



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:22 AM UTC

PDB ID : 6TIY / pdb_00006tiy
Title : DROSOPHILA GMPCPP-TUBULIN
Authors : Gigant, B.
Deposited on : 2019-11-22
Resolution : 2.29 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

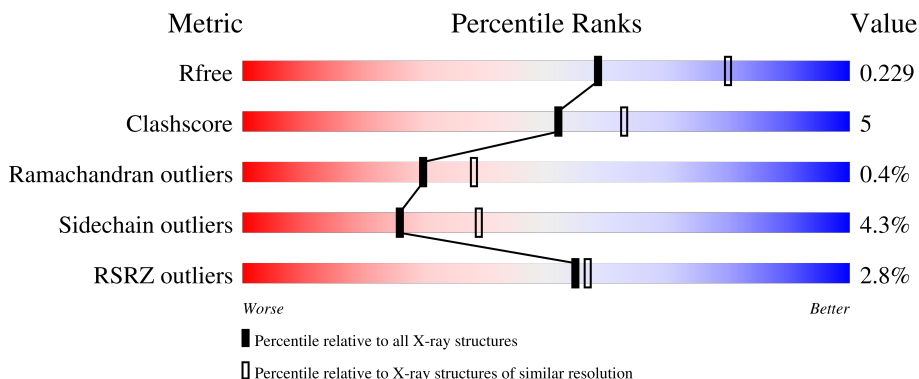
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	5% 80% 15% ..
2	B	447	% 81% 15% ..
2	D	447	% 84% 12% .
3	E	143	6% 78% 13% .. 7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15210 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	434	Total	C	N	O	S	0	0	0
			3392	2148	577	644	23			
1	C	434	Total	C	N	O	S	0	2	0
			3386	2144	575	642	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	430	Total	C	N	O	S	0	0	0
			3362	2112	573	651	26			
2	D	427	Total	C	N	O	S	0	3	0
			3362	2117	570	648	27			

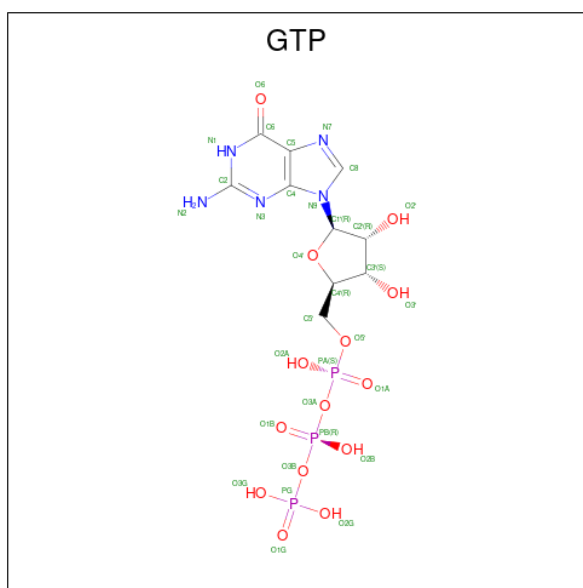
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	133	Total	C	N	O	S	0	0	0
			1085	670	197	214	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	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

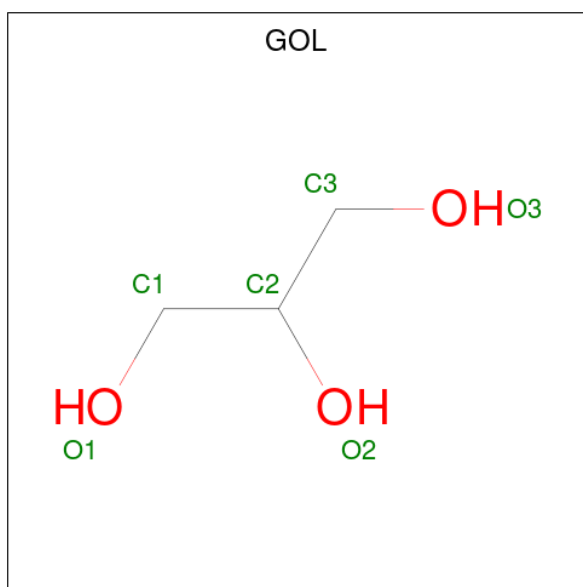
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

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



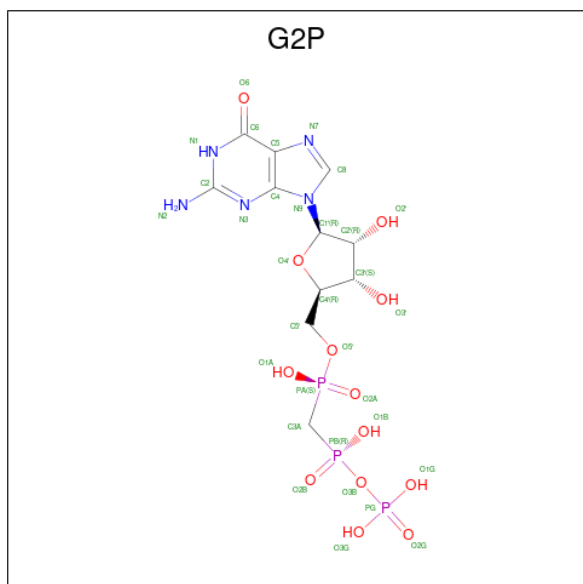
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	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: $C_3H_8O_3$).



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

- Molecule 8 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 32	C 11	N 5	O 13	P 3	0	0
8	D	1	Total 32	C 11	N 5	O 13	P 3	0	0

