



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:28 AM UTC

PDB ID : 8BDG / pdb_00008bdg
Title : Tubulin-taxane-2b complex
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Deposited on : 2022-10-19
Resolution : 2.35 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

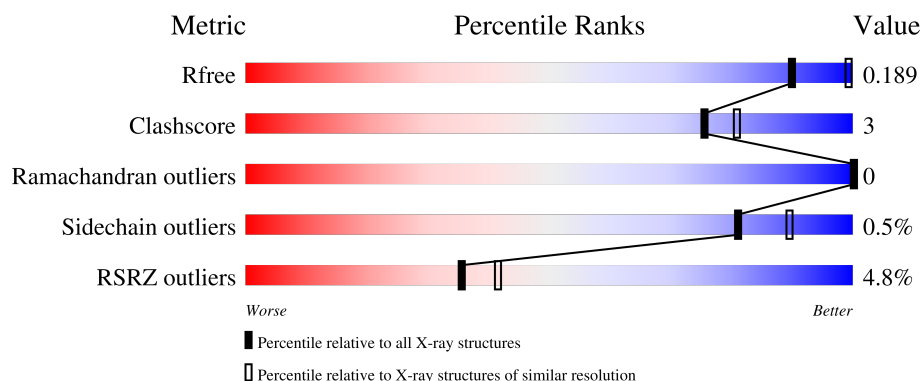
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	3% 89% 9% .
1	C	451	3% 91% 6% .
2	B	445	3% 86% 10% .
2	D	445	4% 86% 9% .

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Mol	Chain	Length	Quality of chain
3	E	143	
4	F	384	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17628 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	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
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
3	E	120	Total	C	N	O	S	0	0	0
			994	614	180	195	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

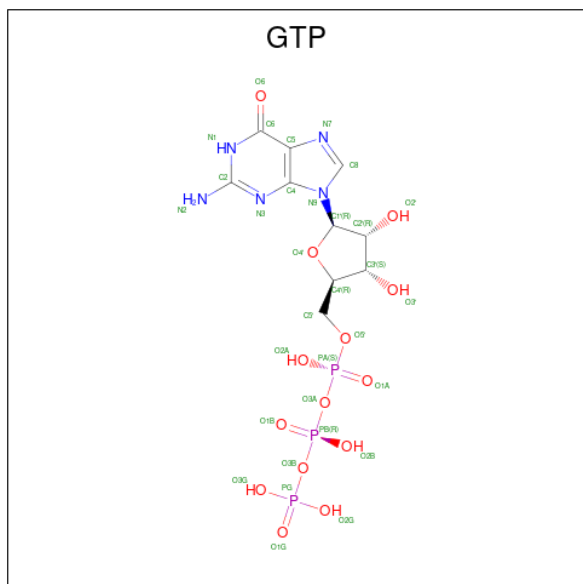
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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: $C_{10}H_{16}N_5O_{14}P_3$).



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

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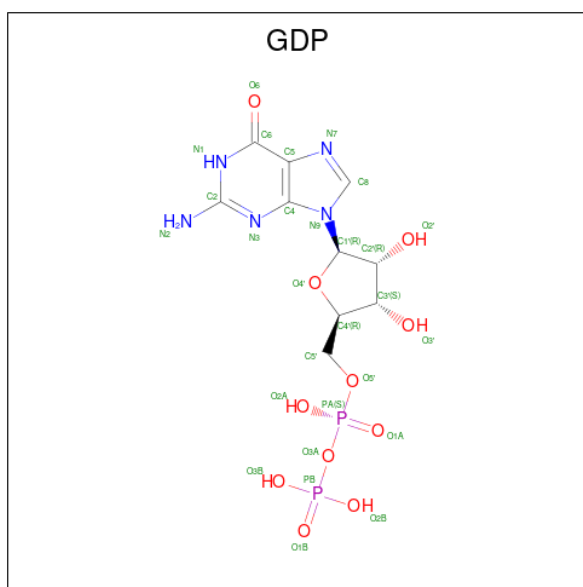
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

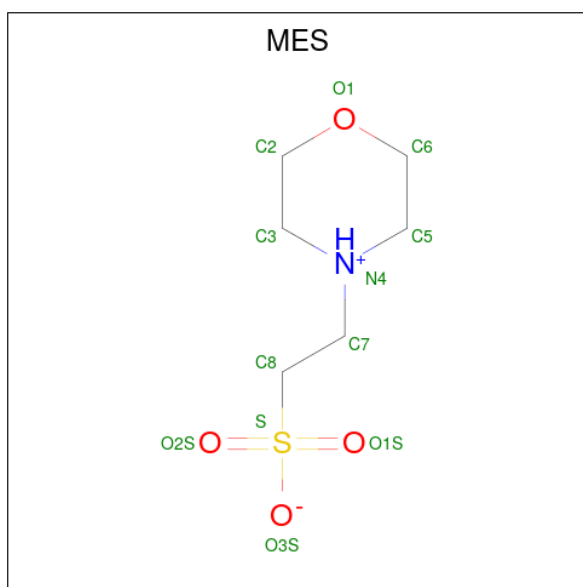
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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



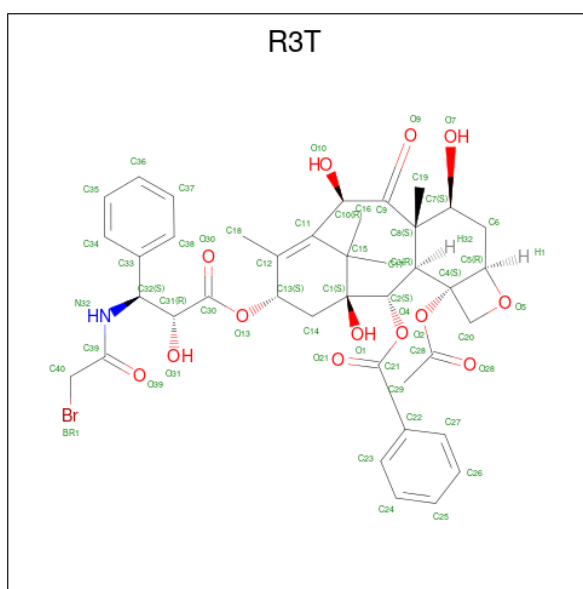
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- 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-(2-bromanylethanoylamino)-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: R3T) (formula: C₄₀H₄₆BrNO₁₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	Br	C	N	O	0	0
			55	1	40	1	13		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	Br	C	N	O	0	0
			55	1	40	1	13		

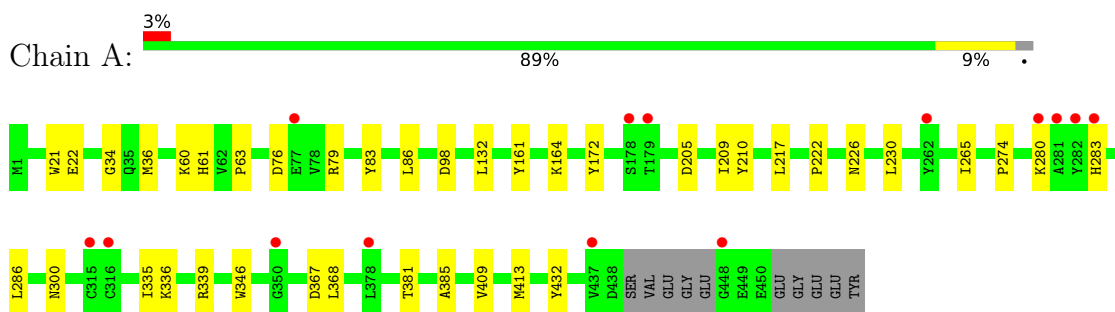
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	29	Total	O	0	0
			29	29		
11	B	35	Total	O	0	0
			35	35		
11	C	89	Total	O	0	0
			89	89		
11	D	8	Total	O	0	0
			8	8		
11	E	4	Total	O	0	0
			4	4		
11	F	1	Total	O	0	0
			1	1		

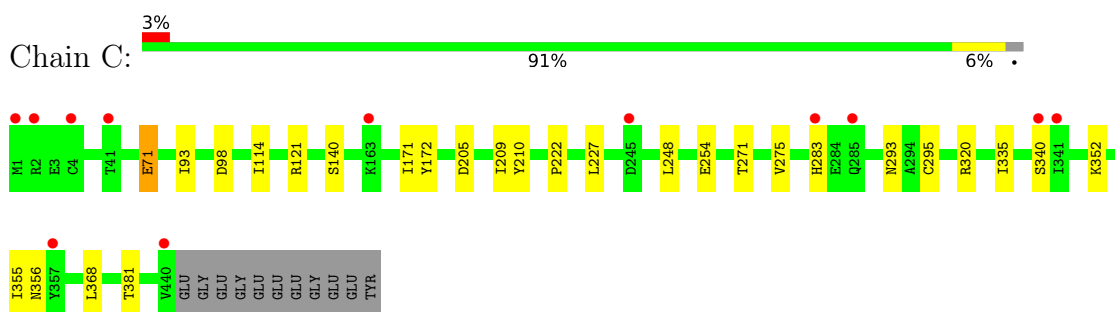
3 Residue-property plots [i](#)

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.

