



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:54 AM UTC

PDB ID : 6TIZ / pdb_00006tiz
Title : DROSOPHILA GDP-TUBULIN Y222F MUTANT
Authors : Gigant, B.
Deposited on : 2019-11-22
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

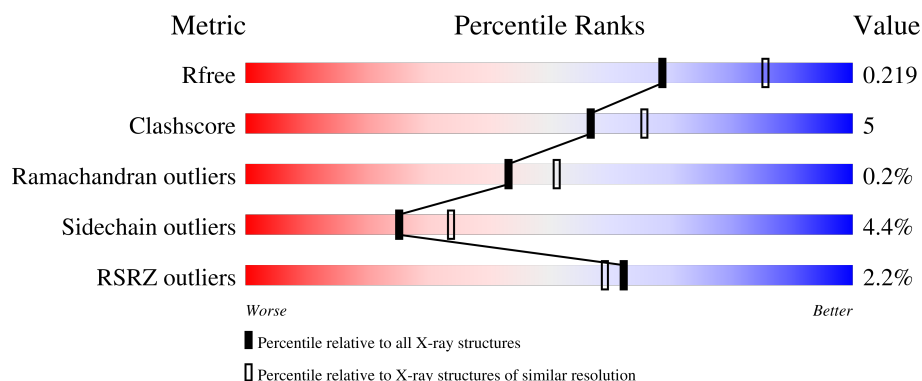
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	450	2% 81% 14% • •
1	C	450	2% 83% 11% • •
2	B	447	2% 81% 14% •
2	D	447	2% 84% 11% •
3	E	143	5% 74% 13% • 10%

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
6	SO4	A	504	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15487 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-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3359	2127	570	639	23			
1	C	430	Total	C	N	O	S	0	3	0
			3372	2137	571	639	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ARG	LYS	engineered mutation	UNP P06603
C	40	ARG	LYS	engineered mutation	UNP P06603

- Molecule 2 is a protein called Tubulin beta-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	1	0
			3359	2111	574	648	26			
2	D	427	Total	C	N	O	S	0	6	0
			3384	2126	577	655	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	PHE	TYR	engineered mutation	UNP Q24560
D	222	PHE	TYR	engineered mutation	UNP Q24560

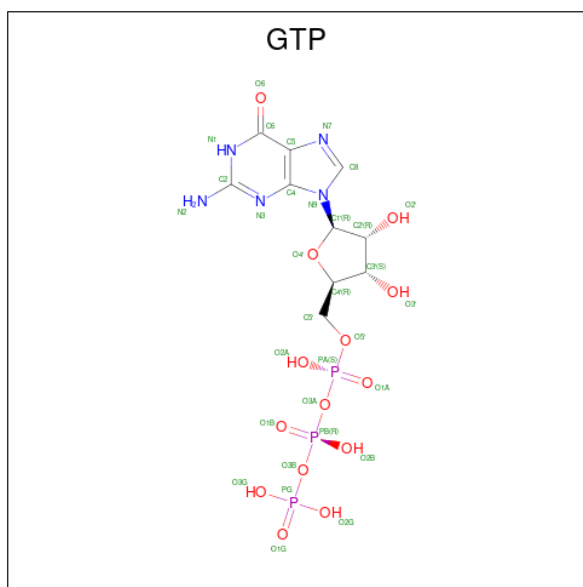
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	129	Total	C	N	O	S	0	1	0
			1055	653	192	206	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	SER	engineered mutation	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

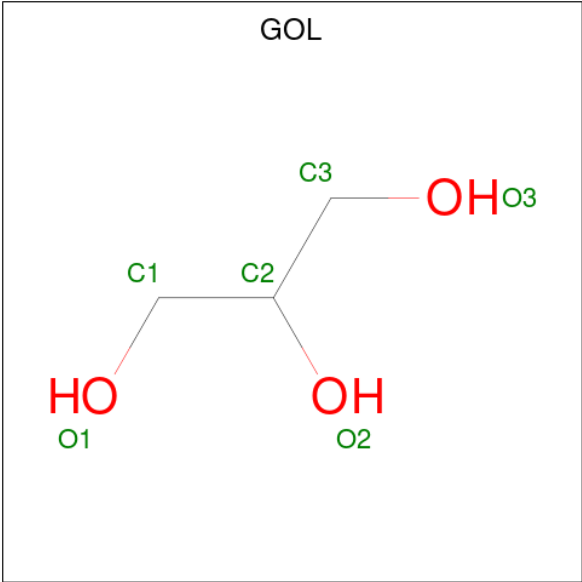
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg		
			1	1	0	0
5	C	1	Total	Mg		
			1	1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



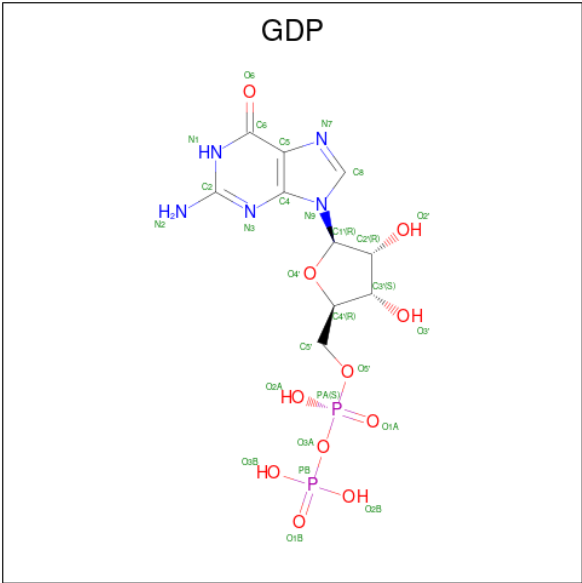
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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



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

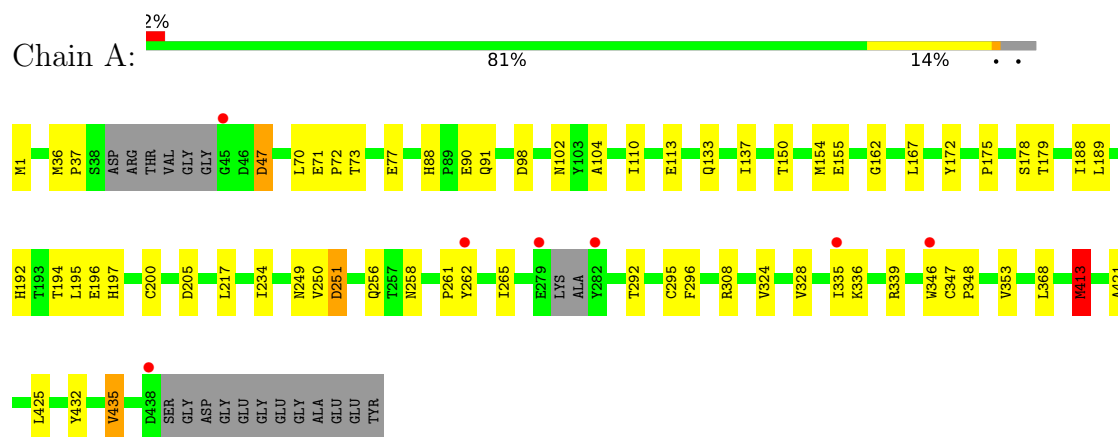
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	218	Total 218	O 218	0	0
9	B	164	Total 164	O 164	0	0
9	C	147	Total 147	O 147	0	0
9	D	185	Total 185	O 185	0	2
9	E	45	Total 45	O 45	0	0

