



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:08 PM UTC

PDB ID : 5JH7 / pdb_00005jh7
Title : Tubulin-Eribulin complex
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Deposited on : 2016-04-20
Resolution : 2.25 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](#) ①) were used in the production of this report:

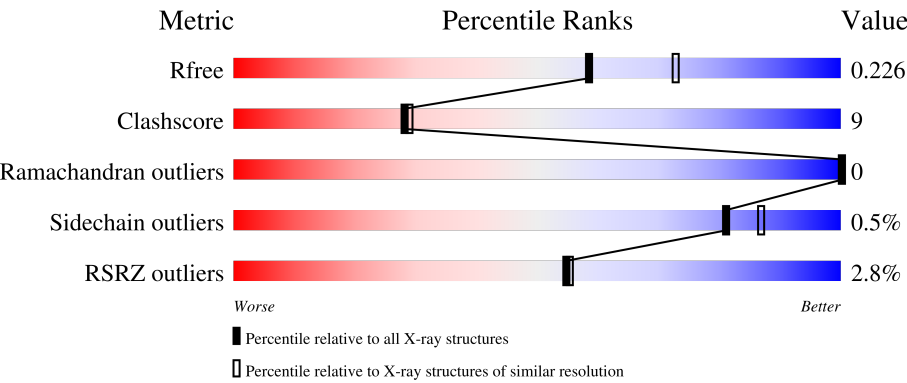
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	% 82%15%..
1	C	450	% 83%14%..
2	B	445	4% 76%20%.
2	D	445	3% 73%22%5%
3	E	143	3% 69%15%15%

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	IMD	B	507	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18483 atoms, of which 118 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	439	Total	C	N	O	S	0	2	0
			3436	2174	583	655	24			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- 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	1	0
			3360	2112	573	648	27			
2	D	424	Total	C	N	O	S	0	1	0
			3335	2095	568	644	28			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

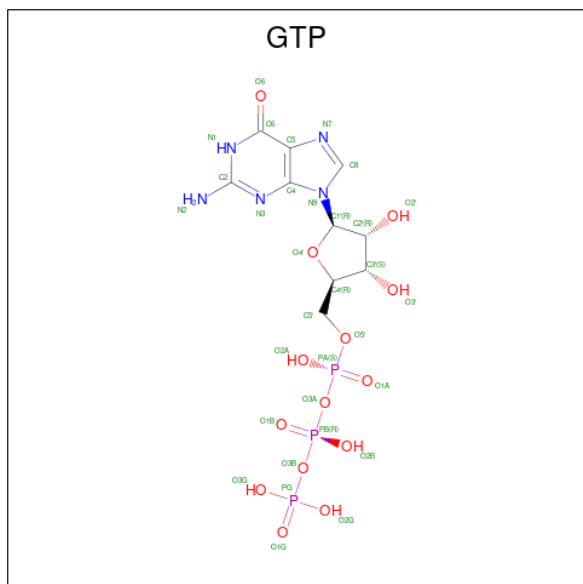
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	342	Total	C	N	O	S	0	0	0
			2800	1797	477	512	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 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

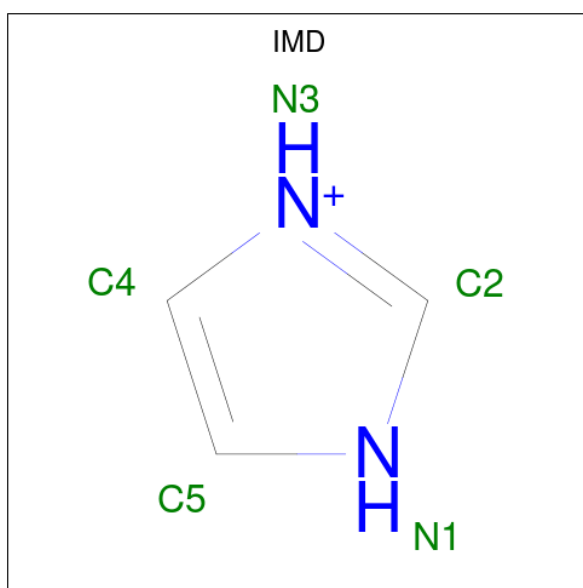
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

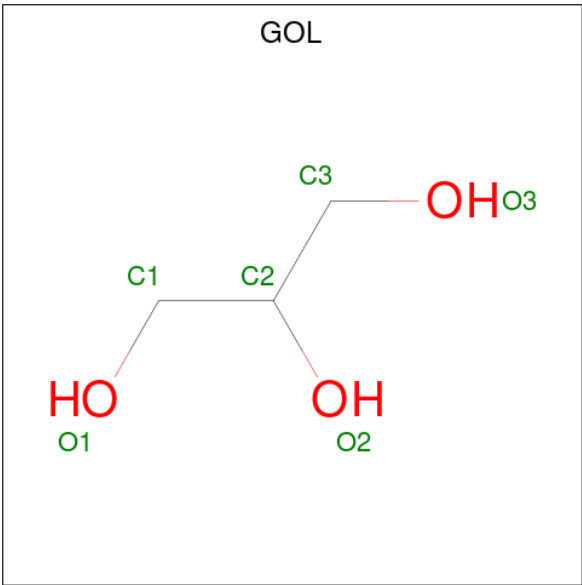
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	2	Total Ca 2 2	0	0
7	E	1	Total Ca 1 1	0	0

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



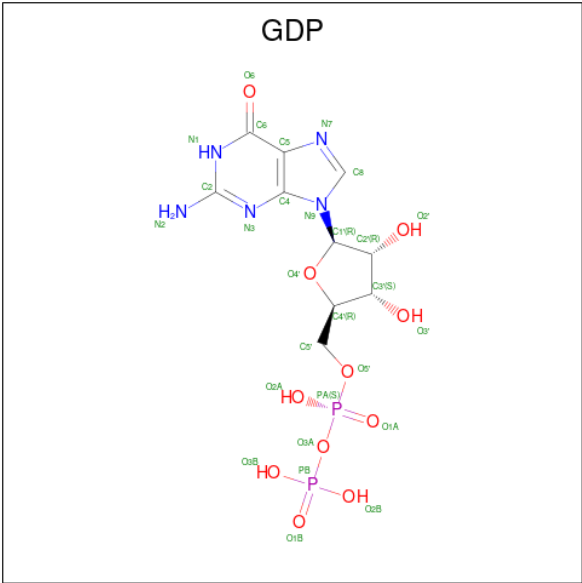
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N 5 3 2	0	0
8	B	1	Total C N 5 3 2	0	0
8	B	1	Total C N 5 3 2	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



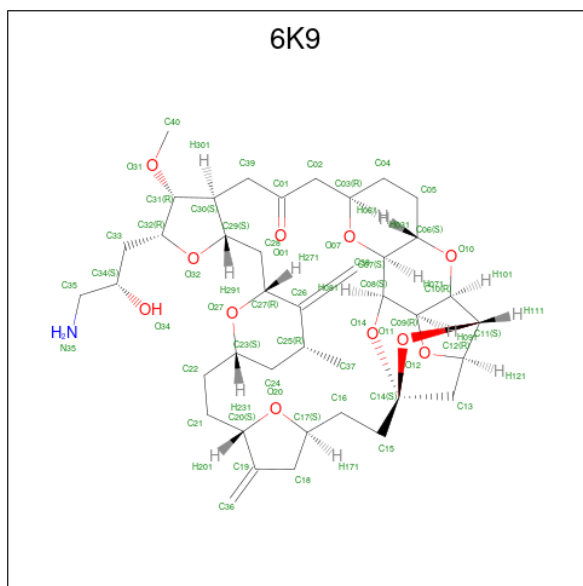
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



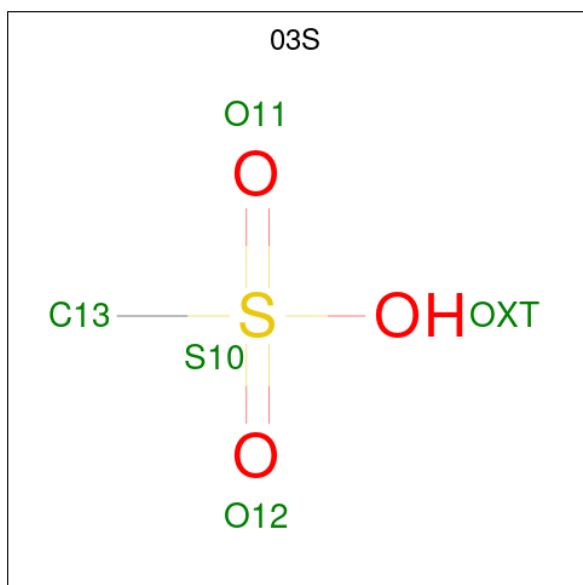
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	D	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 11 is (1S,3S,6S,9S,12S,14R,16R,18S,20R,21R,22S,26R,29S,31R,32S,33R,35R,36S)-20-[(2S)-3-amino-2-hydroxypropyl]-21-methoxy-14-methyl-8,15-dimethylidene-2,19,30,34,37,39,40,41-octaoxononacyclo[24.9.2.1^{3,32}.1^{3,33}.1^{6,9}.1^{12,16}.0^{18,22}.0^{29,36}.0^{31,35}]hen tetracontan-24-one (non-preferred name) (CCD ID: 6K9) (formula: C₄₀H₅₉NO₁₁).



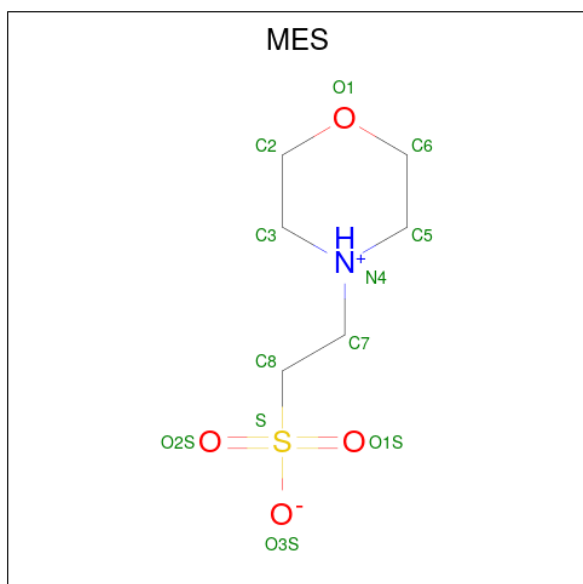
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	0	0
			111	40	59	1	11		
11	D	1	Total	C	H	N	O	0	0
			111	40	59	1	11		

- Molecule 12 is methanesulfonic acid (CCD ID: 03S) (formula: CH₄O₃S).



