



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:26 AM UTC

PDB ID : 5LXS / pdb_00005lxs
Title : Tubulin-KS-1-199-32 complex
Authors : Prota, A.E.; Steinmetz, M.O.
Deposited on : 2016-09-22
Resolution : 2.20 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

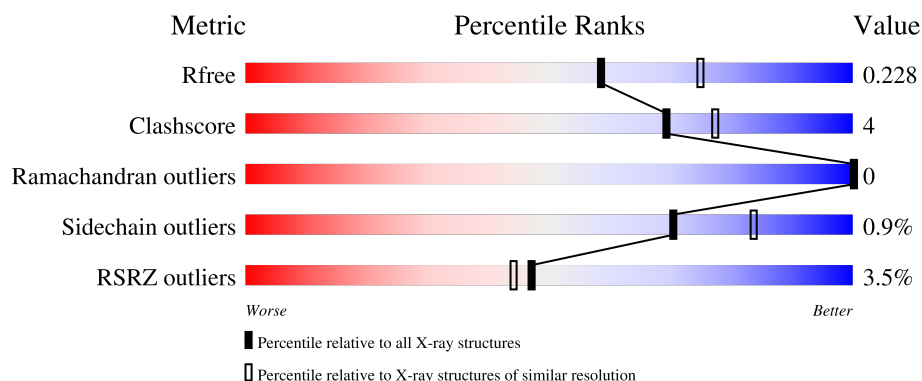
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	2% 89% 8% .
1	C	451	2% 89% 8% .
2	B	445	4% 88% 8% .
2	D	445	4% 87% 10% .
3	E	143	6% 81% 5% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	4% 80% 10% 10%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18850 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	434	Total	C	N	O	S	0	11	0
			3436	2184	580	647	25			
1	C	440	Total	C	N	O	S	0	16	0
			3507	2224	587	671	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	9	0
			3403	2139	577	659	28			
2	D	431	Total	C	N	O	S	0	4	0
			3404	2138	580	658	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	4	0
			1034	639	186	204	5			

There are 2 discrepancies between the modelled and reference sequences:

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

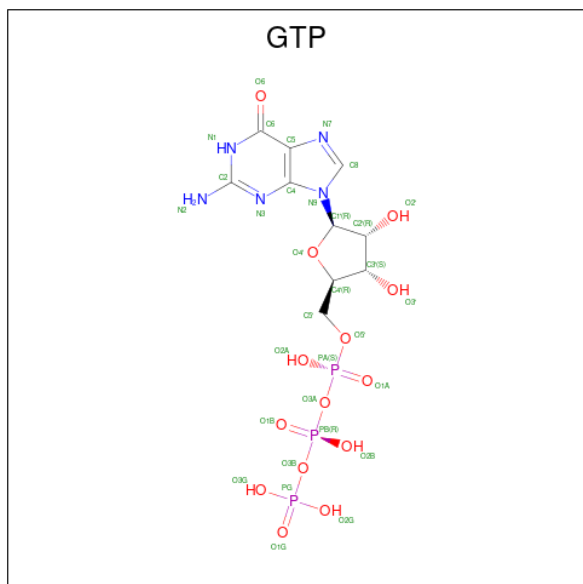
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	345	Total	C	N	O	S	0	7	0
			2869	1847	489	518	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		

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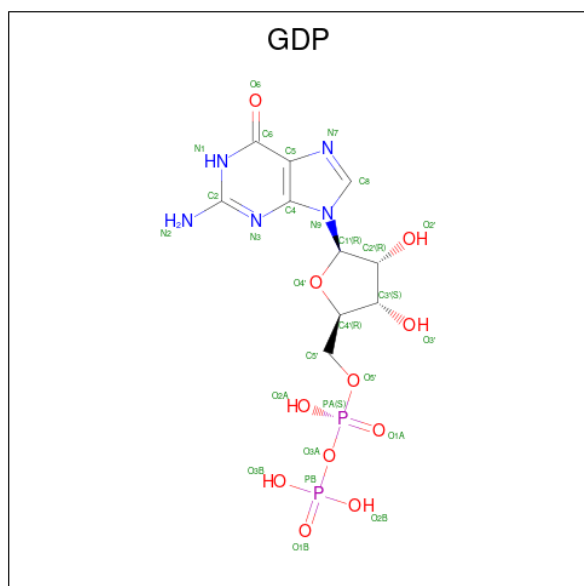
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

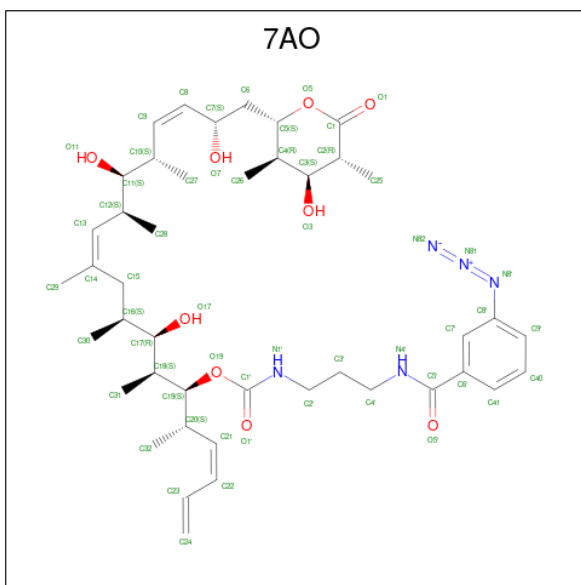
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

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



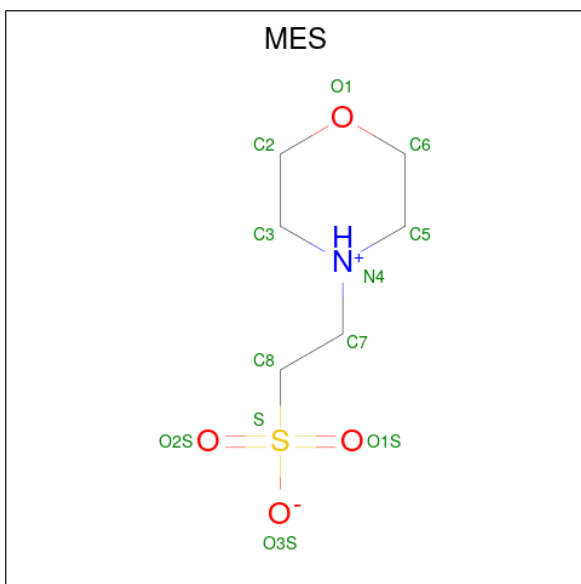
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is [(3 {Z},5 {S},6 {S},7 {S},8 {R},9 {S},11 {Z},13 {S},14 {S},15 {S},16 {Z},18 {S})-19-[(2 {S},3 {R},4 {S},5 {R})-3,5-dimethyl-4-oxidanyl-6-oxidanylidene-oxan-2-yl]-5,7,9,11,13,15-hexamethyl-8,14,18-tris(oxidanyl)nonadeca-1,3,11,16-tetraen-6-yl] {N}-[3-[(3-azidophenyl)carbonylamino]propyl]carbamate (CCD ID: 7AO) (formula: C₄₃H₆₅N₅O₉).



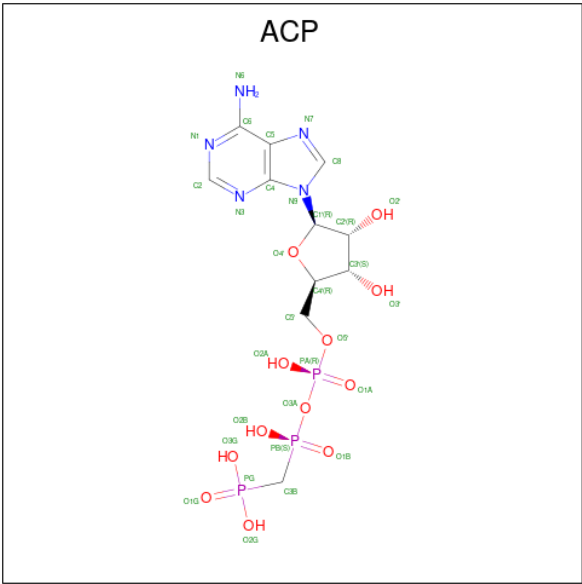
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			57	43	5	9		
9	D	1	Total	C	N	O	0	0
			57	43	5	9		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