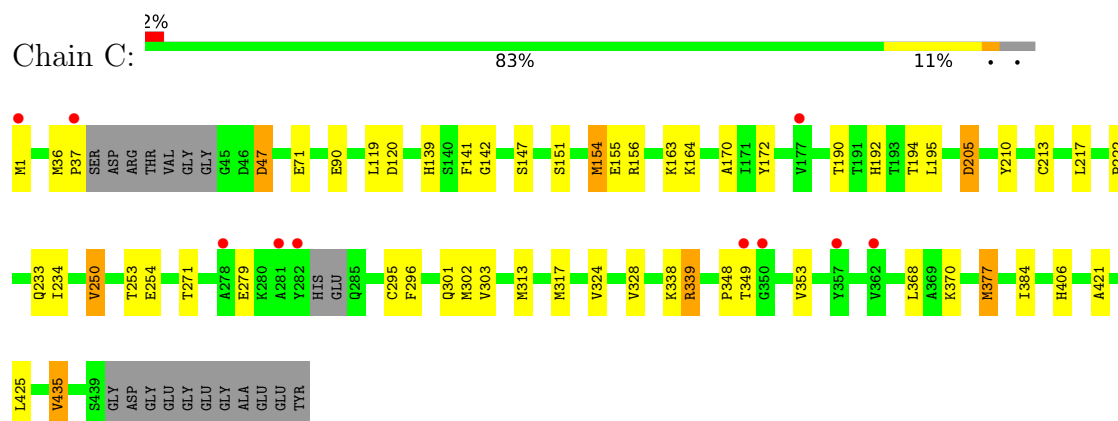
3 Residue-property plots [i](#)

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.

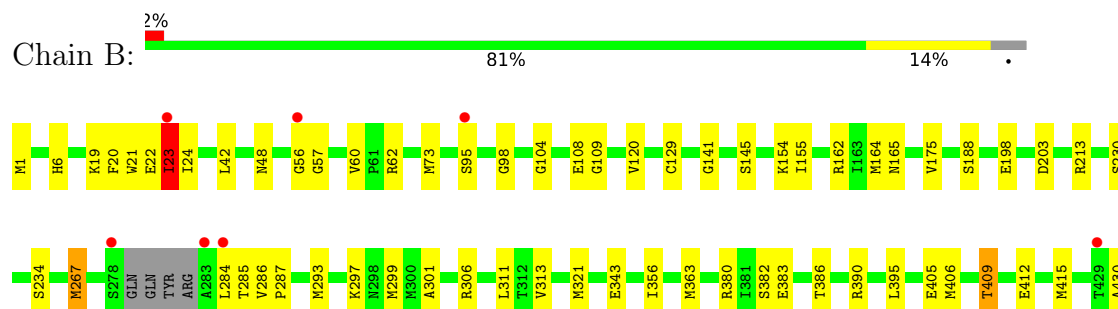
- Molecule 1: Tubulin alpha-1 chain

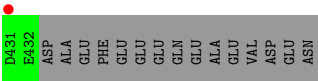


- Molecule 1: Tubulin alpha-1 chain

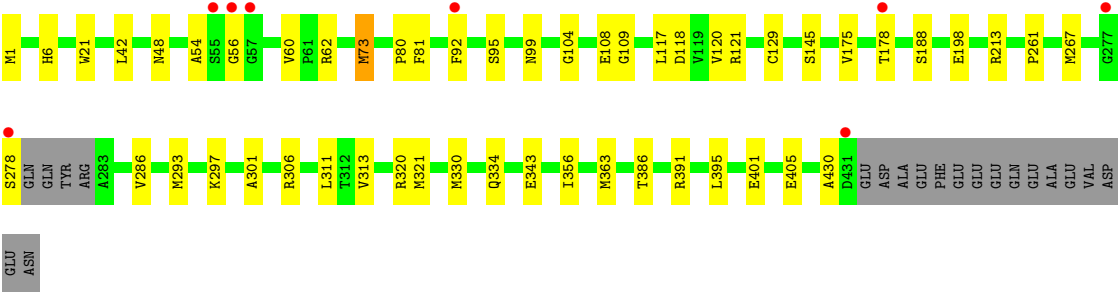
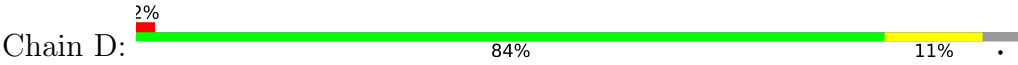


- Molecule 2: Tubulin beta-1 chain

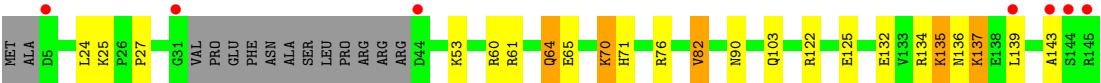




● Molecule 2: Tubulin beta-1 chain



● Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.18Å 126.73Å 250.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.20 32.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (32.00-2.20) 97.0 (32.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.175 , 0.208 0.183 , 0.219	Depositor DCC
R_{free} test set	5278 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.998	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15487	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: GTP, MG, GOL, GDP, SO4