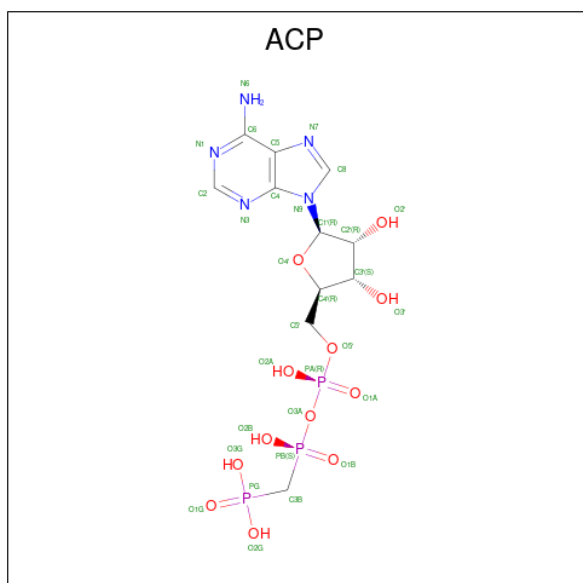
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	O	S	0	0
			5	1	3	1		

- Molecule 13 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

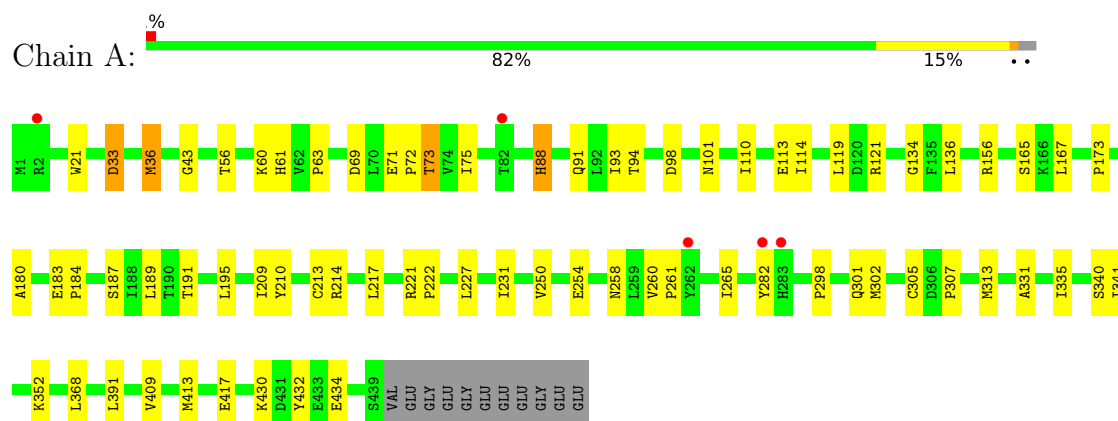
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	150	Total	O	0	0
			150	150		
15	B	112	Total	O	0	0
			112	112		
15	C	231	Total	O	0	0
			231	231		
15	D	99	Total	O	0	0
			99	99		
15	E	34	Total	O	0	0
			34	34		
15	F	64	Total	O	0	0
			64	64		

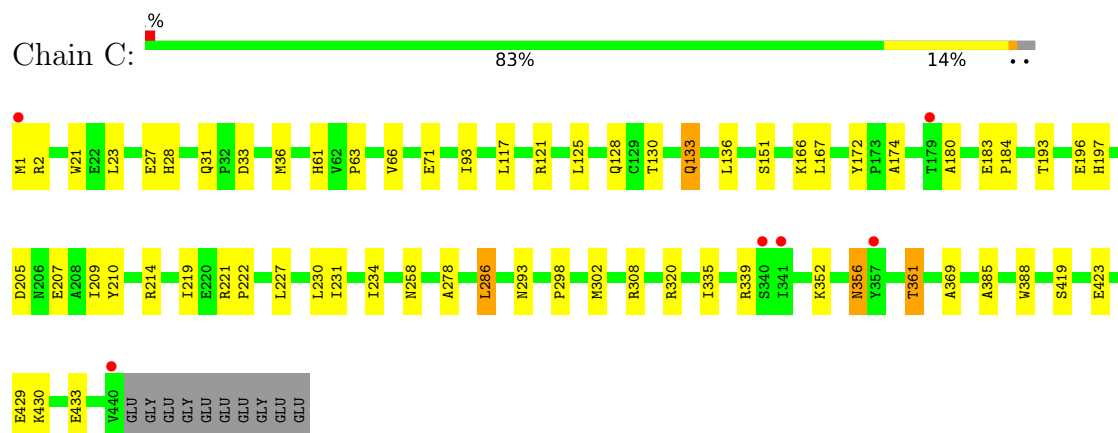
3 Residue-property plots [i](#)

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.

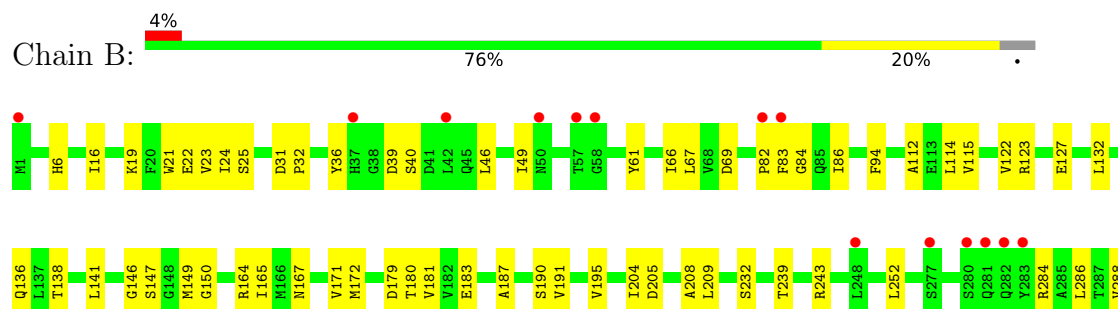
• Molecule 1: Tubulin alpha-1B chain

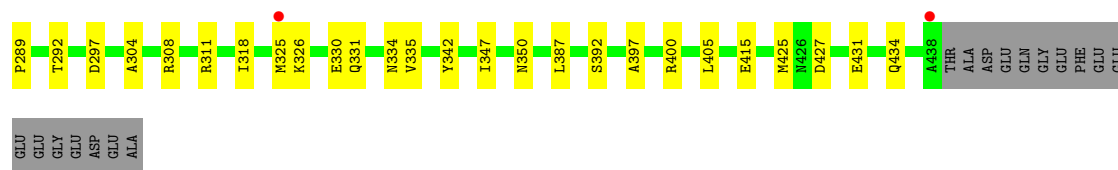


• Molecule 1: Tubulin alpha-1B chain

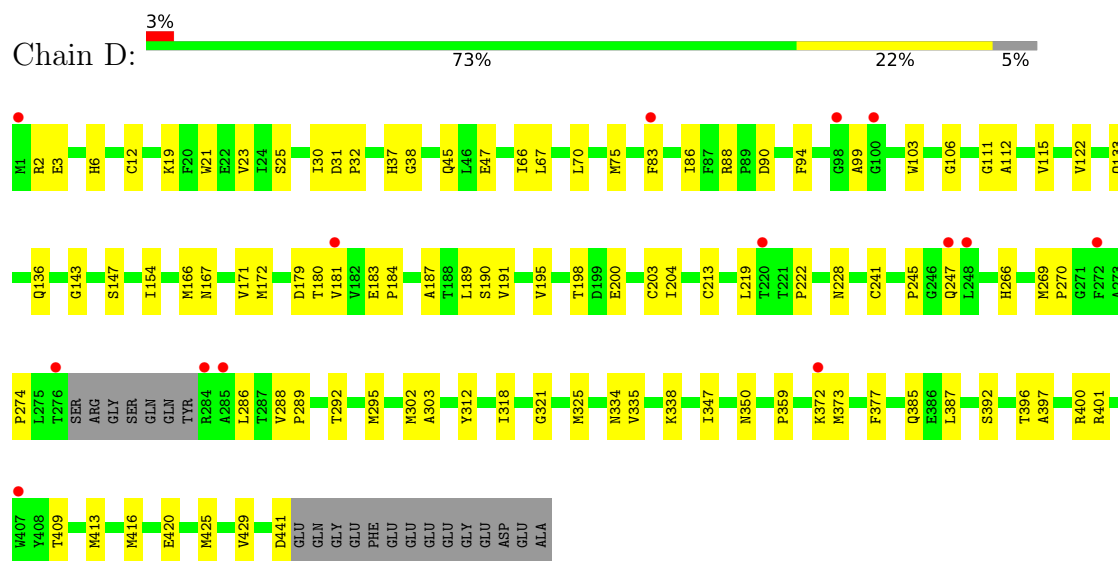


• Molecule 2: Tubulin beta-2B chain

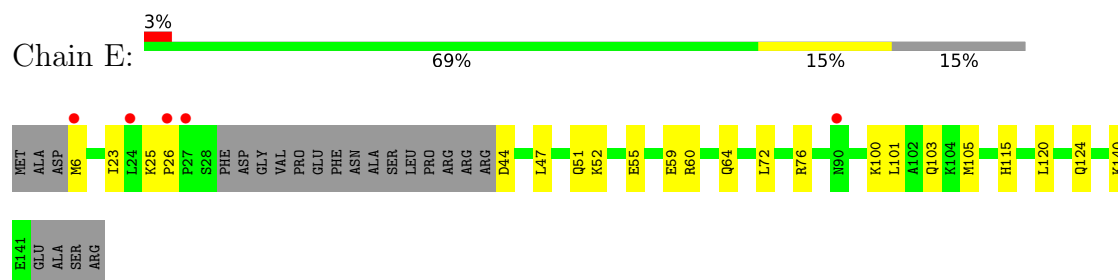




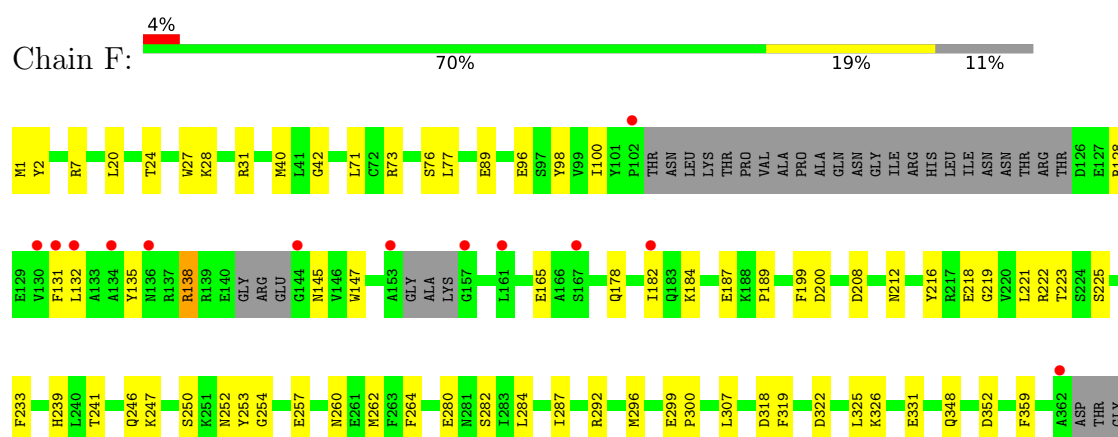
• Molecule 2: Tubulin beta-2B chain

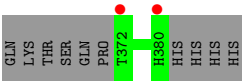


• Molecule 3: Stathmin-4



• 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	105.22Å 157.13Å 182.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.18 – 2.25 72.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.18-2.25) 99.9 (72.18-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.181 , 0.220 0.192 , 0.226	Depositor DCC
R_{free} test set	7166 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	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	18483	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6K9, 03S, GTP, CA, ACP, GOL, MES, GDP, IMD

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	0.27	0/3520	0.72	6/4778 (0.1%)
1	C	0.28	0/3515	0.69	0/4772
2	B	0.27	0/3438	0.68	0/4658
2	D	0.26	0/3411	0.69	0/4620
3	E	0.25	0/1008	0.59	0/1337
4	F	0.24	0/2863	0.66	0/3866
All	All	0.26	0/17755	0.68	6/24031 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	HIS	CA-C-N	5.60	126.84	119.84
1	A	88	HIS	C-N-CA	5.60	126.84	119.84
1	A	260	VAL	CA-C-N	5.28	124.46	118.97
1	A	260	VAL	C-N-CA	5.28	124.46	118.97
1	A	36	MET	CA-C-N	5.12	125.15	119.32
1	A	36	MET	C-N-CA	5.12	125.15	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3436	0	3349	54	0
1	C	3437	0	3348	47	0
2	B	3360	0	3232	73	0
2	D	3335	0	3219	70	0
3	E	1000	0	1018	16	0
4	F	2800	0	2764	54	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	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	2	0	0	0	0
7	E	1	0	0	0	0
8	A	5	0	5	0	0
8	B	10	0	10	4	0
9	A	6	0	8	0	0
9	C	6	0	8	1	0
10	B	28	0	12	1	0
10	D	28	0	12	3	0
11	B	52	59	0	0	0
11	D	52	59	0	0	0
12	B	5	0	4	1	0
13	B	12	0	12	2	0
14	F	31	0	14	3	0
15	A	150	0	0	3	0
15	B	112	0	0	3	0
15	C	231	0	0	2	0
15	D	99	0	0	5	0
15	E	34	0	0	4	0
15	F	64	0	0	0	0
All	All	18365	118	17039	310	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 9.