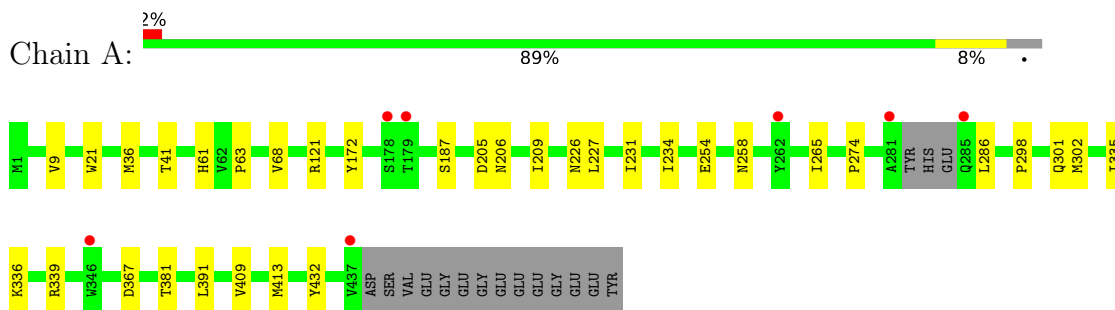
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	181	Total	O	0	0
			181	181		
12	B	154	Total	O	0	0
			154	154		
12	C	256	Total	O	0	0
			256	256		
12	D	161	Total	O	0	0
			161	161		
12	E	61	Total	O	0	0
			61	61		
12	F	98	Total	O	0	0
			98	98		

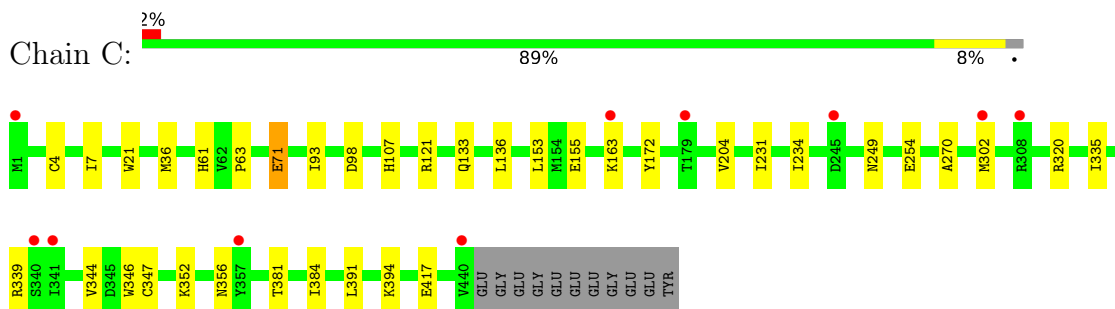
3 Residue-property plots [i](#)

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.

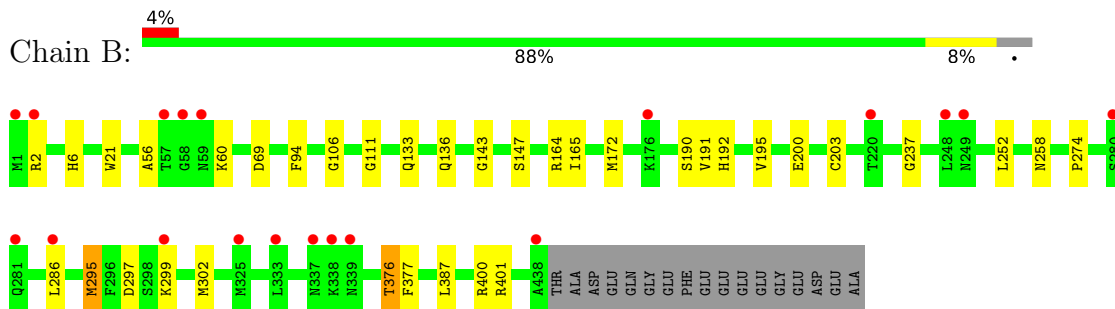
- Molecule 1: Tubulin alpha-1B chain



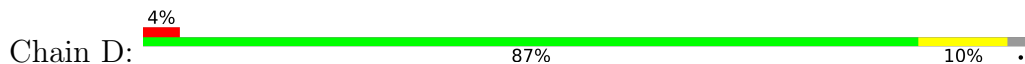
- Molecule 1: Tubulin alpha-1B chain

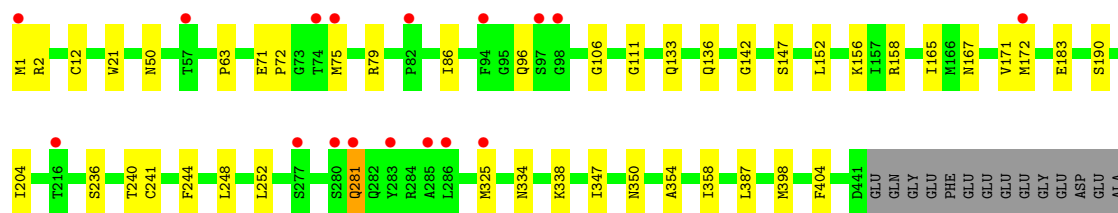


- Molecule 2: Tubulin beta-2B chain

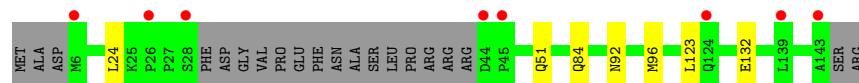
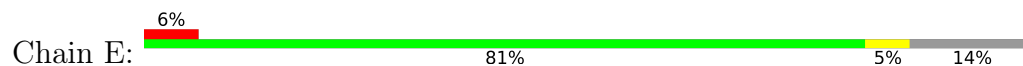


- Molecule 2: Tubulin beta-2B chain

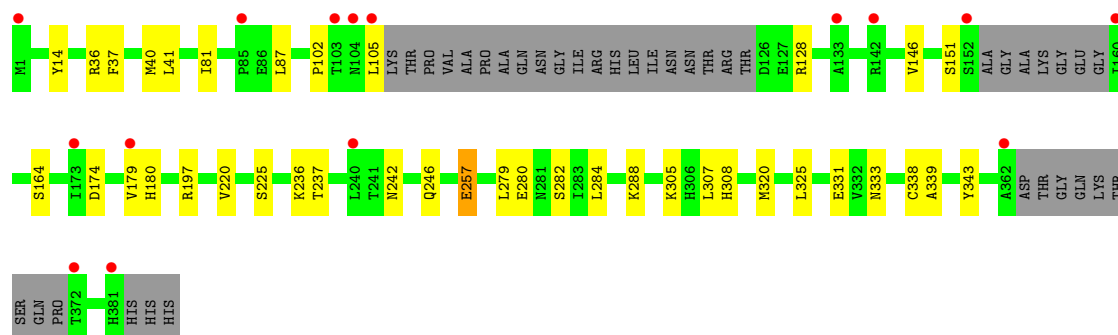
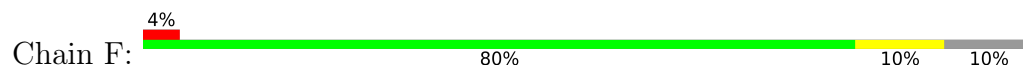




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin 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	104.58Å 157.80Å 179.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.23 – 2.20 72.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.23-2.20) 100.0 (72.23-2.20)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.20Å)	Xtriage
Refinement program	PHENIX (dev_2875: ???)	Depositor
R, R_{free}	0.186 , 0.227 0.189 , 0.228	Depositor DCC
R_{free} test set	7568 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18850	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: CA, MG, GDP, GTP, ACP, MES, 7AO

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	0/3544	0.33	0/4809
1	C	0.15	0/3633	0.37	0/4934
2	B	0.14	0/3505	0.33	0/4747
2	D	0.14	0/3491	0.32	0/4729
3	E	0.12	0/1055	0.27	0/1401
4	F	0.11	0/2955	0.32	0/3992
All	All	0.14	0/18183	0.33	0/24612