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	0.74	1/3436 (0.0%)	1.05	4/4664 (0.1%)
1	C	0.75	2/3455 (0.1%)	1.05	5/4687 (0.1%)
2	B	0.77	2/3434 (0.1%)	1.04	5/4649 (0.1%)
2	D	0.73	0/3462	1.02	5/4688 (0.1%)
3	E	0.68	0/1069	1.13	1/1422 (0.1%)
All	All	0.74	5/14856 (0.0%)	1.04	20/20110 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	MET	SD-CE	-8.26	1.58	1.79
2	B	267	MET	SD-CE	-7.83	1.59	1.79
1	A	413	MET	SD-CE	-7.83	1.59	1.79
1	C	154	MET	SD-CE	-6.09	1.64	1.79
1	C	377	MET	SD-CE	-5.25	1.66	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	ASP	CA-CB-CG	7.24	119.84	112.60
1	A	162	GLY	N-CA-C	6.27	120.22	112.64
1	C	338	LYS	CA-C-N	6.12	128.76	120.38
1	C	338	LYS	C-N-CA	6.12	128.76	120.38
1	A	47	ASP	CA-CB-CG	5.91	118.51	112.60
2	B	23	ILE	N-CA-CB	5.74	117.92	110.57
2	B	356	ILE	N-CA-C	5.64	112.69	107.56
2	D	356	ILE	N-CA-C	5.49	112.56	107.56
2	B	213	ARG	N-CA-C	5.40	116.98	111.14
1	C	142	GLY	N-CA-C	5.37	121.91	113.86
2	D	213	ARG	N-CA-C	5.33	116.90	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	311	LEU	N-CA-C	-5.25	105.00	111.40
2	D	95	SER	N-CA-C	5.24	118.14	111.69
2	B	95	SER	N-CA-C	5.24	118.13	111.69
2	B	311	LEU	N-CA-C	-5.17	105.10	111.40
3	E	82	VAL	N-CA-CB	5.15	118.31	110.58
1	A	251	ASP	CA-CB-CG	5.08	117.67	112.60
1	C	205	ASP	CA-CB-CG	5.07	117.67	112.60
2	D	118	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	102	ASN	CA-CB-CG	5.01	117.61	112.60

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	3359	0	3264	41	0
1	C	3372	0	3296	31	0
2	B	3359	0	3249	35	0
2	D	3384	0	3273	19	0
3	E	1055	0	1056	17	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	15	0	0	2	0
6	B	10	0	0	0	0
6	C	15	0	0	0	0
6	D	20	0	0	0	0
6	E	5	0	0	0	0
7	A	12	0	16	1	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	A	218	0	0	2	0
9	B	164	0	0	2	0
9	C	147	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	185	0	0	0	0
9	E	45	0	0	0	0
All	All	15487	0	14202	132	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 5.