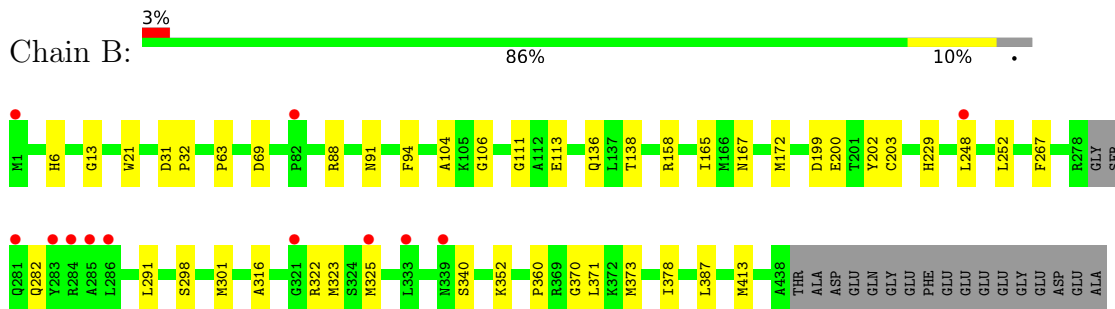
- Molecule 1: Tubulin alpha-1B chain



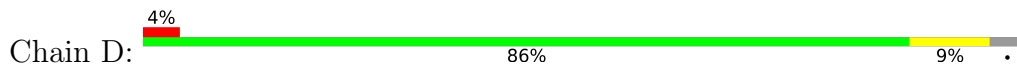
- Molecule 1: Tubulin alpha-1B chain

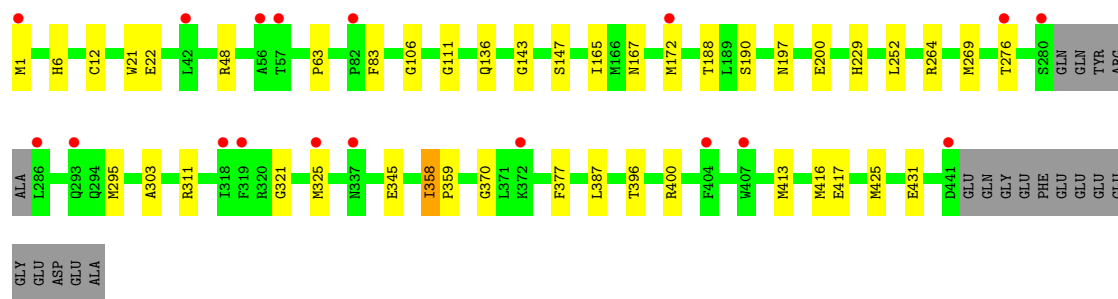


- Molecule 2: Tubulin beta-2B chain

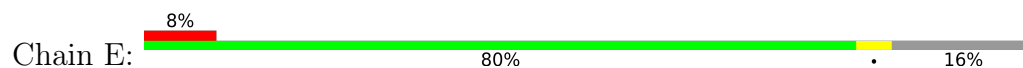


- Molecule 2: Tubulin beta-2B chain

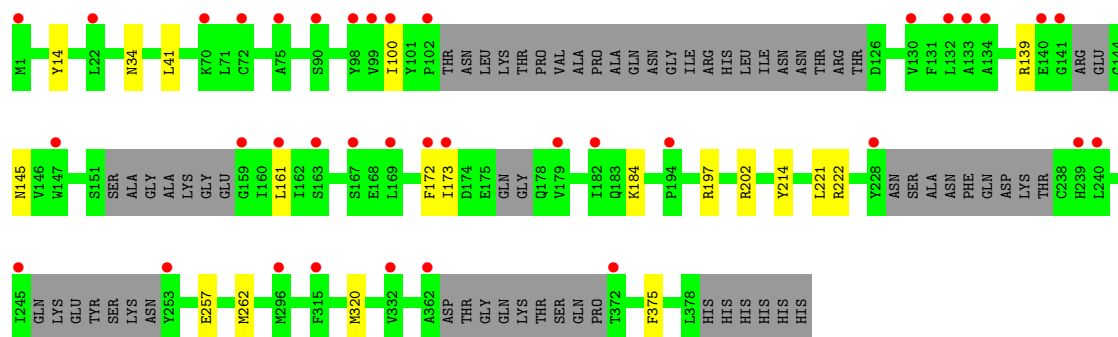
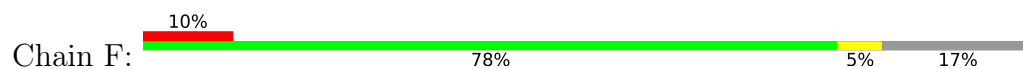




• Molecule 3: Stathmin-4



• 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	105.25Å 158.64Å 179.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.35 49.37 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.37-2.35) 100.0 (49.37-2.35)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.183 , 0.214 (Not available) , 0.189	Depositor DCC
R_{free} test set	6173 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	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	0.96	EDS
Total number of atoms	17628	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: MES, MG, GTP, CA, R3T, GDP

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	0.12	0/3523	0.30	0/4780
1	C	0.14	0/3528	0.34	0/4790
2	B	0.12	0/3433	0.31	0/4648
2	D	0.11	0/3427	0.29	0/4640
3	E	0.12	0/1002	0.25	0/1329
4	F	0.10	0/2670	0.28	0/3603
All	All	0.12	0/17583	0.30	0/23790

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3446	0	3348	23	0
1	C	3447	0	3360	13	1
2	B	3359	0	3241	26	1
2	D	3354	0	3234	28	0
3	E	994	0	1013	3	0
4	F	2614	0	2597	11	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
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	55	0	0	2	0
10	D	55	0	0	3	0
11	A	29	0	0	1	0
11	B	35	0	0	0	0
11	C	89	0	0	0	0
11	D	8	0	0	0	0
11	E	4	0	0	0	0
11	F	1	0	0	0	0
All	All	17628	0	16853	102	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 3.