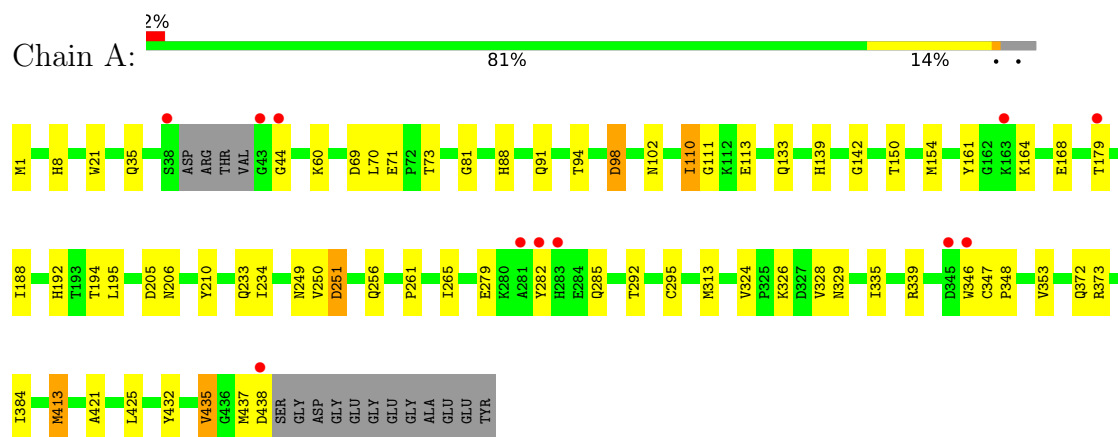
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	143	Total 143	O 143	0	0
9	B	92	Total 92	O 92	0	0
9	C	85	Total 85	O 85	0	0
9	D	96	Total 96	O 96	0	0
9	E	14	Total 14	O 14	0	0

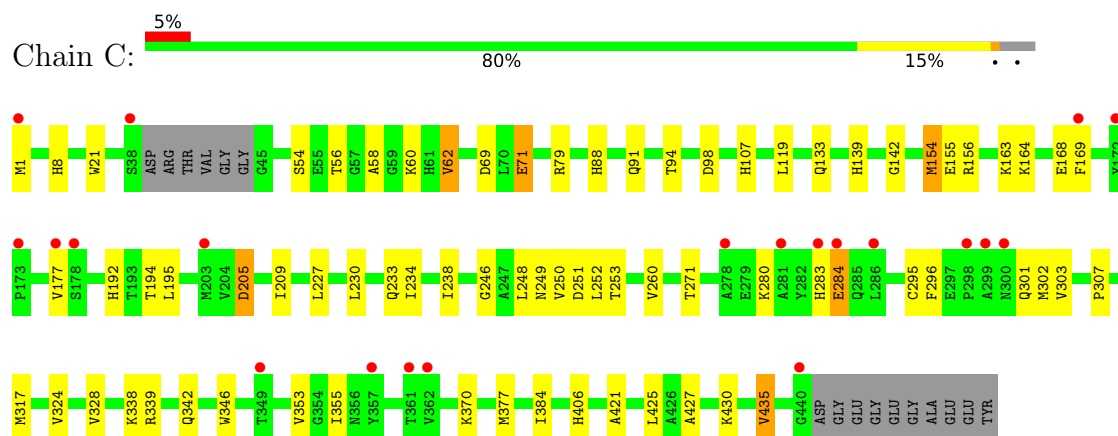
3 Residue-property plots

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.

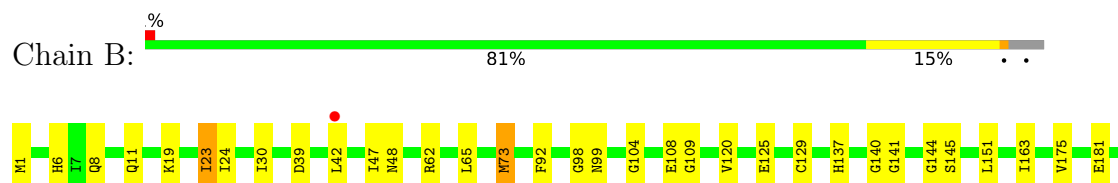
• Molecule 1: Tubulin alpha-1 chain

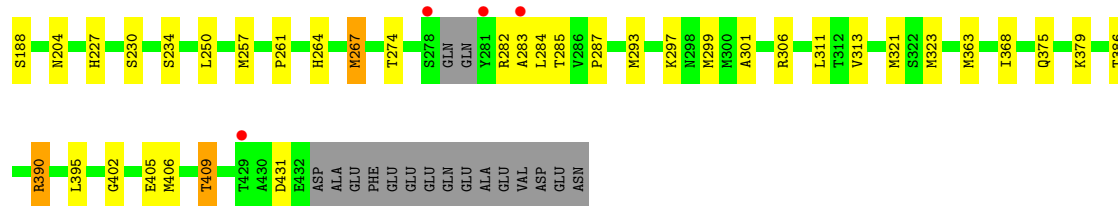


• Molecule 1: Tubulin alpha-1 chain

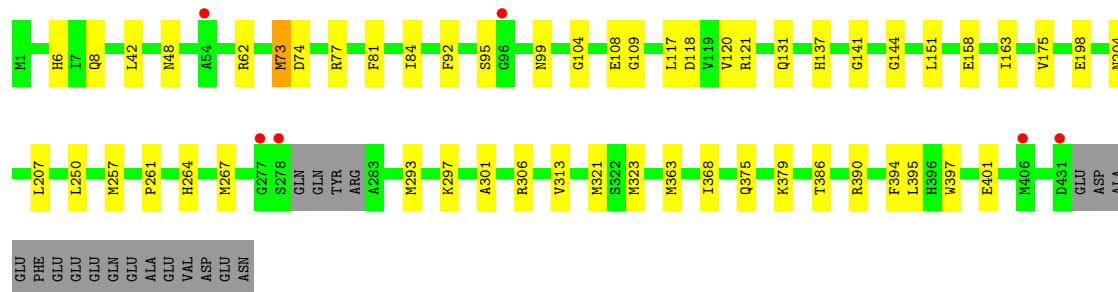
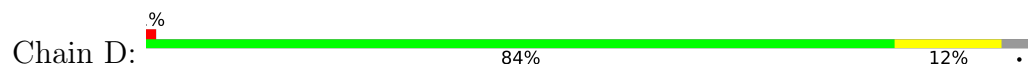


• Molecule 2: Tubulin beta-1 chain

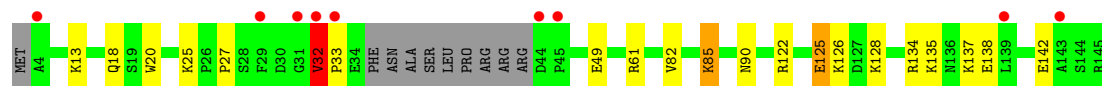
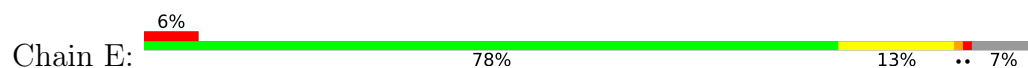




