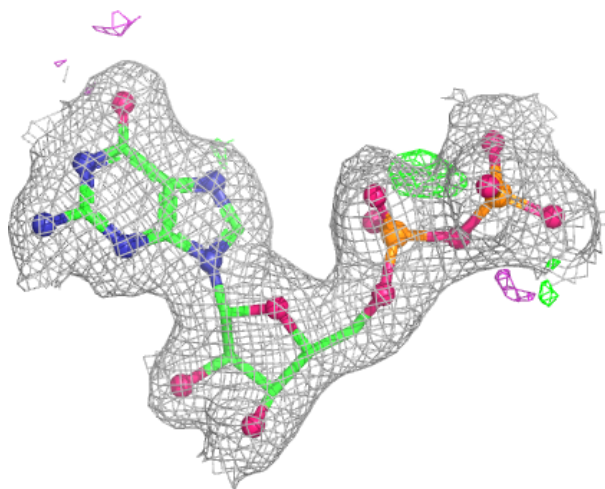
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

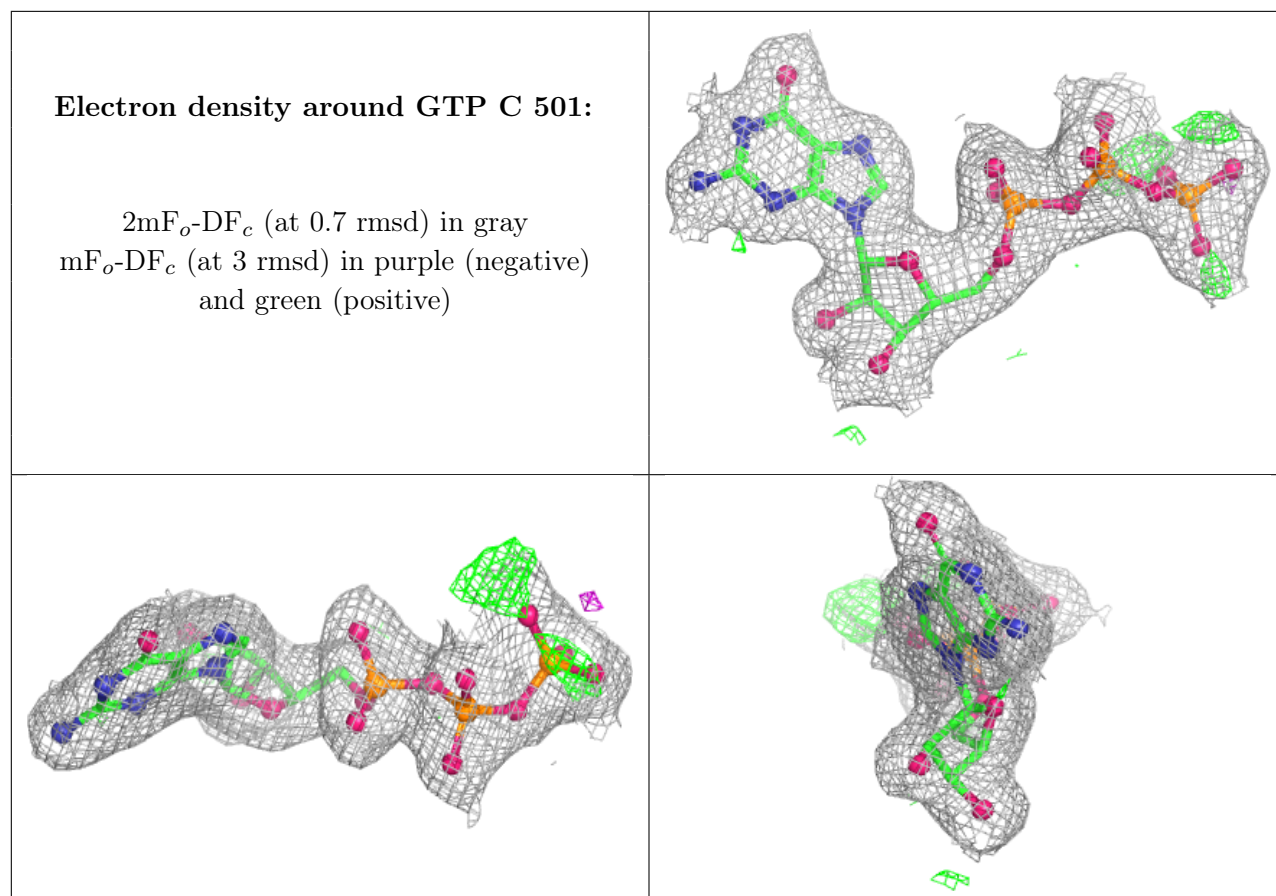




Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.