All (102) 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:167:ASN:HD22	2:B:200:GLU:HB2	1.53	0.73
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.77	0.66
4:F:139:ARG:HB2	4:F:145:ASN:HD21	1.63	0.64
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.81	0.63
2:B:370:GLY:N	10:B:504:R3T:O31	2.31	0.62
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.81	0.62
2:D:229:HIS:NE2	10:D:503:R3T:O39	2.28	0.61
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.66	0.61
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.85	0.59
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.21	0.58
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.86	0.58
4:F:145:ASN:HA	4:F:184:LYS:HE2	1.87	0.57
2:B:158:ARG:CZ	9:B:503:MES:H21	2.34	0.57
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.87	0.56
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.37	0.56
2:D:370:GLY:N	10:D:503:R3T:O31	2.22	0.56
2:B:199:ASP:OD2	9:B:503:MES:H52	2.07	0.55
1:A:280:LYS:HB2	1:A:283:HIS:NE2	2.21	0.54
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.89	0.54
2:D:321:GLY:HA2	2:D:359:PRO:HG3	1.89	0.54
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.92	0.51
2:D:311[B]:ARG:NH2	2:D:345:GLU:OE2	2.41	0.51
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.93	0.51
2:B:136:GLN:HA	2:B:167:ASN:O	2.12	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.49
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.49
2:B:298:SER:HA	2:B:301:MET:HE2	1.94	0.49
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.94	0.49
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.47	0.49
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.94	0.49
4:F:202:ARG:HB2	4:F:222:ARG:HH21	1.78	0.49
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.13	0.49
2:B:229:HIS:HB3	10:B:504:R3T:C25	2.42	0.49
2:D:147:SER:HG	2:D:190:SER:HG	1.60	0.48
4:F:100:ILE:HD11	4:F:173:ILE:HD13	1.95	0.48
2:D:197:ASN:HD21	3:E:126:LYS:HE2	1.79	0.48
2:D:136:GLN:HA	2:D:167:ASN:O	2.14	0.48
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.48
2:D:396:THR:O	2:D:400:ARG:HB2	2.14	0.48
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.95	0.47
2:B:167:ASN:HD21	2:B:202:TYR:HE2	1.62	0.47
2:B:291:LEU:HD12	2:B:373:MET:HE2	1.96	0.47
2:B:13:GLY:HA2	2:B:138:THR:HG22	1.95	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.47
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.14	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.47
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.50	0.46
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.97	0.46
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.96	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.51	0.46
2:D:106:GLY:O	2:D:111:GLY:HA3	2.15	0.46
2:B:340:SER:HB3	4:F:34:ASN:HD21	1.81	0.46
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:HA	1:A:413:MET:O	2.16	0.46
2:D:229:HIS:HB3	10:D:503:R3T:C25	2.46	0.46
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.98	0.45
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.50	0.45
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.97	0.45
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.97	0.45
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.51	0.45
4:F:161:LEU:HD12	4:F:172:PHE:CG	2.51	0.45
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.45
2:B:322:ARG:HD3	2:B:322:ARG:HA	1.73	0.45
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.99	0.45
1:A:300:ASN:ND2	11:A:602:HOH:O	2.47	0.45
2:B:360:PRO:HG2	2:B:371:LEU:HB2	1.99	0.45
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.99	0.44
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.58	0.44
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.52	0.44
3:E:101:LEU:O	3:E:105:MET:HG2	2.17	0.44
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.98	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.43
1:C:293:ASN:HA	1:C:335:ILE:HD11	1.99	0.43
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.54	0.43
1:A:132:LEU:O	1:A:164:LYS:NZ	2.51	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HD3	2.01	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.59	0.43
2:D:416:MET:HA	2:D:416:MET:HE2	2.01	0.42
1:A:63:PRO:HD3	1:A:86:LEU:HG	2.01	0.42
1:C:271:THR:HG21	1:C:295:CYS:O	2.19	0.42
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.42
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.55	0.42
1:A:280:LYS:HB2	1:A:283:HIS:CE1	2.54	0.42
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.01	0.42
2:B:88:ARG:HD2	2:B:91:ASN:OD1	2.20	0.41
1:A:346:TRP:CD1	1:A:346:TRP:H	2.37	0.41
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.01	0.41
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.01	0.41
2:D:325:MET:HE2	2:D:325:MET:HB3	1.98	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.56	0.41
2:B:323:MET:HE2	2:B:373:MET:HG2	2.02	0.41
2:D:358:ILE:H	2:D:358:ILE:HG12	1.64	0.41
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:THR:HA	2:D:425:MET:HE1	2.04	0.40
2:D:413:MET:HE3	2:D:417:GLU:CD	2.47	0.40
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.53	0.40
2:D:1:MET:HE1	2:D:48:ARG:HG2	2.03	0.40
4:F:320:MET:HE2	4:F:320:MET:HB3	1.92	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]	2.14	0.06

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	437/451 (97%)	427 (98%)	10 (2%)	0	100	100
1	C	440/451 (98%)	433 (98%)	7 (2%)	0	100	100
2	B	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
2	D	423/445 (95%)	414 (98%)	9 (2%)	0	100	100
3	E	116/143 (81%)	114 (98%)	2 (2%)	0	100	100
4	F	303/384 (79%)	295 (97%)	8 (3%)	0	100	100
All	All	2141/2319 (92%)	2097 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/379 (98%)	369 (100%)	2 (0%)	81	89
1	C	373/379 (98%)	370 (99%)	3 (1%)	73	84
2	B	369/383 (96%)	367 (100%)	2 (0%)	81	89
2	D	369/383 (96%)	367 (100%)	2 (0%)	81	89
3	E	108/127 (85%)	107 (99%)	1 (1%)	70	82
4	F	287/342 (84%)	287 (100%)	0	100	100
All	All	1877/1993 (94%)	1867 (100%)	10 (0%)	81	89

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

Mol	Chain	Res	Type
1	A	336	LYS
1	A	381	THR
2	B	282	GLN
2	B	325	MET
1	C	71	GLU
1	C	340	SER
1	C	381	THR
2	D	276	THR
2	D	358	ILE
3	E	59	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	101	ASN
1	A	300	ASN
2	B	11	GLN
2	B	167	ASN
2	B	192	HIS
2	B	281	GLN

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Mol	Chain	Res	Type
2	B	336	GLN
2	B	339	ASN
2	B	349	ASN
2	B	434	GLN
1	C	15	GLN
1	C	293	ASN
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	59	ASN
2	D	96	GLN
2	D	167	ASN
2	D	197	ASN
3	E	12	ASN
3	E	84	GLN
3	E	108	ASN
4	F	269	GLN
4	F	348	GLN

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 13 ligands modelled in this entry, 6 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	$\# Z > 2$
8	GDP	B	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.68	6 (13%)
5	GTP	C	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.53	9 (18%)
8	GDP	D	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.67	6 (13%)
5	GTP	A	501	6	33,34,34	0.92	1 (3%)	50,54,54	1.56	10 (20%)
10	R3T	D	503	-	60,60,60	0.96	3 (5%)	93,94,94	2.00	27 (29%)
9	MES	B	503	-	12,12,12	2.32	1 (8%)	15,16,16	1.86	3 (20%)
10	R3T	B	504	-	60,60,60	0.97	4 (6%)	93,94,94	1.93	23 (24%)