• Molecule 2: Tubulin beta-1 chain



• 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	66.67Å 126.56Å 251.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.29 33.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.3 (33.00-2.29) 95.2 (33.00-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.187 , 0.217 0.196 , 0.229	Depositor DCC
R_{free} test set	4565 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	1.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	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	15210	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: GTP, MG, GOL, G2P, 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	0.76	1/3469 (0.0%)	1.12	11/4708 (0.2%)
1	C	0.78	2/3467 (0.1%)	1.13	5/4705 (0.1%)
2	B	0.78	3/3434 (0.1%)	1.09	1/4651 (0.0%)
2	D	0.74	0/3444	1.09	2/4663 (0.0%)
3	E	0.74	1/1096 (0.1%)	1.24	0/1459
All	All	0.76	7/14910 (0.0%)	1.12	19/20186 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	MET	SD-CE	-9.15	1.56	1.79
2	B	73	MET	SD-CE	-6.91	1.62	1.79
2	B	267	MET	SD-CE	-6.84	1.62	1.79
2	B	283	ALA	CA-C	6.13	1.60	1.52
1	C	154	MET	SD-CE	-5.42	1.66	1.79
1	C	177	VAL	CA-C	5.16	1.57	1.52
3	E	32	VAL	CA-C	5.02	1.58	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASN	CA-CB-CG	6.94	119.54	112.60
1	C	338	LYS	CA-C-N	6.14	128.51	120.28
1	C	338	LYS	C-N-CA	6.14	128.51	120.28
1	A	81	GLY	CA-C-N	5.70	127.92	120.28
1	A	81	GLY	C-N-CA	5.70	127.92	120.28
1	C	142	GLY	N-CA-C	5.66	122.35	113.86
2	D	95	SER	N-CA-C	5.66	118.30	111.40
1	A	205	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	260	VAL	N-CA-C	5.44	113.54	108.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	GLY	CA-C-N	5.44	128.32	120.38
1	A	111	GLY	C-N-CA	5.44	128.32	120.38
2	D	118	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	205	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	251	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	142	GLY	N-CA-C	5.31	121.83	113.86
1	A	98	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	311	LEU	N-CA-C	-5.10	105.17	111.40
1	A	249	ASN	CA-C-N	5.09	128.64	120.30
1	A	249	ASN	C-N-CA	5.09	128.64	120.30