All (132) 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)
1:C:339:ARG:H	1:C:339:ARG:HD3	1.37	0.86
1:A:336:LYS:HE3	3:E:25:LYS:HZ1	1.42	0.85
1:C:295:CYS:HB3	1:C:377:MET:HE3	1.63	0.78
1:A:71:GLU:OE2	1:A:73:THR:HB	1.84	0.78
1:C:296:PHE:CE2	1:C:377:MET:HE1	2.24	0.73
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.72	0.70
1:C:163:LYS:HG2	3:E:90:ASN:OD1	1.91	0.70
1:C:295:CYS:CB	1:C:377:MET:HE3	2.23	0.68
1:A:336:LYS:HE3	3:E:25:LYS:NZ	2.09	0.68
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.75	0.67
1:A:308:ARG:NH1	6:A:504:SO4:O3	2.29	0.65
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.15	0.64
2:D:73:MET:HE2	2:D:92:PHE:HB3	1.80	0.64
3:E:132:GLU:HA	3:E:135:LYS:HD3	1.80	0.64
1:A:110:ILE:O	1:A:113:GLU:HG2	1.99	0.62
2:B:48:ASN:O	2:B:62:ARG:NH2	2.31	0.62
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.00	0.62
1:A:292:THR:O	1:A:295:CYS:HB2	2.01	0.60
1:C:295:CYS:HB3	1:C:377:MET:CE	2.33	0.59
1:C:317:MET:SD	1:C:377:MET:HE2	2.44	0.58
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.86	0.58
2:D:395:LEU:HD21	2:D:405:GLU:HG3	1.85	0.58
2:B:104:GLY:O	2:B:109:GLY:HA3	2.06	0.56
9:B:640:HOH:O	1:C:348:PRO:HD2	2.05	0.56
2:B:1:MET:N	2:B:129:CYS:SG	2.77	0.55
2:B:162:ARG:HA	2:B:162:ARG:HE	1.72	0.55
2:B:23:ILE:HG12	2:B:230:SER:HB2	1.89	0.55
2:B:395:LEU:HD21	2:B:405:GLU:HG3	1.89	0.55
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.89	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.41	0.55
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:60:ARG:O	3:E:64:GLN:HG2	2.07	0.54
2:D:104:GLY:O	2:D:109:GLY:HA3	2.07	0.54
1:A:71:GLU:OE2	1:A:73:THR:CB	2.55	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.26	0.53
1:C:154:MET:HE2	1:C:194:THR:HG23	1.90	0.53
2:D:48:ASN:O	2:D:62:ARG:NH2	2.39	0.53
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.91	0.52
2:B:382:SER:O	2:B:386:THR:HG23	2.08	0.52
3:E:70:LYS:NZ	3:E:71[A]:HIS:CE1	2.78	0.52
2:B:406:MET:HA	2:B:409:THR:HG23	1.93	0.51
1:A:339:ARG:NH2	6:A:504:SO4:O4	2.43	0.50
2:D:1:MET:N	2:D:129:CYS:SG	2.79	0.50
2:B:19:LYS:O	2:B:23:ILE:HG13	2.12	0.50
2:B:154:LYS:HD3	3:E:76:ARG:CZ	2.41	0.50
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.93	0.50
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.78	0.49
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.94	0.49
2:B:23:ILE:HD12	2:B:24:ILE:HG23	1.95	0.49
2:D:293:MET:HE3	2:D:313:VAL:HG11	1.94	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.94	0.49
2:B:23:ILE:HD13	2:B:234:SER:HB2	1.95	0.49
1:C:271:THR:OG1	1:C:377:MET:HB3	2.13	0.49
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.94	0.49
1:C:271:THR:HG22	1:C:301:GLN:HA	1.94	0.48
2:B:293:MET:HE3	2:B:313:VAL:HG11	1.95	0.48
1:A:249:ASN:ND2	1:A:258:ASN:HD22	2.11	0.48
1:C:192:HIS:CG	1:C:421:ALA:HA	2.49	0.48
2:D:117:LEU:O	2:D:121:ARG:HG3	2.14	0.48
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.95	0.48
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.96	0.47
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.96	0.47
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.08	0.47
1:A:189:LEU:HD13	1:A:413:MET:HE1	1.96	0.46
2:D:80:PRO:O	2:D:81:PHE:HB2	2.15	0.46
2:D:145:SER:HB2	2:D:188:SER:OG	2.15	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.51	0.46
2:B:267:MET:HE2	2:B:299:MET:HG3	1.98	0.46
2:B:343:GLU:HG3	2:B:430:ALA:HB2	1.98	0.46
3:E:135:LYS:NZ	3:E:136:ASN:ND2	2.63	0.46
1:A:336:LYS:CE	3:E:25:LYS:NZ	2.78	0.45
2:B:386:THR:O	2:B:390:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:135:LYS:HZ3	3:E:136:ASN:CG	2.24	0.45
2:D:321:MET:HE3	2:D:363:MET:HE3	1.97	0.45
7:A:506:GOL:H2	3:E:61:ARG:HG3	1.98	0.45
1:A:296:PHE:O	1:A:339:ARG:NH1	2.49	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.45
1:A:346:TRP:CE3	1:A:347:CYS:SG	3.10	0.45
2:B:165:ASN:ND2	9:B:605:HOH:O	2.49	0.45
1:C:213:CYS:HA	1:C:217:LEU:HD12	1.99	0.45
1:A:150:THR:O	1:A:154:MET:HG2	2.17	0.44
1:C:233:GLN:NE2	9:C:601:HOH:O	2.49	0.44
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.46	0.44
2:D:330:MET:O	2:D:334:GLN:HG2	2.17	0.44
2:B:267:MET:HE2	2:B:299:MET:SD	2.58	0.44
1:C:313:MET:SD	1:C:435:VAL:CG1	3.05	0.44
2:B:141:GLY:O	2:B:145:SER:OG	2.33	0.44
1:C:217:LEU:HD21	1:C:368:LEU:HD23	1.99	0.44
2:B:380:ARG:O	2:B:383:GLU:HG2	2.17	0.43
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.53	0.43
2:D:99:ASN:HB3	2:D:178[A]:THR:HG21	2.00	0.43
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.43
1:A:88:HIS:O	1:A:91:GLN:HG2	2.18	0.43
1:A:137:ILE:HD13	1:A:154:MET:SD	2.59	0.43
1:C:151:SER:O	1:C:155:GLU:HG3	2.19	0.43
3:E:139:LEU:O	3:E:143:ALA:HB3	2.19	0.43
2:B:321:MET:HE3	2:B:363:MET:HE3	1.99	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.42
2:B:267:MET:HE2	2:B:299:MET:CG	2.49	0.42
2:B:286:VAL:HG22	2:B:321:MET:HE3	2.02	0.42
1:A:262:TYR:HB2	1:A:265:ILE:HD12	2.00	0.42
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.20	0.42
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.01	0.42
1:C:339:ARG:HD3	1:C:339:ARG:N	2.19	0.42
1:A:179:THR:HG21	9:A:693:HOH:O	2.20	0.42
1:C:250:VAL:HG23	1:C:254:GLU:HB2	2.01	0.42
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.42
1:A:36:MET:HA	1:A:37:PRO:HD3	1.93	0.42
2:B:382:SER:HB2	2:B:415:MET:HE3	2.02	0.42
1:C:36:MET:HA	1:C:37:PRO:HD3	1.94	0.42
1:A:175:PRO:HA	1:A:178:SER:HB2	2.02	0.41
2:B:23:ILE:HG13	2:B:23:ILE:H	1.69	0.41
1:C:141:PHE:O	1:C:147:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:72:PRO:HD2	2.02	0.41
2:B:203:ASP:HB2	2:B:301:ALA:HA	2.02	0.41
2:B:145:SER:HB2	2:B:188:SER:OG	2.19	0.41
2:B:155:ILE:HG21	2:B:164:MET:HE1	2.03	0.41
1:C:139:HIS:O	1:C:170:ALA:HA	2.21	0.41
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.50	0.41
2:D:401:GLU:C	3:E:137:LYS:HB2	2.46	0.41
2:B:406:MET:HA	2:B:409:THR:CG2	2.50	0.41
2:D:286:VAL:HG22	2:D:321:MET:HE3	2.03	0.41
1:C:163:LYS:HE3	3:E:90:ASN:HA	2.02	0.40
3:E:132:GLU:HG3	3:E:135:LYS:NZ	2.35	0.40
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.40
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.56	0.40
1:A:154:MET:HE2	1:A:194:THR:HG23	2.03	0.40
2:B:20:PHE:HA	2:B:23:ILE:HD11	2.03	0.40
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.51	0.40
2:D:54:ALA:O	2:D:56:GLY:O	2.39	0.40
1:A:261:PRO:HD2	9:A:615:HOH:O	2.21	0.40
2:B:98:GLY:HA3	1:C:253:THR:HG22	2.03	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	425/450 (94%)	411 (97%)	14 (3%)	0	100	100
1	C	426/450 (95%)	408 (96%)	18 (4%)	0	100	100
2	B	425/447 (95%)	413 (97%)	9 (2%)	3 (1%)	18	19
2	D	429/447 (96%)	419 (98%)	10 (2%)	0	100	100
3	E	126/143 (88%)	122 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1831/1937 (94%)	1773 (97%)	55 (3%)	3 (0%)	43 51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	GLY
2	B	284	LEU
2	B	57	GLY

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	361/375 (96%)	347 (96%)	14 (4%)	28 39
1	C	364/375 (97%)	344 (94%)	20 (6%)	19 24
2	B	366/382 (96%)	355 (97%)	11 (3%)	36 49
2	D	370/382 (97%)	356 (96%)	14 (4%)	29 40
3	E	111/126 (88%)	100 (90%)	11 (10%)	7 8
All	All	1572/1640 (96%)	1502 (96%)	70 (4%)	25 33

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	47	ASP
1	A	77	GLU
1	A	90	GLU
1	A	188	ILE
1	A	195	LEU
1	A	196	GLU
1	A	234	ILE
1	A	250	VAL
1	A	256	GLN
1	A	324	VAL

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Mol	Chain	Res	Type
1	A	413	MET
1	A	425	LEU
1	A	435	VAL
2	B	22	GLU
2	B	23	ILE
2	B	42	LEU
2	B	60	VAL
2	B	108	GLU
2	B	120	VAL
2	B	175	VAL
2	B	198	GLU
2	B	297	LYS
2	B	306	ARG
2	B	409	THR
1	C	1[A]	MET
1	C	1[B]	MET
1	C	47	ASP
1	C	71	GLU
1	C	90	GLU
1	C	120	ASP
1	C	164	LYS
1	C	190	THR
1	C	195	LEU
1	C	234	ILE
1	C	250	VAL
1	C	279	GLU
1	C	302	MET
1	C	324	VAL
1	C	339	ARG
1	C	349	THR
1	C	370	LYS
1	C	384	ILE
1	C	425	LEU
1	C	435	VAL
2	D	42	LEU
2	D	60	VAL
2	D	73	MET
2	D	108	GLU
2	D	120	VAL
2	D	175[A]	VAL
2	D	175[B]	VAL
2	D	198	GLU