All (310) 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)
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.44	0.99
3:E:25:LYS:HD2	3:E:26:PRO:HD2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.51	0.91
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.53	0.89
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.52	0.89
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.55	0.88
2:D:213:CYS:HB3	2:D:219:LEU:HD11	1.59	0.83
1:C:221:ARG:HD2	2:D:325:MET:HE3	1.62	0.80
2:B:46:LEU:HD12	2:B:49:ILE:HG21	1.64	0.79
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.17	0.78
2:B:82:PRO:HA	2:B:84:GLY:H	1.48	0.78
1:A:110:ILE:O	15:A:601:HOH:O	2.07	0.73
1:C:27:GLU:HG2	1:C:361:THR:CG2	2.18	0.73
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.36	0.72
1:C:128:GLN:NE2	15:C:601:HOH:O	2.23	0.72
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.72	0.71
2:D:241[B]:CYS:SG	15:D:693:HOH:O	2.47	0.71
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.71	0.70
2:D:147:SER:OG	2:D:190:SER:OG	2.10	0.70
2:D:372:LYS:HE3	2:D:373:MET:HE3	1.74	0.70
1:A:114:ILE:N	15:A:601:HOH:O	2.23	0.70
2:B:331:GLN:HA	2:B:334:ASN:ND2	2.08	0.68
4:F:7:ARG:CD	4:F:40:MET:HE3	2.22	0.68
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.78	0.66
3:E:25:LYS:CD	3:E:26:PRO:HD2	2.26	0.65
3:E:120:LEU:O	3:E:124:GLN:HG2	1.96	0.65
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.79	0.65
1:C:27:GLU:HG2	1:C:361:THR:HG23	1.78	0.65
4:F:98:TYR:HB2	4:F:182:ILE:CG2	2.27	0.65
1:C:133:GLN:HG2	9:C:505:GOL:H2	1.79	0.64
4:F:89:GLU:N	4:F:89:GLU:OE1	2.31	0.64
4:F:348:GLN:NE2	4:F:352:ASP:OD2	2.30	0.64
2:B:132:LEU:O	2:B:164:ARG:NH1	2.28	0.63
2:D:136:GLN:HA	2:D:167:ASN:O	1.99	0.63
2:B:23:VAL:HG21	2:B:232:SER:OG	1.99	0.62
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.80	0.62
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.35	0.62
1:A:33:ASP:N	1:A:33:ASP:OD1	2.34	0.60
2:B:46:LEU:HD12	2:B:49:ILE:CG2	2.31	0.60
2:D:247:GLN:NE2	15:D:601:HOH:O	2.23	0.60
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.19	0.60
2:D:2:ARG:HB3	2:D:133:GLN:HG3	1.84	0.60
1:C:286:LEU:H	1:C:286:LEU:HD12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:SER:HB3	2:D:30:ILE:HD11	1.83	0.60
2:D:321:GLY:HA2	2:D:359:PRO:HG3	1.83	0.60
2:B:284:ARG:NH1	15:B:605:HOH:O	2.35	0.60
8:B:506:IMD:H2	8:B:507:IMD:H5	1.84	0.60
3:E:47:LEU:O	3:E:51:GLN:HG2	2.01	0.60
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.38	0.59
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.83	0.59
1:C:221:ARG:CD	2:D:325:MET:HE3	2.31	0.59
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.85	0.58
2:B:83:PHE:O	2:B:86:ILE:HG12	2.03	0.58
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.38	0.58
1:A:180:ALA:O	1:A:183:GLU:HG3	2.03	0.58
2:B:397:ALA:HA	2:B:400:ARG:NH1	2.18	0.58
2:D:219:LEU:HD12	2:D:219:LEU:O	2.04	0.58
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.86	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.85	0.57
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.87	0.57
2:D:274:PRO:HB3	2:D:286:LEU:CD1	2.33	0.57
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.86	0.57
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.87	0.57
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.86	0.57
1:C:180:ALA:O	1:C:183:GLU:HG3	2.04	0.57
2:D:83:PHE:O	2:D:86:ILE:HG22	2.05	0.57
3:E:6:MET:N	3:E:23:ILE:O	2.38	0.56
2:B:82:PRO:HA	2:B:84:GLY:N	2.18	0.56
8:B:506:IMD:H2	8:B:507:IMD:C5	2.36	0.56
4:F:178:GLN:N	4:F:178:GLN:OE1	2.39	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.56
4:F:71:LEU:HD12	4:F:77:LEU:HD13	1.88	0.56
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.06	0.55
1:A:110:ILE:O	1:A:113:GLU:HG2	2.06	0.55
2:B:46:LEU:HD11	2:B:61:TYR:OH	2.06	0.55
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.70	0.55
4:F:241:THR:OG1	14:F:400:ACP:O3'	2.19	0.55
2:D:143:GLY:HA3	10:D:501:GDP:O3A	2.07	0.55
2:B:171:VAL:HA	2:B:204:ILE:O	2.06	0.55
4:F:98:TYR:HB2	4:F:182:ILE:HG23	1.88	0.55
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.89	0.55
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.42	0.54
2:D:25:SER:HB3	2:D:30:ILE:CD1	2.36	0.54
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:318:ASP:OD2	14:F:400:ACP:O3G	2.26	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.07	0.54
2:B:331:GLN:HA	2:B:334:ASN:HD21	1.72	0.54
1:A:71:GLU:OE2	1:A:73:THR:HB	2.07	0.54
2:B:431:GLU:O	2:B:434:GLN:HG2	2.07	0.54
4:F:73:ARG:HB2	4:F:76:SER:HB2	1.89	0.54
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.90	0.54
4:F:331:GLU:OE2	14:F:400:ACP:O1G	2.27	0.54
2:D:198:THR:HG1	2:D:266:HIS:HE2	1.56	0.53
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.91	0.53
4:F:225:SER:HB3	4:F:252:ASN:HB2	1.90	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
3:E:72:LEU:O	3:E:76:ARG:HG2	2.09	0.53
2:B:179:ASP:OD2	15:B:601:HOH:O	2.19	0.53
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.91	0.53
2:B:297:ASP:HA	8:B:507:IMD:C4	2.39	0.53
4:F:184:LYS:NZ	4:F:187:GLU:OE2	2.42	0.53
2:D:409:THR:O	3:E:140:LYS:NZ	2.40	0.53
2:B:392:SER:HB2	2:B:425:MET:HE3	1.91	0.52
1:C:234:ILE:HD13	1:C:302:MET:SD	2.48	0.52
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.90	0.52
2:B:181:VAL:HB	1:C:258:ASN:OD1	2.10	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.09	0.52
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.40	0.52
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.09	0.52
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.92	0.52
4:F:131:PHE:CE1	4:F:182:ILE:HG12	2.45	0.52
2:D:292:THR:O	2:D:295:MET:HG2	2.10	0.51
3:E:44:ASP:N	15:E:304:HOH:O	2.42	0.51
3:E:55:GLU:O	3:E:59:GLU:HG2	2.10	0.51
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.92	0.51
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.92	0.51
1:C:1:MET:HG2	1:C:130:THR:OG1	2.10	0.51
4:F:40:MET:HE2	4:F:42:GLY:HA3	1.93	0.51
1:A:430:LYS:O	1:A:434:GLU:HG3	2.11	0.51
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.26	0.51
2:B:39:ASP:OD1	2:B:40:SER:N	2.43	0.51
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.51
2:D:274:PRO:HB3	2:D:286:LEU:HD11	1.92	0.51
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.92	0.51
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:219:LEU:CD1	2:D:222:PRO:HB3	2.41	0.50
3:E:100:LYS:O	3:E:103:GLN:HG3	2.10	0.50
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.35	0.50
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.41	0.50
3:E:100:LYS:NZ	15:E:305:HOH:O	2.43	0.50
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.46	0.50
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.93	0.50
1:C:151:SER:HB3	1:C:193:THR:HG21	1.92	0.50
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.93	0.50
2:D:191:VAL:O	2:D:195:VAL:HG23	2.12	0.49
4:F:1:MET:CE	4:F:28:LYS:HB2	2.35	0.49
4:F:247:LYS:HE2	4:F:253:TYR:OH	2.12	0.49
2:D:67:LEU:N	2:D:67:LEU:HD12	2.26	0.49
4:F:299:GLU:N	4:F:300:PRO:HD2	2.27	0.49
2:B:164:ARG:O	13:B:505:MES:H71	2.12	0.49
10:B:501:GDP:O1A	12:B:504:03S:H313	2.13	0.49
2:B:67:LEU:N	2:B:67:LEU:HD12	2.27	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.49
2:B:427:ASP:O	2:B:431:GLU:HG3	2.13	0.49
2:D:25:SER:CB	2:D:30:ILE:HD11	2.43	0.49
2:D:180:THR:O	2:D:181:VAL:HB	2.12	0.49
4:F:40:MET:HE2	4:F:42:GLY:CA	2.43	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.49
2:D:179:ASP:O	2:D:181:VAL:HG23	2.12	0.49
1:C:286:LEU:HD12	1:C:286:LEU:N	2.28	0.48
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.96	0.48
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.13	0.48
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.43	0.48
1:A:409:VAL:HA	1:A:413:MET:O	2.14	0.48
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.95	0.48
2:D:30:ILE:HD13	2:D:86:ILE:HD11	1.96	0.48
4:F:135:TYR:OH	4:F:165:GLU:HA	2.14	0.48
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.43	0.48
2:B:308:ARG:HG3	2:B:342:TYR:CZ	2.49	0.48
2:D:187:ALA:O	2:D:191:VAL:HG23	2.14	0.48
1:A:189:LEU:HD21	1:A:413:MET:HE1	1.95	0.47
1:A:210:TYR:CD2	1:A:214:ARG:HD2	2.49	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
1:A:340:SER:C	1:A:341:ILE:HD12	2.38	0.47
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.47
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.13	0.47
13:B:505:MES:H51	13:B:505:MES:H81	1.67	0.47
1:A:213:CYS:O	1:A:217:LEU:HB2	2.15	0.47
1:C:27:GLU:HG2	1:C:361:THR:HG21	1.96	0.47
2:D:396:THR:O	2:D:400:ARG:HG2	2.15	0.47
4:F:292:ARG:HG2	4:F:296:MET:SD	2.55	0.47
1:A:341:ILE:HD12	1:A:341:ILE:N	2.29	0.47
2:D:66:ILE:HD12	2:D:122:VAL:HG22	1.95	0.47
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.97	0.47
2:D:213:CYS:O	2:D:219:LEU:HG	2.15	0.47
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.49	0.47
1:A:331:ALA:O	1:A:335:ILE:HG13	2.15	0.47
2:B:123:ARG:O	2:B:127:GLU:HG3	2.14	0.47
4:F:135:TYR:HD1	4:F:145:ASN:HD21	1.63	0.46
2:D:37:HIS:HB2	15:D:692:HOH:O	2.15	0.46
1:A:221:ARG:HG3	2:B:325:MET:CB	2.45	0.46
2:D:441:ASP:HA	15:D:673:HOH:O	2.15	0.46
2:B:36:TYR:OH	2:B:40:SER:O	2.33	0.46
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.98	0.46
1:A:136:LEU:CD2	1:A:167:LEU:HB2	2.46	0.46
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.22	0.46
4:F:138:ARG:NH1	4:F:184:LYS:HE2	2.30	0.46
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.51	0.45
1:C:419:SER:O	1:C:423:GLU:HG3	2.17	0.45
2:D:213:CYS:HB3	2:D:219:LEU:CD1	2.41	0.45
1:A:227:LEU:O	1:A:231:ILE:HG13	2.17	0.45
1:A:33:ASP:O	1:A:60:LYS:HE2	2.16	0.45
1:A:69:ASP:O	1:A:94:THR:HA	2.17	0.45
1:A:71:GLU:HG2	1:A:72:PRO:N	2.32	0.45
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.46	0.45
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.85	0.45
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.51	0.45
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.98	0.45
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.16	0.45
2:B:318:ILE:N	2:B:318:ILE:HD12	2.32	0.45
1:C:196:GLU:HB2	15:C:685:HOH:O	2.15	0.45
1:C:430:LYS:HB3	1:C:430:LYS:HE2	1.86	0.45
4:F:20:LEU:O	4:F:24:THR:HG23	2.17	0.45
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.45
1:C:352:LYS:HB3	1:C:352:LYS:HE3	1.80	0.45
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLY:HA2	1:A:56:THR:O	2.17	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.45
2:B:387:LEU:C	2:B:387:LEU:HD23	2.42	0.45
2:D:19:LYS:O	2:D:23:VAL:HG23	2.16	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.17	0.44
1:A:173:PRO:HB3	1:A:183:GLU:OE2	2.18	0.44
1:A:305:CYS:O	1:A:307:PRO:HD3	2.17	0.44
2:B:187:ALA:O	2:B:191:VAL:HG23	2.18	0.44
2:D:274:PRO:HB3	2:D:286:LEU:HD12	1.98	0.44
2:B:331:GLN:O	2:B:335:VAL:HG23	2.17	0.44
3:E:60:ARG:O	3:E:64:GLN:HG3	2.18	0.44
4:F:246:GLN:O	4:F:250:SER:HB3	2.17	0.44
2:B:83:PHE:HB3	2:B:86:ILE:HD13	1.98	0.44
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.44
1:C:166:LYS:HE2	1:C:197:HIS:O	2.16	0.44
3:E:101:LEU:O	3:E:105:MET:HG2	2.16	0.44
2:B:22:GLU:HB2	2:B:83:PHE:CD1	2.53	0.44
3:E:52:LYS:HE3	3:E:52:LYS:HB2	1.86	0.44
2:B:19:LYS:HG3	2:B:232:SER:HB2	1.99	0.44
2:D:409:THR:HA	2:D:413:MET:O	2.17	0.43
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.53	0.43
2:B:180:THR:O	2:B:183:GLU:HG3	2.18	0.43
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.54	0.43
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.54	0.43
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.43
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.43
2:D:112:ALA:O	2:D:115:VAL:HG12	2.19	0.43
3:E:115:HIS:HA	15:E:307:HOH:O	2.18	0.43
4:F:128:ARG:O	4:F:132:LEU:HG	2.18	0.43
2:B:22:GLU:HB2	2:B:83:PHE:CE1	2.54	0.43
2:B:311:ARG:NH1	4:F:31:ARG:HH12	2.17	0.43
2:B:21:TRP:CZ3	2:B:24:ILE:HD11	2.53	0.43
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.43
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.00	0.43
1:C:227:LEU:O	1:C:231:ILE:HG13	2.19	0.43
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.34	0.43
3:E:115:HIS:HB3	15:E:334:HOH:O	2.18	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.42
2:B:325:MET:HE2	15:B:703:HOH:O	2.18	0.42
1:C:31:GLN:HB2	1:C:33:ASP:OD1	2.19	0.42
2:D:75:MET:SD	2:D:94:PHE:HB3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:416:MET:O	2:D:420:GLU:HG3	2.19	0.42
2:B:286:LEU:N	2:B:286:LEU:HD12	2.35	0.42
2:D:392:SER:HB2	2:D:425:MET:HE3	2.01	0.42
1:A:114:ILE:HG22	15:A:601:HOH:O	2.18	0.42
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.49	0.42
4:F:208:ASP:OD2	4:F:212:ASN:HB2	2.20	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.42
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.19	0.42
2:B:239:THR:O	2:B:243:ARG:HG2	2.19	0.42
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.55	0.42
4:F:145:ASN:ND2	4:F:147:TRP:HE1	2.18	0.42
4:F:322:ASP:OD2	4:F:326:LYS:HB3	2.20	0.42
4:F:200:ASP:OD2	4:F:222:ARG:NH1	2.53	0.42
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.50	0.42
4:F:199:PHE:HA	4:F:241:THR:HG21	2.01	0.42
2:B:334:ASN:OD1	2:B:335:VAL:N	2.53	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.42
1:A:191:THR:O	1:A:195:LEU:HB2	2.21	0.41
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.02	0.41
2:D:172:MET:HE3	2:D:203:CYS:SG	2.60	0.41
2:B:21:TRP:O	2:B:25:SER:OG	2.31	0.41
2:B:179:ASP:OD1	1:C:352:LYS:HD2	2.21	0.41
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.20	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HG3	2.03	0.41
1:A:221:ARG:HG3	2:B:325:MET:HB3	2.02	0.41
1:C:28:HIS:O	1:C:36:MET:HE3	2.19	0.41
1:A:136:LEU:HD23	1:A:167:LEU:HB2	2.02	0.41
2:B:191:VAL:O	2:B:195:VAL:HG23	2.20	0.41
1:C:151:SER:HB3	1:C:193:THR:CG2	2.50	0.41
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.55	0.41
2:B:46:LEU:HD11	2:B:61:TYR:CZ	2.56	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.02	0.41
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.35	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.45	0.41
2:B:326:LYS:O	2:B:330:GLU:HG3	2.20	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.41
2:D:318:ILE:HD13	15:D:606:HOH:O	2.20	0.41
2:B:16:ILE:HD11	2:B:138:THR:HB	2.01	0.41
2:B:405:LEU:HD21	2:B:415:GLU:HG2	2.03	0.41
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.41
2:B:82:PRO:CA	2:B:84:GLY:H	2.28	0.41
2:D:228:ASN:OD1	10:D:501:GDP:N1	2.32	0.41
4:F:254:GLY:HA2	4:F:257:GLU:O	2.20	0.41
2:B:112:ALA:O	2:B:115:VAL:HG12	2.20	0.41
2:B:146:GLY:O	2:B:150:GLY:HA3	2.20	0.41
2:B:205:ASP:O	2:B:209:LEU:HG	2.20	0.41
4:F:257:GLU:HG2	4:F:260:ASN:HA	2.03	0.41
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.37	0.40
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.03	0.40
1:C:2:ARG:HA	1:C:2:ARG:HD2	1.77	0.40
1:C:429:GLU:O	1:C:433:GLU:HG3	2.21	0.40
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.40	0.40
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.57	0.40
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.03	0.40
2:D:3:GLU:O	2:D:133:GLN:HB2	2.21	0.40
2:D:397:ALA:O	2:D:401:ARG:HD3	2.21	0.40
4:F:189:PRO:HA	4:F:322:ASP:HA	2.03	0.40
4:F:233:PHE:HD1	4:F:239:HIS:NE2	2.19	0.40
2:B:297:ASP:HA	8:B:507:IMD:H4	2.04	0.40
4:F:222:ARG:HH12	4:F:318:ASP:CG	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/450 (98%)	422 (96%)	17 (4%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
2	D	421/445 (95%)	414 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	332/384 (86%)	318 (96%)	14 (4%)	0	100	100
All	All	2174/2317 (94%)	2119 (98%)	55 (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	372/378 (98%)	369 (99%)	3 (1%)	73	80
1	C	371/378 (98%)	365 (98%)	6 (2%)	55	66
2	B	367/383 (96%)	367 (100%)	0	100	100
2	D	367/383 (96%)	367 (100%)	0	100	100
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	307/342 (90%)	306 (100%)	1 (0%)	86	90
All	All	1893/1991 (95%)	1883 (100%)	10 (0%)	81	87

