



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:12 AM UTC

PDB ID : 7Z7D / pdb_00007z7d
Title : Tubulin-Todalam-Vinblastine-complex
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Deposited on : 2022-03-15
Resolution : 2.00 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

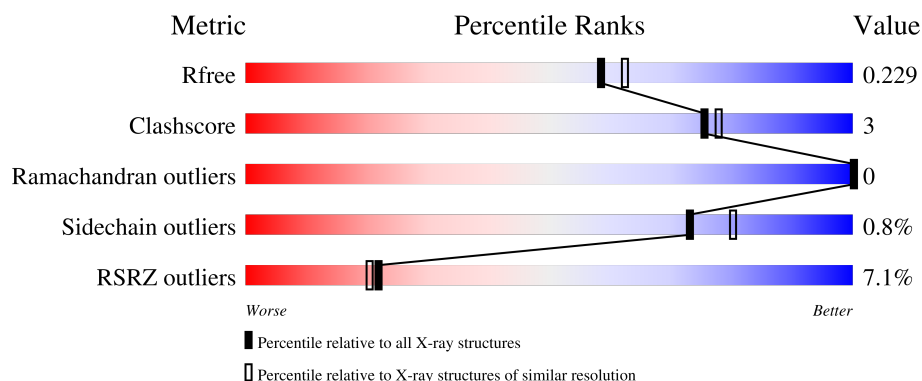
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 7% .
1	C	451	 4% 90% 8% .
2	B	445	 5% 88% 9% .
2	D	445	 6% 84% 11% 5%
3	E	143	 8% 81% . 15%

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Mol	Chain	Length	Quality of chain
4	F	384	15% 82% 7% 11%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	2	0
			3428	2169	583	652	24			
1	C	440	Total	C	N	O	S	0	7	0
			3493	2206	597	666	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	4	0
			3408	2136	588	657	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	1	0
			1019	628	185	201	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

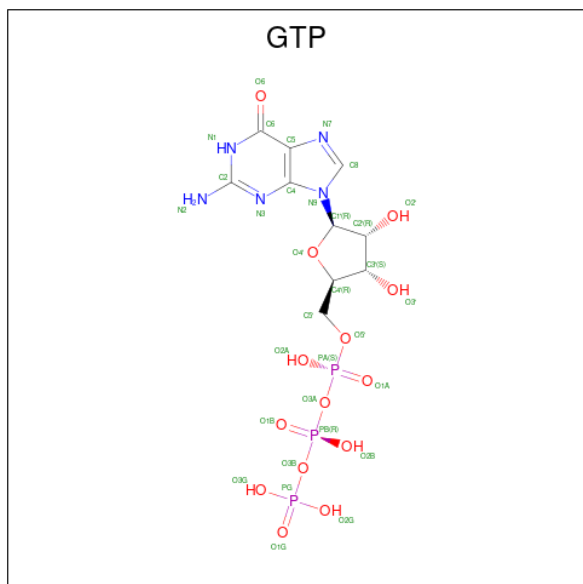
- Molecule 4 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	341	Total	C	N	O	S	0	0	0
			2786	1788	476	508	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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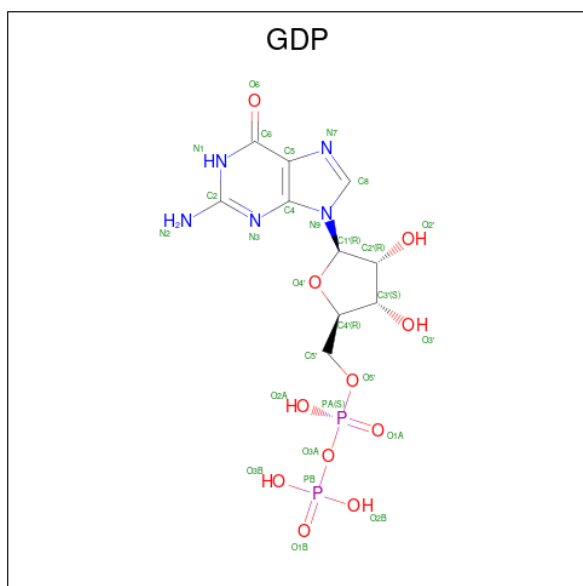
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

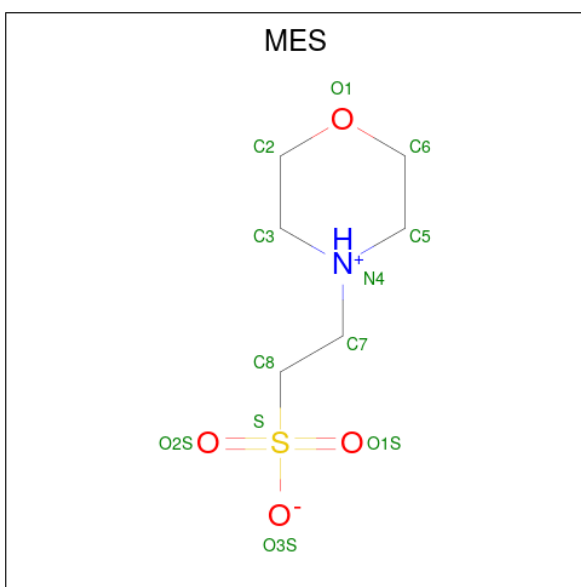
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

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



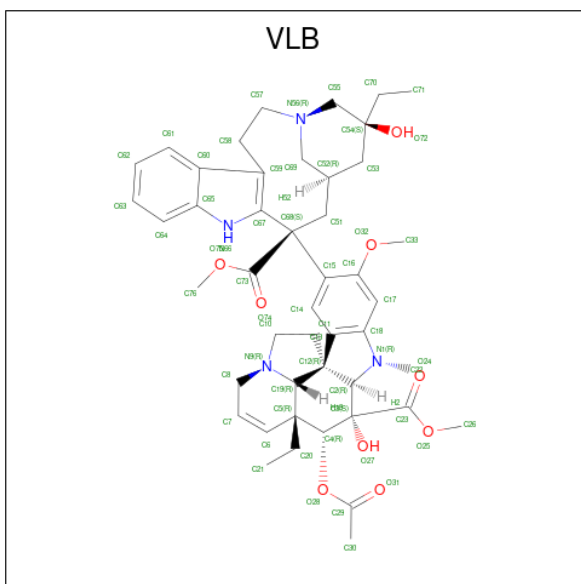
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



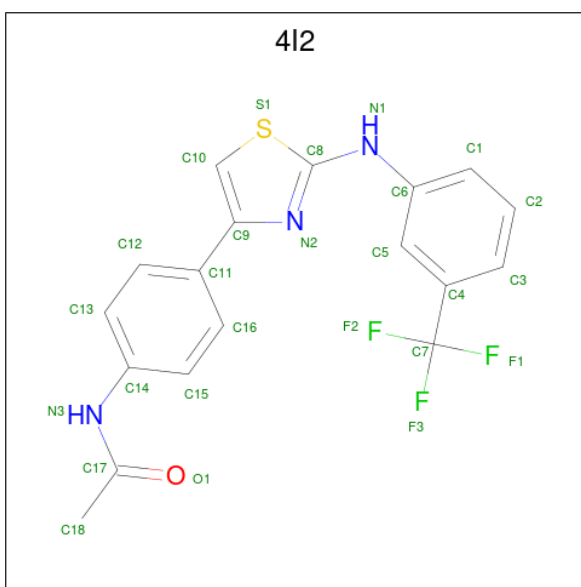
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (CCD ID: VLB) (formula: $C_{46}H_{58}N_4O_9$) (labeled as "Ligand of Interest" by depositor).



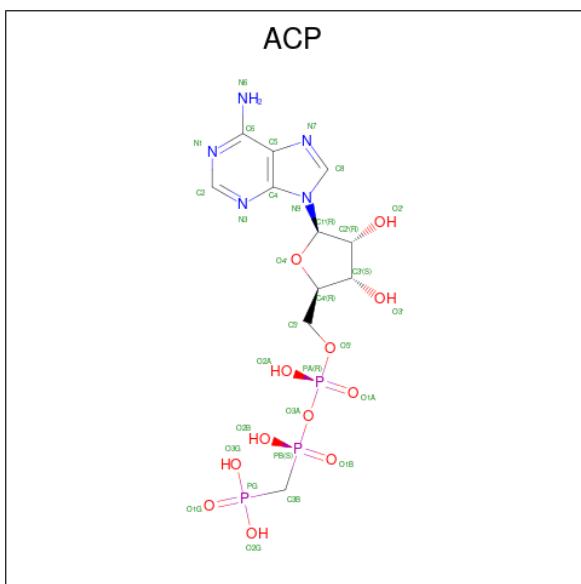
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O		0	0
			59	46	4	9			

- Molecule 11 is N-(4-{2-[3-(trifluoromethyl)anilino]-1,3-thiazol-4-yl}phenyl)acetamide (CCD ID: 4I2) (formula: $C_{18}H_{14}F_3N_3OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	F	N	O	S	0
			26	18	3	3	1	1	