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	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
8	GDP	D	501	6	-	4/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
10	R3T	D	503	-	-	2/35/121/121	0/6/6/6
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
10	R3T	B	504	-	-	2/35/121/121	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.79	1.66	1.77
10	B	504	R3T	O39-C39	3.15	1.29	1.23
8	D	501	GDP	C5-C4	3.14	1.47	1.38
10	D	503	R3T	O39-C39	3.08	1.29	1.23
8	B	501	GDP	C5-C4	3.06	1.47	1.38
10	D	503	R3T	C4-C3	2.55	1.60	1.54
10	B	504	R3T	O13-C13	-2.53	1.41	1.45
8	D	501	GDP	C6-N1	-2.45	1.34	1.38
8	B	501	GDP	C6-N1	-2.39	1.34	1.38
10	B	504	R3T	C4-C3	2.38	1.60	1.54
5	C	501	GTP	PA-O3A	2.35	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	R3T	C22-C21	-2.21	1.45	1.50
8	B	501	GDP	PA-O3A	2.21	1.61	1.59
5	C	501	GTP	C2-N3	2.14	1.38	1.33
10	B	504	R3T	C22-C21	-2.14	1.45	1.50
5	A	501	GTP	C2-N3	2.09	1.38	1.33
8	D	501	GDP	C5-N7	-2.08	1.34	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	R3T	O4-C28-C29	6.74	122.10	110.67
10	B	504	R3T	O4-C28-C29	6.67	121.97	110.67
8	D	501	GDP	C5-C4-N3	-5.74	119.25	128.39
8	B	501	GDP	C5-C4-N3	-5.71	119.31	128.39
10	B	504	R3T	C31-C32-N32	5.17	121.99	109.27
10	B	504	R3T	C2-O2-C21	5.05	127.02	117.80
9	B	503	MES	C5-N4-C3	4.95	119.51	108.84
10	D	503	R3T	C2-O2-C21	4.90	126.75	117.80
5	A	501	GTP	C5-C4-N3	-4.79	120.76	128.39
8	B	501	GDP	C2-N3-C4	4.77	120.52	112.30
10	D	503	R3T	C31-C32-N32	4.70	120.83	109.27
5	C	501	GTP	C5-C4-N3	-4.70	120.91	128.39
8	D	501	GDP	C2-N3-C4	4.67	120.34	112.30
5	A	501	GTP	C2-N3-C4	4.53	120.10	112.30
5	C	501	GTP	C2-N3-C4	4.42	119.90	112.30
10	B	504	R3T	O10-C10-C9	4.33	116.73	109.51
10	D	503	R3T	O10-C10-C9	4.32	116.72	109.51
10	B	504	R3T	C11-C10-C9	-4.28	109.12	114.05
8	D	501	GDP	N9-C4-N3	4.27	134.49	125.95
10	D	503	R3T	C8-C9-C10	4.25	129.01	122.69
10	D	503	R3T	C20-C4-C5	-4.07	81.18	85.38
8	B	501	GDP	N9-C4-N3	4.06	134.06	125.95
10	B	504	R3T	C17-C15-C16	-4.05	94.79	106.29
10	B	504	R3T	C20-C4-C5	-3.96	81.29	85.38
10	D	503	R3T	C17-C15-C16	-3.90	95.23	106.29
10	D	503	R3T	C11-C10-C9	-3.89	109.57	114.05
10	B	504	R3T	C8-C9-C10	3.86	128.44	122.69
10	D	503	R3T	C4-O4-C28	3.84	128.89	119.17
10	B	504	R3T	O4-C28-O28	-3.65	117.25	123.61
10	B	504	R3T	C4-O4-C28	3.62	128.35	119.17
10	D	503	R3T	O5-C5-C4	3.52	94.43	90.58
8	B	501	GDP	C6-C5-N7	3.51	136.68	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	R3T	O4-C28-O28	-3.47	117.56	123.61
8	D	501	GDP	C6-C5-N7	3.31	136.32	130.29
10	B	504	R3T	O5-C5-C4	3.31	94.20	90.58
10	D	503	R3T	C18-C12-C11	-3.15	121.57	125.32
10	D	503	R3T	C4-C3-C2	3.05	117.58	111.70
10	D	503	R3T	O1-C1-C2	3.05	112.15	105.54
10	D	503	R3T	C3-C8-C9	3.04	121.31	116.30
5	C	501	GTP	N9-C4-N3	2.99	131.92	125.95
5	A	501	GTP	N9-C4-N3	2.84	131.63	125.95
5	C	501	GTP	C2-N1-C6	-2.79	120.06	125.11
5	A	501	GTP	C2-N1-C6	-2.77	120.09	125.11
5	C	501	GTP	N9-C8-N7	-2.74	108.33	113.40
8	B	501	GDP	C4-C5-N7	-2.71	106.38	110.67
10	B	504	R3T	C4-C3-C2	2.68	116.87	111.70
5	A	501	GTP	N9-C8-N7	-2.65	108.48	113.40
10	B	504	R3T	C17-C15-C1	2.61	116.64	111.13
8	D	501	GDP	C4-C5-N7	-2.60	106.55	110.67
10	D	503	R3T	O10-C10-C11	-2.58	107.31	111.48
10	B	504	R3T	O1-C1-C2	2.53	111.03	105.54
5	A	501	GTP	C8-N7-C5	2.53	108.77	104.26
10	D	503	R3T	O13-C13-C12	2.52	115.83	109.85
10	D	503	R3T	O1-C1-C15	-2.50	103.19	108.86
5	C	501	GTP	O6-C6-C5	-2.49	119.95	126.53
5	C	501	GTP	C8-N7-C5	2.49	108.70	104.26
10	D	503	R3T	C17-C15-C1	2.46	116.32	111.13
10	B	504	R3T	O10-C10-C11	-2.44	107.54	111.48
5	C	501	GTP	C5-C6-N1	2.43	119.43	113.25
10	B	504	R3T	C3-C8-C9	2.42	120.30	116.30
5	A	501	GTP	O3G-PG-O3B	2.40	112.67	104.64
10	D	503	R3T	C33-C32-C31	2.38	117.37	111.46
5	A	501	GTP	C5-C6-N1	2.36	119.27	113.25
10	B	504	R3T	C18-C12-C11	-2.36	122.51	125.32
10	D	503	R3T	C10-C11-C12	-2.35	117.10	120.65
5	C	501	GTP	O2A-PA-O3A	2.33	113.57	107.27
5	A	501	GTP	O6-C6-C5	-2.31	120.44	126.53
10	B	504	R3T	O13-C13-C12	2.28	115.27	109.85
10	D	503	R3T	O9-C9-C10	-2.25	114.81	117.37
9	B	503	MES	C7-N4-C5	2.23	117.17	111.24
10	D	503	R3T	O5-C20-C4	2.22	94.37	91.94
10	D	503	R3T	C16-C15-C11	2.22	121.63	112.78
10	B	504	R3T	C16-C15-C11	2.21	121.59	112.78
9	B	503	MES	C6-C5-N4	-2.18	106.81	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	R3T	O13-C30-O30	-2.17	120.04	123.95
8	B	501	GDP	O6-C6-C5	-2.16	120.84	126.53
10	D	503	R3T	O13-C30-C31	2.10	114.47	111.13
10	B	504	R3T	O1-C1-C15	-2.10	104.09	108.86
10	D	503	R3T	C4-C3-C8	2.09	113.76	110.78
10	B	504	R3T	C33-C32-C31	2.07	116.61	111.46
10	B	504	R3T	O5-C20-C4	2.07	94.20	91.94
5	A	501	GTP	O2B-PB-O3A	2.03	112.76	107.27
10	B	504	R3T	O9-C9-C10	-2.01	115.07	117.37
8	D	501	GDP	O6-C6-C5	-2.01	121.23	126.53

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
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
5	C	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	PA-O3A-PB-O3B
10	B	504	R3T	C31-C32-N32-C39
10	D	503	R3T	C31-C32-N32-C39
9	B	503	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3A-PA-O2A
10	B	504	R3T	O31-C31-C32-N32
5	C	501	GTP	C4'-C5'-O5'-PA
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G