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

Mol	Chain	Res	Type
1	A	33	ASP
1	A	73	THR
1	A	282	TYR
1	C	71	GLU
1	C	133	GLN
1	C	286	LEU
1	C	293	ASN
1	C	356	ASN
1	C	361	THR
4	F	138	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	309	HIS
1	A	356	ASN
1	A	393	HIS
2	B	15	GLN
2	B	91	ASN
2	B	294	GLN
1	C	283	HIS
1	C	342	GLN
1	C	372	GLN
1	C	393	HIS
2	D	8	GLN
2	D	37	HIS
2	D	85	GLN
2	D	136	GLN
2	D	167	ASN
2	D	300	ASN
3	E	136	ASN
4	F	145	ASN
4	F	242	ASN
4	F	243	HIS
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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$
9	GOL	C	505	-	5,5,5	0.36	0	5,5,5	0.38	0
8	IMD	A	504	-	5,5,5	0.65	0	5,5,5	0.44	0
9	GOL	A	505	-	5,5,5	0.39	0	5,5,5	0.29	0
10	GDP	D	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.71	6 (13%)
10	GDP	B	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
14	ACP	F	400	6	31,33,33	2.00	7 (22%)	47,52,52	2.31	14 (29%)
8	IMD	B	506	-	5,5,5	0.63	0	5,5,5	0.43	0
5	GTP	A	501	6	33,34,34	1.02	3 (9%)	50,54,54	1.55	8 (16%)
5	GTP	C	501	6	33,34,34	0.96	3 (9%)	50,54,54	1.52	9 (18%)
8	IMD	B	507	-	5,5,5	0.63	0	5,5,5	0.43	0
13	MES	B	505	-	12,12,12	2.31	1 (8%)	15,16,16	1.85	2 (13%)
11	6K9	B	503	-	57,60,60	2.22	14 (24%)	61,92,92	1.81	14 (22%)
12	03S	B	504	-	4,4,4	1.97	2 (50%)	6,6,6	0.58	0
11	6K9	D	502	-	57,60,60	2.22	14 (24%)	61,92,92	1.74	15 (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
9	GOL	C	505	-	-	2/4/4/4	-
8	IMD	A	504	-	-	-	0/1/1/1
9	GOL	A	505	-	-	2/4/4/4	-
10	GDP	D	501	-	-	5/16/32/32	0/3/3/3
10	GDP	B	501	-	-	4/16/32/32	0/3/3/3
14	ACP	F	400	6	-	10/19/38/38	0/3/3/3
8	IMD	B	506	-	-	-	0/1/1/1
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
13	MES	B	505	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	IMD	B	507	-	-	-	0/1/1/1
11	6K9	B	503	-	-	2/31/131/131	-
11	6K9	D	502	-	-	3/31/131/131	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	505	MES	C8-S	-7.72	1.66	1.77
11	D	502	6K9	C18-C19	-7.34	1.40	1.51
11	B	503	6K9	C18-C19	-7.33	1.40	1.51
11	D	502	6K9	C02-C01	-7.10	1.41	1.51
11	B	503	6K9	C02-C01	-6.86	1.41	1.51
14	F	400	ACP	PG-O1G	5.67	1.61	1.50
11	D	502	6K9	C39-C01	-5.50	1.43	1.51
11	B	503	6K9	C39-C01	-5.45	1.43	1.51
14	F	400	ACP	C6-N6	5.44	1.48	1.34
11	B	503	6K9	O11-C11	4.66	1.50	1.43
11	B	503	6K9	C38-C26	4.47	1.39	1.32
11	D	502	6K9	O11-C11	4.40	1.50	1.43
11	D	502	6K9	C38-C26	4.32	1.39	1.32
11	B	503	6K9	C20-C19	-3.47	1.43	1.51
11	B	503	6K9	C33-C32	3.44	1.58	1.52
11	D	502	6K9	C20-C19	-3.44	1.43	1.51
11	D	502	6K9	C33-C32	3.40	1.58	1.52
10	D	501	GDP	C5-C4	3.20	1.47	1.38
14	F	400	ACP	C2'-C3'	-3.07	1.45	1.53
10	B	501	GDP	C5-C4	3.07	1.47	1.38
11	B	503	6K9	C30-C29	3.05	1.59	1.53
11	D	502	6K9	C30-C29	2.95	1.59	1.53
11	D	502	6K9	C27-C26	-2.94	1.43	1.52
11	B	503	6K9	C08-C07	-2.93	1.46	1.52
11	D	502	6K9	C08-C07	-2.87	1.46	1.52
11	B	503	6K9	C27-C26	-2.85	1.43	1.52
11	B	503	6K9	C33-C34	2.65	1.58	1.52
11	D	502	6K9	C33-C34	2.62	1.58	1.52
12	B	504	03S	O11-S10	2.62	1.53	1.44
12	B	504	03S	O12-S10	2.60	1.53	1.44
11	D	502	6K9	C24-C25	2.47	1.57	1.53
10	B	501	GDP	C6-N1	-2.45	1.34	1.38
10	D	501	GDP	C6-N1	-2.37	1.34	1.38
5	A	501	GTP	PA-O3A	2.37	1.62	1.59
11	D	502	6K9	O07-C03	2.37	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	400	ACP	PG-O3G	2.36	1.60	1.55
11	B	503	6K9	C24-C25	2.34	1.57	1.53
11	B	503	6K9	O07-C03	2.33	1.48	1.44
14	F	400	ACP	O5'-C5'	-2.32	1.35	1.44
5	A	501	GTP	PB-O3B	2.27	1.61	1.59
14	F	400	ACP	O3'-C3'	-2.15	1.37	1.43
5	A	501	GTP	C2-N3	2.14	1.38	1.33
5	C	501	GTP	PB-O3B	2.11	1.61	1.59
14	F	400	ACP	C5-N7	-2.10	1.35	1.39
11	B	503	6K9	C05-C04	2.09	1.58	1.52
10	D	501	GDP	PA-O3A	2.08	1.61	1.59
11	D	502	6K9	C05-C04	2.07	1.57	1.52
5	C	501	GTP	C2-N3	2.04	1.38	1.33
10	D	501	GDP	C5-N7	-2.03	1.35	1.39
10	B	501	GDP	C5-N7	-2.03	1.35	1.39
5	C	501	GTP	PA-O3A	2.02	1.61	1.59

