



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:23 PM UTC

PDB ID : 7Q1F / pdb_00007q1f
Title : CPAP:TUBULIN:IE5 ALPHAREP COMPLEX
Authors : Campanacci, V.; Gigant, b.
Deposited on : 2021-10-19
Resolution : 2.35 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

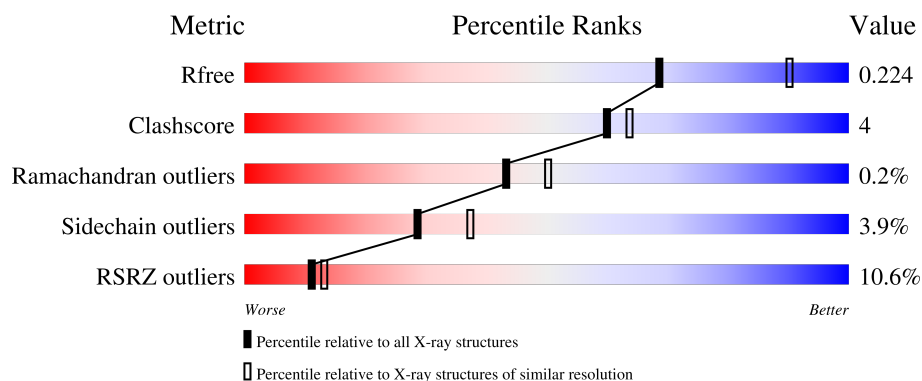
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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

Mol	Chain	Length	Quality of chain
1	A	451	2% 83% 11% . .
1	R	451	2% 84% 11% . .
2	B	445	2% 82% 14% .
2	S	445	5% 82% 15% .
3	C	232	3% 80% 13% 6%

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Mol	Chain	Length	Quality of chain
3	D	232	30% 63% 6% 31%
3	T	232	5% 82% 12% 5%
3	U	232	41% 59% 5% 37%
4	P	75	33% 49% 17% 33%
4	V	75	28% 45% 11% 44%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20341 atoms, of which 79 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3380	2141	575	642	22			
1	R	432	Total	C	N	O	S	0	2	0
			3396	2151	577	646	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3367	2112	575	653	27			
2	S	431	Total	C	N	O	S	0	0	0
			3389	2126	580	656	27			

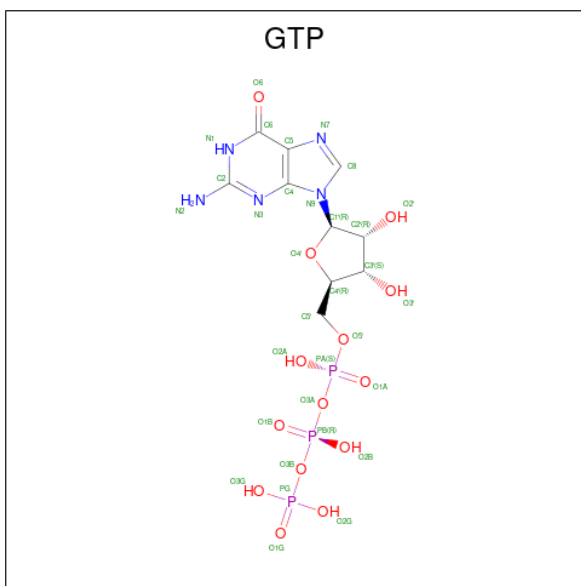
- Molecule 3 is a protein called IE5 ALPHAREP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1633	1011	299	321	2			
3	D	160	Total	C	N	O	S	0	0	0
			1011	621	189	200	1			
3	T	220	Total	C	N	O	S	0	0	0
			1655	1027	303	323	2			
3	U	147	Total	C	N	O	S	0	0	0
			837	507	162	167	1			

- Molecule 4 is a protein called Centromere protein J.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	50	Total	C	N	O	0	0	0
			369	232	65	72			
4	V	42	Total	C	N	O	0	0	0
			320	202	54	64			