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



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

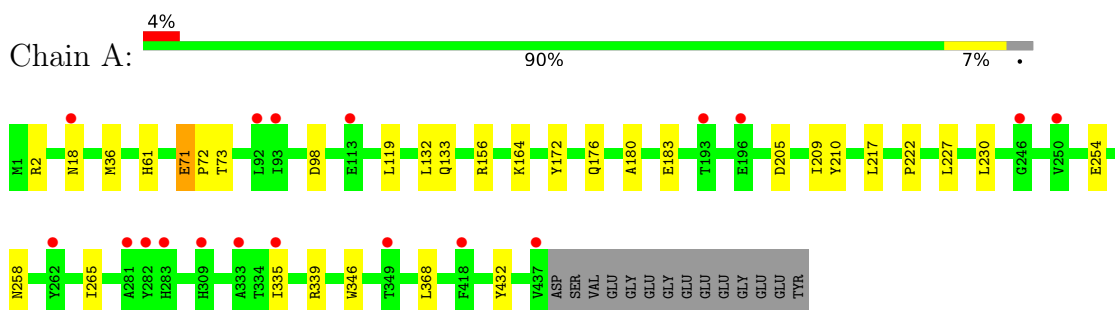
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	141	Total 141	O 141	0	0
13	B	214	Total 214	O 214	0	0
13	C	317	Total 317	O 317	0	0
13	D	86	Total 86	O 86	0	0
13	E	42	Total 42	O 42	0	0
13	F	56	Total 56	O 56	0	0

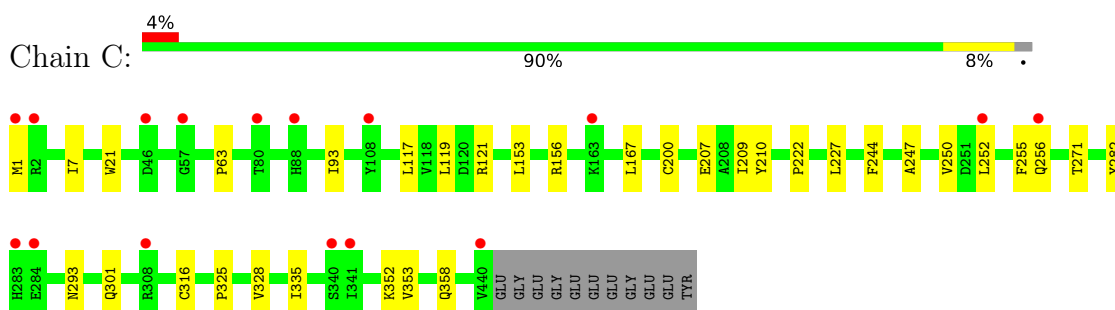
3 Residue-property plots [i](#)

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.

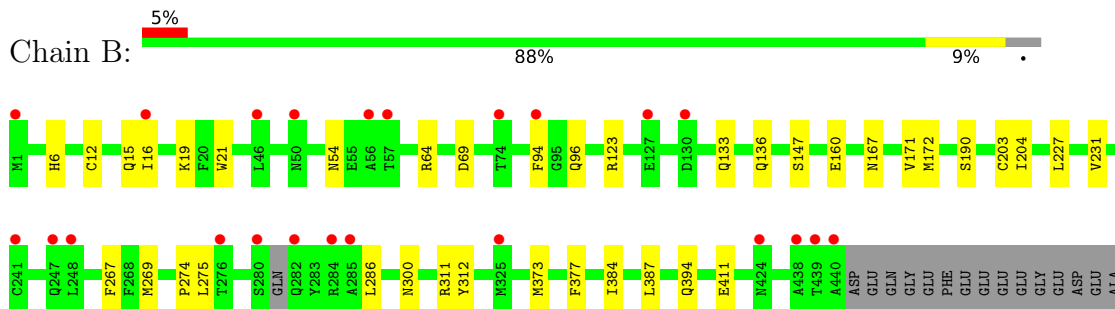
- Molecule 1: Tubulin alpha-1B chain



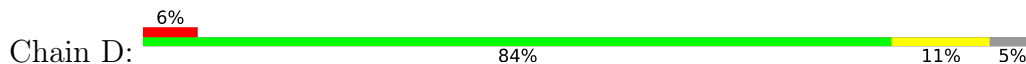
- Molecule 1: Tubulin alpha-1B chain

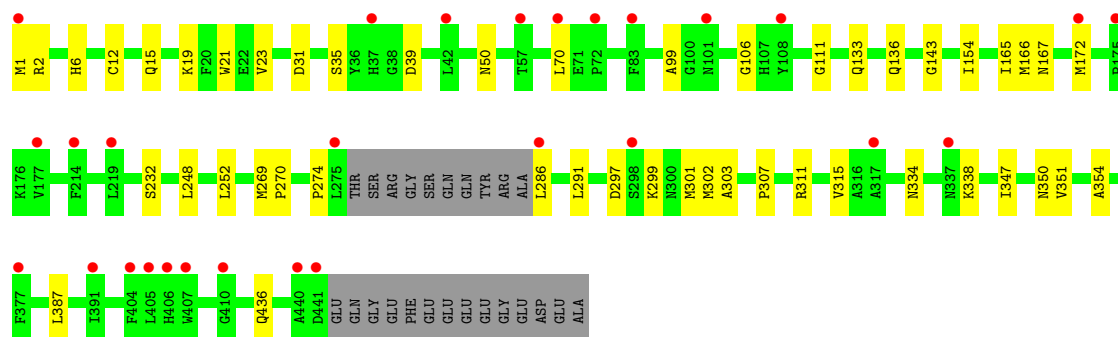


- Molecule 2: Tubulin beta-2B chain

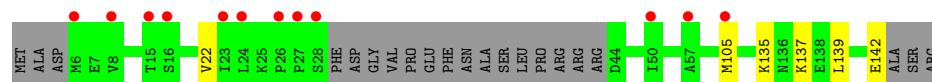
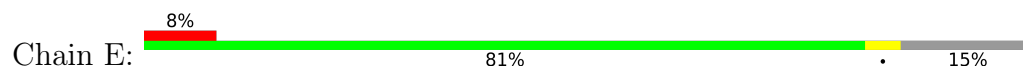


- Molecule 2: Tubulin beta-2B chain

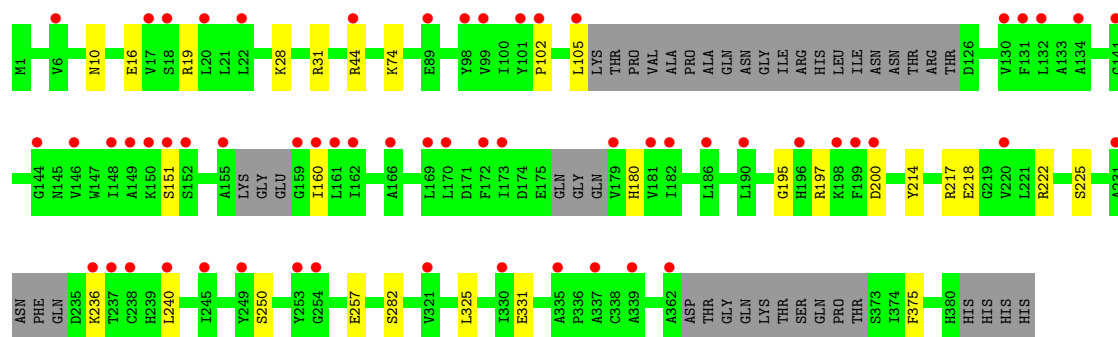
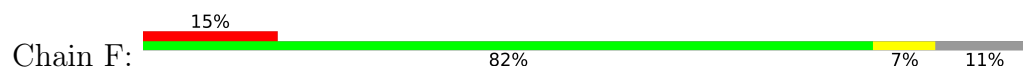




● Molecule 3: Stathmin-4



● 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	105.29Å 157.30Å 182.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.60 – 2.00 45.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (45.60-2.00) 98.3 (45.60-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.204 , 0.236 (Not available) , 0.229	Depositor DCC
R_{free} test set	10682 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18556	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: 4I2, GTP, MES, VLB, ACP, MG, CA, 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	0.10	0/3506	0.28	0/4759
1	C	0.13	0/3571	0.32	0/4847
2	B	0.12	0/3481	0.29	0/4710
2	D	0.09	0/3382	0.25	0/4581
3	E	0.08	0/1028	0.20	0/1364
4	F	0.08	0/2847	0.25	0/3843
All	All	0.11	0/17815	0.28	0/24104