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	400	ACP	O4'-C1'-N9	-7.53	93.63	108.09
10	B	501	GDP	C5-C4-N3	-6.21	118.51	128.39
10	D	501	GDP	C5-C4-N3	-6.03	118.79	128.39
14	F	400	ACP	C5-C4-N3	-5.42	119.25	126.72
14	F	400	ACP	C2'-C1'-N9	5.14	126.08	113.30
10	B	501	GDP	C2-N3-C4	5.11	121.10	112.30
10	D	501	GDP	C2-N3-C4	4.90	120.74	112.30
5	A	501	GTP	C5-C4-N3	-4.85	120.67	128.39
5	C	501	GTP	C5-C4-N3	-4.70	120.90	128.39
11	B	503	6K9	C16-C15-C14	-4.68	107.94	114.43
10	B	501	GDP	N9-C4-N3	4.54	135.03	125.95
5	A	501	GTP	C2-N3-C4	4.53	120.09	112.30
5	C	501	GTP	C2-N3-C4	4.50	120.05	112.30
10	D	501	GDP	N9-C4-N3	4.42	134.80	125.95
14	F	400	ACP	N3-C2-N1	-4.42	121.89	128.58
14	F	400	ACP	N3-C4-N9	4.42	134.69	127.17
13	B	505	MES	C5-N4-C3	4.35	118.20	108.84
11	D	502	6K9	C16-C15-C14	-3.93	108.98	114.43
11	B	503	6K9	O27-C23-C24	-3.89	104.22	110.14
11	B	503	6K9	C33-C34-C35	3.88	115.24	111.87
14	F	400	ACP	PB-O3A-PA	-3.74	120.16	132.37
11	D	502	6K9	O27-C23-C24	-3.55	104.74	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	400	ACP	C2-N3-C4	3.50	120.38	111.83
11	D	502	6K9	C10-O10-C06	3.44	121.68	113.83
11	D	502	6K9	C33-C34-C35	3.43	114.85	111.87
11	B	503	6K9	C10-O10-C06	3.41	121.63	113.83
11	D	502	6K9	C18-C19-C36	-3.39	120.19	126.31
10	B	501	GDP	C6-C5-N7	3.31	136.32	130.29
11	D	502	6K9	C04-C03-C02	-3.30	106.65	113.11
11	B	503	6K9	C18-C19-C36	-3.30	120.36	126.31
11	B	503	6K9	C04-C03-C02	-3.28	106.70	113.11
11	B	503	6K9	C23-O27-C27	3.25	117.55	112.39
14	F	400	ACP	N9-C8-N7	-3.22	109.37	113.94
10	D	501	GDP	C6-C5-N7	3.20	136.12	130.29
5	A	501	GTP	N9-C4-N3	3.09	132.13	125.95
11	D	502	6K9	C23-O27-C27	3.07	117.27	112.39
11	B	503	6K9	O20-C17-C16	3.01	113.55	109.17
14	F	400	ACP	C4-N9-C8	2.92	108.81	105.74
5	C	501	GTP	N9-C4-N3	2.91	131.78	125.95
11	B	503	6K9	C37-C25-C24	-2.90	106.84	111.51
5	A	501	GTP	C2-N1-C6	-2.81	120.01	125.11
14	F	400	ACP	O5'-C5'-C4'	2.79	118.48	108.99
5	C	501	GTP	N9-C8-N7	-2.78	108.24	113.40
5	A	501	GTP	N9-C8-N7	-2.78	108.24	113.40
10	B	501	GDP	C4-C5-N7	-2.66	106.45	110.67
5	C	501	GTP	C2-N1-C6	-2.66	120.29	125.11
5	A	501	GTP	C8-N7-C5	2.63	108.95	104.26
11	D	502	6K9	C37-C25-C24	-2.62	107.30	111.51
14	F	400	ACP	C5-N7-C8	2.59	107.51	103.45
5	C	501	GTP	C8-N7-C5	2.58	108.86	104.26
11	B	503	6K9	C32-C33-C34	-2.57	108.75	114.49
11	B	503	6K9	O12-C12-C11	-2.57	99.49	104.92
10	D	501	GDP	C4-C5-N7	-2.57	106.60	110.67
13	B	505	MES	C6-C5-N4	-2.56	106.23	110.12
14	F	400	ACP	C3'-C2'-C1'	2.47	106.13	101.46
11	D	502	6K9	O12-C12-C11	-2.47	99.71	104.92
11	D	502	6K9	O20-C17-C16	2.47	112.76	109.17
11	B	503	6K9	C10-C11-C12	2.44	109.44	103.78
5	A	501	GTP	C5-C6-N1	2.41	119.40	113.25
5	C	501	GTP	C5-C6-N1	2.39	119.34	113.25
11	B	503	6K9	C40-O31-C31	-2.32	108.52	114.47
11	D	502	6K9	C10-C11-C12	2.31	109.14	103.78
5	A	501	GTP	O6-C6-C5	-2.30	120.47	126.53
11	D	502	6K9	C32-C33-C34	-2.23	109.51	114.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O6-C6-C5	-2.23	120.63	126.53
11	D	502	6K9	C40-O31-C31	-2.21	108.80	114.47
11	D	502	6K9	O07-C03-C04	2.20	112.22	109.91
14	F	400	ACP	C5'-C4'-C3'	-2.14	107.50	115.21
10	D	501	GDP	O6-C6-C5	-2.10	120.99	126.53
11	D	502	6K9	C05-C06-C07	-2.09	106.75	110.87
5	C	501	GTP	O2A-PA-O3A	2.05	112.82	107.27
14	F	400	ACP	C4-C5-N7	-2.04	108.25	110.58
10	B	501	GDP	O6-C6-C5	-2.04	121.16	126.53
11	B	503	6K9	O31-C31-C30	-2.02	107.35	114.76

There are no chirality outliers.

All (45) 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
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	A	505	GOL	O1-C1-C2-O2
9	A	505	GOL	O1-C1-C2-C3
10	B	501	GDP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O1A
10	D	501	GDP	C5'-O5'-PA-O2A
11	B	503	6K9	C33-C34-C35-N35
11	B	503	6K9	O34-C34-C35-N35
11	D	502	6K9	C33-C34-C35-N35
11	D	502	6K9	O34-C34-C35-N35
14	F	400	ACP	PB-C3B-PG-O2G
14	F	400	ACP	PG-C3B-PB-O1B
14	F	400	ACP	PG-C3B-PB-O2B
14	F	400	ACP	PG-C3B-PB-O3A
14	F	400	ACP	C5'-O5'-PA-O1A
14	F	400	ACP	C5'-O5'-PA-O2A
14	F	400	ACP	C5'-O5'-PA-O3A
9	C	505	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O1G
14	F	400	ACP	PB-C3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O2A
14	F	400	ACP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C4'-C5'-O5'-PA
14	F	400	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
10	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
11	D	502	6K9	C31-C32-C33-C34
5	A	501	GTP	PB-O3B-PG-O1G
9	C	505	GOL	O1-C1-C2-O2
10	D	501	GDP	PB-O3A-PA-O1A

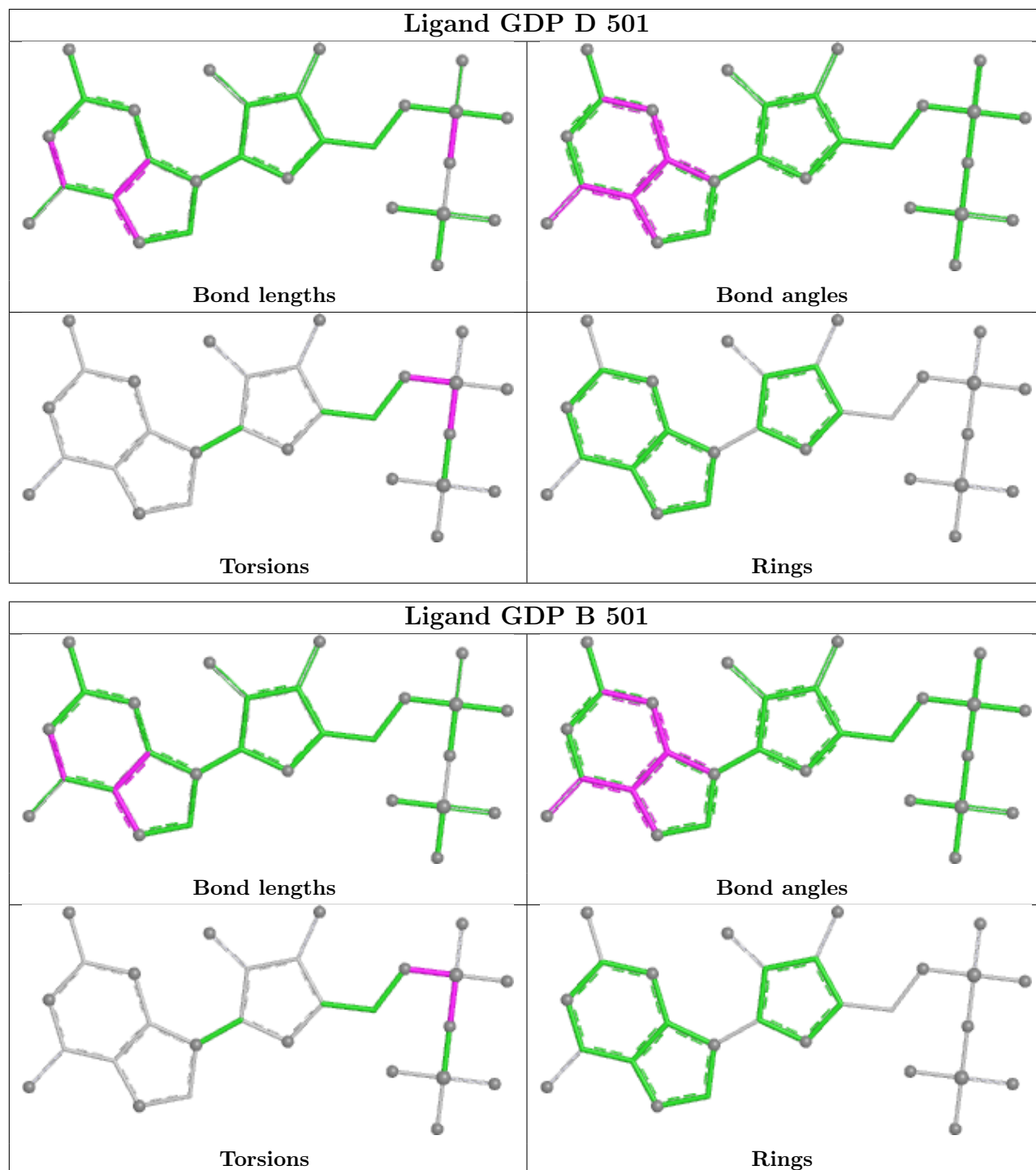
There are no ring outliers.