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	3436	0	3402	21	0
1	C	3507	0	3447	19	0
2	B	3403	0	3301	23	0
2	D	3404	0	3294	31	0
3	E	1034	0	1056	5	0
4	F	2869	0	2868	23	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	4	0
9	B	57	0	0	0	0
9	D	57	0	0	1	0
10	B	12	0	13	1	0
11	F	31	0	14	2	0
12	A	181	0	0	0	0
12	B	154	0	0	3	0
12	C	256	0	0	2	0
12	D	161	0	0	7	0
12	E	61	0	0	2	0
12	F	98	0	0	3	0
All	All	18850	0	17443	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (124) 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)
11:F:401:ACP:H8	11:F:401:ACP:H5'1	1.67	0.76
2:D:147[B]:SER:HG	2:D:190:SER:HG	1.37	0.73
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.72	0.71
8:D:501:GDP:O3B	12:D:601:HOH:O	2.10	0.67
4:F:242:ASN:OD1	11:F:401:ACP:H3B2	1.97	0.65
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.80	0.64
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.80	0.64
2:B:274:PRO:HB3	2:B:286:LEU:HD11	1.82	0.62
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	1.83	0.59
4:F:331:GLU:OE2	4:F:333:ASN:ND2	2.36	0.59
8:D:501:GDP:O3B	12:D:602:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.37	0.57
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.87	0.57
2:D:281:GLN:HG3	9:D:503:7AO:C41	2.34	0.56
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.88	0.56
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.10	0.56
2:D:167:ASN:ND2	12:D:609:HOH:O	2.39	0.56
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.38	0.56
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.87	0.55
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.88	0.55
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.89	0.55
3:E:84[B]:GLN:OE1	12:E:301:HOH:O	2.18	0.54
2:D:136:GLN:HA	2:D:167:ASN:O	2.07	0.54
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.90	0.54
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.89	0.54
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.47	0.54
1:C:417:GLU:OE1	12:C:601:HOH:O	2.19	0.52
2:D:2:ARG:NH1	12:D:610:HOH:O	2.39	0.52
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.92	0.52
2:D:75:MET:HG3	2:D:79:ARG:HH12	1.75	0.51
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.91	0.51
4:F:36:ARG:NH2	12:F:504:HOH:O	2.40	0.51
2:B:297:ASP:OD2	2:B:299:LYS:NZ	2.44	0.51
2:D:398:MET:HE3	2:D:404:PHE:HD2	1.75	0.51
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.41	0.51
2:D:241[B]:CYS:SG	12:D:718:HOH:O	2.59	0.51
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.92	0.51
8:B:501:GDP:O1A	12:B:601:HOH:O	2.20	0.51
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.92	0.51
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.92	0.50
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.45	0.50
3:E:51:GLN:NE2	12:E:302:HOH:O	2.32	0.50
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.93	0.50
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	1.94	0.50
2:D:236:SER:O	2:D:240[B]:THR:HG23	2.13	0.49
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
2:B:191:VAL:O	2:B:195[B]:VAL:HG13	2.12	0.49
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.94	0.49
2:B:192:HIS:O	2:B:195[B]:VAL:HG22	2.13	0.48
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.28	0.48
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.96	0.48
1:C:107:HIS:HE1	1:C:155:GLU:OE1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.49	0.48
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.54	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.47
4:F:320:MET:HE3	4:F:320:MET:HB3	1.83	0.47
2:D:142:GLY:O	2:D:183:GLU:HG2	2.14	0.47
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.40	0.47
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.96	0.47
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.30	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.47
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.96	0.46
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.16	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.46
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.51	0.46
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.98	0.46
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.20	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.96	0.46
4:F:220[A]:VAL:HG11	4:F:339:ALA:HB2	1.97	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.45
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.98	0.45
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.51	0.45
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.99	0.45
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.82	0.45
2:D:398:MET:HE3	2:D:404:PHE:CD2	2.51	0.45
3:E:92:ASN:O	3:E:96:MET:HG2	2.16	0.45
2:B:258:ASN:OD1	12:B:602:HOH:O	2.21	0.44
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.99	0.44
1:A:298:PRO:HA	1:A:301:GLN:CD	2.41	0.44
1:C:204:VAL:HG11	1:C:231:ILE:HG12	1.99	0.44
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.98	0.44
1:A:121:ARG:HA	1:A:121:ARG:HD3	1.80	0.44
4:F:288:LYS:NZ	12:F:507:HOH:O	2.47	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.53	0.44
2:B:172:MET:HE3	2:B:203:CYS:SG	2.58	0.44
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.44
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.48	0.43
2:D:158:ARG:NH1	12:D:626:HOH:O	2.51	0.43
2:D:72:PRO:HG3	2:D:96:GLN:HA	2.01	0.43
4:F:237:THR:O	4:F:246:GLN:NE2	2.46	0.43
1:C:133:GLN:NE2	12:C:629:HOH:O	2.52	0.43
1:C:234:ILE:HG21	1:C:302:MET:SD	2.59	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LYS:HE3	12:D:743:HOH:O	2.18	0.43
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.53	0.42
4:F:305:LYS:NZ	12:F:508:HOH:O	2.48	0.42
2:B:164:ARG:O	10:B:505:MES:H31	2.19	0.42
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.53	0.42
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.42
4:F:151:SER:HB2	4:F:179:VAL:O	2.18	0.42
2:D:325:MET:HE2	2:D:325:MET:HB2	1.97	0.42
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.55	0.42
1:A:336:LYS:HG3	3:E:24:LEU:HD13	2.02	0.42
2:B:106:GLY:O	2:B:111:GLY:HA3	2.21	0.41
2:D:106:GLY:O	2:D:111:GLY:HA3	2.20	0.41
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.56	0.41
2:B:2:ARG:HB3	2:B:133:GLN:HG3	2.03	0.41
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.36	0.41
2:B:274:PRO:CB	2:B:286:LEU:HD11	2.49	0.41
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.41
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.02	0.41
4:F:151:SER:HB3	4:F:180:HIS:CG	2.56	0.41
1:A:9:VAL:HA	1:A:68[B]:VAL:HG13	2.03	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.87	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
2:B:136:GLN:NE2	12:B:610:HOH:O	2.34	0.40
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.56	0.40
2:D:152:LEU:O	2:D:156:LYS:HG2	2.22	0.40
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.57	0.40
4:F:236:LYS:HE3	4:F:236:LYS:HB2	1.90	0.40
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.03	0.40
2:D:183:GLU:OE2	8:D:501:GDP:O3'	2.34	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	441/451 (98%)	432 (98%)	9 (2%)	0	100	100
1	C	454/451 (101%)	445 (98%)	9 (2%)	0	100	100
2	B	435/445 (98%)	426 (98%)	9 (2%)	0	100	100
2	D	433/445 (97%)	422 (98%)	11 (2%)	0	100	100
3	E	123/143 (86%)	122 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	334 (97%)	10 (3%)	0	100	100
All	All	2230/2319 (96%)	2181 (98%)	49 (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	376/379 (99%)	373 (99%)	3 (1%)	73	85
1	C	387/379 (102%)	382 (99%)	5 (1%)	61	76
2	B	379/383 (99%)	375 (99%)	4 (1%)	65	79
2	D	376/383 (98%)	373 (99%)	3 (1%)	73	85
3	E	114/127 (90%)	113 (99%)	1 (1%)	70	84
4	F	319/342 (93%)	317 (99%)	2 (1%)	78	89
All	All	1951/1993 (98%)	1933 (99%)	18 (1%)	70	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	234	ILE
1	A	381	THR
2	B	200	GLU

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Mol	Chain	Res	Type
2	B	295	MET
2	B	302	MET
2	B	376	THR
1	C	71	GLU
1	C	163	LYS
1	C	347	CYS
1	C	381	THR
1	C	384	ILE
2	D	71	GLU
2	D	86	ILE
2	D	281	GLN
3	E	132	GLU
4	F	225	SER
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	216	ASN
2	B	50	ASN
2	B	192	HIS
2	B	385	GLN
1	C	11	GLN
1	C	101	ASN
1	C	393	HIS
2	D	247	GLN
2	D	293	GLN
2	D	349	ASN
4	F	269	GLN
4	F	306	HIS
4	F	310	GLN
4	F	379	HIS