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

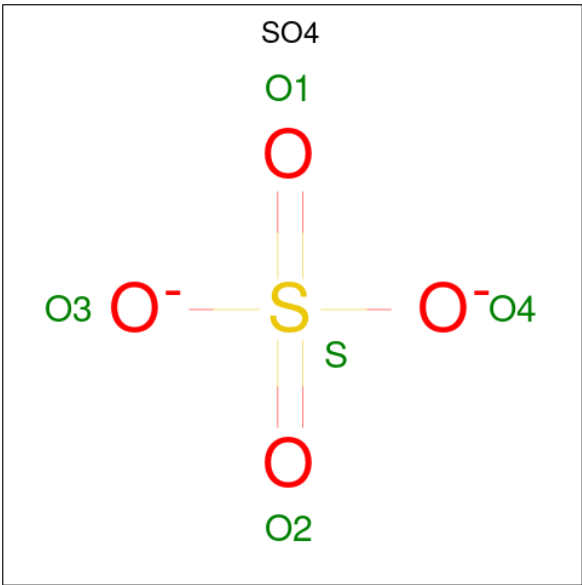


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
5	R	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

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

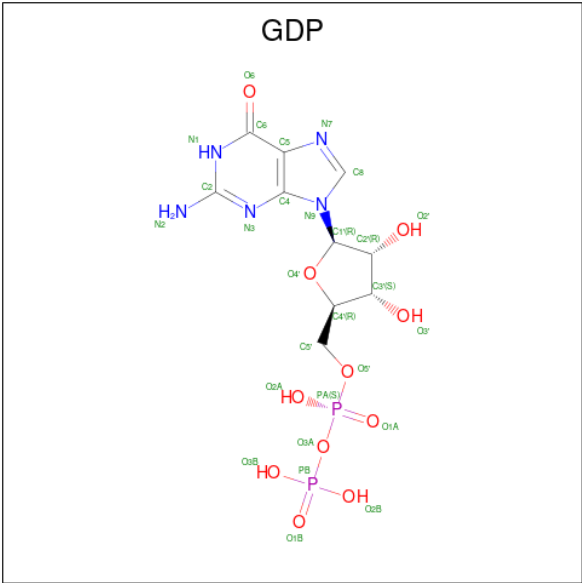
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	R	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



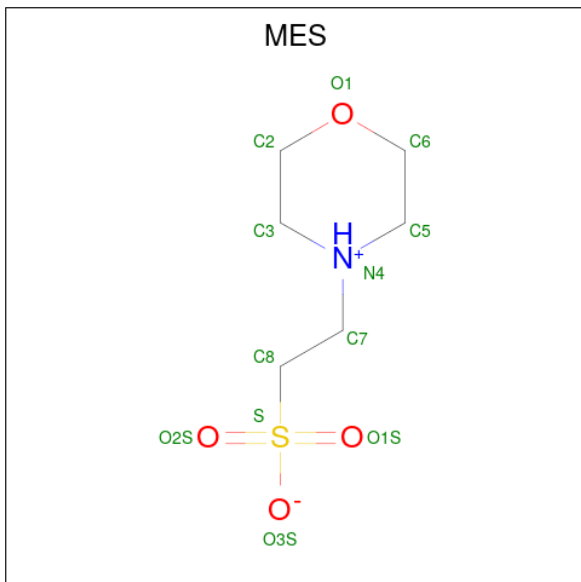
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	R	1	Total	O	S	0	0
			5	4	1		