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	3428	0	3339	17	0
1	C	3493	0	3395	21	1
2	B	3408	0	3285	21	1
2	D	3309	0	3189	26	0
3	E	1019	0	1030	2	0
4	F	2786	0	2759	16	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
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	2	0
9	B	12	0	12	0	0
10	B	59	0	58	5	0
11	C	26	0	0	0	0
12	F	31	0	14	0	0
13	A	141	0	0	0	0
13	B	214	0	0	1	0
13	C	317	0	0	2	0
13	D	86	0	0	0	0
13	E	42	0	0	1	0
13	F	56	0	0	1	0
All	All	18556	0	17129	104	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 (104) 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:D:270:PRO:HG2	2:D:302:MET:HB2	1.72	0.71
3:E:135:LYS:HE3	3:E:139:LEU:HD11	1.75	0.69
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.82	0.62
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.82	0.60
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.68	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.21	0.59
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.84	0.58
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.19	0.58
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.84	0.58
1:C:209:ILE:HD12	1:C:227:LEU:HB3	1.87	0.57
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.87	0.55
1:C:328:VAL:HG11	1:C:353[A]:VAL:HG11	1.87	0.55
10:B:505:VLB:C59	10:B:505:VLB:H691	2.37	0.55
4:F:28:LYS:NZ	13:F:507:HOH:O	2.41	0.54
1:C:293[A]:ASN:HA	1:C:335:ILE:HD11	1.89	0.53
10:B:505:VLB:H691	10:B:505:VLB:C67	2.38	0.53
1:C:293[B]:ASN:HA	1:C:335:ILE:HD11	1.89	0.53
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.90	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.93	0.51
1:C:271:THR:OG1	1:C:301[B]:GLN:OE1	2.28	0.51
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.93	0.51
2:D:311:ARG:NH1	2:D:436:GLN:O	2.43	0.50
1:C:207:GLU:OE1	13:C:601:HOH:O	2.20	0.50
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.93	0.50
2:B:136:GLN:HA	2:B:167:ASN:O	2.11	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.93	0.49
1:A:132:LEU:O	1:A:164:LYS:NZ	2.45	0.49
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.95	0.49
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.95	0.48
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.94	0.48
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.95	0.48
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.95	0.48
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.94	0.48
4:F:200:ASP:OD2	4:F:222:ARG:NH2	2.47	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.49	0.48
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.78	0.48
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.96	0.47
1:C:250:VAL:HA	1:C:255:PHE:HE1	1.78	0.47
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.41	0.47
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.97	0.47
2:D:301:MET:HE3	2:D:307:PRO:HG3	1.96	0.47
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.18	0.47
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.47
10:B:505:VLB:C65	1:C:325:PRO:HB3	2.45	0.46
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.15	0.46
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.50	0.46
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.97	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.51	0.46
2:B:373:MET:HE2	2:B:373:MET:HB3	1.70	0.46
3:E:137:LYS:NZ	13:E:303:HOH:O	2.43	0.45
2:D:106:GLY:O	2:D:111:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.45
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.97	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.45
2:D:136:GLN:HA	2:D:167:ASN:O	2.17	0.45
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.98	0.45
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.51	0.45
2:D:2:ARG:HB3	2:D:133:GLN:HG3	1.98	0.45
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.48	0.44
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.17	0.44
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.44
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.52	0.44
2:D:31:ASP:OD1	2:D:35:SER:N	2.46	0.44
2:B:311:ARG:NH2	4:F:31:ARG:HH12	2.16	0.44
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.00	0.44
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.98	0.44
1:C:252:LEU:HD12	1:C:256[A]:GLN:HG2	1.99	0.43
2:B:227:LEU:HD22	10:B:505:VLB:H711	2.00	0.43
4:F:151:SER:HB3	4:F:180:HIS:CG	2.53	0.43
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.00	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.19	0.43
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.53	0.43
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.43
1:C:252:LEU:HD22	13:C:800:HOH:O	2.18	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.43
1:C:247:ALA:HB1	1:C:250:VAL:CG1	2.49	0.43
2:B:15:GLN:O	2:B:19:LYS:HG2	2.19	0.43
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.44	0.43
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.01	0.42
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.01	0.42
1:C:316:CYS:HA	1:C:352:LYS:O	2.20	0.42
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.00	0.42
4:F:160:ILE:O	4:F:236:LYS:NZ	2.40	0.42
2:B:394:GLN:NE2	13:B:601:HOH:O	2.26	0.42
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.01	0.42
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.35	0.42
2:B:269:MET:HG2	2:B:384:ILE:HD13	2.02	0.41
10:B:505:VLB:H213	10:B:505:VLB:H19	1.81	0.41
4:F:195:GLY:HA3	4:F:197:ARG:HD3	2.02	0.41
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.02	0.41
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.02	0.41
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.56	0.41
2:D:286:LEU:HD23	2:D:291:LEU:HD13	2.02	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.41
1:A:346:TRP:CD1	1:A:346:TRP:H	2.39	0.41
2:D:15:GLN:O	2:D:19:LYS:HG2	2.20	0.41
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.39	0.41
4:F:225:SER:OG	4:F:250:SER:OG	2.35	0.41
2:D:39:ASP:OD1	2:D:39:ASP:N	2.54	0.41
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.48	0.40
4:F:197:ARG:NH2	4:F:257:GLU:OE1	2.45	0.40
2:D:297:ASP:OD2	2:D:299:LYS:HE2	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:411:GLU:OE1	1:C:282:TYR:OH[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%)	422 (97%)	15 (3%)	0	100	100
1	C	445/451 (99%)	439 (99%)	6 (1%)	0	100	100
2	B	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
2	D	417/445 (94%)	412 (99%)	5 (1%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	329/384 (86%)	317 (96%)	12 (4%)	0	100	100
All	All	2174/2319 (94%)	2131 (98%)	43 (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	370/379 (98%)	367 (99%)	3 (1%)	73	80
1	C	22/379 (6%)	22 (100%)	0	100	100
2	B	374/383 (98%)	373 (100%)	1 (0%)	86	91
2	D	34/383 (9%)	34 (100%)	0	100	100
3	E	111/127 (87%)	108 (97%)	3 (3%)	39	42
4	F	21/342 (6%)	21 (100%)	0	100	100
All	All	932/1993 (47%)	925 (99%)	7 (1%)	73	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	71	GLU
1	A	176	GLN
2	B	133	GLN
3	E	22	VAL
3	E	105	MET
3	E	142	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	85	GLN
1	A	393	HIS
2	B	247	GLN
2	B	282	GLN
2	B	349	ASN
2	D	436	GLN

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Mol	Chain	Res	Type
3	E	103	GLN
3	E	136	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
8	GDP	B	501	6	29,30,30	1.14	2 (6%)	45,47,47	1.69	6 (13%)
5	GTP	A	501	6	33,34,34	0.99	2 (6%)	50,54,54	1.50	8 (16%)
11	4I2	C	504	-	28,28,28	1.64	5 (17%)	40,40,40	1.44	6 (15%)
5	GTP	C	501	6	33,34,34	0.95	2 (6%)	50,54,54	1.50	9 (18%)
8	GDP	D	501	6	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
10	VLB	B	505	-	66,67,67	2.39	13 (19%)	82,108,108	2.61	26 (31%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	15,16,16	1.73	3 (20%)
12	ACP	F	401	6	31,33,33	0.67	1 (3%)	47,52,52	1.01	1 (2%)

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	-	4/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
11	4I2	C	504	-	-	3/18/18/18	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
8	GDP	D	501	6	-	5/16/32/32	0/3/3/3
10	VLB	B	505	-	-	8/40/131/131	0/7/9/9
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
12	ACP	F	401	6	-	5/19/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	VLB	C67-C59	11.21	1.54	1.37
9	B	504	MES	C8-S	-7.51	1.67	1.77
10	B	505	VLB	C16-C15	6.29	1.51	1.39
10	B	505	VLB	O75-C73	6.09	1.44	1.33
10	B	505	VLB	O25-C23	5.69	1.43	1.33
11	C	504	4I2	C8-N2	5.20	1.39	1.31
10	B	505	VLB	C18-C13	4.73	1.44	1.39
10	B	505	VLB	O28-C29	4.52	1.45	1.35
10	B	505	VLB	C60-C65	4.33	1.46	1.41
11	C	504	4I2	C8-N1	3.40	1.41	1.36
11	C	504	4I2	C17-N3	3.36	1.42	1.36
12	F	401	ACP	PB-O3A	3.36	1.62	1.58
10	B	505	VLB	C58-C59	3.16	1.56	1.51
8	D	501	GDP	C5-C4	3.11	1.47	1.38
10	B	505	VLB	C57-C58	3.06	1.58	1.52
8	B	501	GDP	C5-C4	2.98	1.46	1.38
10	B	505	VLB	C68-C67	2.81	1.57	1.52
10	B	505	VLB	C57-N56	2.67	1.53	1.47
8	B	501	GDP	C6-N1	-2.51	1.34	1.38
10	B	505	VLB	C65-N66	-2.33	1.34	1.38
11	C	504	4I2	C9-N2	2.32	1.43	1.39
8	D	501	GDP	C6-N1	-2.31	1.34	1.38
5	C	501	GTP	PA-O3A	2.29	1.62	1.59
5	A	501	GTP	PA-O3A	2.26	1.61	1.59
5	A	501	GTP	C2-N3	2.15	1.38	1.33
10	B	505	VLB	C51-C52	2.12	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C5-N7	-2.05	1.35	1.39
5	C	501	GTP	C2-N3	2.03	1.38	1.33
11	C	504	4I2	C14-N3	2.00	1.45	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	VLB	C52-C69-N56	11.33	130.17	111.20
12	F	401	ACP	PB-O3A-PA	-6.70	110.51	132.37
10	B	505	VLB	O32-C16-C15	6.30	122.83	116.59
8	D	501	GDP	C5-C4-N3	-6.09	118.70	128.39
8	B	501	GDP	C5-C4-N3	-5.71	119.30	128.39
10	B	505	VLB	O75-C73-C68	5.27	119.72	111.21
10	B	505	VLB	C64-C65-C60	-5.26	117.10	122.19
8	D	501	GDP	C2-N3-C4	5.14	121.14	112.30
10	B	505	VLB	C33-O32-C16	5.13	125.03	117.51
5	A	501	GTP	C5-C4-N3	-4.85	120.68	128.39
8	B	501	GDP	C2-N3-C4	4.80	120.57	112.30
5	C	501	GTP	C5-C4-N3	-4.67	120.95	128.39
5	A	501	GTP	C2-N3-C4	4.57	120.17	112.30
10	B	505	VLB	C19-C5-C6	4.56	112.82	108.27
5	C	501	GTP	C2-N3-C4	4.53	120.09	112.30
9	B	504	MES	C5-N4-C3	4.43	118.39	108.84
8	D	501	GDP	N9-C4-N3	4.41	134.77	125.95
10	B	505	VLB	O25-C23-C3	4.38	119.42	112.21
10	B	505	VLB	C60-C59-C67	-4.30	101.37	106.84
8	B	501	GDP	N9-C4-N3	4.30	134.54	125.95
11	C	504	4I2	C8-N2-C9	4.17	113.33	109.96
11	C	504	4I2	S1-C8-N2	-4.17	111.31	115.69
10	B	505	VLB	C12-C19-C5	-4.11	115.16	118.20
10	B	505	VLB	O32-C16-C17	-4.08	117.06	124.08
10	B	505	VLB	C2-C12-C19	3.94	120.73	114.07
10	B	505	VLB	O28-C29-C30	3.74	117.75	111.09
11	C	504	4I2	C10-S1-C8	3.65	91.24	88.40
10	B	505	VLB	C22-N1-C2	3.63	127.93	119.14
8	B	501	GDP	C6-C5-N7	3.43	136.53	130.29
10	B	505	VLB	C54-C53-C52	3.42	119.29	109.98
8	D	501	GDP	C6-C5-N7	3.41	136.50	130.29
10	B	505	VLB	C3-C2-N1	3.36	117.43	112.81
10	B	505	VLB	C8-N9-C19	3.32	120.87	112.48
10	B	505	VLB	O75-C73-O74	-3.30	118.28	123.95
10	B	505	VLB	C5-C19-N9	3.26	118.59	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	VLB	C61-C60-C65	3.18	122.14	118.84
5	A	501	GTP	N9-C4-N3	3.14	132.22	125.95
10	B	505	VLB	O25-C23-O24	-3.10	118.61	123.95
10	B	505	VLB	C20-C5-C6	-3.09	104.31	107.99
5	C	501	GTP	N9-C4-N3	2.92	131.79	125.95
5	C	501	GTP	N9-C8-N7	-2.71	108.38	113.40
8	D	501	GDP	C4-C5-N7	-2.69	106.41	110.67
5	A	501	GTP	N9-C8-N7	-2.67	108.45	113.40
10	B	505	VLB	C11-C12-C13	-2.66	107.52	112.36
11	C	504	4I2	C10-C9-N2	-2.66	111.47	114.53
10	B	505	VLB	C69-N56-C55	2.64	114.44	110.87
5	A	501	GTP	C2-N1-C6	-2.61	120.37	125.11
5	C	501	GTP	C8-N7-C5	2.52	108.75	104.26
8	B	501	GDP	C4-C5-N7	-2.51	106.70	110.67
5	A	501	GTP	C8-N7-C5	2.47	108.66	104.26
5	C	501	GTP	C2-N1-C6	-2.47	120.64	125.11
9	B	504	MES	O2S-S-C8	2.41	110.37	106.73
5	A	501	GTP	C5-C6-N1	2.40	119.36	113.25
10	B	505	VLB	C61-C60-C59	-2.31	129.79	133.73
11	C	504	4I2	S1-C8-N1	2.30	128.07	121.37
5	A	501	GTP	O6-C6-C5	-2.28	120.50	126.53
5	C	501	GTP	C5-C6-N1	2.25	118.98	113.25
5	C	501	GTP	O2A-PA-O3A	2.22	113.29	107.27
5	C	501	GTP	O6-C6-C5	-2.22	120.67	126.53
8	B	501	GDP	O6-C6-C5	-2.20	120.73	126.53
10	B	505	VLB	C76-O75-C73	2.14	119.42	115.91
10	B	505	VLB	C11-C12-C2	-2.07	108.15	112.17
9	B	504	MES	O1S-S-C8	2.04	109.81	106.73
11	C	504	4I2	F3-C7-C4	-2.04	108.53	112.90
8	D	501	GDP	O6-C6-C5	-2.03	121.19	126.53