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	3392	0	3301	33	0
1	C	3386	0	3303	45	0
2	B	3362	0	3240	37	0
2	D	3362	0	3254	31	0
3	E	1085	0	1089	11	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	15	0	0	0	0
6	E	5	0	0	0	0
7	A	6	0	8	1	0
8	B	32	0	14	4	0
8	D	32	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	143	0	0	2	0
9	B	92	0	0	0	0
9	C	85	0	0	1	0
9	D	96	0	0	1	0
9	E	14	0	0	0	0
All	All	15210	0	14247	149	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 (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.10	0.97
2:D:204:ASN:HD21	8:D:501:G2P:H2N2	1.07	0.96
2:B:204:ASN:HD21	8:B:501:G2P:H2N2	1.12	0.90
2:D:141:GLY:HA3	8:D:501:G2P:H3A1	1.52	0.89
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.15	0.89
1:C:296:PHE:CE1	1:C:377:MET:HE1	2.08	0.88
1:A:71:GLU:OE2	1:A:73:THR:HB	1.76	0.86
2:B:6:HIS:CE1	2:B:8:GLN:HE21	1.98	0.80
1:C:339:ARG:H	1:C:339:ARG:HD3	1.44	0.80
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.00	0.80
2:D:261:PRO:O	2:D:264:HIS:HD2	1.71	0.73
2:B:261:PRO:O	2:B:264:HIS:HD2	1.74	0.70
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.74	0.68
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.75	0.68
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.44	0.66
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.79	0.64
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.00	0.61
2:B:227:HIS:HE1	2:B:274:THR:HG23	1.66	0.60
7:A:506:GOL:H2	3:E:61:ARG:HG3	1.83	0.60
1:A:110:ILE:O	1:A:113:GLU:HG2	2.03	0.58
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.84	0.58
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.85	0.58
2:B:23:ILE:HD13	2:B:234:SER:HB2	1.86	0.57
2:B:145:SER:HG	2:B:188:SER:HG	1.52	0.57
1:C:427:ALA:O	1:C:430:LYS:HG3	2.03	0.57
1:C:317:MET:SD	1:C:377:MET:HE2	2.44	0.57
1:A:71:GLU:OE2	1:A:73:THR:CB	2.52	0.56
2:B:406:MET:HA	2:B:409:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:HG2	3:E:90:ASN:OD1	2.06	0.56
2:D:48:ASN:O	2:D:62:ARG:NH2	2.37	0.56
2:B:11:GLN:HB3	8:B:501:G2P:O2A	2.06	0.56
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.52	0.56
1:A:292:THR:O	1:A:295:CYS:HB2	2.05	0.55
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.72	0.55
1:A:346:TRP:CZ3	1:A:347:CYS:SG	2.99	0.55
2:D:73[A]:MET:HG3	2:D:74:ASP:N	2.23	0.54
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.89	0.54
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.26	0.54
2:B:104:GLY:O	2:B:109:GLY:HA3	2.08	0.53
1:C:283:HIS:O	1:C:284:GLU:O	2.26	0.53
2:D:73[A]:MET:SD	2:D:77:ARG:NH1	2.80	0.53
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.90	0.53
2:D:293:MET:HE3	2:D:313:VAL:HG11	1.90	0.53
1:C:427:ALA:HA	1:C:430:LYS:HG2	1.90	0.53
1:C:209:ILE:HD11	1:C:302:MET:HG3	1.91	0.53
2:B:141:GLY:HA3	8:B:501:G2P:H3A1	1.89	0.53
2:B:267:MET:HE2	2:B:299:MET:HG3	1.91	0.53
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.91	0.52
1:A:437:MET:HG3	1:A:438:ASP:N	2.23	0.52
1:C:296:PHE:CZ	1:C:377:MET:HE1	2.45	0.52
2:D:204:ASN:ND2	8:D:501:G2P:H2N2	1.91	0.52
2:B:48:ASN:O	2:B:62:ARG:NH2	2.41	0.52
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.75	0.51
2:B:293:MET:HE3	2:B:313:VAL:HG11	1.92	0.51
2:B:145:SER:OG	2:B:188:SER:OG	2.24	0.50
1:A:285:GLN:NE2	1:A:372:GLN:H	2.10	0.50
1:A:437:MET:HG3	1:A:438:ASP:H	1.76	0.50
2:D:73[A]:MET:HB3	2:D:92[A]:PHE:CZ	2.46	0.50
2:B:227:HIS:CE1	2:B:274:THR:HG23	2.47	0.50
1:A:139:HIS:HE1	1:A:168:GLU:OE1	1.95	0.50
2:D:321:MET:HE3	2:D:363:MET:HE3	1.94	0.49
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.94	0.49
1:C:133:GLN:HE22	1:C:252:LEU:H	1.60	0.49
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.95	0.48
2:B:65:LEU:O	2:B:73:MET:HE1	2.13	0.48
1:C:133:GLN:NE2	1:C:252:LEU:H	2.11	0.48
2:B:386:THR:O	2:B:390:ARG:HB2	2.13	0.48
1:A:88:HIS:H	1:A:91:GLN:NE2	2.12	0.48
2:D:99:ASN:ND2	9:D:604:HOH:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:MET:HE3	2:B:363:MET:HE3	1.96	0.47
2:D:104:GLY:O	2:D:109:GLY:HA3	2.14	0.47
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.96	0.47
1:C:271:THR:HG21	1:C:295:CYS:O	2.14	0.47
1:C:54:SER:OG	1:C:62:VAL:HG13	2.14	0.47
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.96	0.47
2:B:395:LEU:HD21	2:B:405:GLU:HG3	1.95	0.47
1:C:295:CYS:HB3	1:C:377:MET:HE3	1.97	0.47
2:D:386:THR:O	2:D:390:ARG:HB2	2.14	0.47
1:A:88:HIS:H	1:A:91:GLN:HE21	1.63	0.47
2:D:137:HIS:HD2	2:D:144:GLY:O	1.98	0.47
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.95	0.47
1:A:150:THR:O	1:A:154:MET:HG2	2.14	0.47
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.97	0.47
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.44	0.47
2:B:23:ILE:HD12	2:B:24:ILE:HG23	1.97	0.47
1:C:139:HIS:HE1	1:C:168:GLU:OE1	1.98	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.46
2:D:375:GLN:HE21	2:D:379:LYS:HE3	1.81	0.46
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.80	0.46
2:D:131:GLN:NE2	2:D:250:LEU:H	2.14	0.46
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.80	0.46
1:A:261:PRO:HD2	9:A:609:HOH:O	2.16	0.45
3:E:32:VAL:N	3:E:33:PRO:HD3	2.32	0.45
2:B:137:HIS:HD2	2:B:144:GLY:O	2.00	0.45
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.99	0.45
2:D:73[A]:MET:HB3	2:D:92[A]:PHE:CE1	2.51	0.45
2:D:204:ASN:HD22	2:D:207:LEU:HD12	1.82	0.45
1:C:107:HIS:CE1	1:C:155:GLU:OE2	2.68	0.45
1:A:329:ASN:HD21	3:E:20:TRP:NE1	2.11	0.45
2:D:73[A]:MET:HG3	2:D:74:ASP:H	1.80	0.45
2:D:73[A]:MET:SD	2:D:77:ARG:NH2	2.88	0.45
1:C:154:MET:HE2	1:C:194:THR:HG23	1.99	0.45
1:C:246:GLY:H	1:C:249:ASN:HD21	1.63	0.45
1:C:301:GLN:HE22	1:C:307:PRO:CG	2.30	0.44
2:B:402:GLY:O	3:E:85:LYS:HE2	2.17	0.44
2:B:267:MET:HE2	2:B:299:MET:CG	2.47	0.44
1:C:280:LYS:NZ	1:C:283:HIS:HA	2.33	0.44
2:B:23:ILE:HG12	2:B:230:SER:HB2	2.00	0.43
1:C:280:LYS:HZ2	1:C:283:HIS:HA	1.83	0.43
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:GLN:HE21	2:B:379:LYS:HE3	1.84	0.43
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.99	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.43
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.43
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.43
2:B:1:MET:N	2:B:129:CYS:SG	2.84	0.43
2:B:98:GLY:HA3	1:C:253:THR:HG22	2.01	0.43
3:E:32:VAL:N	3:E:33:PRO:CD	2.82	0.43
1:A:154:MET:HE2	1:A:194:THR:HG23	2.01	0.42
1:C:79:ARG:HD3	9:C:632:HOH:O	2.18	0.42
1:C:69:ASP:O	1:C:94:THR:HA	2.19	0.42
2:B:19:LYS:O	2:B:23:ILE:HG13	2.20	0.42
1:A:69:ASP:O	1:A:94:THR:HA	2.20	0.42
2:B:30:ILE:HD11	2:B:47:ILE:HD11	2.02	0.42
2:D:257:MET:HE2	2:D:368:ILE:HG22	2.02	0.42
1:A:206:ASN:O	1:A:210:TYR:HB2	2.20	0.41
2:D:401:GLU:C	3:E:137:LYS:HB2	2.44	0.41
1:C:56:THR:HG22	1:C:60:LYS:H	1.86	0.41
2:B:140:GLY:HA3	2:B:181:GLU:HG2	2.03	0.41
1:C:56:THR:HG23	1:C:58:ALA:H	1.85	0.41
3:E:125:GLU:HA	3:E:128:LYS:HD2	2.03	0.41
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.55	0.41
1:C:88:HIS:O	1:C:91:GLN:HG2	2.20	0.41
1:C:205:ASP:CB	1:C:303:VAL:HA	2.50	0.41
2:D:73[A]:MET:HB3	2:D:92[A]:PHE:CE2	2.56	0.41
2:B:99:ASN:HA	8:B:501:G2P:O3G	2.21	0.41
1:C:169:PHE:HE2	1:C:238:ILE:HD12	1.85	0.41
1:C:133:GLN:HE22	1:C:251:ASP:HB2	1.86	0.41
2:D:394:PHE:O	2:D:397:TRP:HB2	2.21	0.41
1:A:179:THR:HG21	9:A:657:HOH:O	2.20	0.40
2:D:81:PHE:O	2:D:84:ILE:HG22	2.21	0.40
1:A:35:GLN:OE1	1:A:60:LYS:HG2	2.21	0.40
2:B:257:MET:HE2	2:B:368:ILE:HG22	2.04	0.40
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.39	0.40
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.04	0.40
2:D:117:LEU:O	2:D:121:ARG:HG3	2.21	0.40
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.69	0.40
1:C:427:ALA:HA	1:C:430:LYS:CG	2.51	0.40
3:E:13:LYS:HD3	3:E:18:GLN:HG3	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	430/450 (96%)	417 (97%)	11 (3%)	2 (0%)	24	31
1	C	431/450 (96%)	415 (96%)	15 (4%)	1 (0%)	43	55
2	B	426/447 (95%)	419 (98%)	4 (1%)	3 (1%)	18	23
2	D	426/447 (95%)	420 (99%)	6 (1%)	0	100	100
3	E	129/143 (90%)	125 (97%)	3 (2%)	1 (1%)	16	20
All	All	1842/1937 (95%)	1796 (98%)	39 (2%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR
1	C	284	GLU
1	A	44	GLY
2	B	284	LEU
2	B	282	ARG
3	E	142	GLU
2	B	175	VAL