5.3.3 RNA ⓘ

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 17 ligands modelled in this entry, 9 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$
10	MES	B	505	-	12,12,12	2.29	1 (8%)	15,16,16	1.08	1 (6%)
9	7AO	D	503	-	58,58,58	1.78	7 (12%)	68,78,78	1.57	16 (23%)
8	GDP	B	501	6	29,30,30	1.20	4 (13%)	45,47,47	1.72	5 (11%)
8	GDP	D	501	6	29,30,30	1.22	4 (13%)	45,47,47	1.73	6 (13%)
11	ACP	F	401	6	31,33,33	1.83	8 (25%)	47,52,52	2.10	12 (25%)
5	GTP	A	501	6	33,34,34	1.25	3 (9%)	50,54,54	1.66	6 (12%)
9	7AO	B	504	-	58,58,58	1.79	7 (12%)	68,78,78	1.53	14 (20%)
5	GTP	C	501	6	33,34,34	1.23	4 (12%)	50,54,54	1.60	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	505	-	-	2/6/14/14	0/1/1/1
9	7AO	D	503	-	-	7/64/84/84	0/2/2/2
8	GDP	B	501	6	-	5/16/32/32	0/3/3/3
8	GDP	D	501	6	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	6	-	8/19/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
9	7AO	B	504	-	-	7/64/84/84	0/2/2/2
5	GTP	C	501	6	-	5/22/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	7AO	N82-N81	-7.79	1.07	1.23
9	B	504	7AO	N82-N81	-7.78	1.07	1.23
10	B	505	MES	C8-S	-7.65	1.66	1.77
11	F	401	ACP	C6-N6	5.44	1.48	1.34
9	B	504	7AO	N81-N8'	-5.36	1.07	1.24
9	D	503	7AO	N81-N8'	-5.31	1.07	1.24
9	D	503	7AO	C2-C1	-5.22	1.39	1.51
9	B	504	7AO	C2-C1	-5.14	1.40	1.51
9	B	504	7AO	C6'-C5'	-4.85	1.39	1.50
9	D	503	7AO	C6'-C5'	-4.52	1.40	1.50
9	B	504	7AO	C8'-N8'	-3.55	1.34	1.43
9	D	503	7AO	C8'-N8'	-3.52	1.34	1.43
9	B	504	7AO	C22-C23	3.40	1.52	1.44
9	D	503	7AO	C22-C23	3.38	1.52	1.44
8	D	501	GDP	C5-C4	3.15	1.47	1.38
11	F	401	ACP	C2'-C3'	-3.14	1.44	1.53
5	C	501	GTP	C5-C4	3.12	1.47	1.38
5	A	501	GTP	C5-C4	3.11	1.47	1.38
11	F	401	ACP	PB-O1B	3.06	1.58	1.51
5	A	501	GTP	PB-O3B	3.05	1.62	1.59
8	B	501	GDP	C5-C4	3.03	1.47	1.38
11	F	401	ACP	PG-O2G	2.94	1.61	1.55
8	B	501	GDP	C6-N1	-2.70	1.33	1.38
8	D	501	GDP	PA-O3A	2.45	1.62	1.59
8	D	501	GDP	C6-N1	-2.43	1.34	1.38
5	A	501	GTP	C6-N1	-2.41	1.34	1.38
11	F	401	ACP	O5'-C5'	-2.28	1.36	1.44
5	C	501	GTP	PB-O3B	2.27	1.62	1.59
9	B	504	7AO	O5-C5	-2.25	1.43	1.46
11	F	401	ACP	PG-O3G	2.24	1.60	1.55
5	C	501	GTP	C6-N1	-2.23	1.34	1.38
11	F	401	ACP	C5-N7	-2.19	1.35	1.39
5	C	501	GTP	PA-O3A	2.19	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	7AO	O5-C5	-2.18	1.43	1.46
11	F	401	ACP	O3'-C3'	-2.11	1.37	1.43
8	B	501	GDP	PA-O3A	2.09	1.61	1.59
8	D	501	GDP	C5-N7	-2.07	1.34	1.39
8	B	501	GDP	C5-N7	-2.01	1.35	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	O4'-C1'-N9	-6.03	96.52	108.09
8	D	501	GDP	C5-C4-N3	-5.94	118.94	128.39
8	B	501	GDP	C5-C4-N3	-5.87	119.05	128.39
5	A	501	GTP	C5-C4-N3	-5.86	119.06	128.39
5	C	501	GTP	C5-C4-N3	-5.68	119.35	128.39
11	F	401	ACP	C5-C4-N3	-5.14	119.64	126.72
5	A	501	GTP	C2-N3-C4	5.05	120.99	112.30
8	B	501	GDP	C2-N3-C4	4.98	120.88	112.30
8	D	501	GDP	C2-N3-C4	4.93	120.80	112.30
5	C	501	GTP	C2-N3-C4	4.88	120.70	112.30
11	F	401	ACP	N3-C2-N1	-4.75	121.39	128.58
9	D	503	7AO	O19-C1'-N1'	4.54	118.40	111.01
8	D	501	GDP	N9-C4-N3	4.41	134.77	125.95
5	C	501	GTP	N9-C4-N3	4.31	134.56	125.95
9	B	504	7AO	O19-C1'-N1'	4.30	118.01	111.01
8	B	501	GDP	N9-C4-N3	4.28	134.52	125.95
5	A	501	GTP	N9-C4-N3	4.23	134.41	125.95
11	F	401	ACP	C2'-C1'-N9	4.05	123.36	113.30
11	F	401	ACP	N3-C4-N9	3.94	133.87	127.17
9	D	503	7AO	C29-C14-C13	-3.85	116.58	123.85
9	B	504	7AO	C20-C21-C22	-3.79	118.28	126.11
9	B	504	7AO	C29-C14-C13	-3.59	117.06	123.85
5	A	501	GTP	C6-C5-N7	3.53	136.71	130.29
11	F	401	ACP	C2-N3-C4	3.51	120.41	111.83
11	F	401	ACP	O5'-C5'-C4'	3.50	120.92	108.99
5	C	501	GTP	C6-C5-N7	3.41	136.50	130.29
8	D	501	GDP	C6-C5-N7	3.40	136.48	130.29
8	B	501	GDP	C6-C5-N7	3.39	136.46	130.29
9	B	504	7AO	O1'-C1'-N1'	-3.34	119.91	124.93
11	F	401	ACP	N9-C8-N7	-3.23	109.36	113.94
11	F	401	ACP	PB-O3A-PA	-3.11	122.22	132.37
9	D	503	7AO	O1-C1-C2	-3.09	118.67	124.28
9	D	503	7AO	O1'-C1'-N1'	-3.01	120.41	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	7AO	C26-C4-C3	-2.95	108.05	112.13
9	B	504	7AO	O1-C1-C2	-2.86	119.08	124.28
9	D	503	7AO	C25-C2-C3	-2.82	107.95	112.95
9	D	503	7AO	C28-C12-C13	-2.81	105.31	110.08
9	D	503	7AO	C20-C21-C22	-2.78	120.37	126.11
11	F	401	ACP	C4-N9-C8	2.75	108.63	105.74
5	A	501	GTP	C4-C5-N7	-2.68	106.43	110.67
8	D	501	GDP	C4-C5-N7	-2.66	106.46	110.67
11	F	401	ACP	C5-N7-C8	2.63	107.59	103.45
9	D	503	7AO	C28-C12-C11	-2.63	105.81	111.45
9	B	504	7AO	C25-C2-C3	-2.59	108.36	112.95
9	B	504	7AO	C26-C4-C3	-2.50	108.68	112.13
5	C	501	GTP	C4-C5-N7	-2.47	106.75	110.67
8	B	501	GDP	C4-C5-N7	-2.46	106.77	110.67
9	B	504	7AO	C16-C17-C18	-2.46	112.52	116.20
9	B	504	7AO	O5-C1-O1	2.43	122.04	118.52
11	F	401	ACP	C4-C5-N7	-2.32	107.94	110.58
9	B	504	7AO	O5-C5-C6	2.30	110.38	106.41
9	D	503	7AO	O19-C1'-O1'	-2.28	121.19	124.55
9	B	504	7AO	C29-C14-C15	2.28	120.34	115.28
9	D	503	7AO	C29-C14-C15	2.27	120.31	115.28
9	D	503	7AO	C16-C17-C18	-2.26	112.81	116.20
5	C	501	GTP	O6-C6-C5	-2.25	120.60	126.53
9	D	503	7AO	C30-C16-C17	-2.24	107.40	111.45
9	B	504	7AO	C28-C12-C11	-2.21	106.71	111.45
9	D	503	7AO	C10-C9-C8	-2.15	119.30	125.81
10	B	505	MES	O1S-S-C8	2.15	109.98	106.73
9	D	503	7AO	C7-C8-C9	-2.13	119.72	124.74
5	A	501	GTP	O6-C6-C5	-2.11	120.97	126.53
9	B	504	7AO	C28-C12-C13	-2.08	106.54	110.08
9	D	503	7AO	O5-C1-O1	2.08	121.54	118.52
8	D	501	GDP	O6-C6-C5	-2.06	121.10	126.53
9	B	504	7AO	C30-C16-C17	-2.03	107.77	111.45

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A

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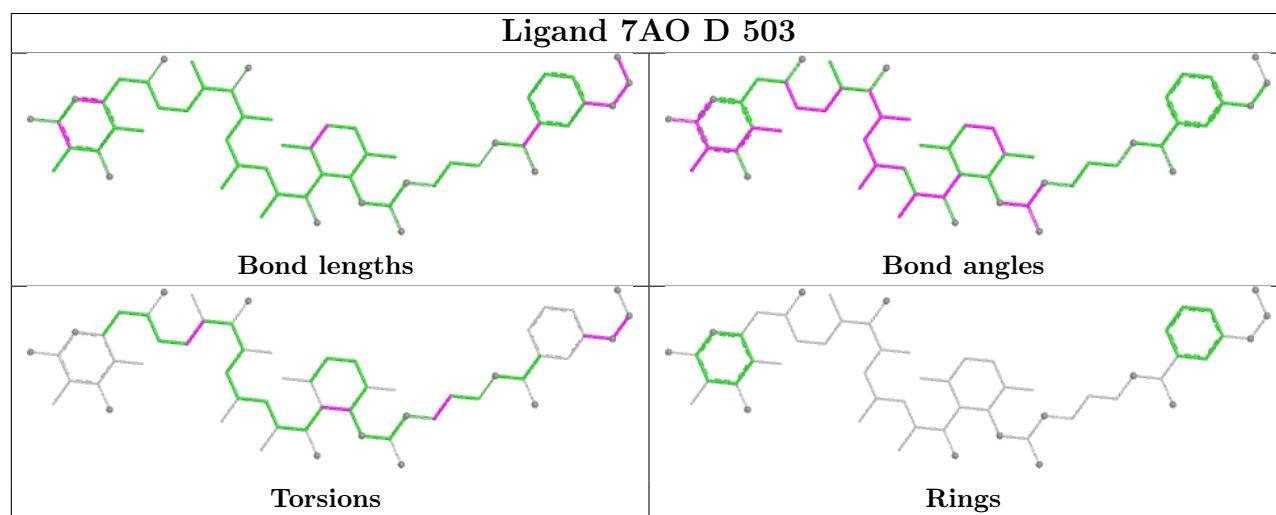
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
9	D	503	7AO	C9'-C8'-N8'-N81
9	D	503	7AO	N1'-C2'-C3'-C4'
9	B	504	7AO	C7'-C8'-N8'-N81
9	D	503	7AO	C7'-C8'-N8'-N81
11	F	401	ACP	PB-O3A-PA-O1A
9	B	504	7AO	C8'-N8'-N81-N82
9	B	504	7AO	C9'-C8'-N8'-N81
10	B	505	MES	C8-C7-N4-C5
11	F	401	ACP	PB-O3A-PA-O5'
9	D	503	7AO	C11-C10-C9-C8
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	504	7AO	O7-C7-C8-C9
11	F	401	ACP	C5'-O5'-PA-O1A
10	B	505	MES	C8-C7-N4-C3
9	B	504	7AO	C17-C18-C19-C20
9	D	503	7AO	C17-C18-C19-C20
9	B	504	7AO	C6-C7-C8-C9
9	B	504	7AO	C31-C18-C19-C20
9	D	503	7AO	C8'-N8'-N81-N82
11	F	401	ACP	PG-C3B-PB-O1B
9	D	503	7AO	C31-C18-C19-C20
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
8	B	501	GDP	PB-O3A-PA-O1A