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



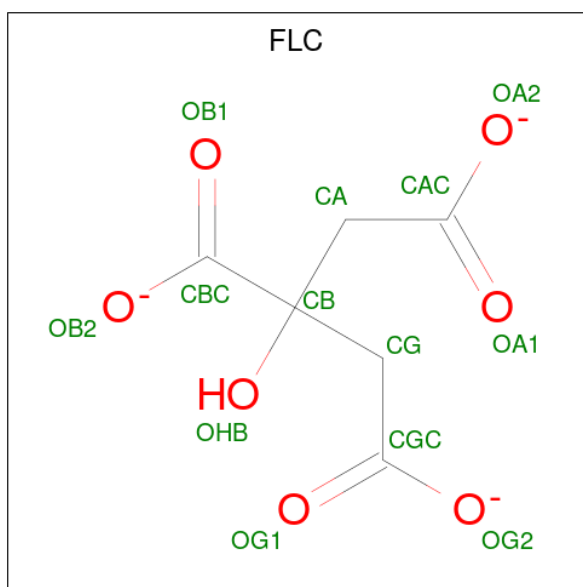
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
8	S	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	B	1	Total 12	C 6	N 1	O 4	S 1	0	0	
9	B	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
9	S	1	Total 12	C 6	N 1	O 4	S 1	0	0	
9	S	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0

- Molecule 10 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	H	O	0	0
			18	6	5	7		

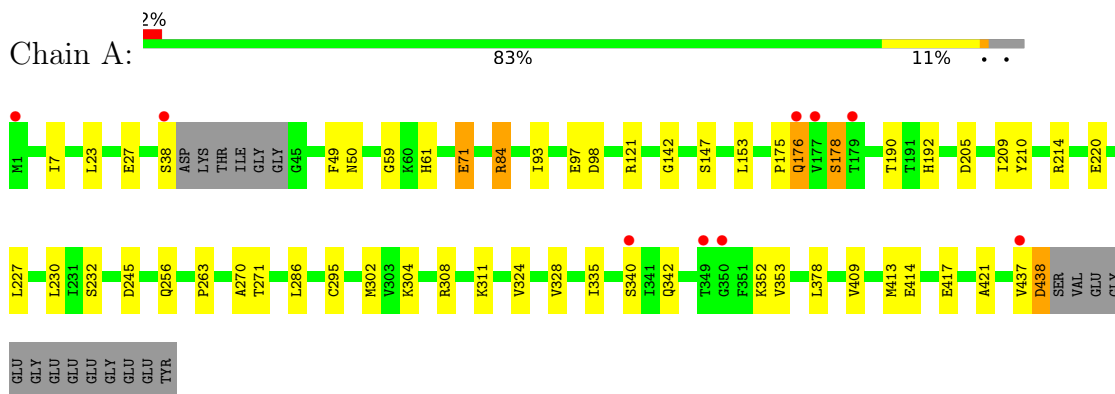
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	226	Total	O	0	0
			226	226		
11	B	108	Total	O	0	0
			108	108		
11	C	37	Total	O	0	0
			37	37		
11	D	6	Total	O	0	0
			6	6		
11	P	5	Total	O	0	0
			5	5		
11	R	225	Total	O	0	0
			225	225		
11	S	62	Total	O	0	0
			62	62		
11	T	36	Total	O	0	0
			36	36		
11	U	2	Total	O	0	0
			2	2		
11	V	5	Total	O	0	0
			5	5		

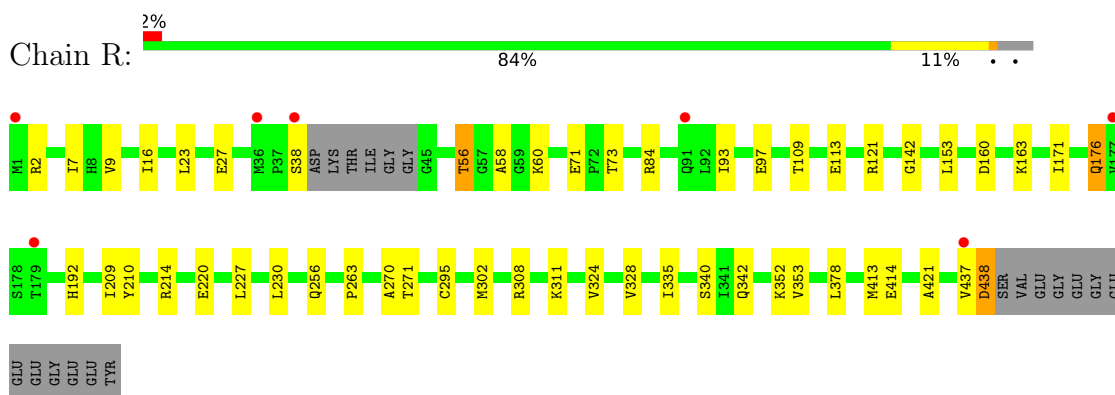
3 Residue-property plots [i](#)