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Mol	Chain	Res	Type
2	D	278	SER
2	D	297	LYS
2	D	306	ARG
2	D	320	ARG
2	D	386	THR
2	D	391	ARG
3	E	53	LYS
3	E	64	GLN
3	E	65	GLU
3	E	70	LYS
3	E	82	VAL
3	E	103	GLN
3	E	122	ARG
3	E	125	GLU
3	E	134	ARG
3	E	135	LYS
3	E	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	249	ASN
1	A	342	GLN
1	A	356	ASN
2	B	11	GLN
2	B	37	HIS
2	B	48	ASN
2	B	292	GLN
2	B	426	GLN
1	C	11	GLN
1	C	15	GLN
1	C	35	GLN
1	C	256	GLN
1	C	380	ASN
2	D	37	HIS
2	D	48	ASN
2	D	99	ASN
2	D	245	GLN

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 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GDP	D	501	-	29,30,30	0.46	0	45,47,47	0.55	1 (2%)
6	SO4	D	504	-	4,4,4	0.26	0	6,6,6	0.06	0
6	SO4	A	505	-	4,4,4	0.30	0	6,6,6	0.09	0
6	SO4	C	503	-	4,4,4	0.25	0	6,6,6	0.15	0
6	SO4	A	503	-	4,4,4	0.26	0	6,6,6	0.18	0
4	GTP	A	501	5	33,34,34	0.49	0	50,54,54	0.52	1 (2%)
6	SO4	C	505	-	4,4,4	0.27	0	6,6,6	0.08	0
6	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.26	0
6	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.14	0
6	SO4	C	504	-	4,4,4	0.27	0	6,6,6	0.13	0
6	SO4	B	503	-	4,4,4	0.25	0	6,6,6	0.14	0
6	SO4	D	505	-	4,4,4	0.24	0	6,6,6	0.12	0
6	SO4	D	503	-	4,4,4	0.28	0	6,6,6	0.15	0
8	GDP	B	501	-	29,30,30	0.50	0	45,47,47	0.55	1 (2%)
6	SO4	E	201	-	4,4,4	0.22	0	6,6,6	0.12	0
7	GOL	A	507	-	5,5,5	0.05	0	5,5,5	0.33	0
7	GOL	A	506	-	5,5,5	0.14	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	C	501	5	33,34,34	0.45	0	50,54,54	0.52	1 (2%)
6	SO4	D	502	-	4,4,4	0.25	0	6,6,6	0.20	0

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	-	-	3/16/32/32	0/3/3/3
8	GDP	D	501	-	-	4/16/32/32	0/3/3/3
7	GOL	A	507	-	-	1/4/4/4	-
7	GOL	A	506	-	-	0/4/4/4	-
4	GTP	C	501	5	-	6/22/38/38	0/3/3/3
4	GTP	A	501	5	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	GTP	O5'-PA-O1A	2.17	117.55	108.94
8	D	501	GDP	O2A-PA-O5'	2.16	117.37	107.57
8	B	501	GDP	O3B-PB-O2B	2.05	115.48	107.80
4	A	501	GTP	O5'-PA-O1A	2.02	116.94	108.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A

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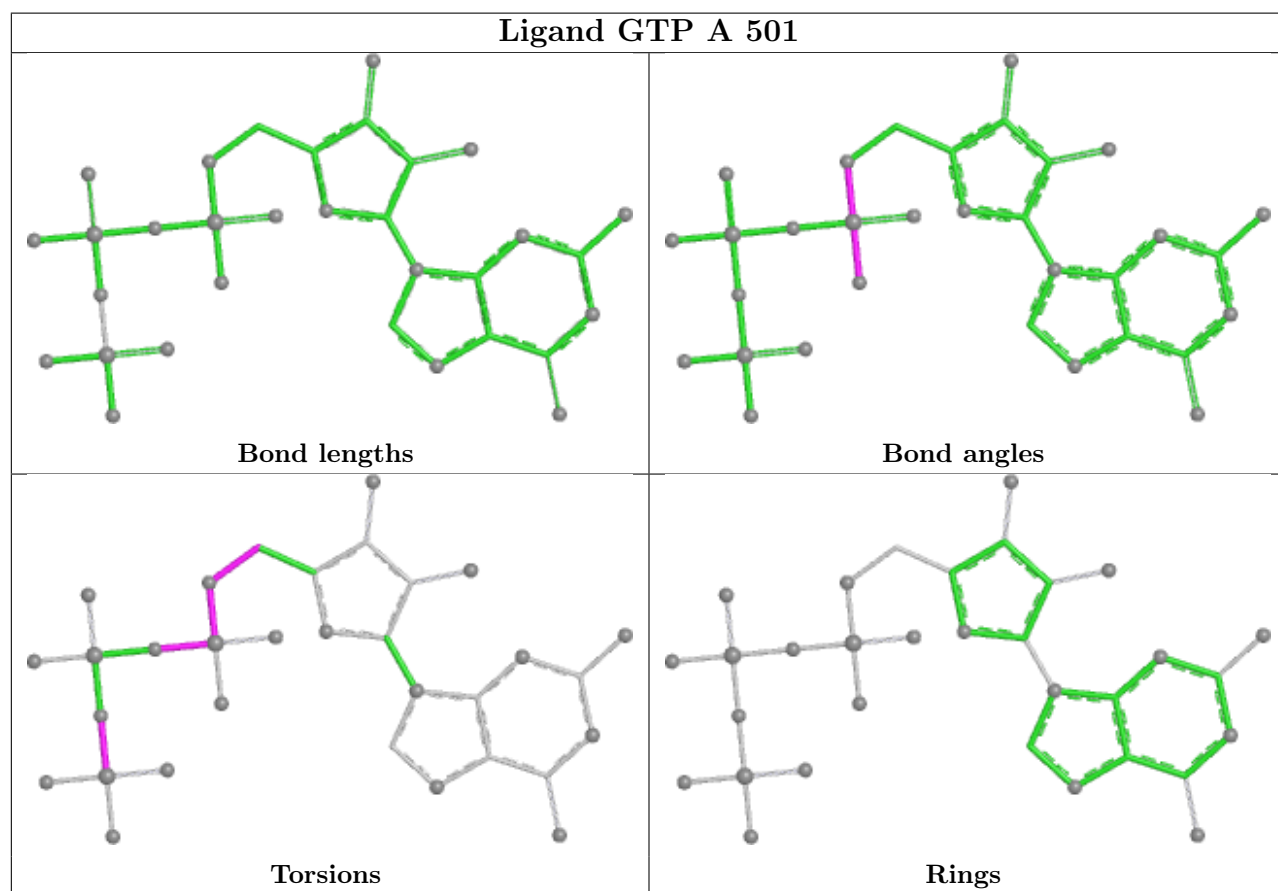
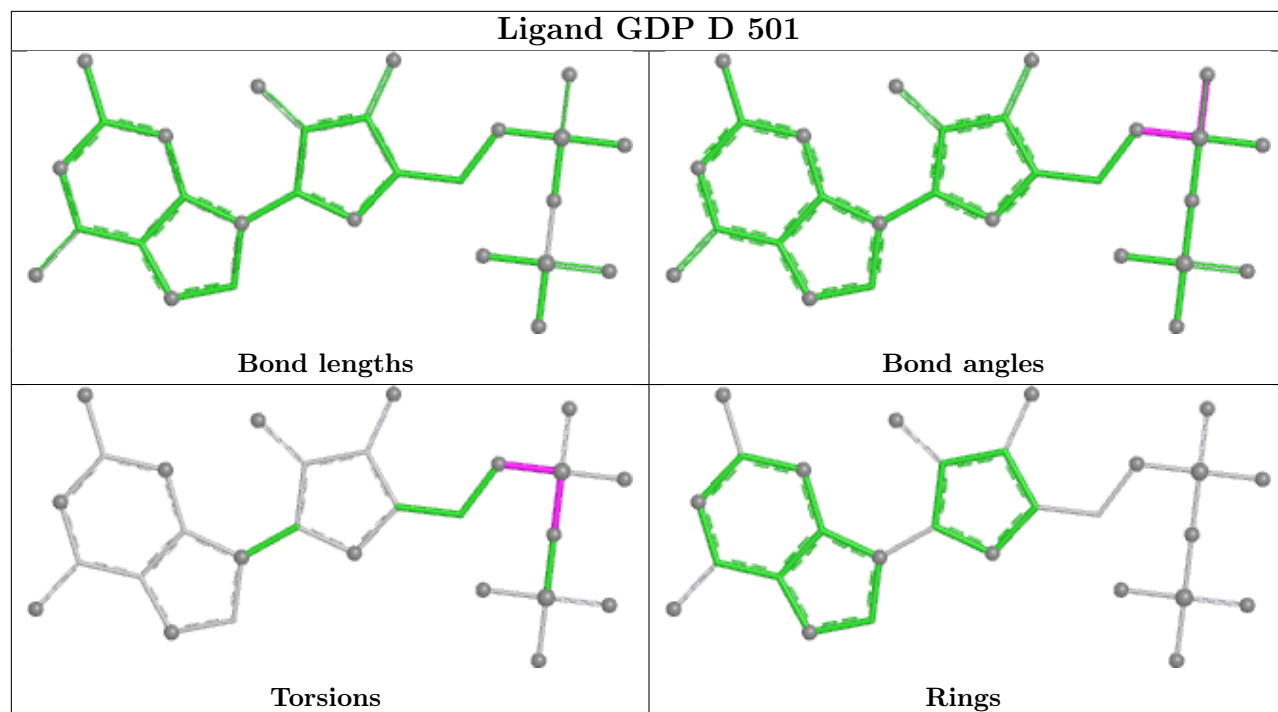
Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	C4'-C5'-O5'-PA
4	C	501	GTP	C4'-C5'-O5'-PA
7	A	507	GOL	O1-C1-C2-O2
4	C	501	GTP	PB-O3A-PA-O2A
8	D	501	GDP	PB-O3A-PA-O2A