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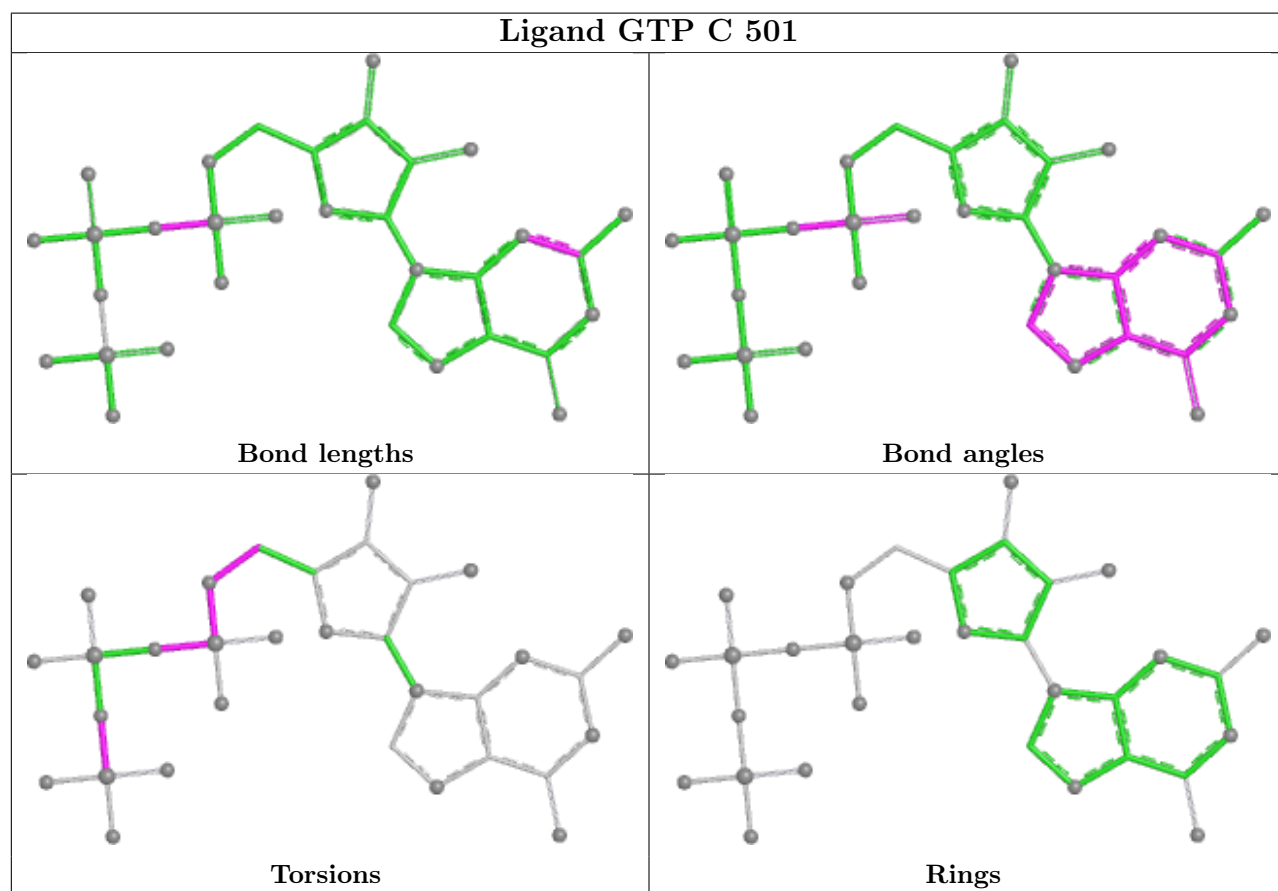
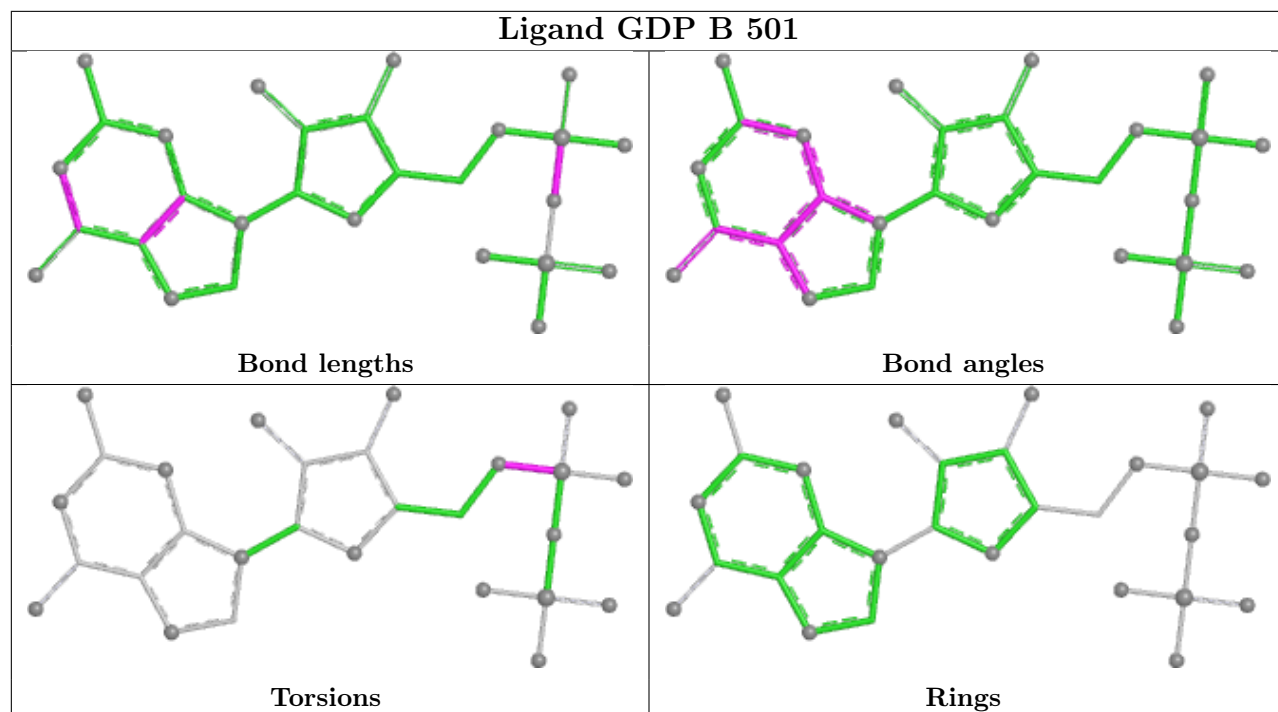
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
10	D	503	R3T	C1-C2-O2-C21
5	A	501	GTP	C4'-C5'-O5'-PA

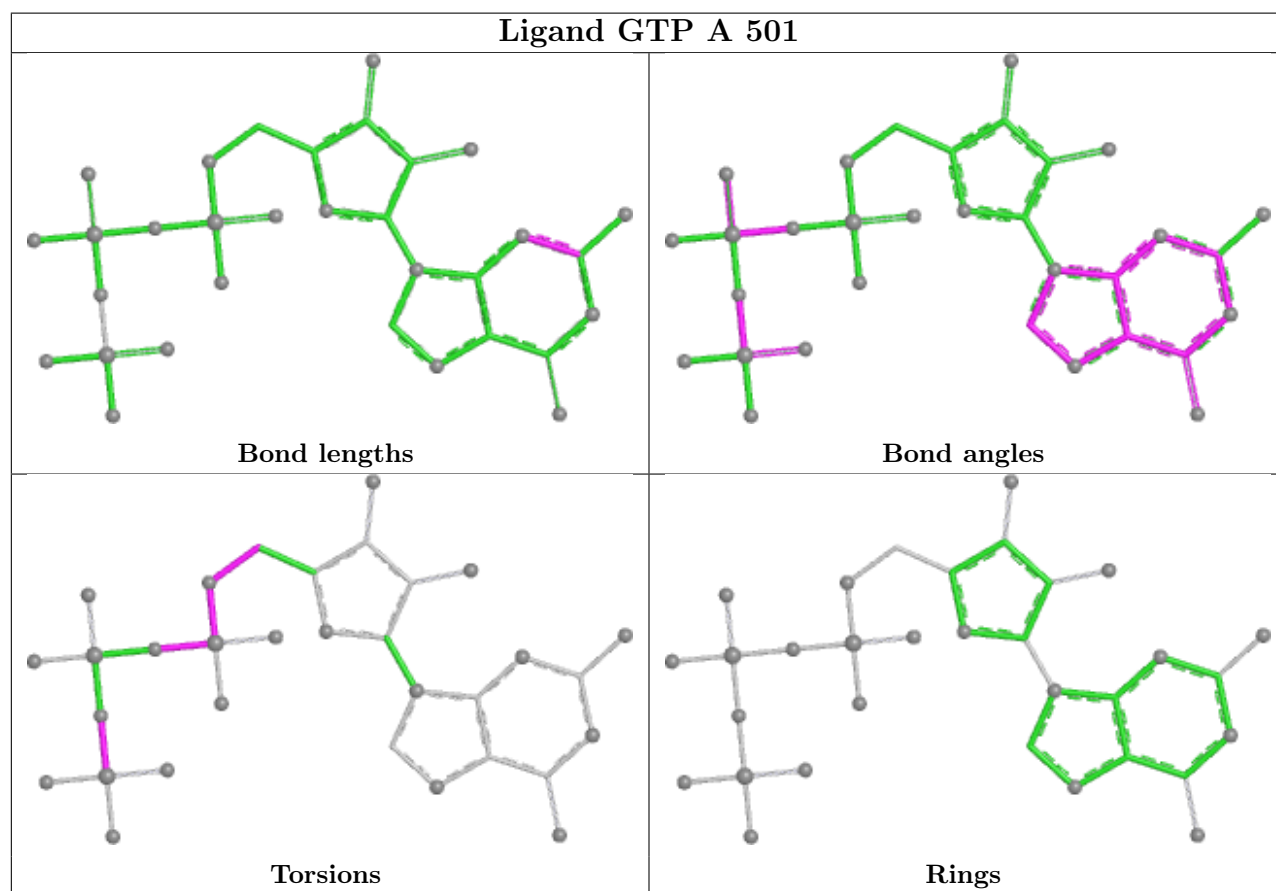
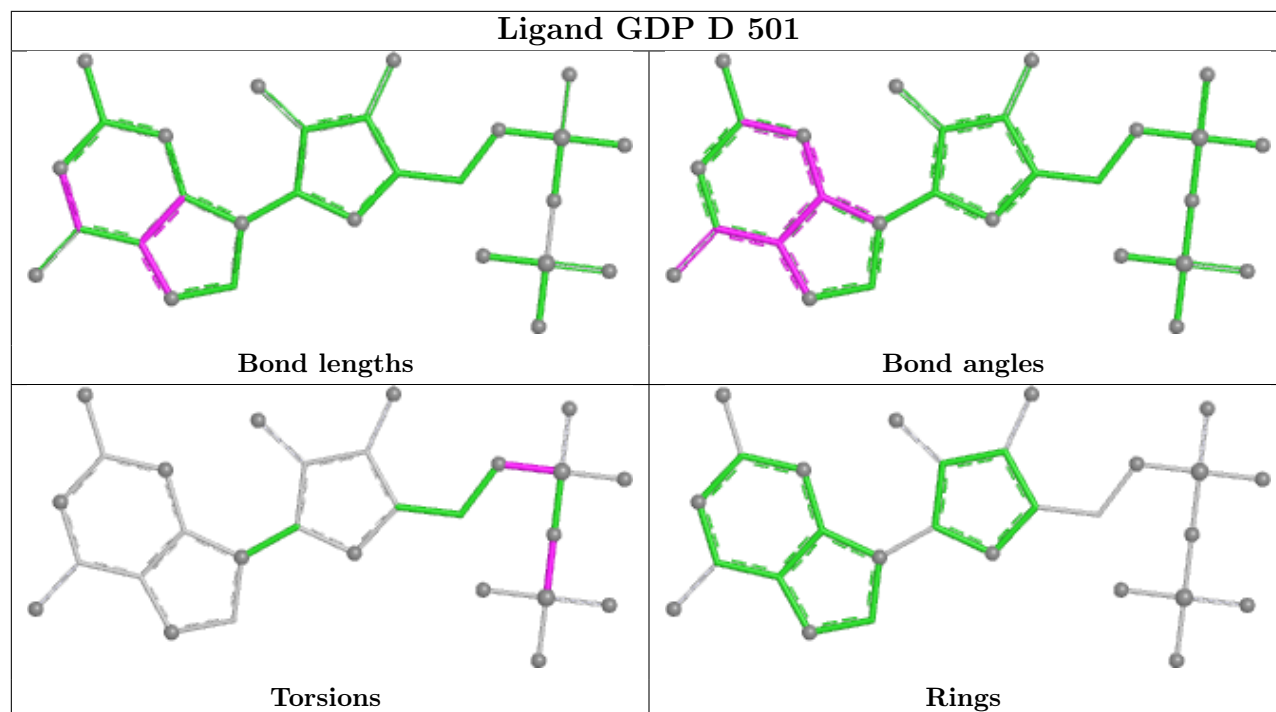
There are no ring outliers.