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.

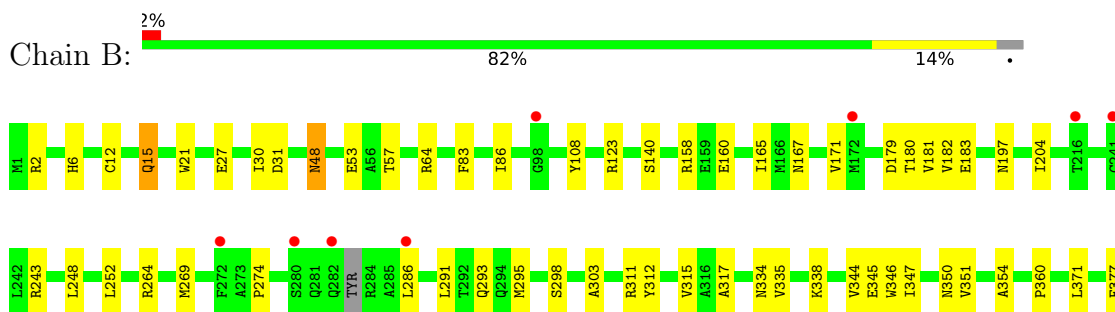
- Molecule 1: Tubulin alpha chain

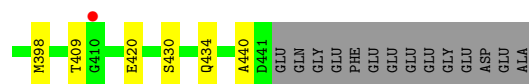


- Molecule 1: Tubulin alpha chain

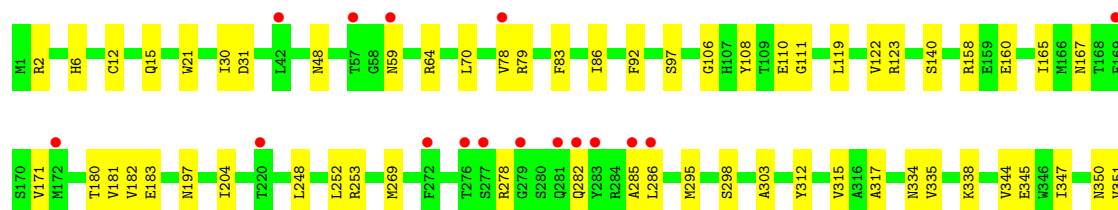
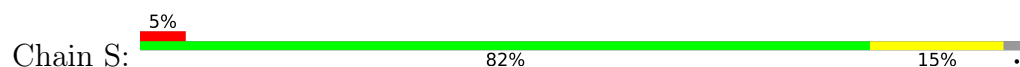


- Molecule 2: Tubulin beta chain

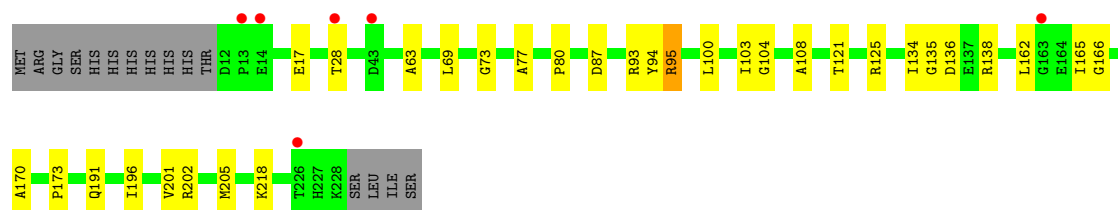
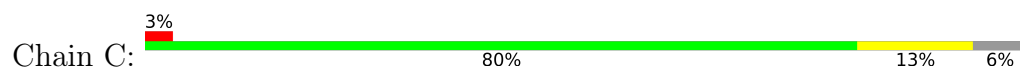