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	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

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Mol	Chain	Res	Type	Atoms
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-O2A
10	B	505	VLB	C53-C54-C70-C71
10	B	505	VLB	C58-C57-N56-C69
10	B	505	VLB	C51-C68-C73-O74
10	B	505	VLB	C51-C68-C73-O75
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	C5'-O5'-PA-O1A
10	B	505	VLB	O72-C54-C70-C71
10	B	505	VLB	C17-C16-O32-C33
10	B	505	VLB	C15-C16-O32-C33
5	A	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	PA-O3A-PB-O1B
11	C	504	4I2	S1-C8-N1-C6
5	A	501	GTP	PB-O3A-PA-O2A
11	C	504	4I2	N2-C8-N1-C6
5	C	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	PA-O3A-PB-O3B
10	B	505	VLB	C67-C68-C73-O74
12	F	401	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
11	C	504	4I2	C5-C6-N1-C8
5	C	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

4 monomers are involved in 9 short contacts:

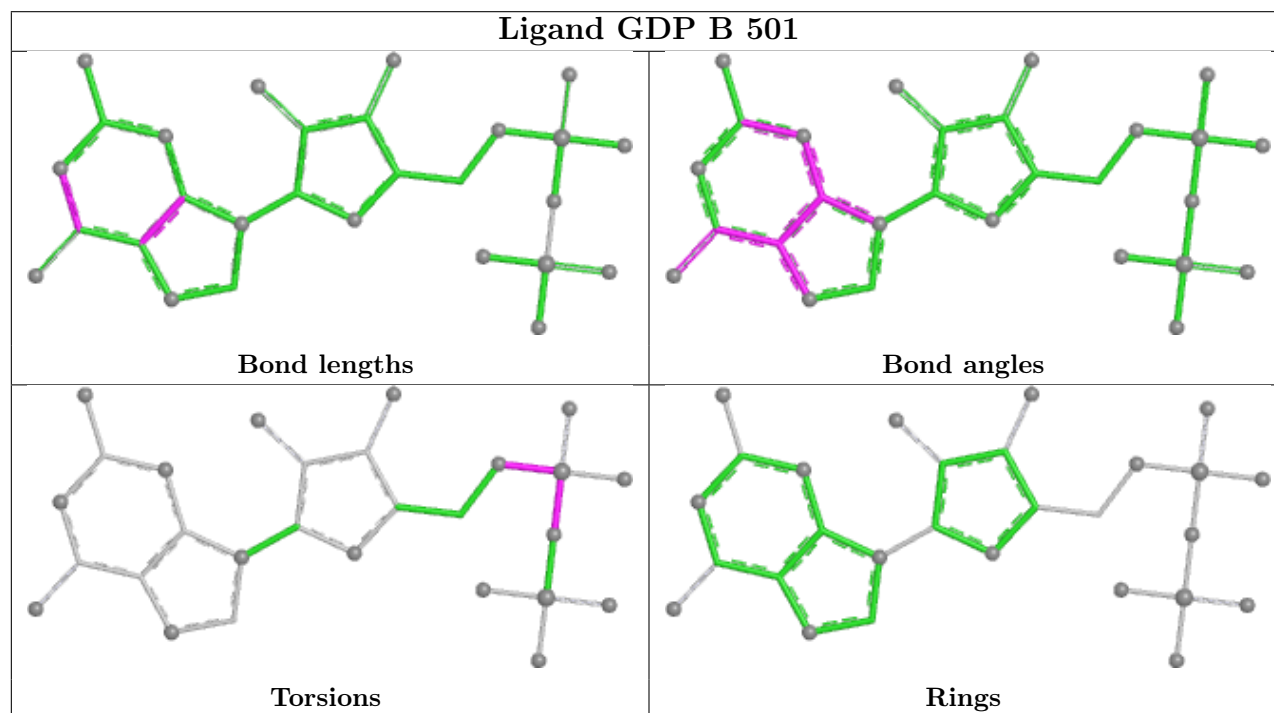
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	1	0
5	A	501	GTP	1	0
8	D	501	GDP	2	0