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	364/375 (97%)	346 (95%)	18 (5%)	22	34
1	C	364/375 (97%)	349 (96%)	15 (4%)	27	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	365/382 (96%)	352 (96%)	13 (4%)	31	47
2	D	367/382 (96%)	354 (96%)	13 (4%)	32	48
3	E	115/126 (91%)	104 (90%)	11 (10%)	8	10
All	All	1575/1640 (96%)	1505 (96%)	70 (4%)	26	38

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	110	ILE
1	A	188	ILE
1	A	195	LEU
1	A	233	GLN
1	A	234	ILE
1	A	250	VAL
1	A	256	GLN
1	A	279	GLU
1	A	313	MET
1	A	324	VAL
1	A	326	LYS
1	A	339	ARG
1	A	373	ARG
1	A	384	ILE
1	A	413	MET
1	A	425	LEU
1	A	435	VAL
2	B	23	ILE
2	B	39	ASP
2	B	42	LEU
2	B	108	GLU
2	B	120	VAL
2	B	125	GLU
2	B	151	LEU
2	B	297	LYS
2	B	306	ARG
2	B	323	MET
2	B	390	ARG
2	B	409	THR
2	B	431	ASP
1	C	1[A]	MET
1	C	1[B]	MET

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Mol	Chain	Res	Type
1	C	62	VAL
1	C	71	GLU
1	C	164	LYS
1	C	195	LEU
1	C	233	GLN
1	C	234	ILE
1	C	250	VAL
1	C	324	VAL
1	C	342	GLN
1	C	370	LYS
1	C	384	ILE
1	C	425	LEU
1	C	435	VAL
2	D	42	LEU
2	D	73[A]	MET
2	D	73[B]	MET
2	D	108	GLU
2	D	120	VAL
2	D	151	LEU
2	D	158	GLU
2	D	175	VAL
2	D	198	GLU
2	D	297	LYS
2	D	306	ARG
2	D	323	MET
2	D	395	LEU
3	E	25	LYS
3	E	32	VAL
3	E	49	GLU
3	E	82	VAL
3	E	85	LYS
3	E	122	ARG
3	E	125	GLU
3	E	126	LYS
3	E	134	ARG
3	E	135	LYS
3	E	138	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS

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Mol	Chain	Res	Type
1	A	50	ASN
1	A	85	GLN
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	256	GLN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	342	GLN
1	A	356	ASN
2	B	6	HIS
2	B	11	GLN
2	B	37	HIS
2	B	48	ASN
2	B	137	HIS
2	B	204	ASN
2	B	227	HIS
2	B	264	HIS
2	B	292	GLN
2	B	298	ASN
2	B	337	ASN
2	B	375	GLN
2	B	423	GLN
2	B	426	GLN
1	C	8	HIS
1	C	35	GLN
1	C	50	ASN
1	C	85	GLN
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	256	GLN
1	C	301	GLN
1	C	329	ASN
1	C	380	ASN
2	D	6	HIS

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Mol	Chain	Res	Type
2	D	37	HIS
2	D	48	ASN
2	D	131	GLN
2	D	137	HIS
2	D	195	ASN
2	D	204	ASN
2	D	264	HIS
2	D	337	ASN
2	D	375	GLN
2	D	396	HIS
2	D	423	GLN
3	E	71	HIS
3	E	111	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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z > 2$
6	SO4	D	503	-	4,4,4	0.26	0	6,6,6	0.15	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	0.52	0	50,54,54	0.58	1 (2%)
6	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.25	0
6	SO4	A	504	-	4,4,4	0.26	0	6,6,6	0.15	0
6	SO4	B	503	-	4,4,4	0.29	0	6,6,6	0.18	0
6	SO4	D	504	-	4,4,4	0.29	0	6,6,6	0.17	0
6	SO4	C	503	-	4,4,4	0.28	0	6,6,6	0.10	0
8	G2P	D	501	5	30,34,34	0.44	0	46,54,54	0.72	2 (4%)
4	GTP	A	501	5	33,34,34	0.51	0	50,54,54	0.51	0
7	GOL	A	506	-	5,5,5	0.11	0	5,5,5	0.26	0
6	SO4	E	201	-	4,4,4	0.25	0	6,6,6	0.10	0
8	G2P	B	501	5	30,34,34	0.46	0	46,54,54	0.82	2 (4%)
6	SO4	D	505	-	4,4,4	0.30	0	6,6,6	0.19	0
6	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.12	0
6	SO4	C	504	-	4,4,4	0.28	0	6,6,6	0.11	0
6	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.22	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
4	GTP	C	501	5	-	6/22/38/38	0/3/3/3
8	G2P	D	501	5	-	6/19/38/38	0/3/3/3
4	GTP	A	501	5	-	6/22/38/38	0/3/3/3
7	GOL	A	506	-	-	0/4/4/4	-
8	G2P	B	501	5	-	5/19/38/38	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	G2P	O2B-PB-C3A	3.47	118.18	109.05
8	B	501	G2P	O2A-PA-C3A	3.37	117.91	109.05
8	D	501	G2P	O2B-PB-C3A	2.83	116.52	109.05
8	D	501	G2P	O2A-PA-C3A	2.80	116.43	109.05
4	C	501	GTP	O5'-PA-O1A	2.43	118.56	108.94

There are no chirality outliers.