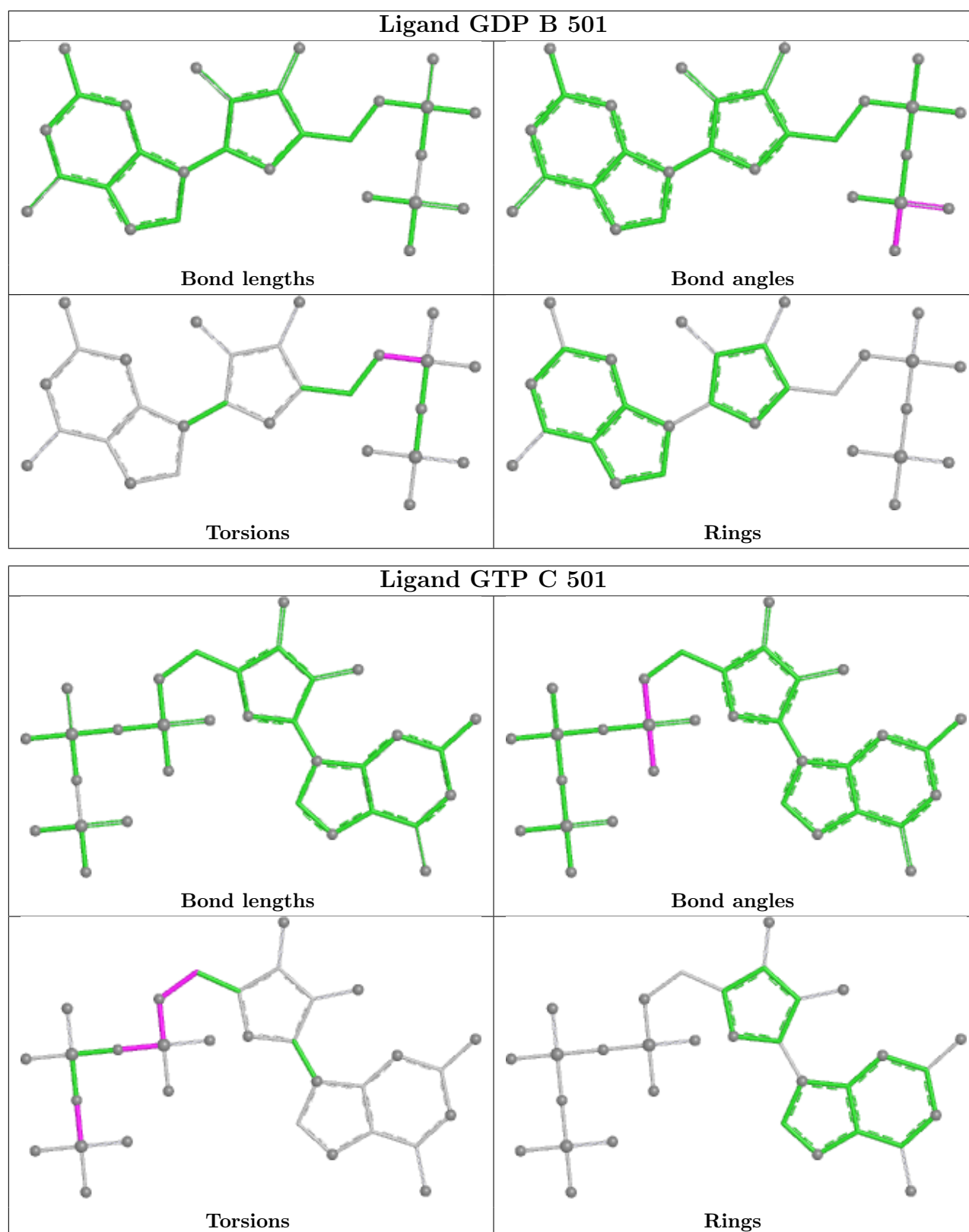
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	SO4	2	0
7	A	506	GOL	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	430/450 (95%)	-0.01	7 (1%) 70 67	32, 48, 69, 89	1 (0%)
1	C	430/450 (95%)	0.28	10 (2%) 61 58	25, 55, 82, 103	3 (0%)
2	B	428/447 (95%)	-0.02	8 (1%) 66 63	23, 48, 75, 99	1 (0%)
2	D	427/447 (95%)	-0.05	8 (1%) 66 63	24, 45, 71, 87	6 (1%)
3	E	129/143 (90%)	0.44	7 (5%) 31 28	34, 61, 86, 98	1 (0%)
All	All	1844/1937 (95%)	0.08	40 (2%) 62 59	23, 50, 77, 103	12 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	TYR	6.8
1	A	346	TRP	4.9
1	C	349	THR	3.7
2	B	283	ALA	3.7
1	C	177	VAL	3.5
1	C	357	TYR	3.5
1	C	362	VAL	3.4
1	A	438	ASP	3.4
3	E	143	ALA	3.3
1	C	1[A]	MET	3.2
2	D	277	GLY	3.2
1	C	37	PRO	2.9
1	C	281	ALA	2.8
2	D	57	GLY	2.8
1	C	278	ALA	2.6
3	E	145	ARG	2.5
3	E	144	SER	2.5
2	D	55	SER	2.5
3	E	31	GLY	2.5
3	E	44	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	56	GLY	2.4
2	D	431	ASP	2.4
2	D	278	SER	2.4
1	C	350	GLY	2.4
2	B	23	ILE	2.4
2	B	95	SER	2.4
2	B	278	SER	2.4
1	A	262	TYR	2.3
3	E	5	ASP	2.3
1	A	279	GLU	2.2
1	A	335	ILE	2.2
2	B	431	ASP	2.2
2	B	56	GLY	2.1
1	A	282	TYR	2.1
2	D	178[A]	THR	2.1
2	B	429	THR	2.1
2	D	92	PHE	2.1
2	B	284	LEU	2.1
3	E	139	LEU	2.1
1	A	45	GLY	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	SO4	D	504	5/5	0.46	0.13	175,175,175,175	0
6	SO4	C	505	5/5	0.62	0.10	142,142,142,142	0
7	GOL	A	506	6/6	0.66	0.19	63,64,65,65	0