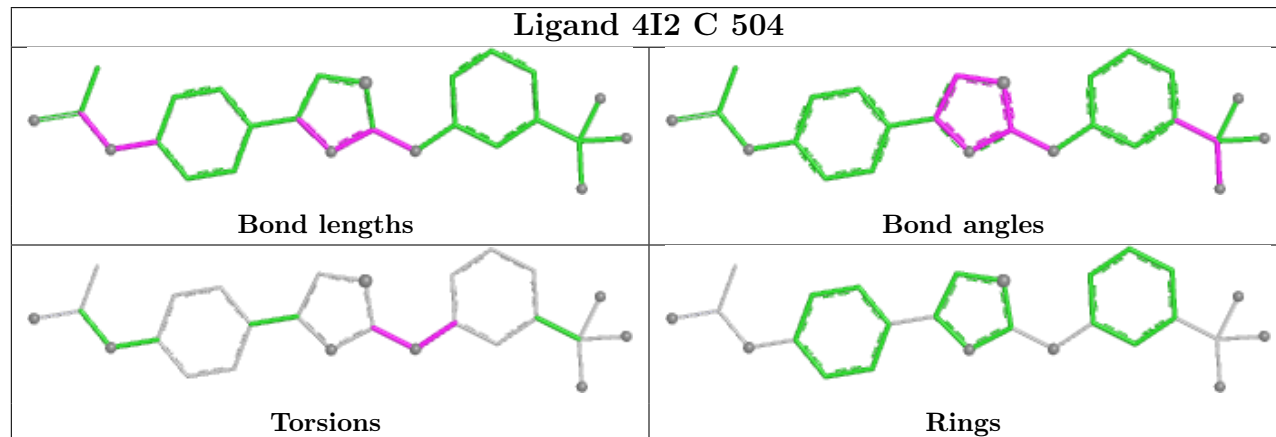
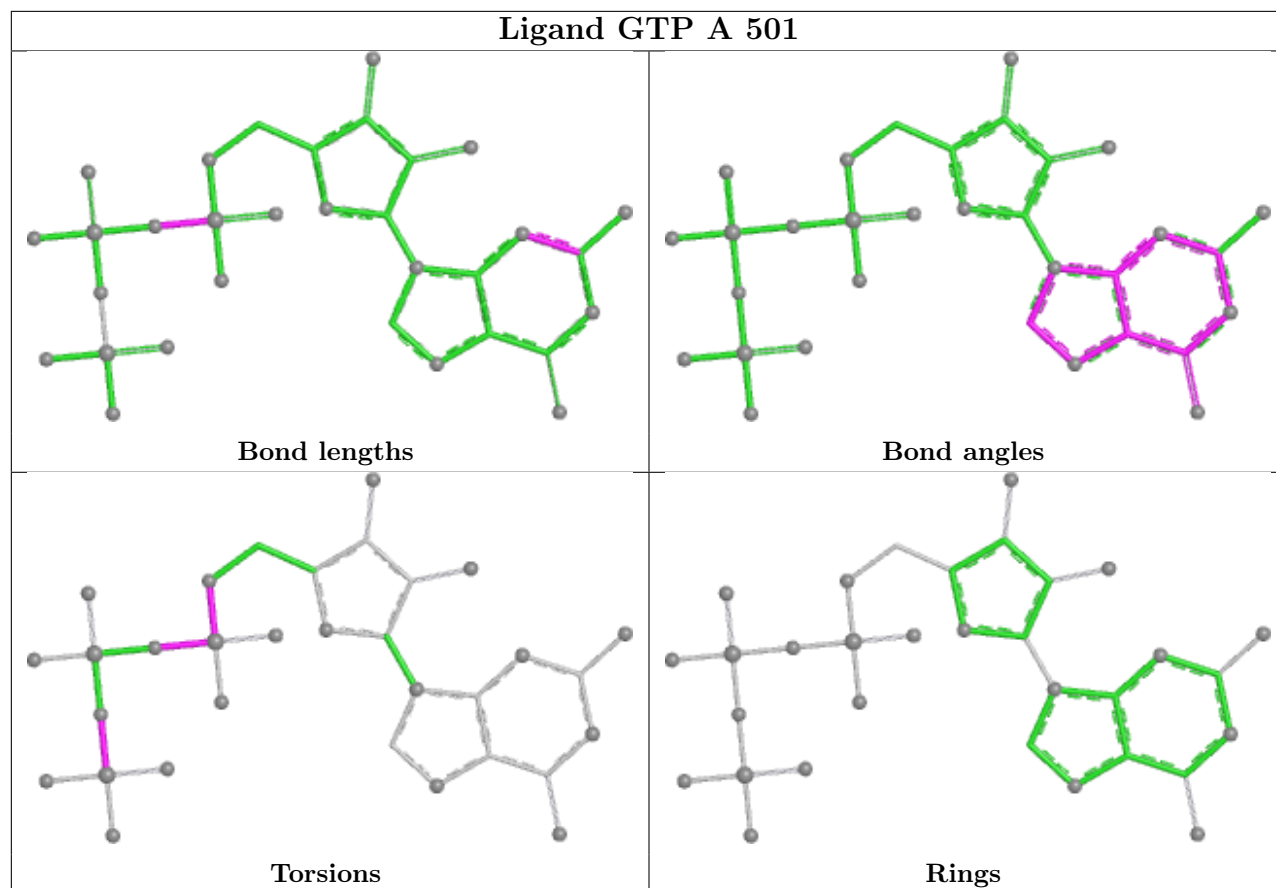
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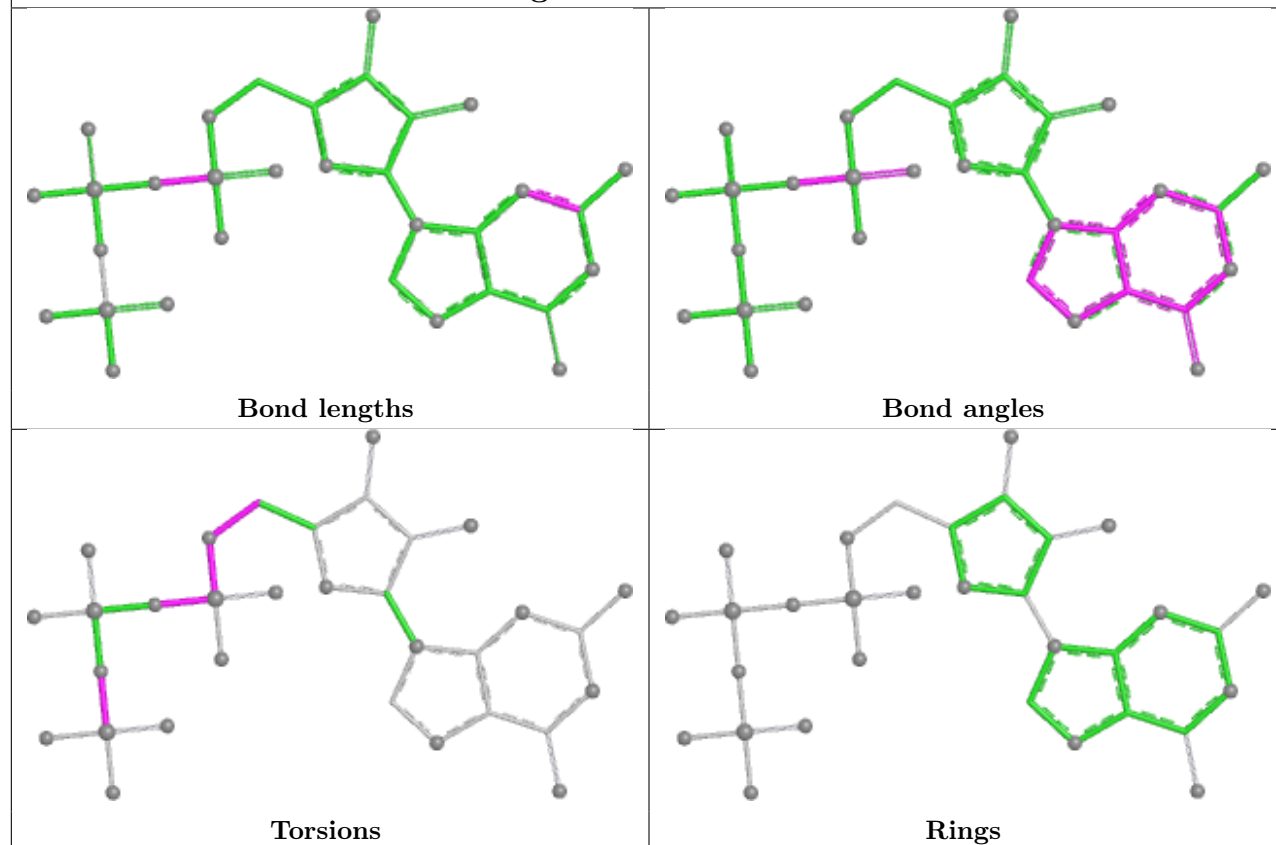
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	VLB	5	0