9 monomers are involved in 15 short contacts:

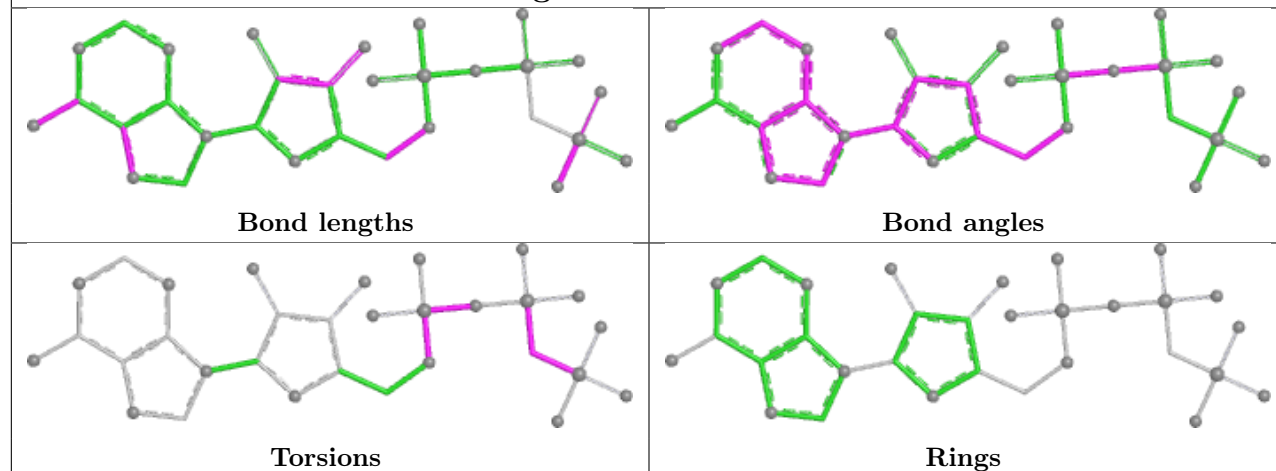
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	505	GOL	1	0
10	D	501	GDP	3	0
10	B	501	GDP	1	0
14	F	400	ACP	3	0
8	B	506	IMD	2	0
5	A	501	GTP	1	0
8	B	507	IMD	4	0
13	B	505	MES	2	0
12	B	504	03S	1	0

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

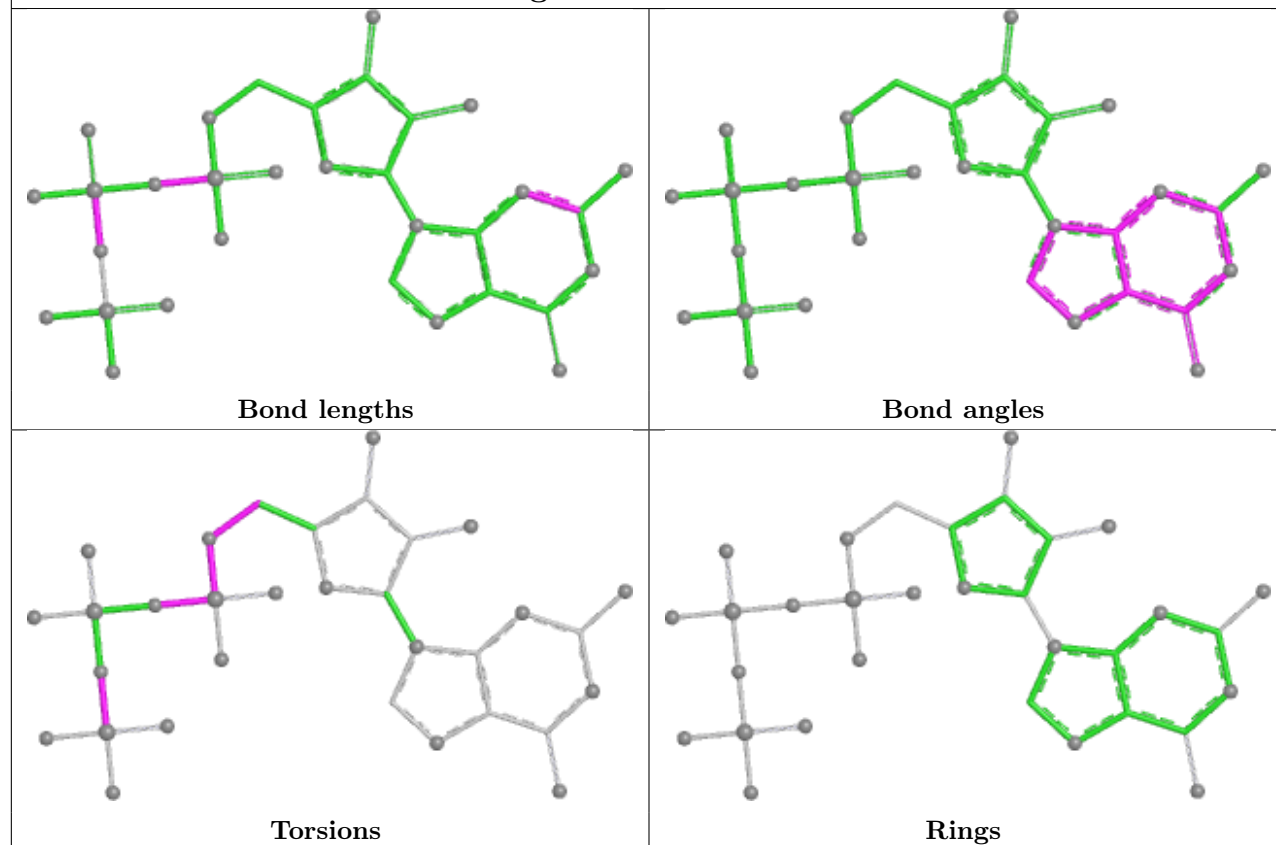
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