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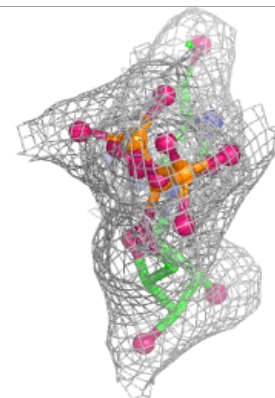
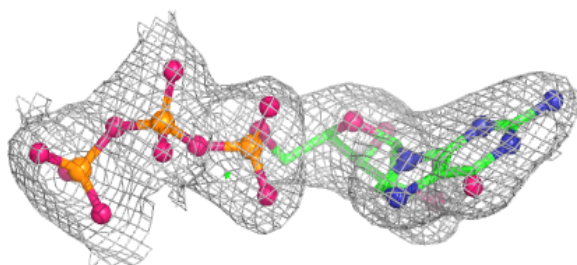
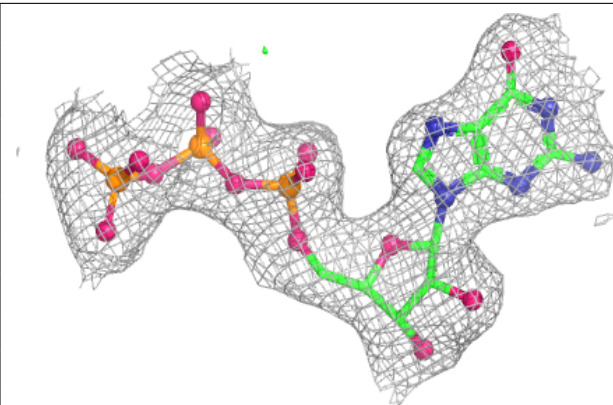
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	C	504	5/5	0.71	0.11	129,129,129,129	0
6	SO4	E	201	5/5	0.72	0.11	131,131,131,131	0
6	SO4	A	505	5/5	0.73	0.17	124,124,124,124	0
6	SO4	D	503	5/5	0.76	0.15	128,128,128,129	0
6	SO4	B	503	5/5	0.76	0.10	154,154,154,154	0
6	SO4	A	504	5/5	0.77	0.12	105,105,106,106	0
7	GOL	A	507	6/6	0.84	0.13	70,71,71,71	0
6	SO4	B	502	5/5	0.85	0.08	102,102,102,102	0
6	SO4	C	503	5/5	0.88	0.14	125,125,125,125	0
6	SO4	A	503	5/5	0.89	0.08	83,83,83,83	0
6	SO4	D	505	5/5	0.92	0.10	111,111,111,111	0
4	GTP	A	501	32/32	0.98	0.04	35,38,41,41	0
4	GTP	C	501	32/32	0.98	0.05	41,47,49,50	0
6	SO4	D	502	5/5	0.98	0.05	59,59,59,59	0
8	GDP	B	501	28/28	0.98	0.04	38,41,42,42	0
8	GDP	D	501	28/28	0.98	0.04	33,35,36,37	0
5	MG	C	502	1/1	0.99	0.02	40,40,40,40	0
5	MG	A	502	1/1	0.99	0.03	39,39,39,39	0