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

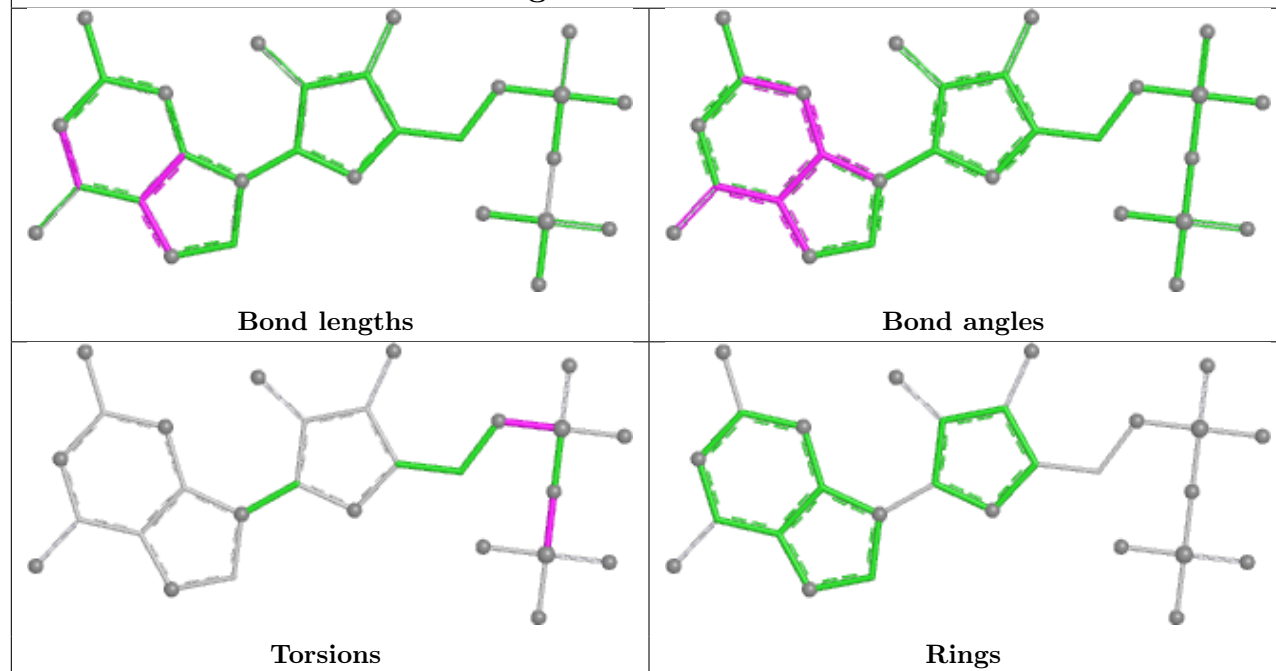


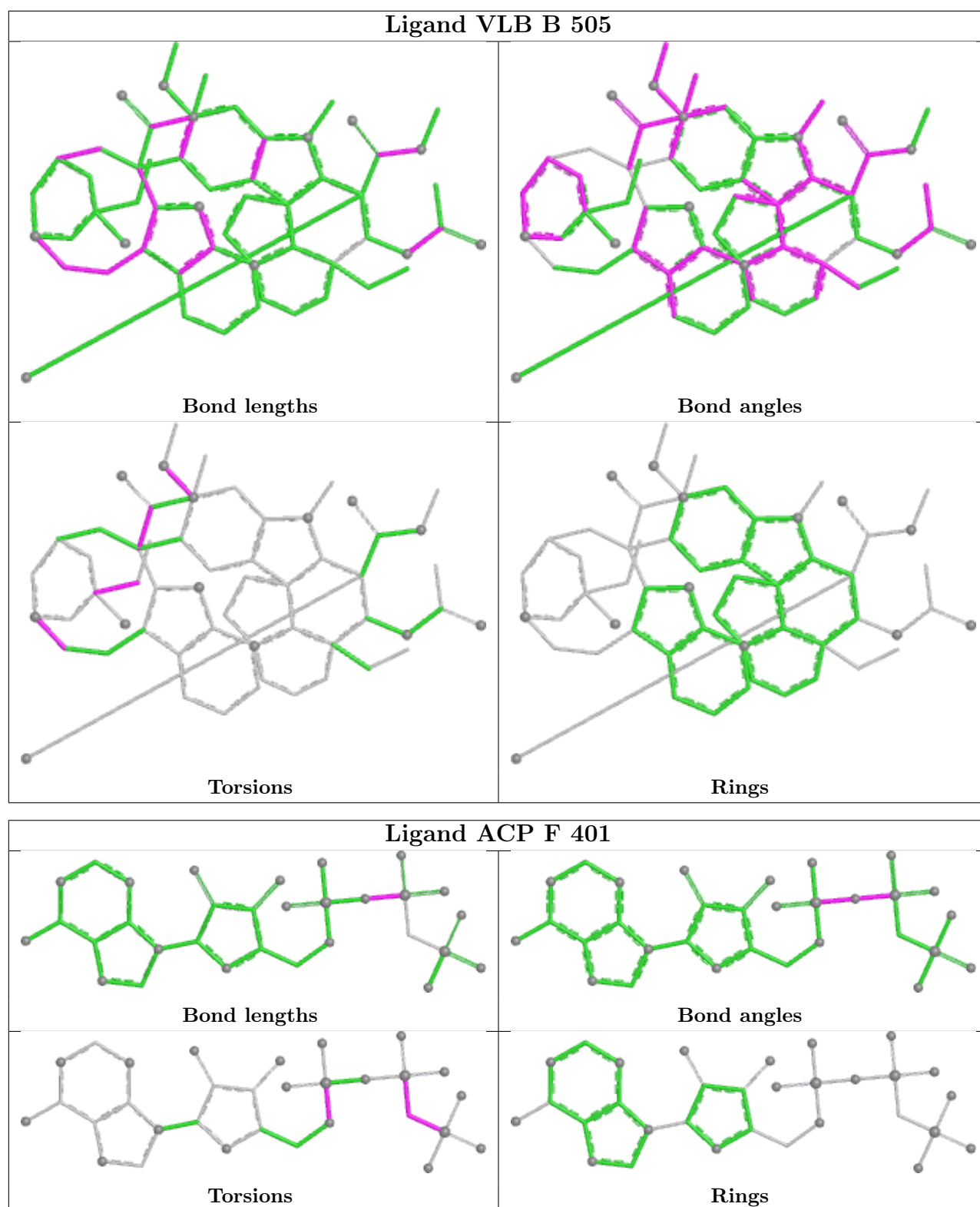


Ligand GTP C 501



Ligand GDP D 501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	437:ASP	C	438:ALA	N	2.96

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	0.54	18 (4%)	41	40	21, 50, 75, 123	2 (0%)
1	C	440/451 (97%)	0.04	16 (3%)	46	45	17, 39, 63, 76	7 (1%)
2	B	429/445 (96%)	0.28	23 (5%)	31	30	14, 42, 75, 121	4 (0%)
2	D	421/445 (94%)	0.75	28 (6%)	24	22	34, 56, 81, 109	0
3	E	122/143 (85%)	0.89	12 (9%)	13	12	22, 61, 94, 114	1 (0%)
4	F	341/384 (88%)	1.11	59 (17%)	4	3	41, 71, 123, 141	0
All	All	2190/2319 (94%)	0.54	156 (7%)	22	20	14, 51, 92, 141	14 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	4.7
4	F	155	ALA	4.5
2	D	177	VAL	4.3
2	B	438	ALA	4.2
1	C	1	MET	4.0
4	F	159	GLY	4.0
2	D	407	TRP	3.8
4	F	169	LEU	3.8
4	F	130	VAL	3.7
4	F	186	LEU	3.7
2	B	424[A]	ASN	3.7
4	F	199	PHE	3.7
1	C	256[A]	GLN	3.7
4	F	231	ALA	3.6
4	F	146	VAL	3.6
4	F	179	VAL	3.5
3	E	8	VAL	3.5
4	F	166	ALA	3.5
1	A	282	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	3.4
4	F	132	LEU	3.4
2	B	74	THR	3.4
4	F	182	ILE	3.4
2	B	248	LEU	3.3
2	B	285	ALA	3.3
4	F	131	PHE	3.3
4	F	160	ILE	3.2
2	D	172	MET	3.2
1	C	2	ARG	3.1
4	F	245	ILE	3.1
1	C	252	LEU	3.0
2	B	57	THR	3.0
1	A	250	VAL	3.0
2	B	1	MET	3.0
2	B	284	ARG	2.9
4	F	337	ALA	2.9
4	F	148	ILE	2.9
3	E	6	MET	2.9
2	D	404	PHE	2.9
4	F	20	LEU	2.9
4	F	141	GLY	2.9
3	E	27	PRO	2.9
3	E	28	SER	2.9
2	B	439	THR	2.8
1	C	340	SER	2.8
2	D	286	LEU	2.8
4	F	105	LEU	2.8
1	A	437	VAL	2.8
3	E	23	ILE	2.8
1	C	88	HIS	2.8
2	D	410	GLY	2.8
4	F	240	LEU	2.8
2	B	440	ALA	2.7
1	C	440	VAL	2.7
2	D	57	THR	2.7
4	F	151	SER	2.7
4	F	134	ALA	2.6
3	E	26	PRO	2.6
4	F	181	VAL	2.6
2	D	1	MET	2.6
4	F	321	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	330	ILE	2.5
2	D	83	PHE	2.5
1	C	108	TYR	2.5
2	B	282	GLN	2.5
4	F	162	ILE	2.5
2	B	276	THR	2.5
3	E	15	THR	2.5
4	F	170	LEU	2.5
2	B	94	PHE	2.5
4	F	172	PHE	2.5
4	F	238	CYS	2.4
1	C	80	THR	2.4
1	A	283	HIS	2.4
1	A	309	HIS	2.4
4	F	17	VAL	2.4
4	F	253	TYR	2.4
2	D	70	LEU	2.4
4	F	6	VAL	2.4
4	F	220	VAL	2.4
1	A	262	TYR	2.4
1	A	281	ALA	2.4
2	B	50	ASN	2.4
2	B	280	SER	2.4
4	F	152	SER	2.4
4	F	196	HIS	2.4
1	A	92	LEU	2.3
2	D	214	PHE	2.3
3	E	50	ILE	2.3
2	D	406	HIS	2.3
1	A	196	GLU	2.3
1	C	283	HIS	2.3
2	D	391	ILE	2.3
4	F	99	VAL	2.3
2	D	175	PRO	2.3
4	F	339	ALA	2.3
4	F	190	LEU	2.3
4	F	200	ASP	2.3
2	D	72	PRO	2.3
1	C	308	ARG	2.3
2	B	56	ALA	2.3
4	F	89	GLU	2.2
1	A	349	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	237	THR	2.2
4	F	198	LYS	2.2
4	F	22	LEU	2.2
1	A	113	GLU	2.2
4	F	18	SER	2.2
1	A	418	PHE	2.2
2	B	16	ILE	2.2
4	F	149	ALA	2.2
2	D	42	LEU	2.2
2	D	275	LEU	2.2
2	D	37	HIS	2.2
2	B	325	MET	2.2
1	A	333	ALA	2.2
2	D	317	ALA	2.2
2	D	405	LEU	2.2
4	F	101	TYR	2.2
1	A	18	ASN	2.2
4	F	102	PRO	2.1
2	D	377	PHE	2.1
4	F	362	ALA	2.1
2	B	46	LEU	2.1
1	C	163	LYS	2.1
1	C	284	GLU	2.1
1	C	57	GLY	2.1
4	F	144	GLY	2.1
3	E	57	ALA	2.1
4	F	335	ALA	2.1
4	F	236	LYS	2.1
2	D	441	ASP	2.1
4	F	98	TYR	2.1
2	B	247	GLN	2.1
1	A	93	ILE	2.1
1	A	335	ILE	2.1
4	F	44	ARG	2.1
2	D	440	ALA	2.1
3	E	24	LEU	2.1
2	B	127	GLU	2.1
2	D	101	ASN	2.1
2	D	108	TYR	2.1
1	C	341	ILE	2.1
2	D	298	SER	2.1
3	E	16	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	246	GLY	2.0
4	F	249	TYR	2.0
4	F	254	GLY	2.0
3	E	105	MET	2.0
2	D	337	ASN	2.0
2	D	219	LEU	2.0
1	C	46	ASP	2.0
2	B	130	ASP	2.0
2	B	241	CYS	2.0
4	F	150	LYS	2.0
1	A	193	THR	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.