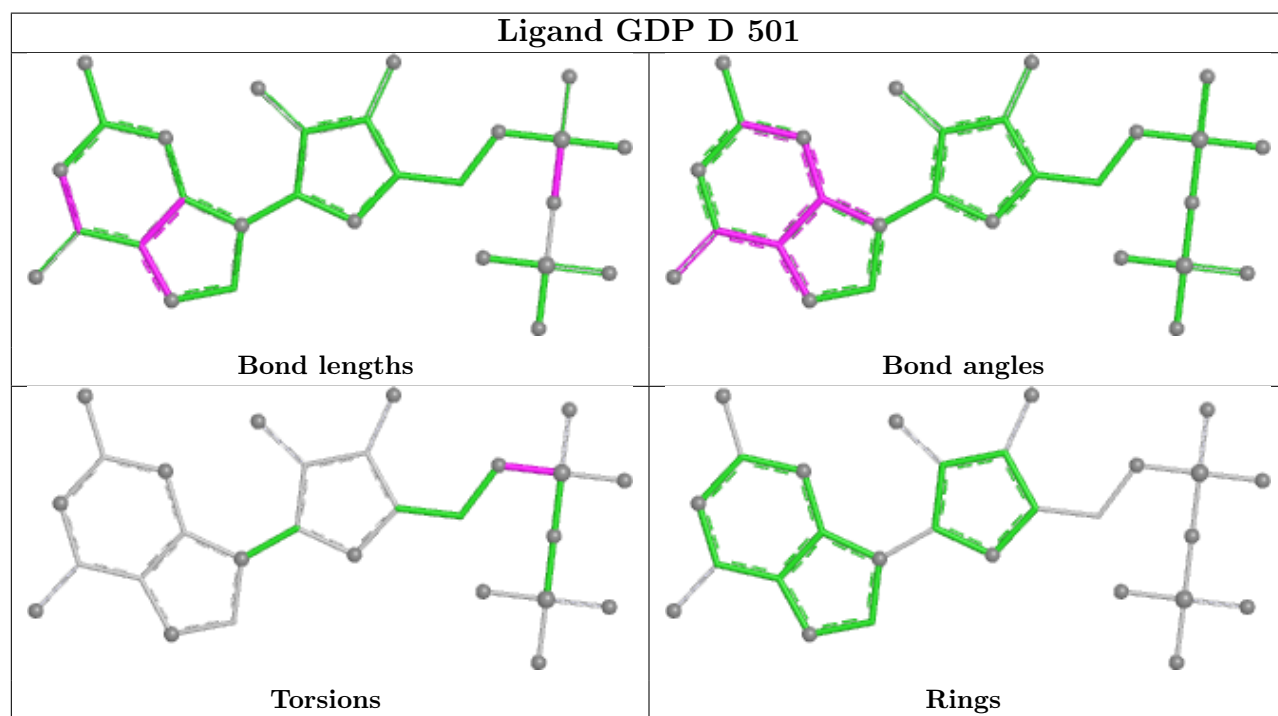
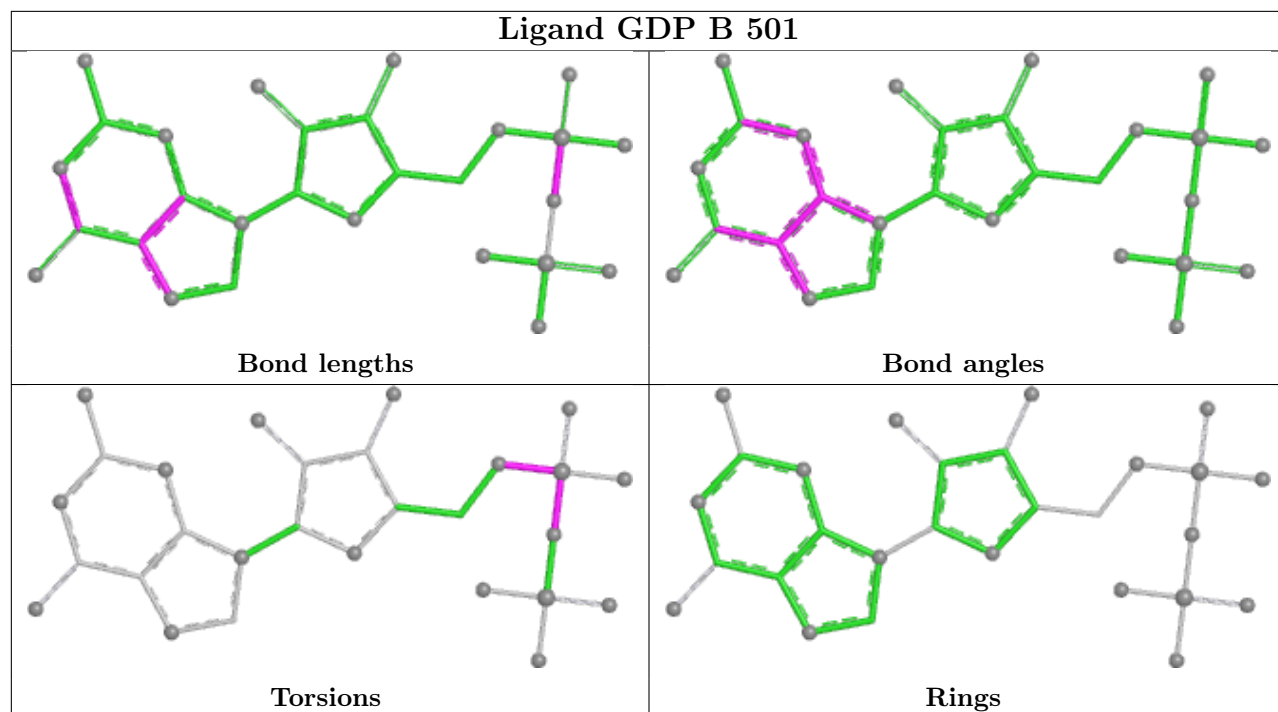
There are no ring outliers.

5 monomers are involved in 9 short contacts:

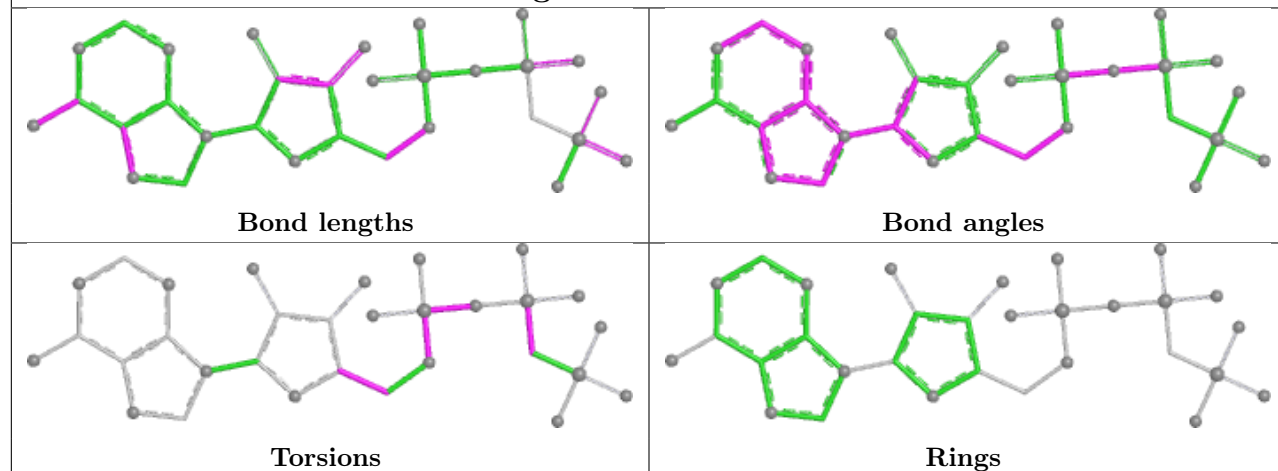
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	MES	1	0
9	D	503	7AO	1	0
8	B	501	GDP	1	0
8	D	501	GDP	4	0
11	F	401	ACP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