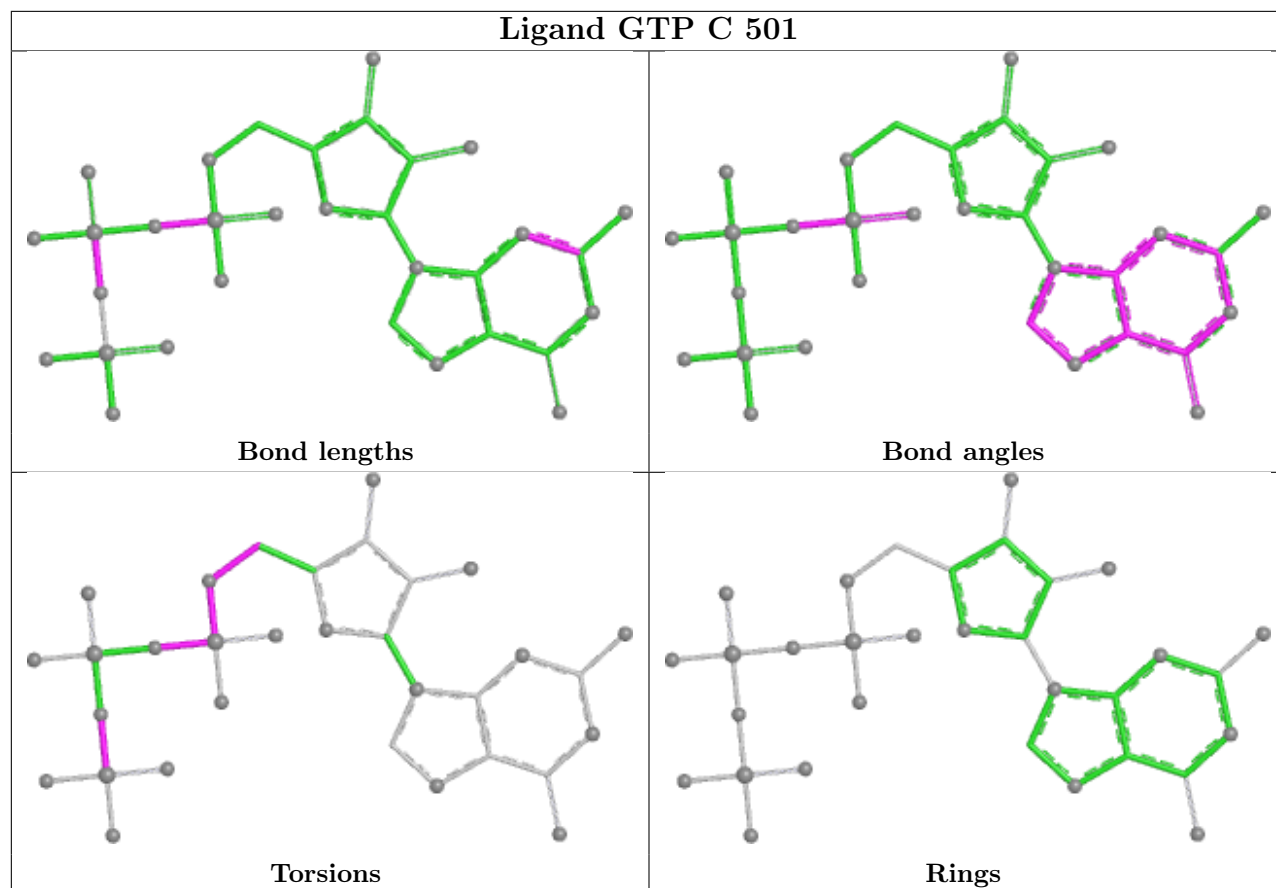
Ligand ACP F 400



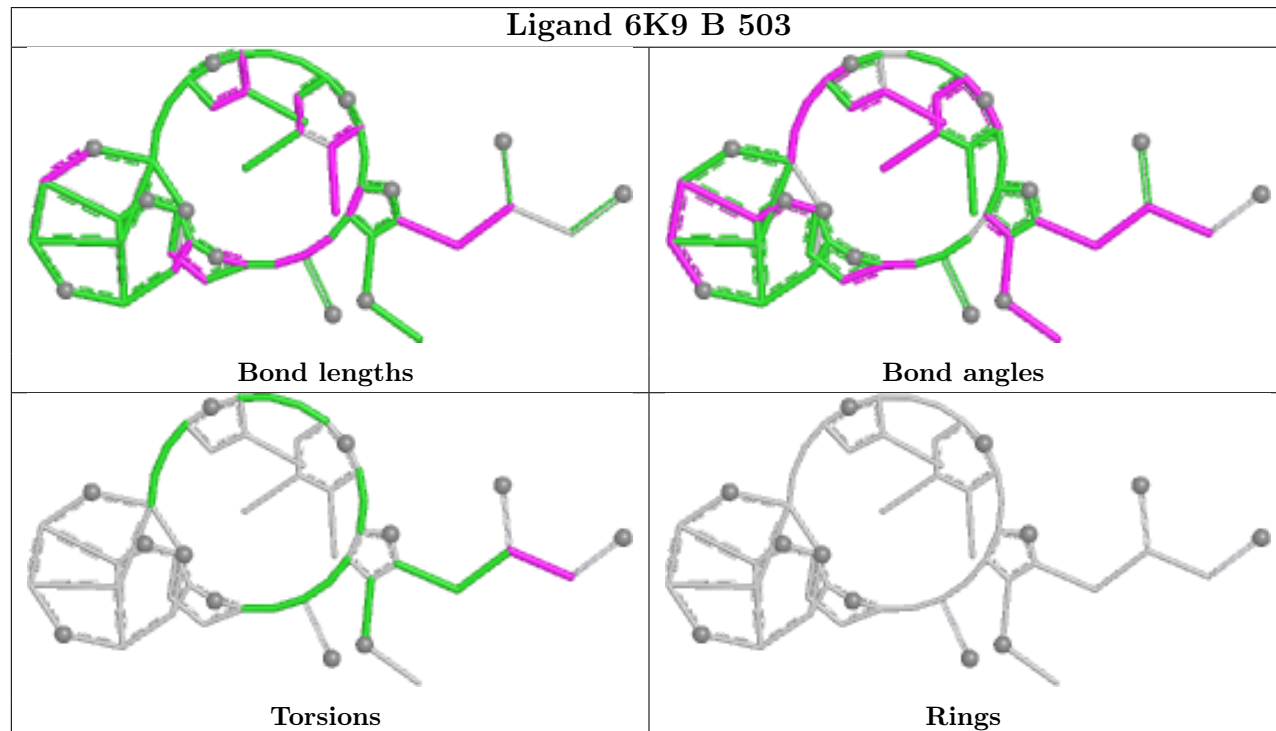
Ligand GTP A 501

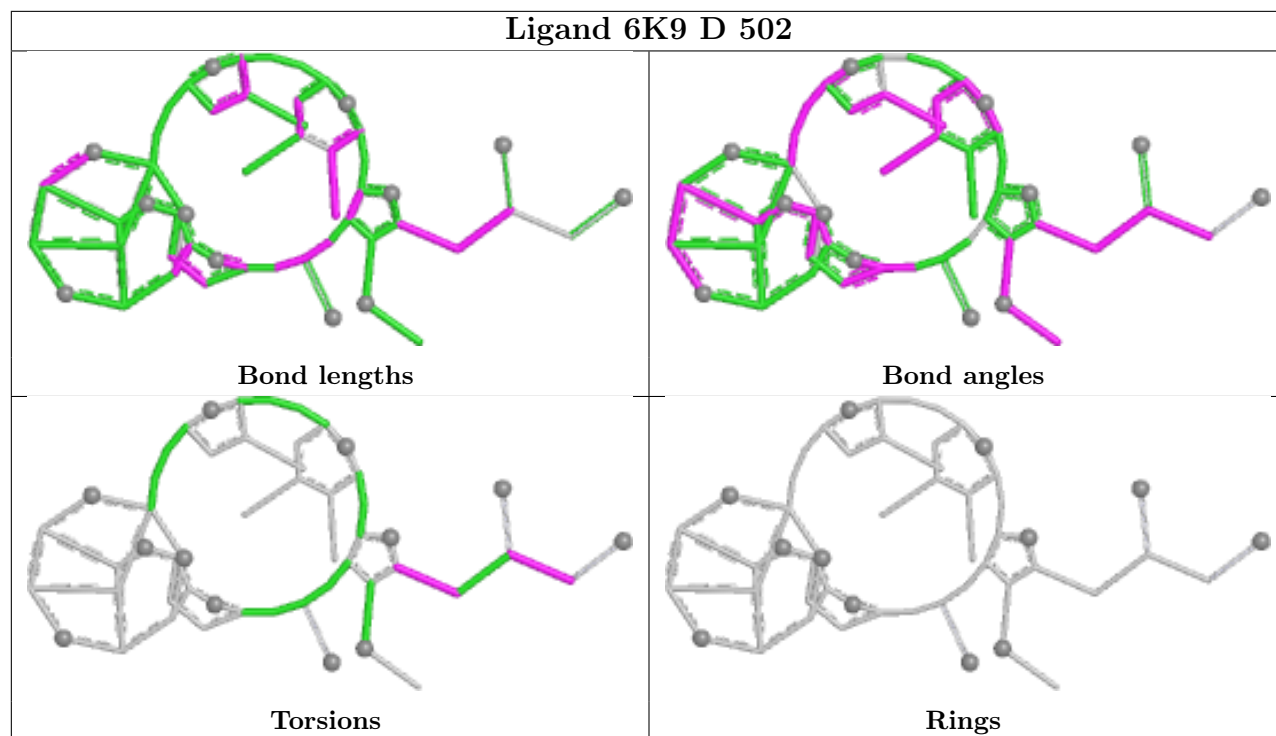


Ligand GTP C 501



Ligand 6K9 B 503





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	439/450 (97%)	0.08	5 (1%) 78 79	37, 66, 99, 145	2 (0%)
1	C	440/450 (97%)	-0.13	6 (1%) 73 74	37, 53, 79, 100	0
2	B	428/445 (96%)	0.22	16 (3%) 45 45	31, 65, 111, 155	3 (0%)
2	D	424/445 (95%)	0.24	14 (3%) 49 49	36, 71, 104, 136	7 (1%)
3	E	121/143 (84%)	0.63	5 (4%) 41 41	49, 83, 106, 119	0
4	F	342/384 (89%)	0.46	15 (4%) 39 38	48, 86, 145, 172	0
All	All	2194/2317 (94%)	0.19	61 (2%) 55 55	31, 68, 115, 172	12 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	153	ALA	5.3
2	B	1	MET	4.3
4	F	132	LEU	3.9
4	F	362	ALA	3.7
3	E	6	MET	3.7
2	D	220	THR	3.7
4	F	157	GLY	3.6
2	B	248	LEU	3.4
2	B	57	THR	3.3
4	F	102	PRO	3.2
1	A	282	TYR	3.1
2	B	82	PRO	3.1
1	C	440	VAL	3.0
3	E	24	LEU	3.0
2	D	248	LEU	3.0
4	F	372	THR	3.0
1	A	2	ARG	3.0
2	B	280	SER	3.0
1	A	283	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	281	GLN	2.8
2	B	58	GLY	2.8
4	F	380	HIS	2.8
3	E	26	PRO	2.8
2	D	407	TRP	2.8
4	F	182	ILE	2.8
4	F	144	GLY	2.8
2	B	438	ALA	2.6
2	B	42	LEU	2.6
3	E	27	PRO	2.5
4	F	130	VAL	2.5
1	C	340	SER	2.5
2	D	284	ARG	2.5
2	B	283	TYR	2.5
2	D	98	GLY	2.5
2	B	325	MET	2.4
2	D	181	VAL	2.4
2	D	285	ALA	2.3
2	D	272	PHE	2.3
4	F	131	PHE	2.3
2	D	247	GLN	2.3
2	D	276	THR	2.3
1	C	341	ILE	2.3
2	B	50	ASN	2.3
1	C	179	THR	2.3
2	B	37	HIS	2.2
2	B	83	PHE	2.2
1	C	1	MET	2.2
2	D	1	MET	2.2
4	F	134	ALA	2.2
2	D	100	GLY	2.2
2	B	277	SER	2.2
3	E	90	ASN	2.1
4	F	167	SER	2.1
2	B	282	GLN	2.1
4	F	161	LEU	2.1
4	F	136	ASN	2.1
1	C	357	TYR	2.1
1	A	82	THR	2.0
1	A	262	TYR	2.0
2	D	83	PHE	2.0
2	D	372	LYS	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](#)

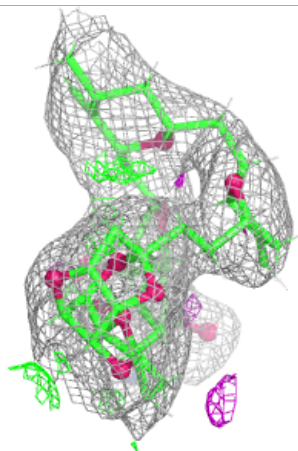
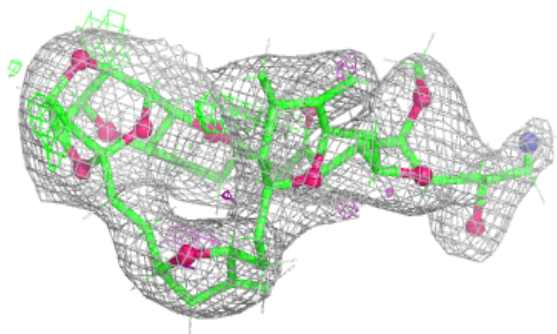
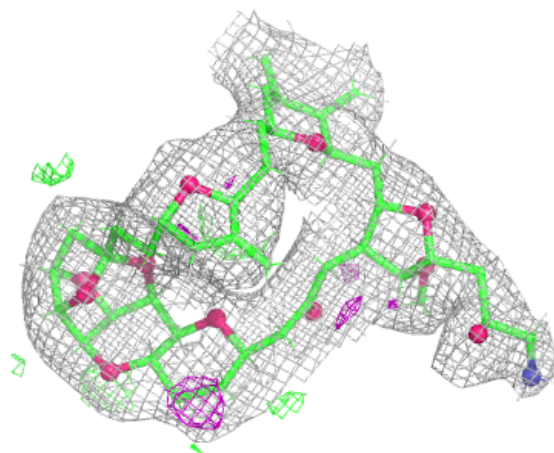
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	03S	B	504	5/5	0.77	0.13	51,102,113,114	0
7	CA	A	503	1/1	0.83	0.17	219,219,219,219	0
9	GOL	A	505	6/6	0.85	0.17	69,85,88,89	0
11	6K9	D	502	52/52	0.86	0.10	63,92,111,115	0
8	IMD	B	507	5/5	0.87	0.13	107,109,111,113	0
13	MES	B	505	12/12	0.89	0.12	57,78,100,112	0
7	CA	E	200	1/1	0.90	0.10	98,98,98,98	0
6	MG	F	401	1/1	0.90	0.07	88,88,88,88	0
8	IMD	B	506	5/5	0.91	0.18	94,96,102,103	0
8	IMD	A	504	5/5	0.91	0.18	85,87,90,90	0
7	CA	C	504	1/1	0.92	0.10	117,117,117,117	0
14	ACP	F	400	31/31	0.92	0.09	71,84,123,146	0
9	GOL	C	505	6/6	0.93	0.14	69,88,89,91	0
10	GDP	D	501	28/28	0.94	0.09	45,61,81,86	0
11	6K9	B	503	52/52	0.94	0.07	42,60,74,79	0
7	CA	B	502	1/1	0.95	0.09	96,96,96,96	0
10	GDP	B	501	28/28	0.96	0.08	40,51,57,60	0
5	GTP	C	501	32/32	0.97	0.06	35,40,51,53	0
5	GTP	A	501	32/32	0.98	0.06	38,49,57,84	0
7	CA	C	503	1/1	0.99	0.04	69,69,69,69	0
6	MG	C	502	1/1	0.99	0.03	40,40,40,40	0
6	MG	A	502	1/1	0.99	0.06	48,48,48,48	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.