All (23) 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	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	G2P	PB-O3B-PG-O1G
8	B	501	G2P	C5'-O5'-PA-C3A
8	D	501	G2P	PB-O3B-PG-O1G
8	D	501	G2P	PB-O3B-PG-O3G
8	D	501	G2P	PB-C3A-PA-O2A
8	D	501	G2P	PB-C3A-PA-O5'
8	B	501	G2P	O4'-C4'-C5'-O5'
8	B	501	G2P	C3'-C4'-C5'-O5'
8	B	501	G2P	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	C5'-O5'-PA-O2A
8	D	501	G2P	C5'-O5'-PA-O1A
4	A	501	GTP	PB-O3A-PA-O2A
4	C	501	GTP	PB-O3A-PA-O2A
8	D	501	G2P	PB-O3B-PG-O2G
4	A	501	GTP	C4'-C5'-O5'-PA
4	C	501	GTP	C4'-C5'-O5'-PA

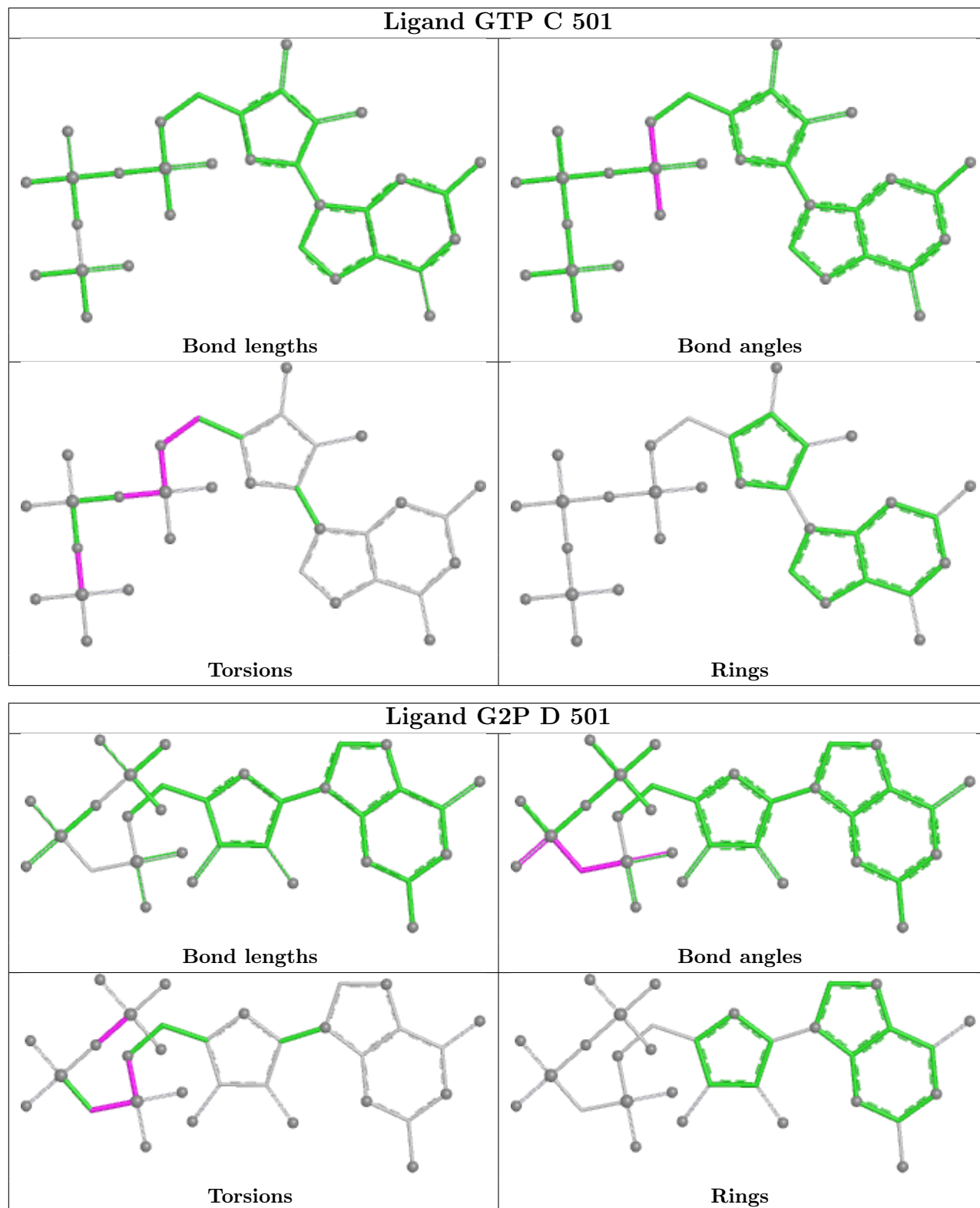
There are no ring outliers.