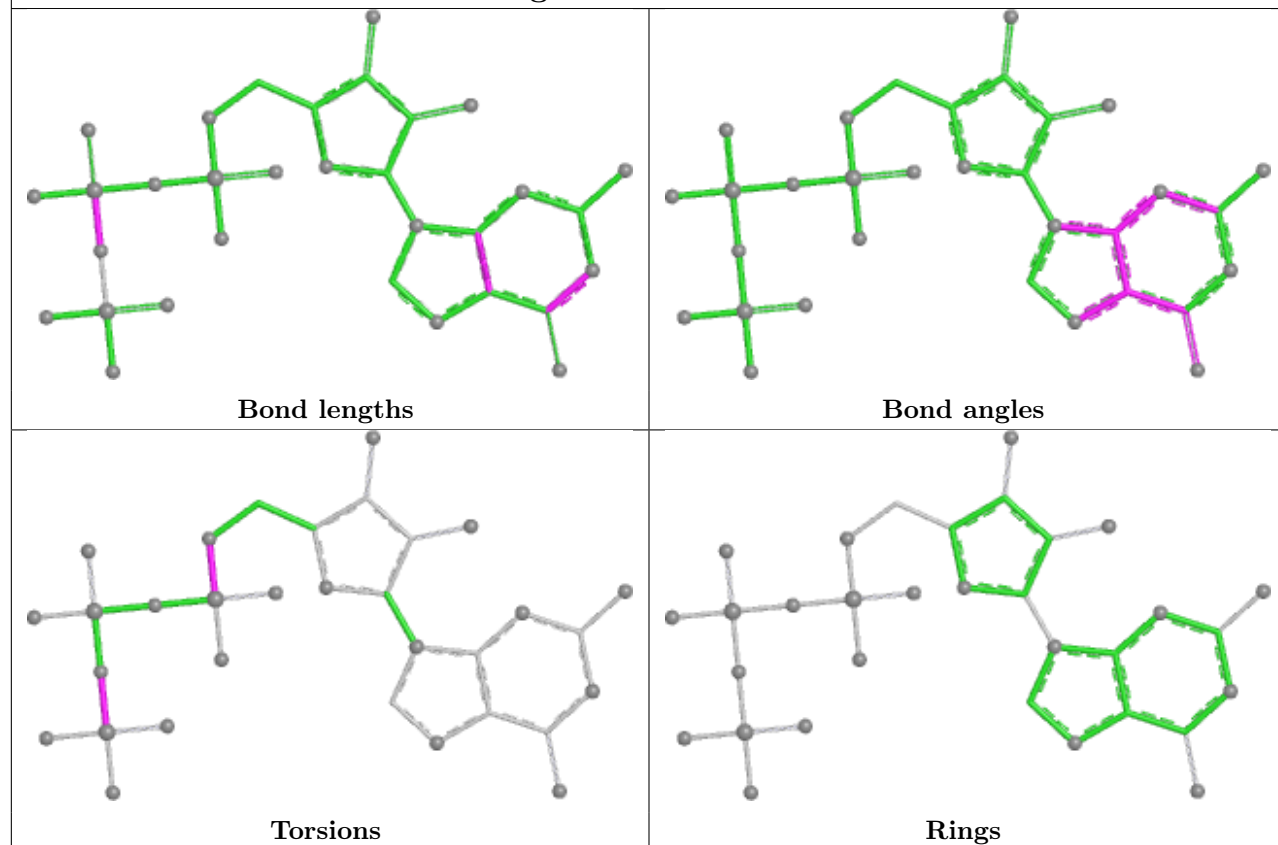


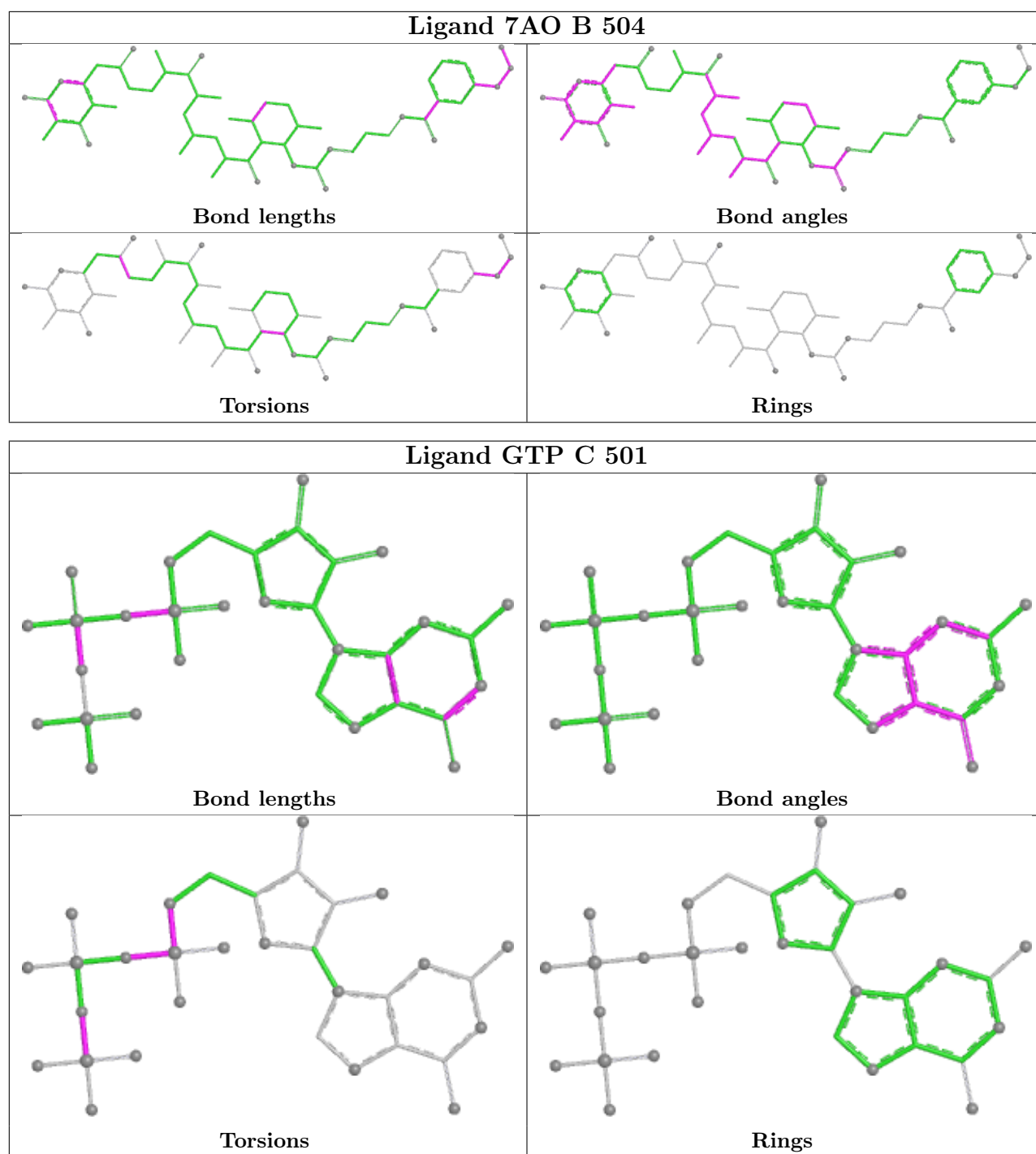


Ligand ACP F 401



Ligand GTP A 501





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	434/451 (96%)	-0.26	7 (1%) 70 67	20, 45, 76, 121	11 (2%)
1	C	440/451 (97%)	-0.39	10 (2%) 61 58	20, 36, 65, 114	16 (3%)
2	B	428/445 (96%)	0.02	19 (4%) 39 36	20, 48, 89, 128	9 (2%)
2	D	431/445 (96%)	-0.07	17 (3%) 43 40	22, 46, 85, 145	4 (0%)
3	E	123/143 (86%)	0.31	8 (6%) 25 22	26, 56, 102, 120	4 (3%)
4	F	345/384 (89%)	0.36	15 (4%) 40 36	24, 67, 117, 170	7 (2%)
All	All	2201/2319 (94%)	-0.07	76 (3%) 47 44	20, 47, 93, 170	51 (2%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	THR	5.7
1	C	340	SER	4.4
2	D	75	MET	4.3
1	A	262	TYR	4.2
1	C	440	VAL	4.1
2	B	1	MET	4.0
4	F	381	HIS	4.0
2	B	333	LEU	3.8
3	E	143	ALA	3.7
1	A	437	VAL	3.7
2	B	248	LEU	3.6
2	D	286	LEU	3.6
1	A	281	ALA	3.5
1	C	1	MET	3.4
2	D	82	PRO	3.3
4	F	152	SER	3.2
2	B	438	ALA	3.2
2	D	1	MET	3.2
4	F	372	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	176	LYS	3.0
4	F	362	ALA	2.9
2	B	325	MET	2.9
2	B	220	THR	2.9
2	D	325	MET	2.8
2	B	249	ASN	2.8
2	D	283	TYR	2.8
4	F	179	VAL	2.8
3	E	6	MET	2.7
2	D	57	THR	2.7
4	F	160	ILE	2.7
2	B	338	LYS	2.6
2	D	285	ALA	2.6
4	F	142	ARG	2.6
2	B	280	SER	2.6
2	B	337	ASN	2.5
2	D	74	THR	2.5
1	C	357	TYR	2.4
1	A	178	SER	2.4
4	F	105	LEU	2.4
3	E	45	PRO	2.4
3	E	28	SER	2.4
1	C	179	THR	2.4
2	B	286	LEU	2.4
2	B	2	ARG	2.4
3	E	44	ASP	2.3
2	B	57	THR	2.3
2	D	216	THR	2.3
4	F	173	ILE	2.3
3	E	124	GLN	2.3
1	C	302	MET	2.3
4	F	1	MET	2.3
2	B	281	GLN	2.3
3	E	139	LEU	2.3
2	D	98	GLY	2.3
2	D	94	PHE	2.3
2	D	172	MET	2.2
2	D	97	SER	2.2
2	D	277	SER	2.2
2	B	339	ASN	2.2
4	F	104	ASN	2.2