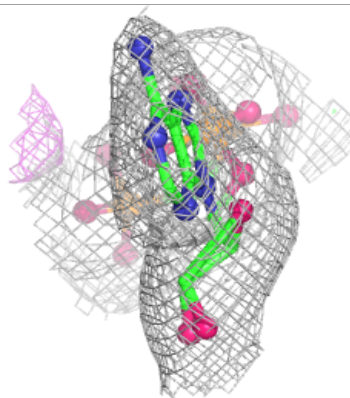
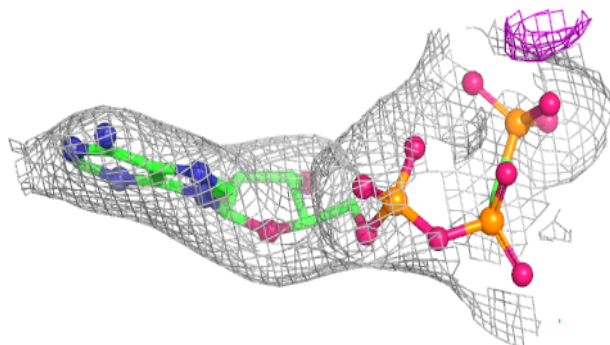
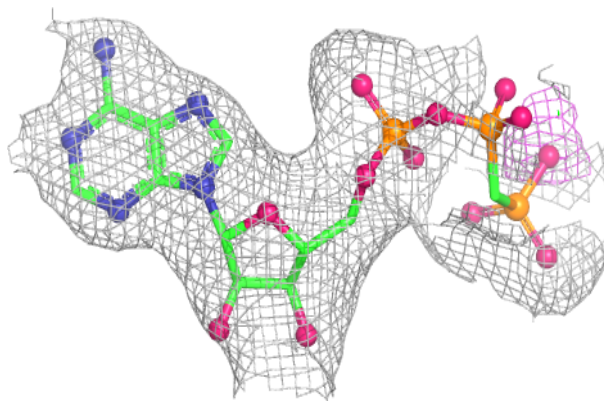
Electron density around 6K9 D 502:

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

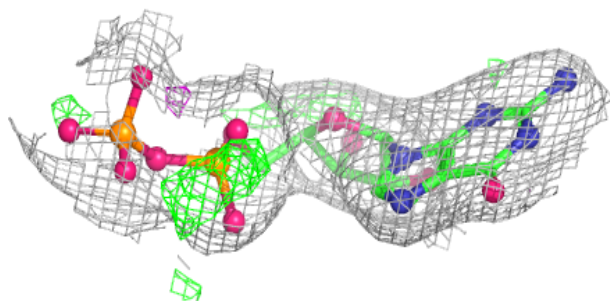
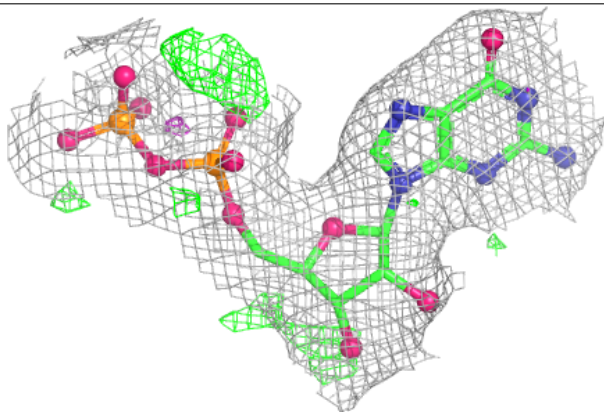


Electron density around ACP F 400:

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

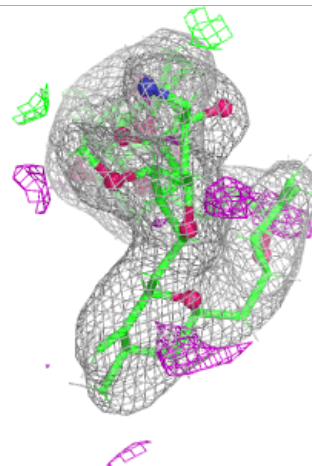
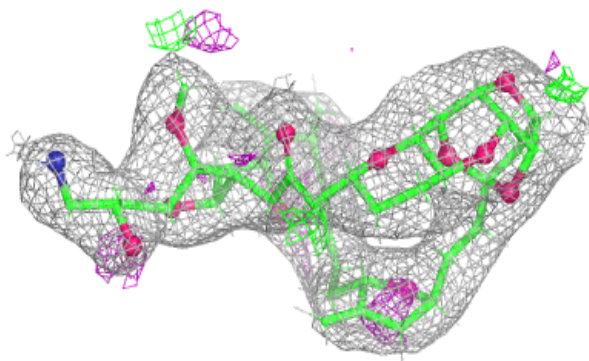
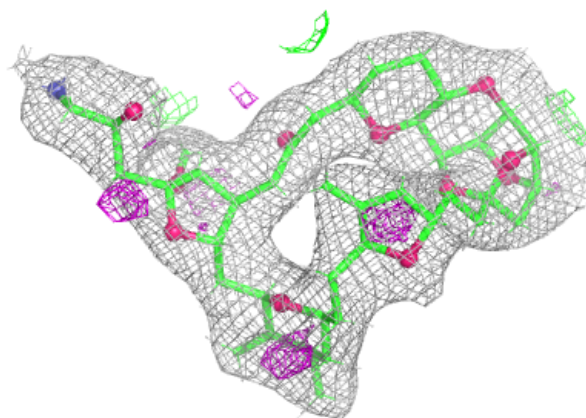
**Electron density around GDP D 501:**

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



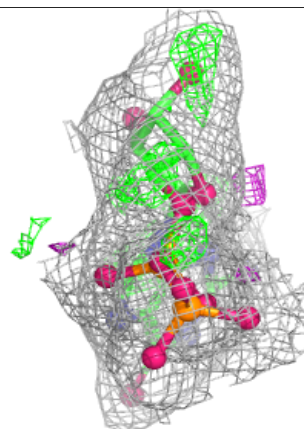
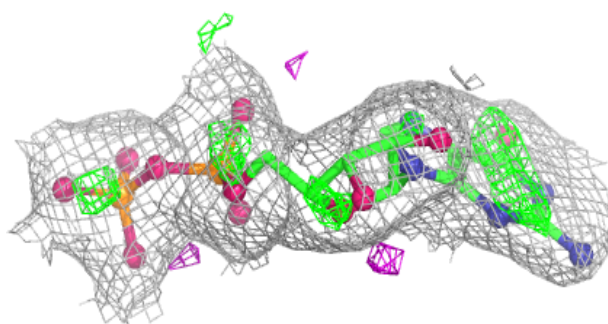
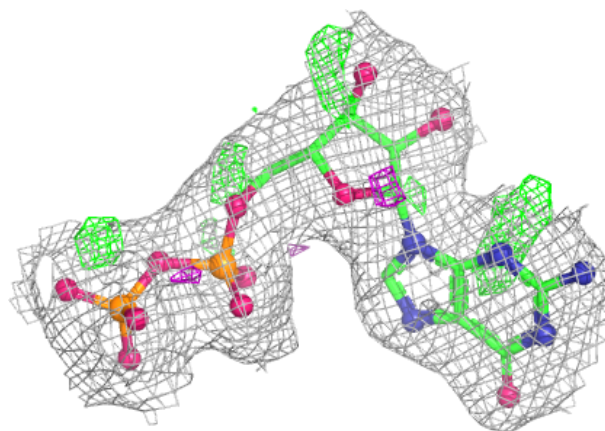
Electron density around 6K9 B 503:

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

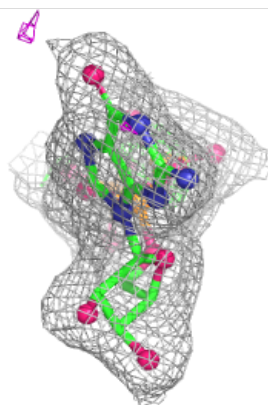
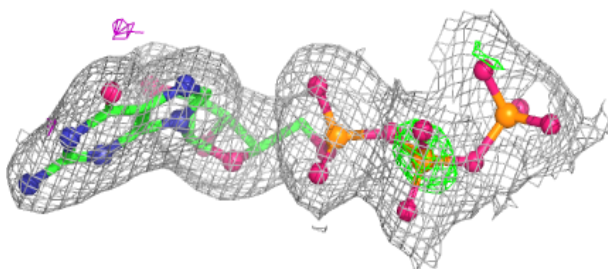
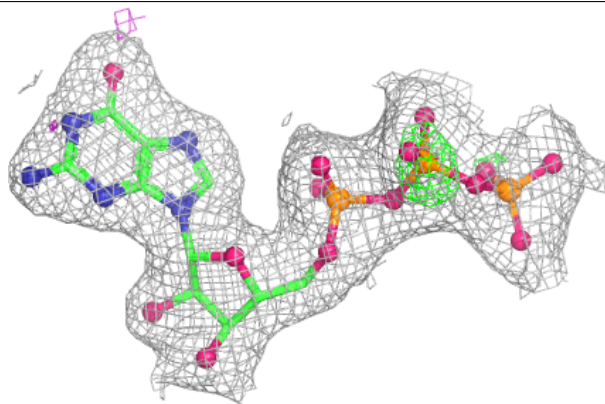


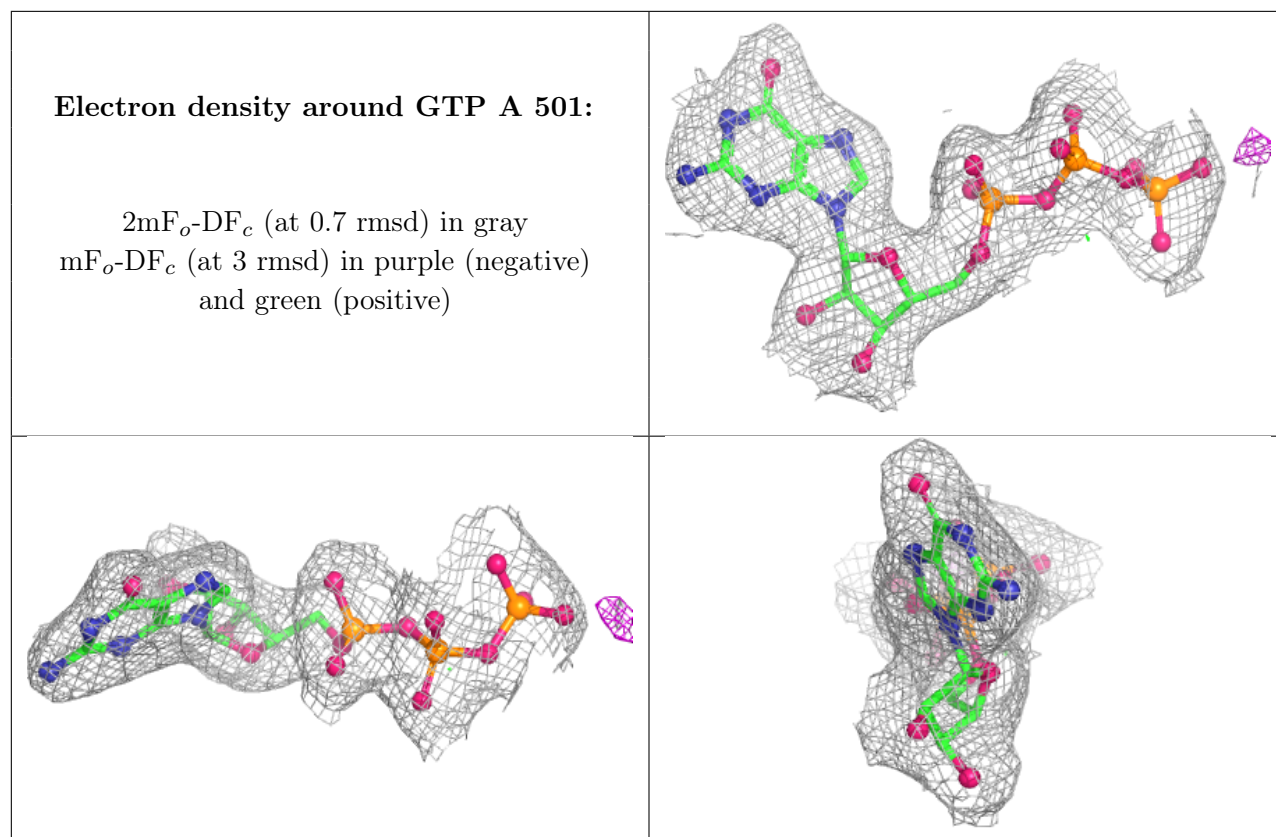
Electron density around GDP B 501:

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 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.