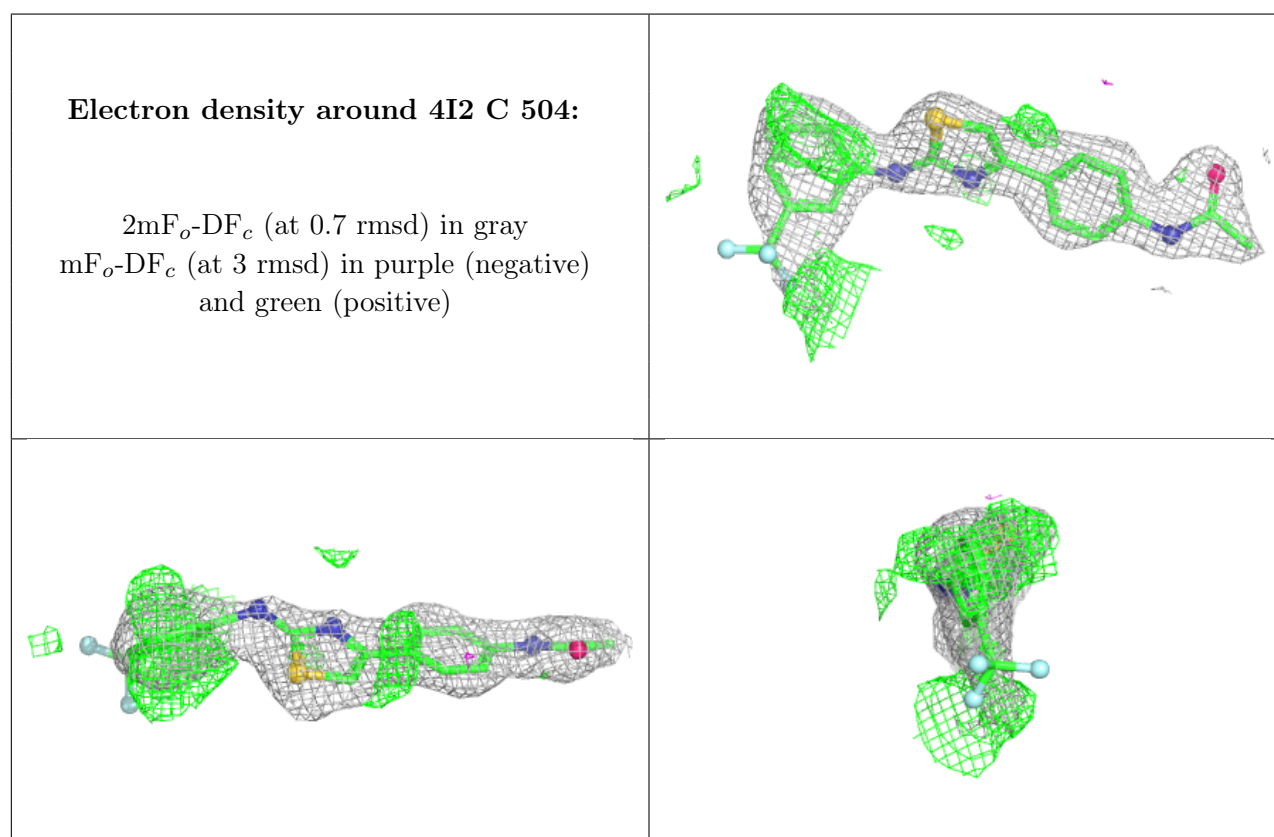
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.82	0.15	61,61,61,61	0
7	CA	B	503	1/1	0.83	0.10	93,93,93,93	0
11	4I2	C	504	26/26	0.84	0.22	29,48,58,69	26
8	GDP	D	501	28/28	0.89	0.12	38,52,72,93	0
7	CA	E	201	1/1	0.89	0.10	98,98,98,98	0
12	ACP	F	401	31/31	0.89	0.10	60,80,101,112	0
9	MES	B	504	12/12	0.91	0.12	39,52,61,62	0
6	MG	F	402	1/1	0.95	0.08	70,70,70,70	0
10	VLB	B	505	59/59	0.95	0.07	28,34,44,54	0
5	GTP	A	501	32/32	0.96	0.07	27,34,42,44	0
7	CA	A	503	1/1	0.97	0.07	66,66,66,66	0
8	GDP	B	501	28/28	0.98	0.05	26,29,31,36	0

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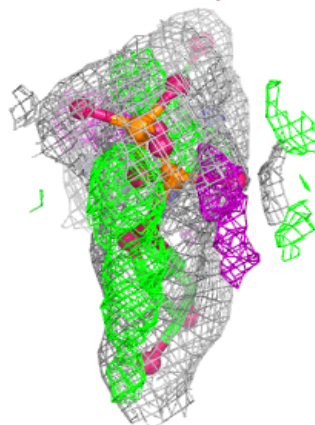
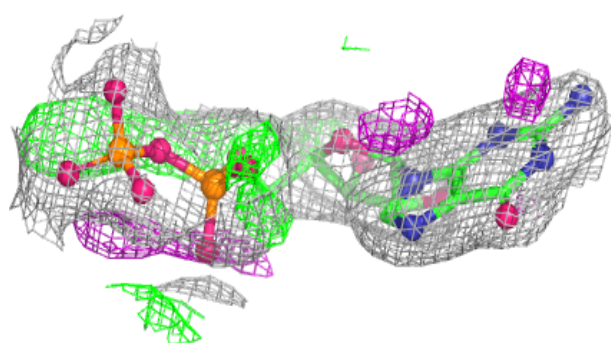
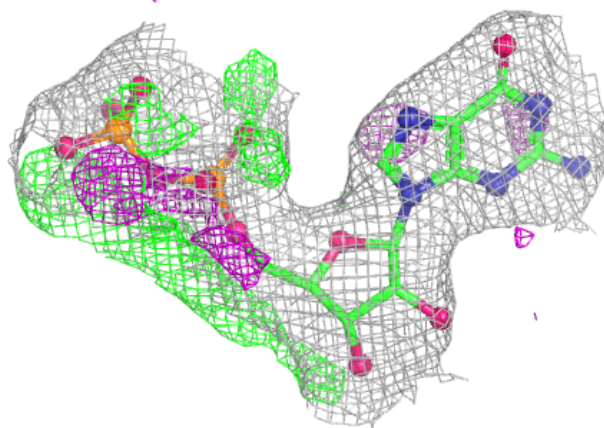
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	502	1/1	0.98	0.03	34,34,34,34	0
5	GTP	C	501	32/32	0.98	0.05	24,29,32,33	0
6	MG	C	502	1/1	0.99	0.03	27,27,27,27	0
7	CA	C	503	1/1	0.99	0.03	58,58,58,58	0
6	MG	B	502	1/1	0.99	0.04	37,37,37,37	0

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.

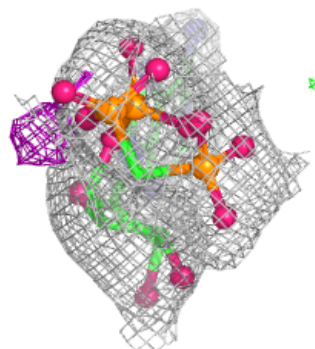
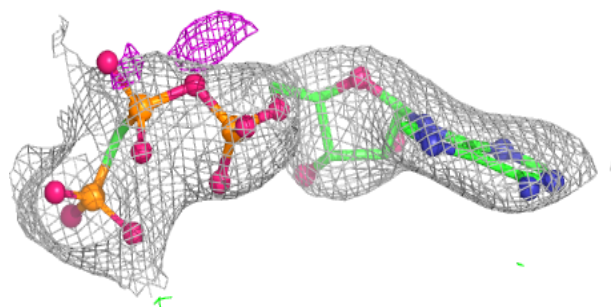
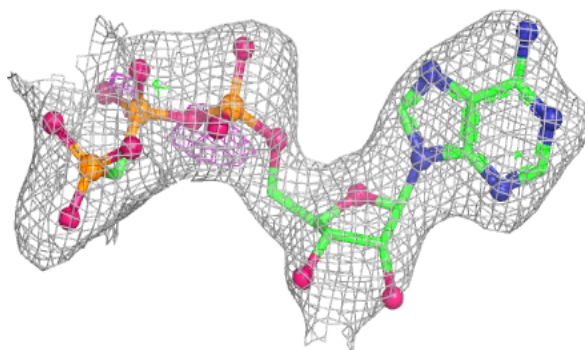


Electron density around GDP D 501:

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

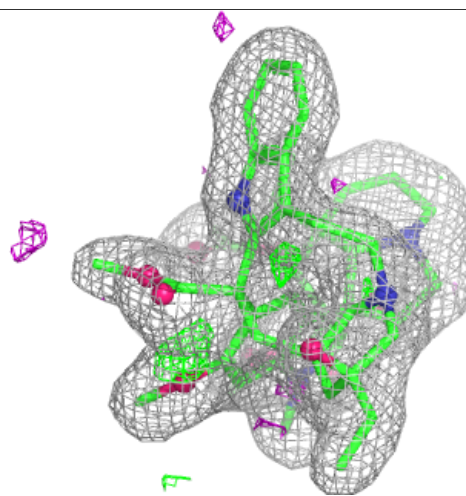
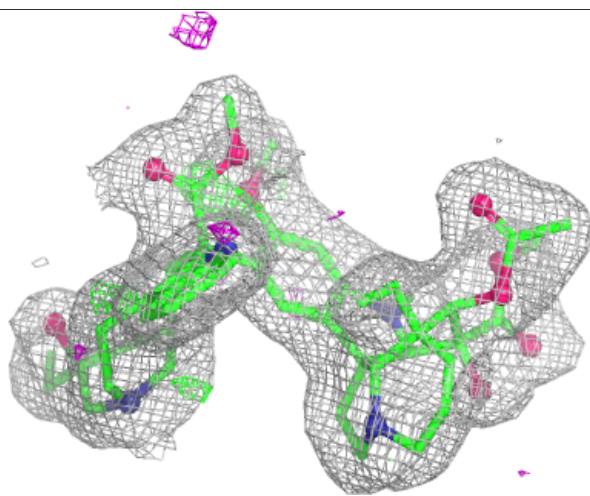
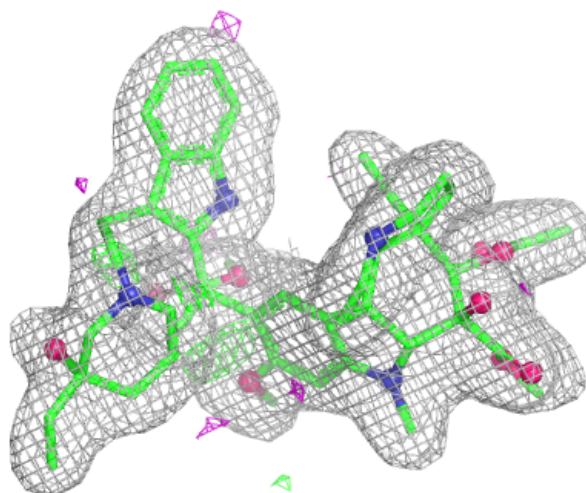
**Electron density around ACP F 401:**

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



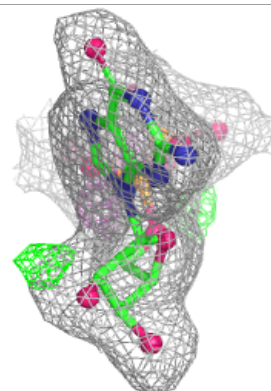
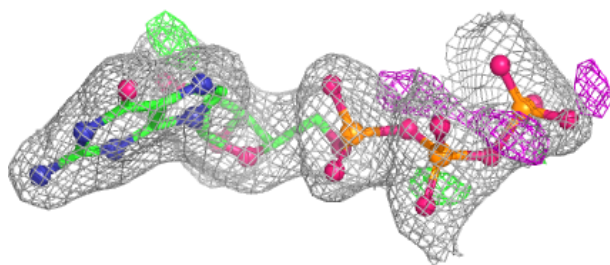
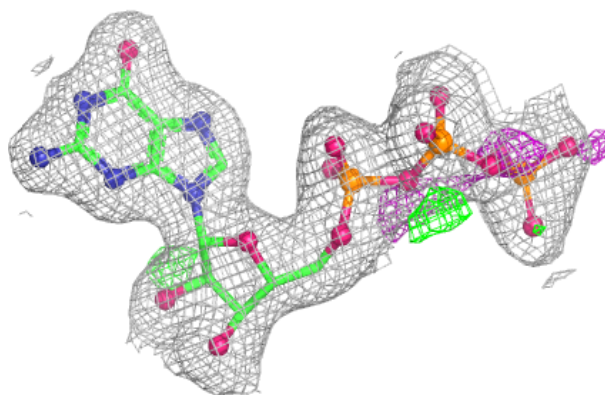
Electron density around VLB B 505:

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



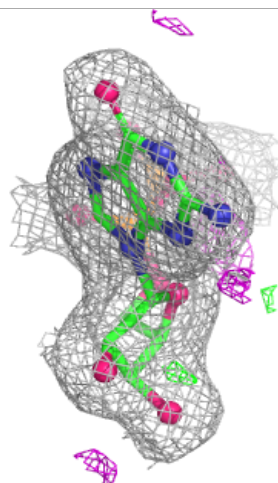
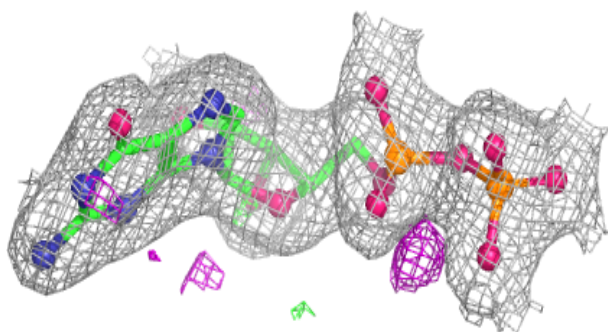
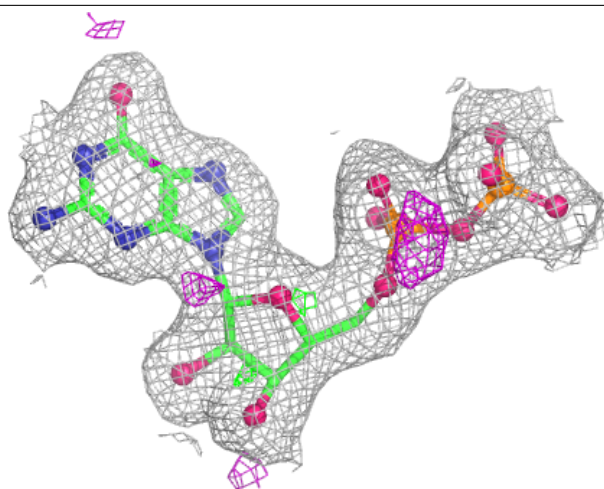
Electron density around GTP A 501:

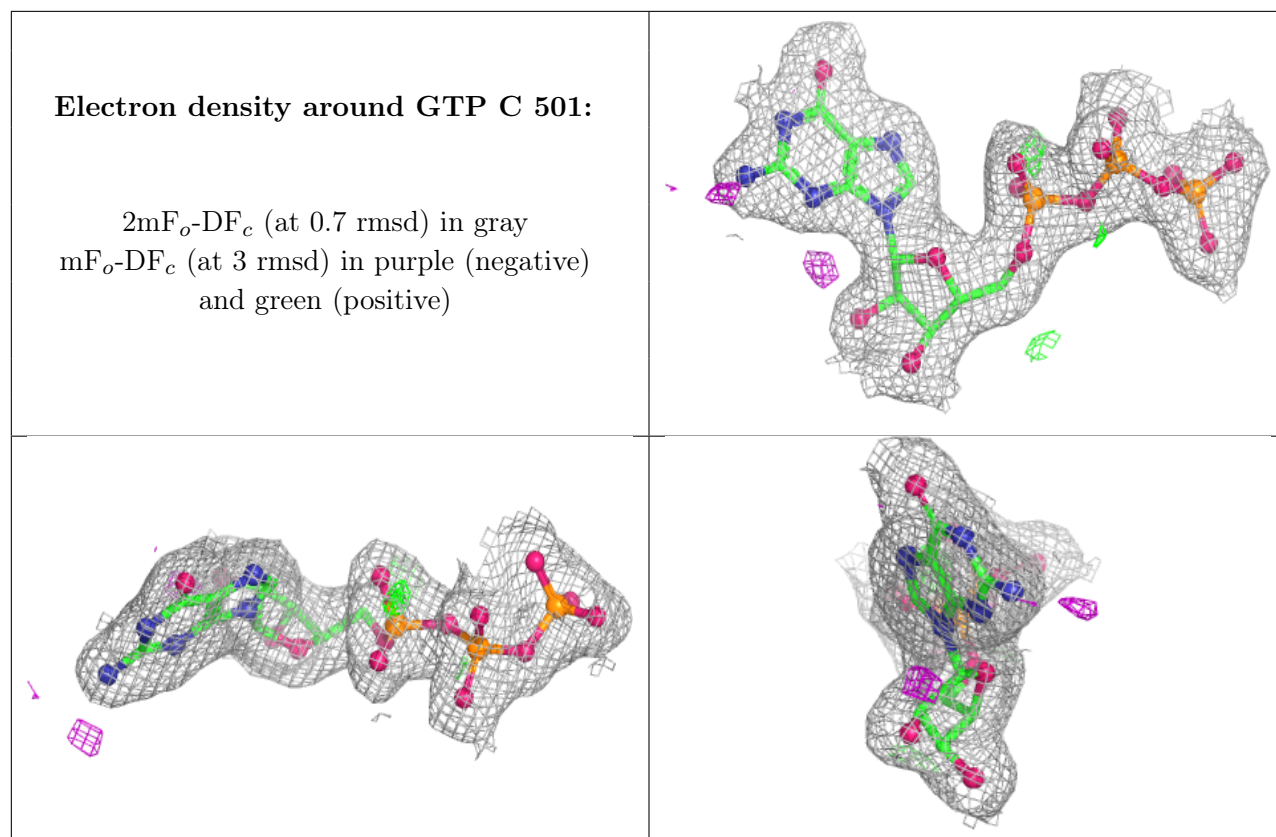
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.