3	E	26	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	85	PRO	2.2
4	F	240	LEU	2.2
2	B	58	GLY	2.2
1	C	163	LYS	2.2
2	D	281	GLN	2.1
1	C	341	ILE	2.1
2	B	299	LYS	2.1
1	C	245	ASP	2.1
1	C	308	ARG	2.1
4	F	133	ALA	2.1
2	D	280	SER	2.1
4	F	103	THR	2.1
1	A	346	TRP	2.1
1	A	285	GLN	2.0
2	B	59	ASN	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	F	402	1/1	0.84	0.12	79,79,79,79	0
6	MG	D	502	1/1	0.85	0.16	65,65,65,65	0
9	7AO	B	504	57/57	0.88	0.15	34,56,129,132	0
10	MES	B	505	12/12	0.90	0.11	38,50,64,66	0
7	CA	B	503	1/1	0.91	0.07	84,84,84,84	0
7	CA	E	201	1/1	0.93	0.14	82,82,82,82	0
11	ACP	F	401	31/31	0.93	0.09	56,66,104,117	0
9	7AO	D	503	57/57	0.94	0.10	27,45,103,106	0

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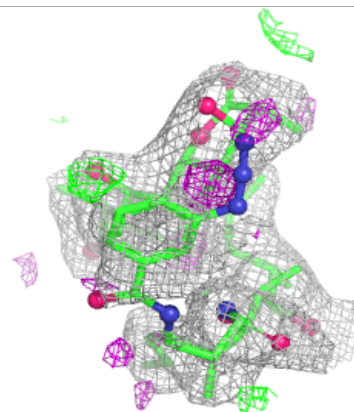
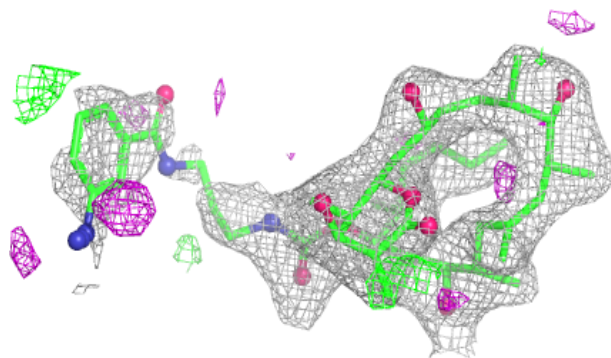
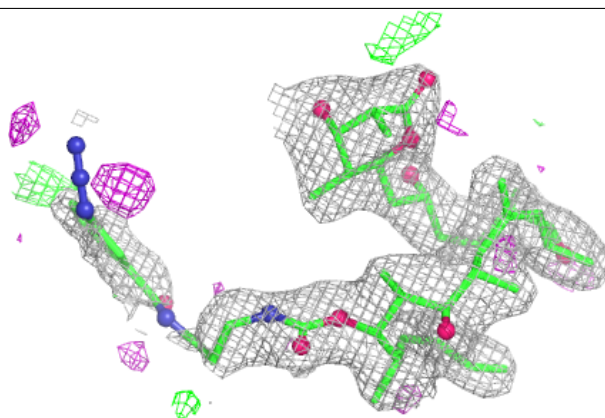
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	502	1/1	0.96	0.06	51,51,51,51	0
8	GDP	D	501	28/28	0.97	0.06	28,39,43,53	0
8	GDP	B	501	28/28	0.98	0.05	23,31,38,41	0
7	CA	C	503	1/1	0.98	0.04	52,52,52,52	0
5	GTP	C	501	32/32	0.99	0.04	22,27,33,48	0
5	GTP	A	501	32/32	0.99	0.05	22,31,36,45	0
7	CA	A	503	1/1	0.99	0.04	59,59,59,59	0
6	MG	A	502	1/1	1.00	0.01	27,27,27,27	0
6	MG	C	502	1/1	1.00	0.05	27,27,27,27	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.

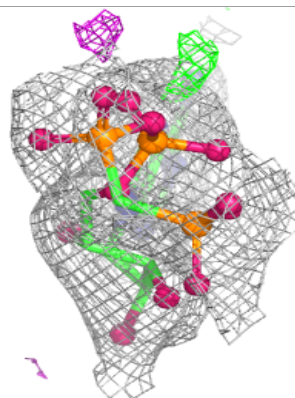
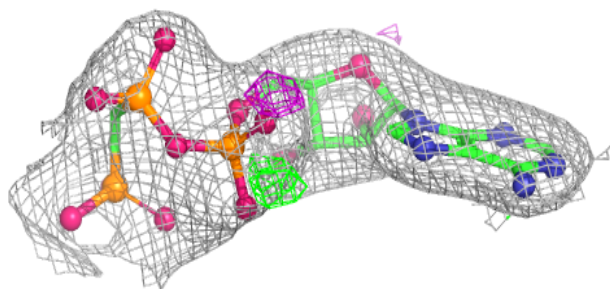
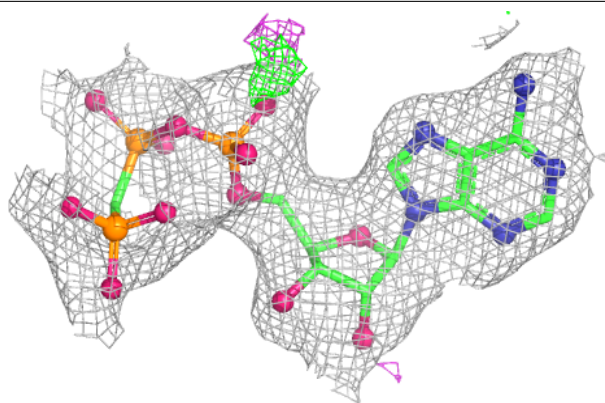
Electron density around 7AO B 504:

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

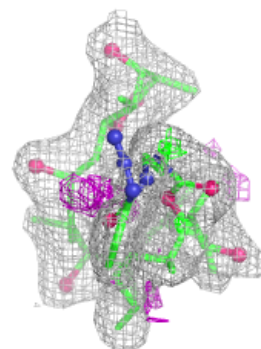
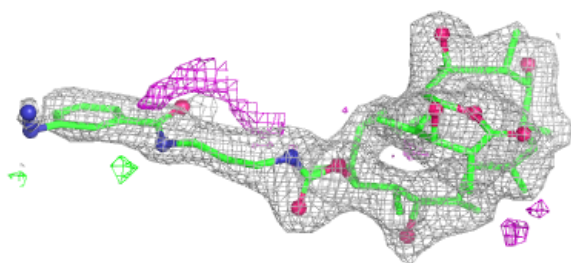
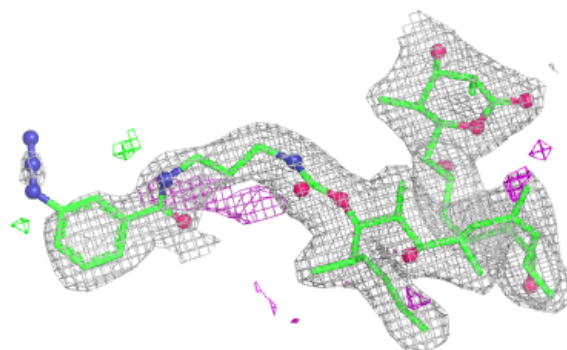


Electron density around ACP F 401:

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

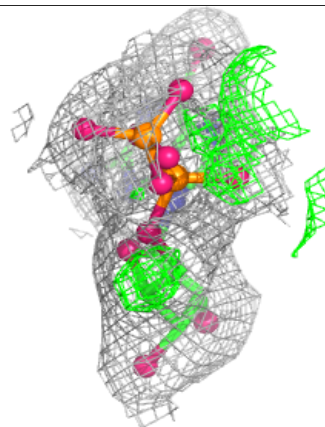
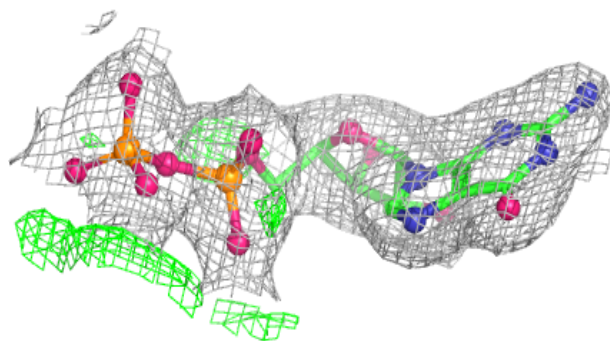
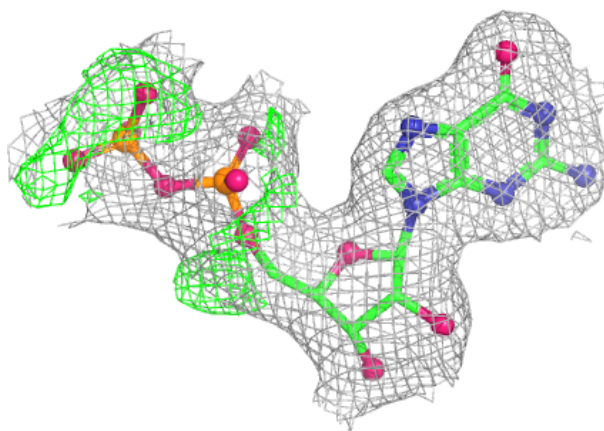
**Electron density around 7AO D 503:**

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



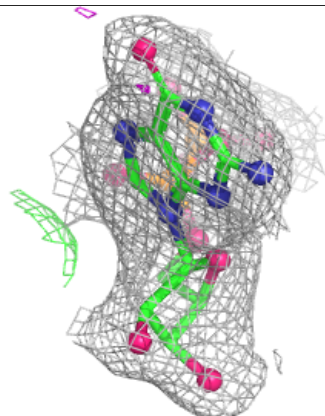
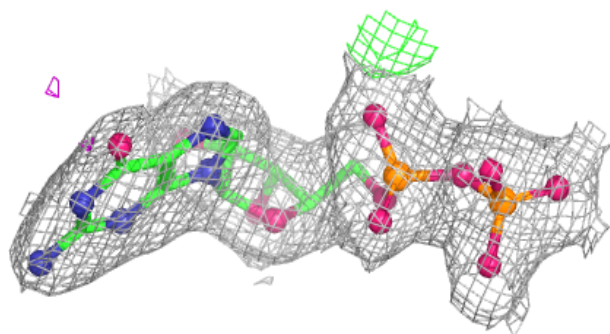
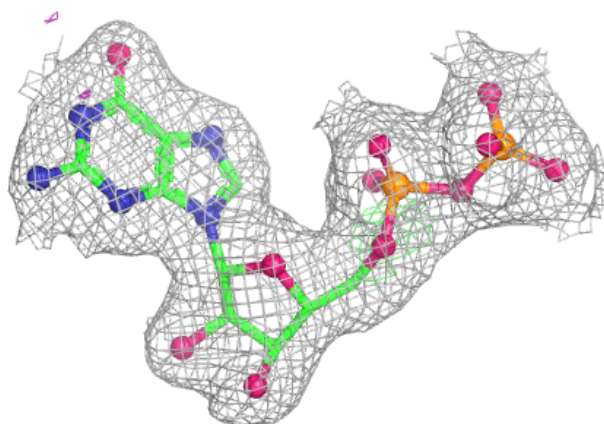
Electron density around GDP D 501:

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

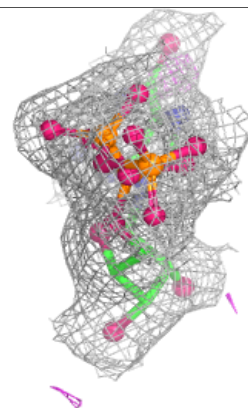
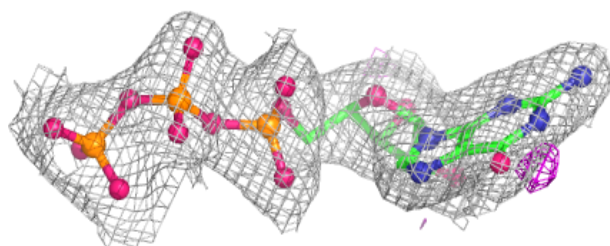
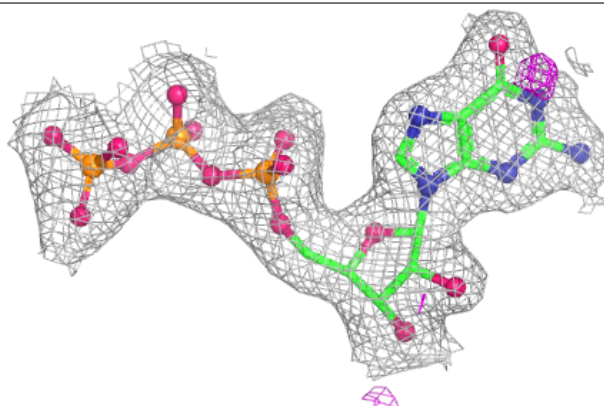


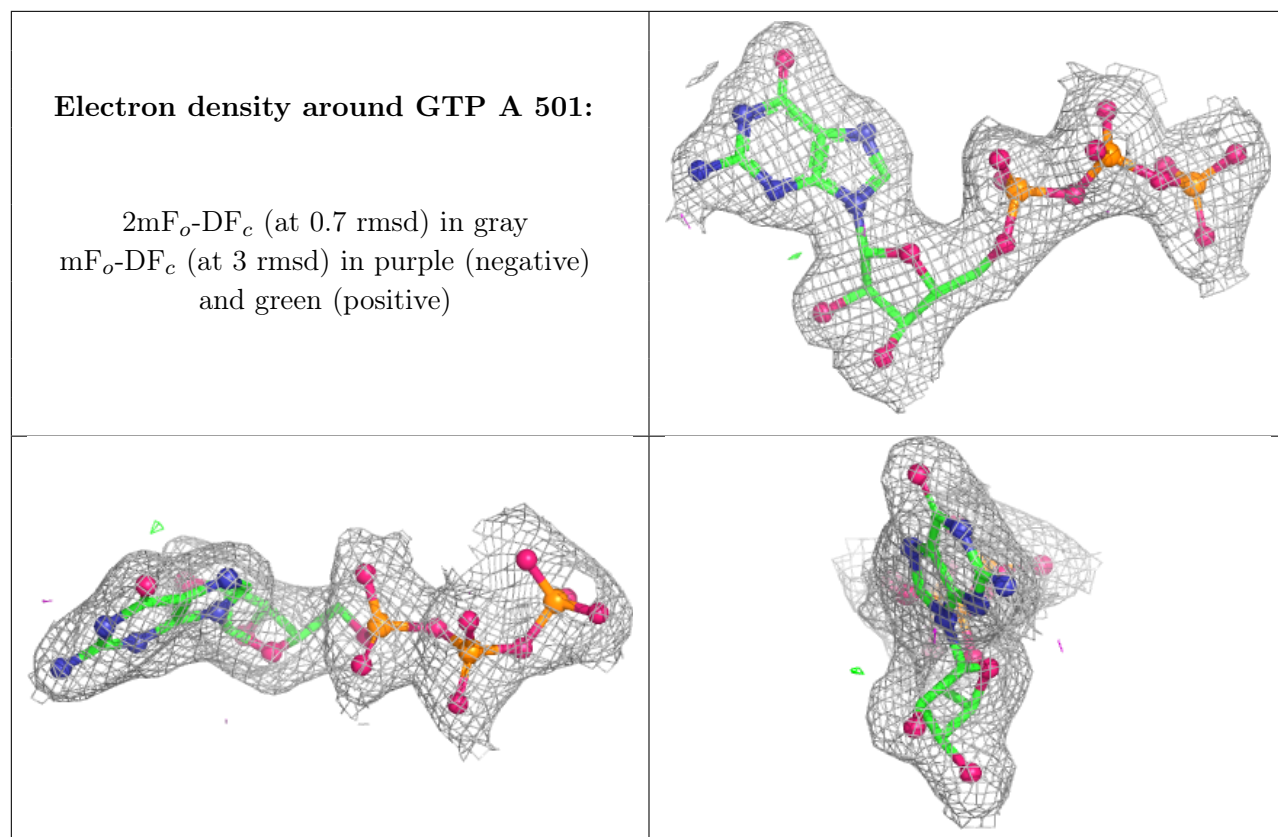
Electron density around GDP B 501:

$2mF_o-DF_c$ (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.