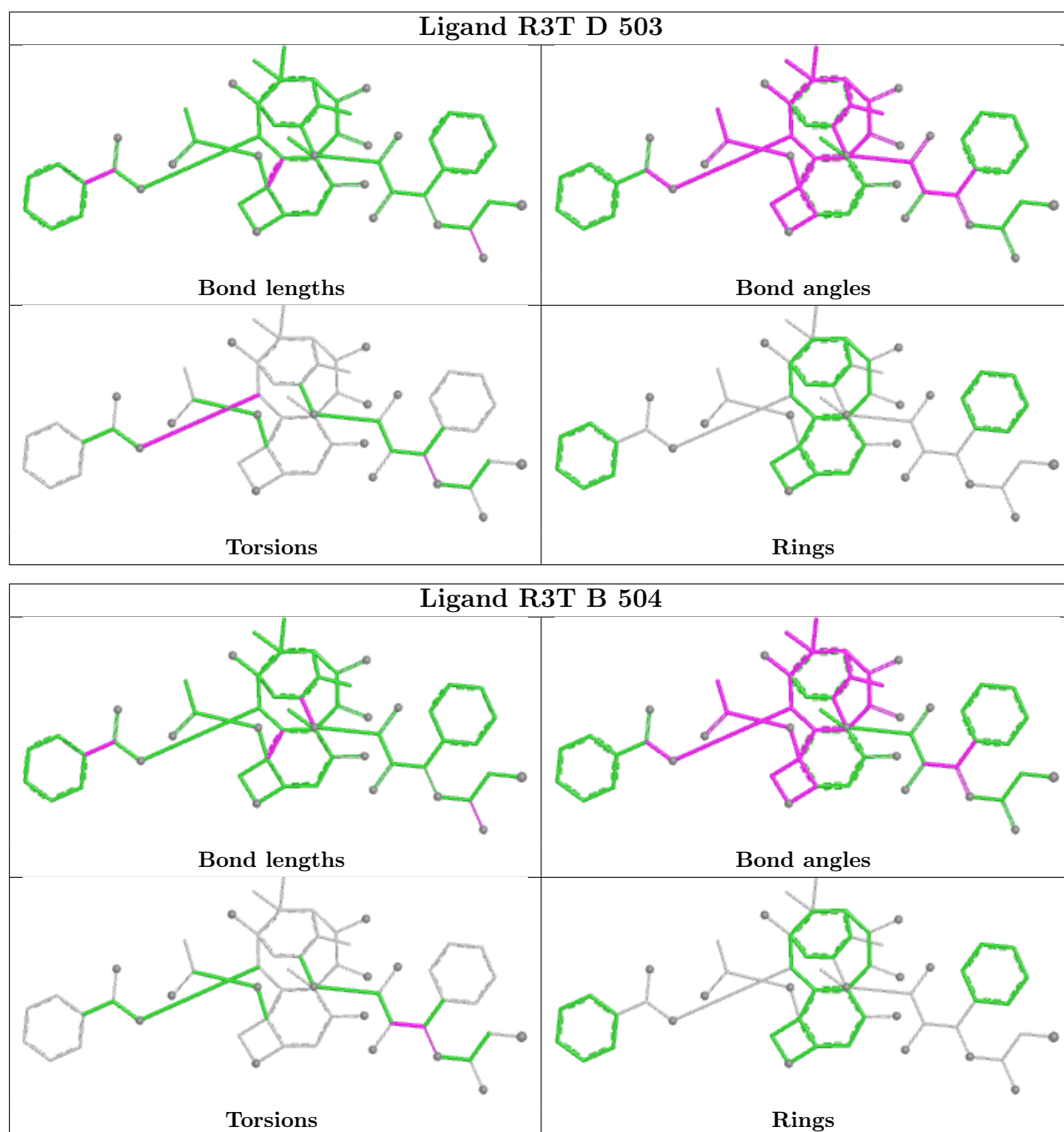
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
5	A	501	GTP	1	0
10	D	503	R3T	3	0
9	B	503	MES	2	0
10	B	504	R3T	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%)	0.18	14 (3%)	50	57	47, 67, 101, 154	0
1	C	440/451 (97%)	-0.09	12 (2%)	56	63	29, 54, 83, 129	2 (0%)
2	B	426/445 (95%)	0.17	12 (2%)	55	61	41, 65, 109, 139	0
2	D	426/445 (95%)	0.41	18 (4%)	40	46	33, 77, 114, 152	1 (0%)
3	E	120/143 (83%)	0.58	11 (9%)	14	17	53, 81, 120, 143	0
4	F	319/384 (83%)	0.78	37 (11%)	9	11	62, 95, 162, 198	0
All	All	2172/2319 (93%)	0.28	104 (4%)	35	41	29, 70, 123, 198	3 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	5.6
4	F	245	ILE	5.1
1	C	440	VAL	4.6
1	A	179	THR	4.3
4	F	161	LEU	4.3
2	B	325	MET	4.1
1	C	340	SER	4.1
2	D	280	SER	4.1
2	B	1	MET	3.8
3	E	15	THR	3.7
2	D	286	LEU	3.6
4	F	240	LEU	3.6
4	F	141	GLY	3.6
1	A	283	HIS	3.4
1	C	41	THR	3.4
4	F	90	SER	3.4
2	D	407	TRP	3.3
2	D	57	THR	3.3
2	B	333	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	296	MET	3.2
2	D	82	PRO	3.0
3	E	27	PRO	3.0
1	A	448	GLY	3.0
3	E	8	VAL	3.0
1	C	357	TYR	3.0
1	A	262	TYR	2.9
3	E	22	VAL	2.9
1	A	316	CYS	2.9
1	C	1	MET	2.9
3	E	6	MET	2.8
2	D	441	ASP	2.8
4	F	133	ALA	2.8
4	F	362	ALA	2.8
3	E	24	LEU	2.8
4	F	253	TYR	2.8
4	F	134	ALA	2.8
1	C	283	HIS	2.7
4	F	159	GLY	2.7
2	B	248	LEU	2.7
1	A	282	TYR	2.7
2	B	283	TYR	2.7
4	F	172	PHE	2.7
4	F	315	PHE	2.7
4	F	130	VAL	2.7
2	D	325	MET	2.6
3	E	139	LEU	2.6
2	D	56	ALA	2.6
1	A	77	GLU	2.6
4	F	179	VAL	2.6
1	C	341	ILE	2.6
1	A	281	ALA	2.5
2	D	404	PHE	2.5
1	C	4	CYS	2.5
4	F	372	THR	2.5
2	D	318	ILE	2.4
4	F	169	LEU	2.4
2	B	285	ALA	2.4
1	A	178	SER	2.4
2	D	319	PHE	2.4
1	C	163	LYS	2.4
2	B	339	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	102	PRO	2.4
3	E	23	ILE	2.4
2	D	42	LEU	2.4
2	D	172	MET	2.4
4	F	1	MET	2.4
3	E	44	ASP	2.3
4	F	100	ILE	2.3
4	F	173	ILE	2.3
2	D	337	ASN	2.3
2	D	372	LYS	2.3
2	B	284	ARG	2.3
3	E	7	GLU	2.3
4	F	99	VAL	2.3
1	A	280	LYS	2.3
1	A	350	GLY	2.3
4	F	75	ALA	2.3
1	C	285	GLN	2.3
2	D	293	GLN	2.3
2	D	276	THR	2.2
4	F	98	TYR	2.2
4	F	167	SER	2.2
4	F	132	LEU	2.2
4	F	194	PRO	2.2
4	F	228	TYR	2.2
1	A	437	VAL	2.2
1	C	2	ARG	2.2
2	B	286	LEU	2.2
4	F	163	SER	2.2
1	C	245	ASP	2.1
4	F	239	HIS	2.1
2	B	321	GLY	2.1
1	A	315	CYS	2.1
1	A	378	LEU	2.1
4	F	140	GLU	2.1
4	F	72	CYS	2.1
4	F	70	LYS	2.1
2	B	82	PRO	2.1
4	F	332	VAL	2.1
2	B	281	GLN	2.1
4	F	22	LEU	2.0
4	F	147	TRP	2.0
3	E	141	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	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](#)