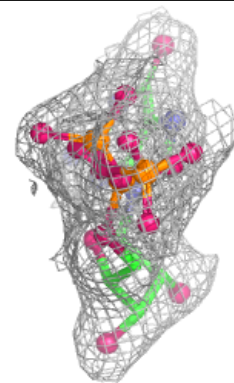
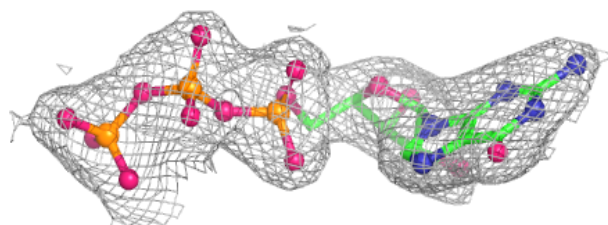
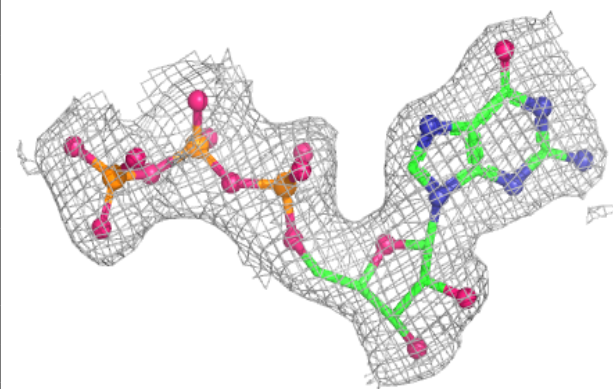
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP A 501:

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

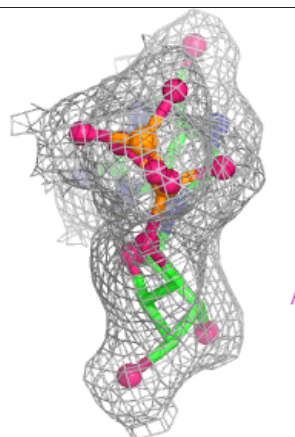
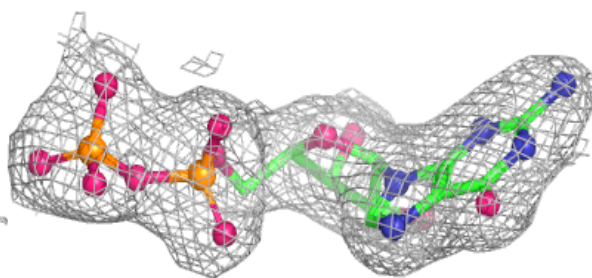
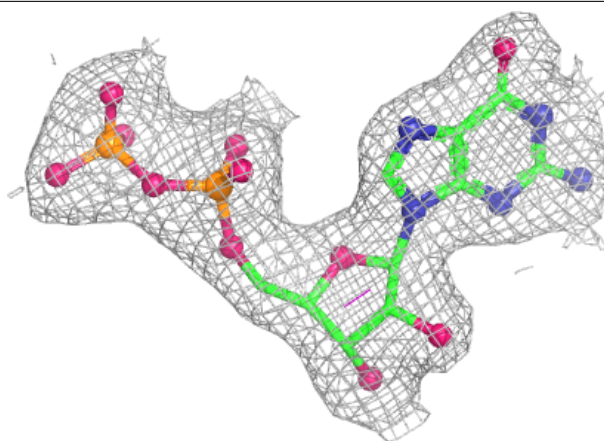
**Electron density around GTP C 501:**

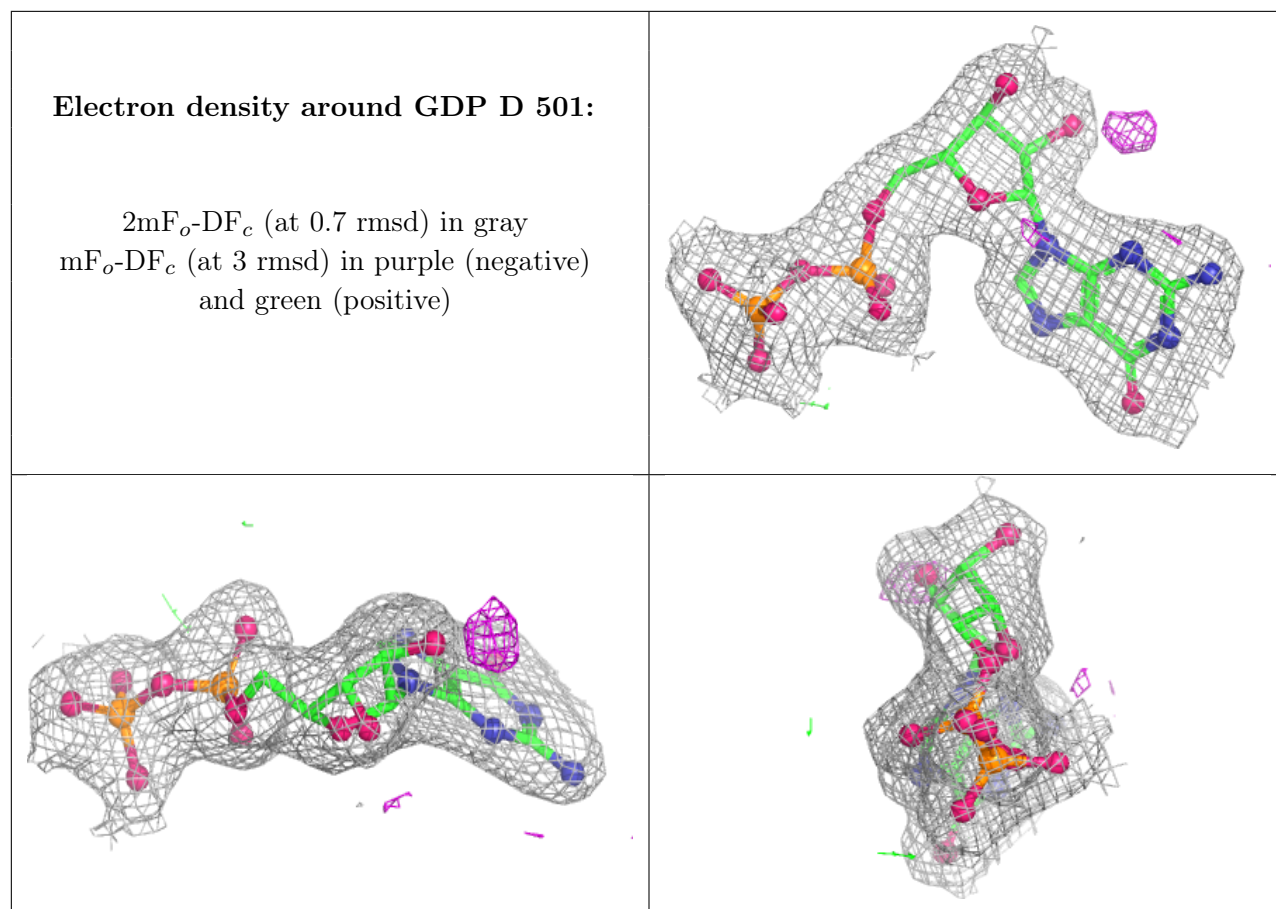
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.