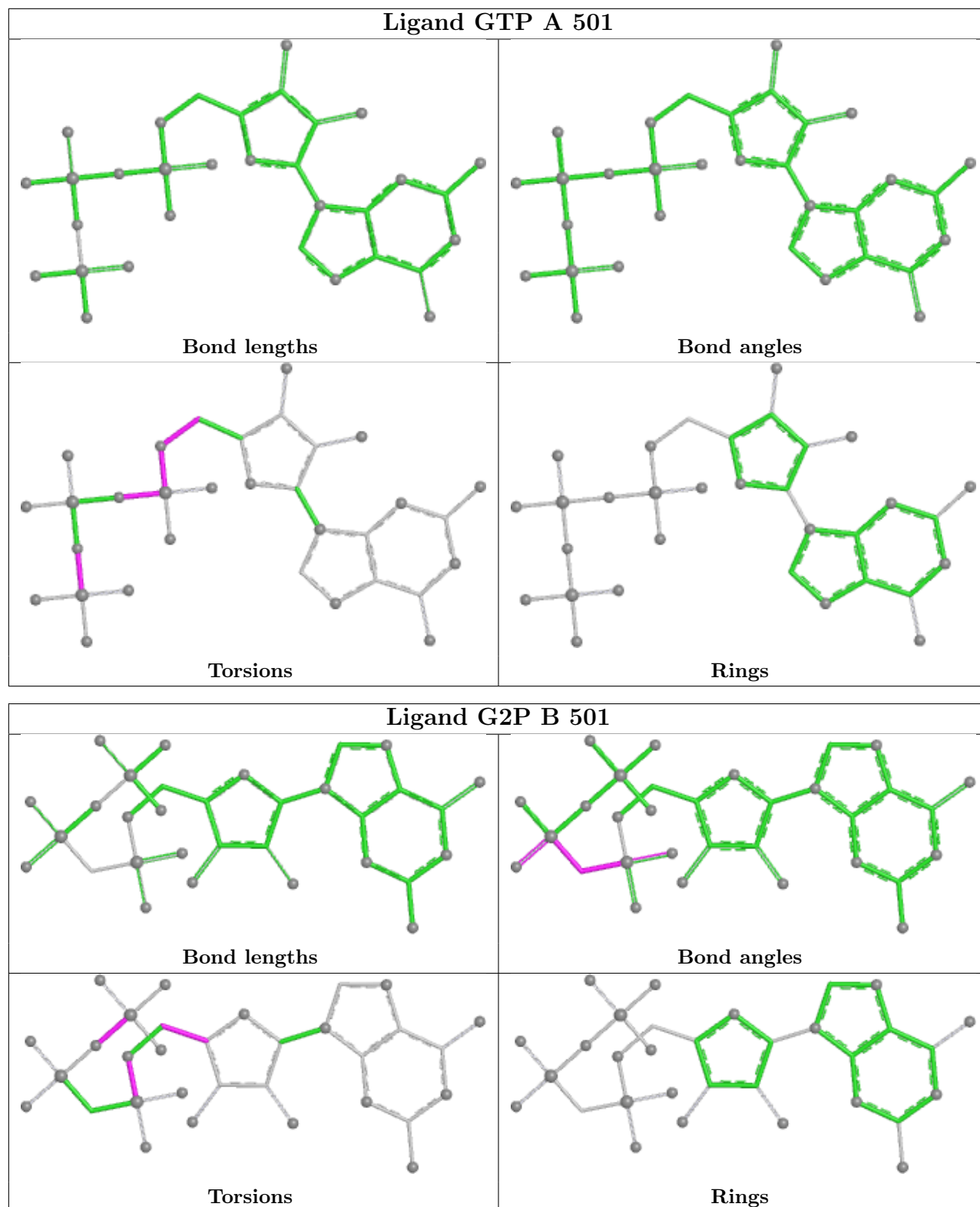
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	G2P	3	0
7	A	506	GOL	1	0
8	B	501	G2P	4	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	434/450 (96%)	0.11	11 (2%) 58 60	45, 59, 82, 105	0
1	C	434/450 (96%)	0.39	21 (4%) 35 37	37, 65, 94, 112	2 (0%)
2	B	430/447 (96%)	0.12	5 (1%) 76 77	44, 60, 89, 112	0
2	D	427/447 (95%)	0.07	6 (1%) 73 75	32, 56, 81, 96	3 (0%)
3	E	133/143 (93%)	0.61	9 (6%) 23 25	58, 75, 113, 125	0
All	All	1858/1937 (95%)	0.20	52 (2%) 55 57	32, 61, 90, 125	5 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	32	VAL	6.7
1	C	362	VAL	4.8
1	C	177	VAL	4.5
1	A	346	TRP	4.3
1	A	43	GLY	4.0
1	A	438	ASP	3.8
1	C	172	TYR	3.6
2	B	281	TYR	3.5
2	D	278	SER	3.2
3	E	44	ASP	3.2
1	C	298	PRO	3.2
1	C	203	MET	3.2
1	A	179	THR	3.1
1	C	169	PHE	3.1
3	E	29	PHE	3.0
2	D	277	GLY	3.0
1	A	281	ALA	2.9
3	E	143	ALA	2.9
1	C	278	ALA	2.9
3	E	4	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	2.8
1	C	284	GLU	2.8
1	C	283	HIS	2.7
1	A	38	SER	2.7
1	C	1[A]	MET	2.6
1	C	357	TYR	2.6
2	B	278	SER	2.6
2	D	96	GLY	2.5
2	D	406	MET	2.5
2	B	283	ALA	2.5
2	D	54	ALA	2.5
2	B	429	THR	2.4
1	C	173	PRO	2.4
3	E	45	PRO	2.4
1	C	349	THR	2.4
1	A	163	LYS	2.3
2	B	42	LEU	2.3
1	A	44	GLY	2.3
1	C	440	GLY	2.3
1	A	345	ASP	2.3
3	E	139	LEU	2.2
3	E	33	PRO	2.2
3	E	31	GLY	2.2
1	C	38	SER	2.2
2	D	431	ASP	2.2
1	A	283	HIS	2.2
1	C	361	THR	2.2
1	C	178	SER	2.1
1	C	299	ALA	2.1
1	C	300	ASN	2.1
1	C	281	ALA	2.0
1	C	286	LEU	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 ⓘ

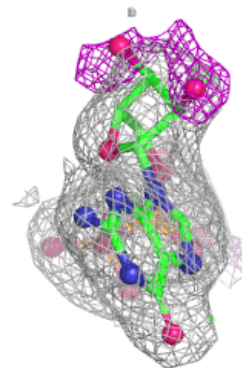
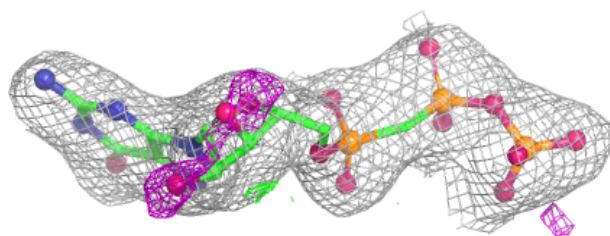
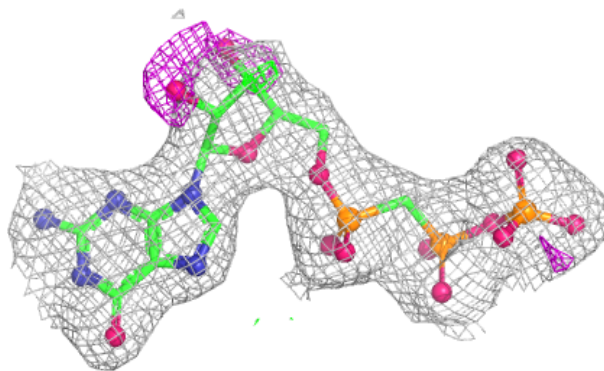
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	C	504	5/5	0.49	0.12	175,175,175,175	0
7	GOL	A	506	6/6	0.59	0.21	82,82,82,83	0
6	SO4	B	504	5/5	0.69	0.11	151,151,151,151	0
6	SO4	A	505	5/5	0.74	0.11	115,116,116,116	0
6	SO4	B	503	5/5	0.77	0.10	118,118,118,119	0
6	SO4	A	503	5/5	0.84	0.10	107,107,107,107	0
6	SO4	D	504	5/5	0.85	0.12	127,127,127,127	0
6	SO4	A	504	5/5	0.85	0.14	131,131,131,131	0
6	SO4	E	201	5/5	0.86	0.08	132,132,132,132	0
6	SO4	D	505	5/5	0.87	0.10	113,113,113,113	0
6	SO4	C	503	5/5	0.89	0.13	140,140,140,140	0
8	G2P	B	501	32/32	0.95	0.07	54,56,61,62	0
8	G2P	D	501	32/32	0.95	0.08	42,49,55,55	0
4	GTP	C	501	32/32	0.96	0.07	52,59,62,64	0
5	MG	B	502	1/1	0.98	0.04	68,68,68,68	0
4	GTP	A	501	32/32	0.98	0.05	45,49,49,50	0
6	SO4	D	503	5/5	0.98	0.04	66,66,66,66	0
5	MG	A	502	1/1	0.99	0.03	52,52,52,52	0
5	MG	C	502	1/1	1.00	0.02	47,47,47,47	0
5	MG	D	502	1/1	1.00	0.03	58,58,58,58	0