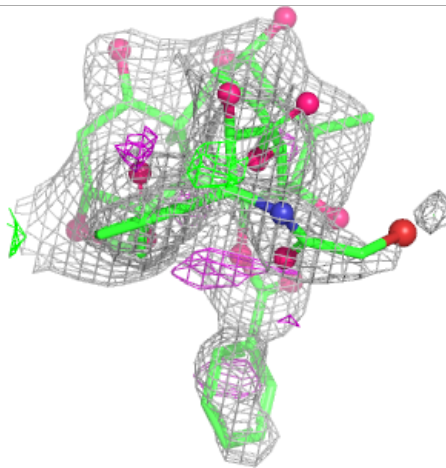
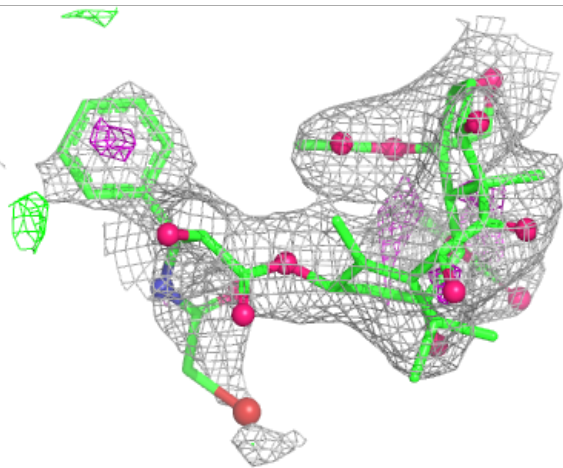
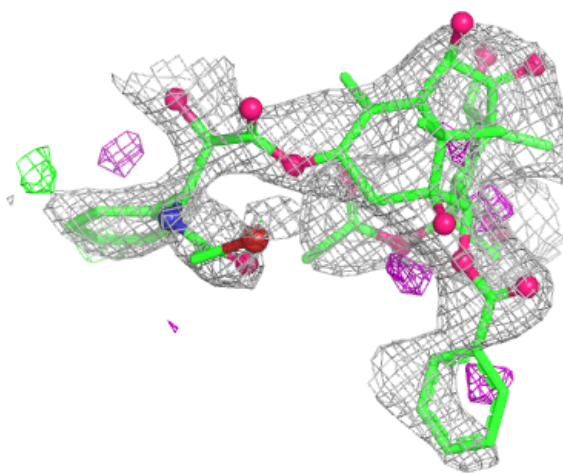
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.71	0.16	93,93,93,93	0
6	MG	F	401	1/1	0.81	0.11	86,86,86,86	0
10	R3T	B	504	55/55	0.83	0.15	102,134,238,328	0
10	R3T	D	503	55/55	0.86	0.15	113,136,250,374	0
8	GDP	D	501	28/28	0.92	0.09	57,67,88,103	0
7	CA	A	503	1/1	0.93	0.10	102,102,102,102	0
9	MES	B	503	12/12	0.94	0.10	61,67,81,81	0
6	MG	B	502	1/1	0.96	0.11	41,41,41,41	0
5	GTP	A	501	32/32	0.97	0.07	40,51,59,66	0
5	GTP	C	501	32/32	0.98	0.06	37,44,54,58	0
8	GDP	B	501	28/28	0.98	0.06	41,49,56,60	0
6	MG	A	502	1/1	0.99	0.02	44,44,44,44	0
6	MG	C	502	1/1	1.00	0.02	42,42,42,42	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.

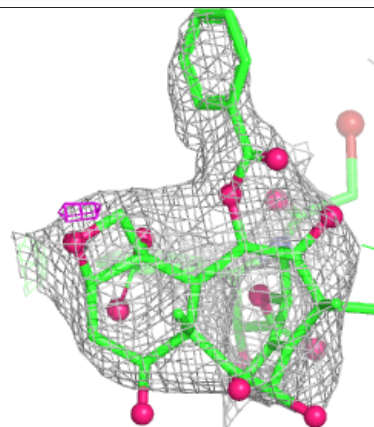
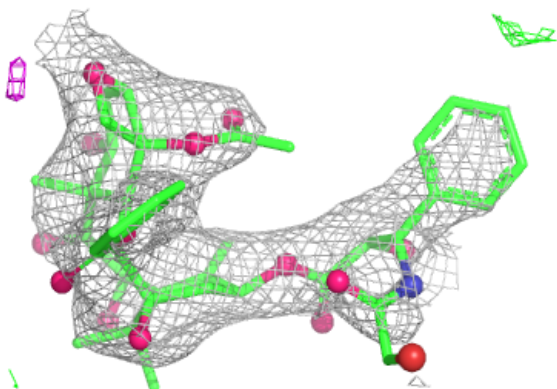
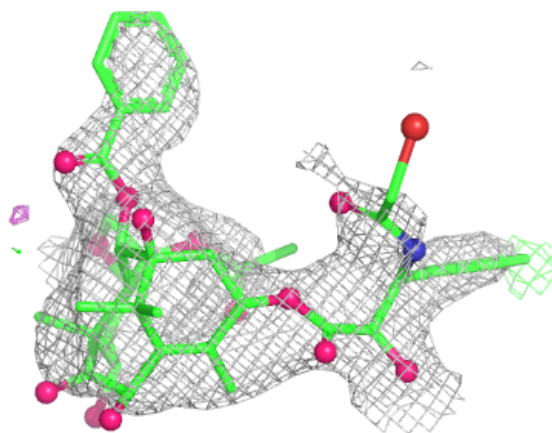
Electron density around R3T B 504:

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



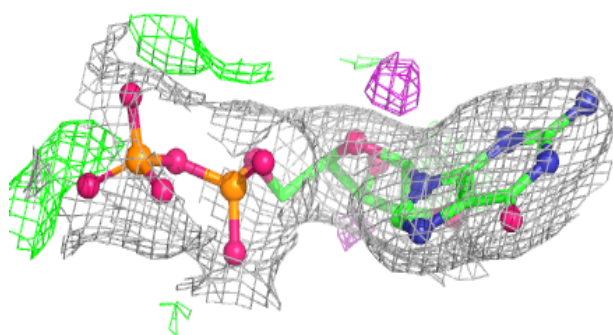
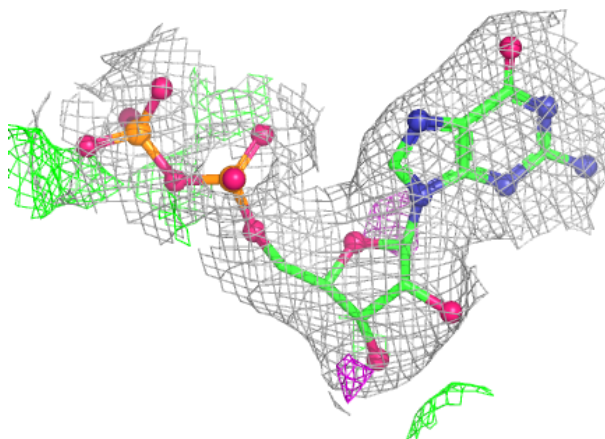
Electron density around R3T D 503:

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



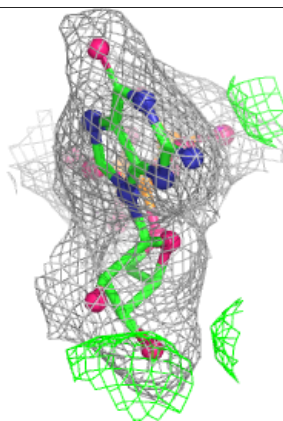
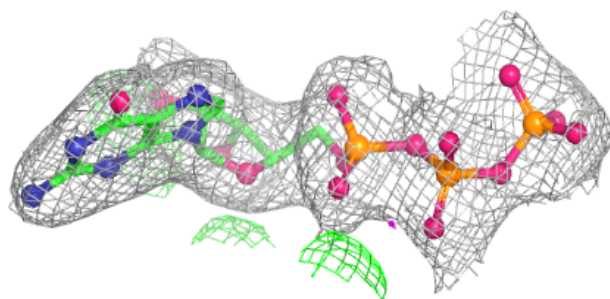
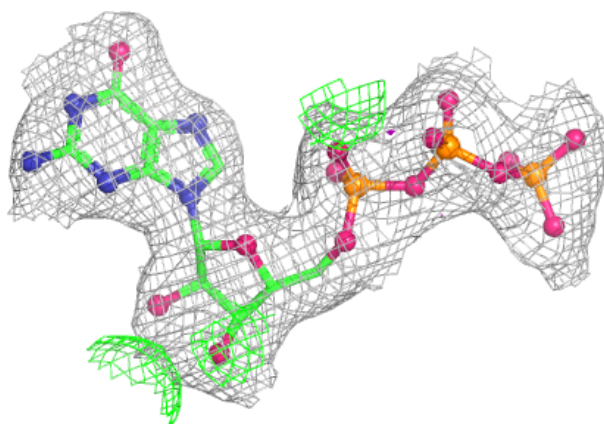
Electron density around GDP D 501:

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

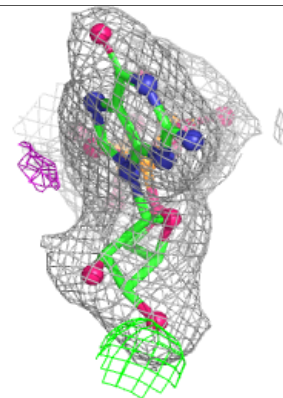
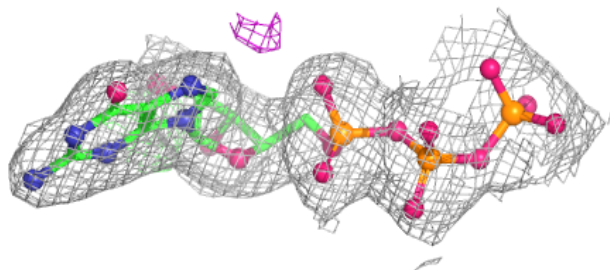
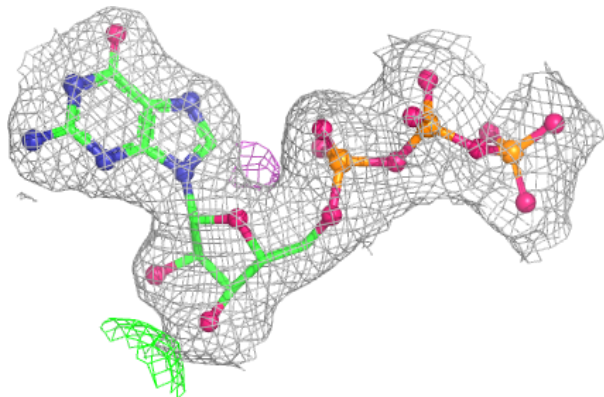


Electron density around GTP A 501:

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

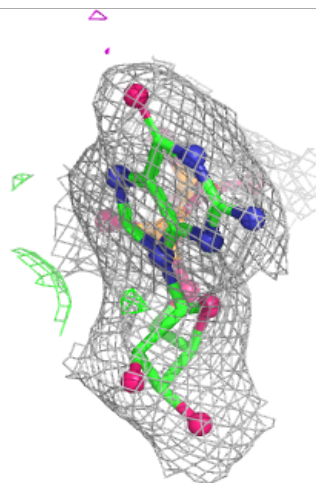
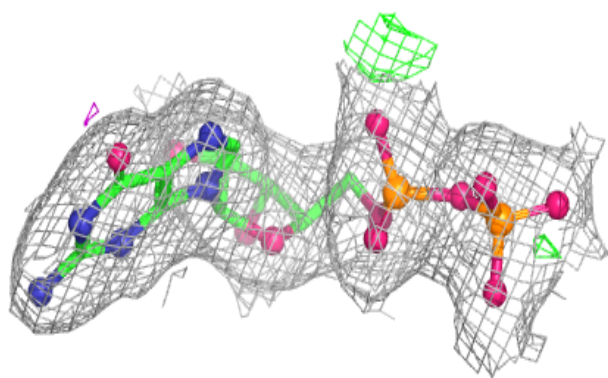
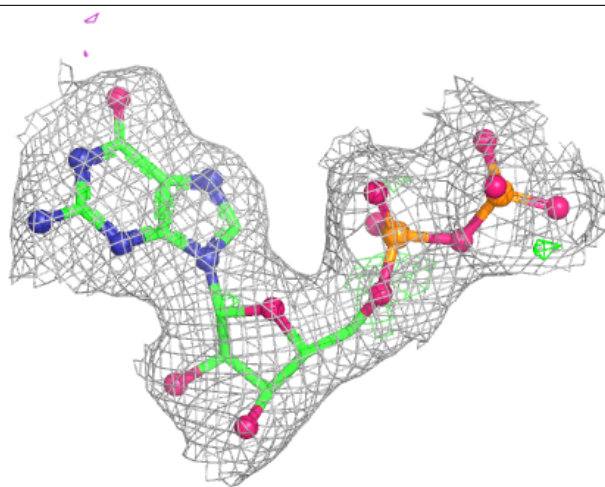
**Electron density around GTP C 501:**

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



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.