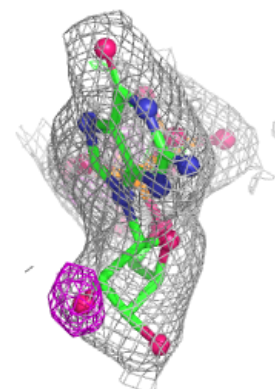
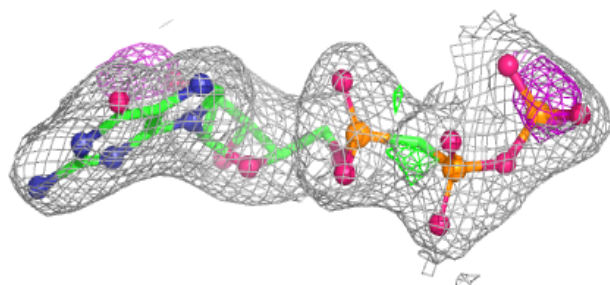
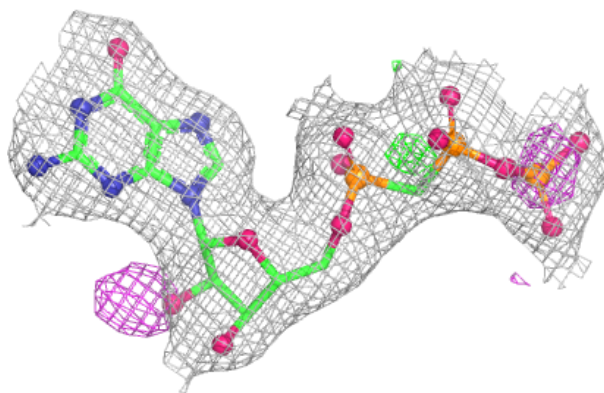
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G2P B 501:

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

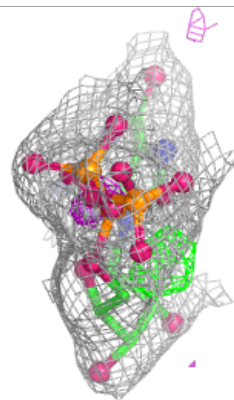
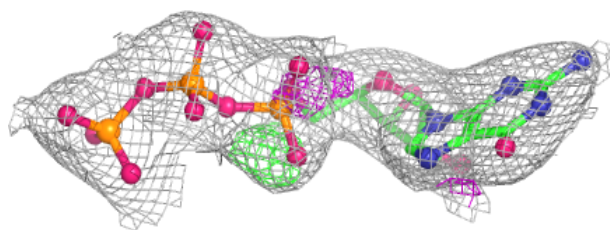
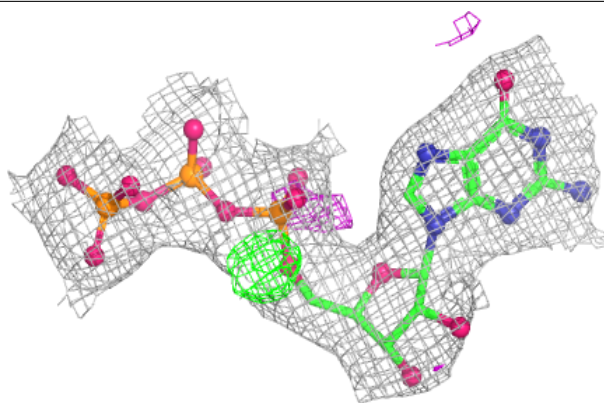
**Electron density around G2P D 501:**

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

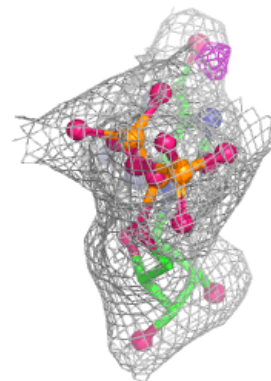
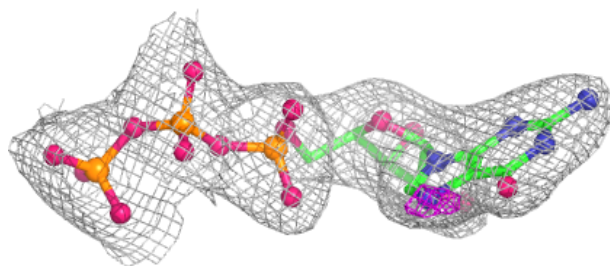
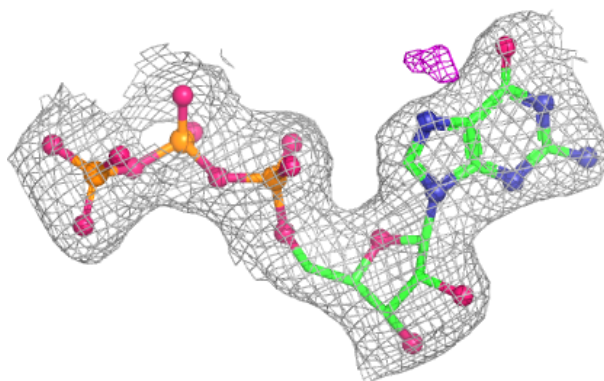


Electron density around GTP C 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.