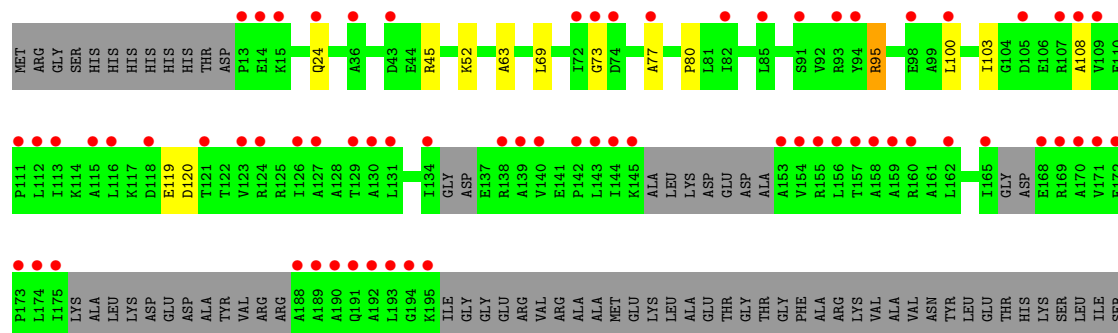
• Molecule 2: Tubulin beta chain



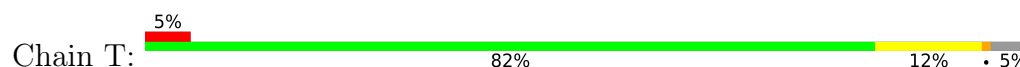
• Molecule 3: IE5 ALPHAREP

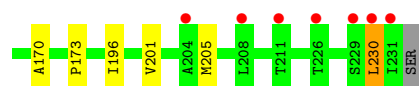


• Molecule 3: IE5 ALPHAREP

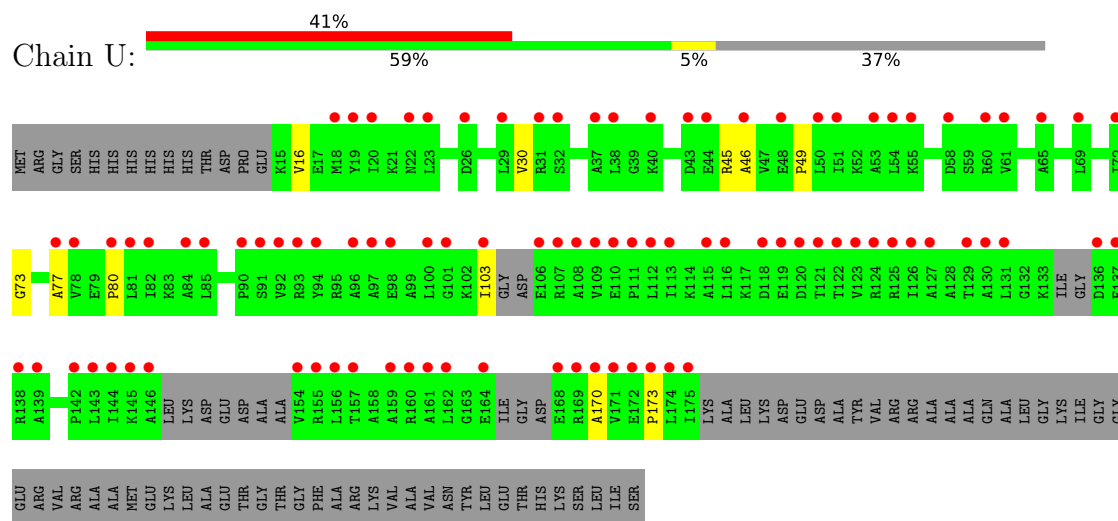


• Molecule 3: IE5 ALPHAREP

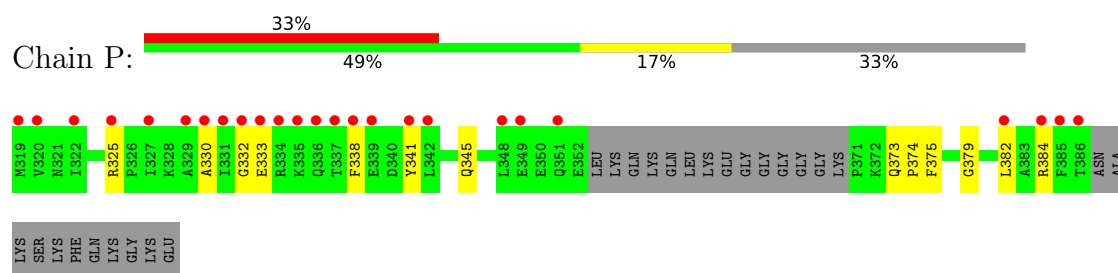




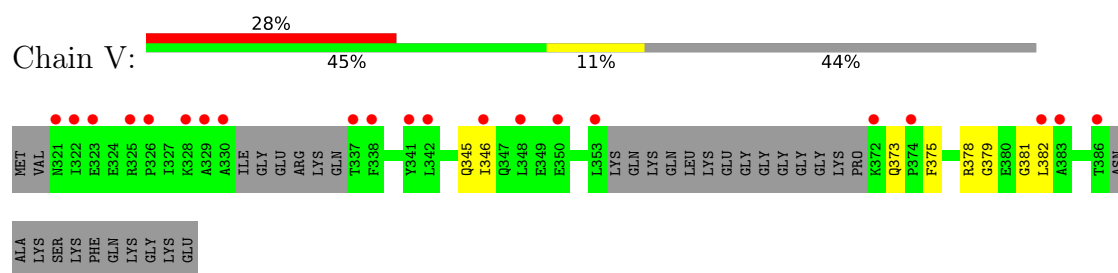
• Molecule 3: IE5 ALPHAREP



• Molecule 4: Centromere protein J



• Molecule 4: Centromere protein J



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.09Å 215.86Å 95.54Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	107.93 – 2.35 107.93 – 2.35	Depositor EDS
% Data completeness (in resolution range)	68.8 (107.93-2.35) 68.8 (107.93-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.188 , 0.220 0.193 , 0.224	Depositor DCC
R_{free} test set	4793 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 73.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20341	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: MES, MG, GTP, SO4, GDP, FLC

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	0.79	0/3457	1.14	3/4693 (0.1%)
1	R	0.80	0/3479	1.14	3/4723 (0.1%)
2	B	0.76	0/3440	1.10	2/4659 (0.0%)
2	S	0.72	0/3464	1.09	4/4692 (0.1%)
3	C	0.75	0/1645	1.11	0/2215
3	D	0.70	0/1014	1.01	0/1383
3	T	0.75	0/1667	1.12	4/2244 (0.2%)
3	U	0.71	0/838	1.08	0/1153
4	P	0.79	0/373	1.21	1/502 (0.2%)
4	V	0.68	0/322	1.08	2/431 (0.5%)
All	All	0.76	0/19699	1.11	19/26695 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CA-CB-CG	7.50	120.10	112.60
1	A	142	GLY	N-CA-C	5.68	120.03	112.77
4	P	332	GLY	N-CA-C	5.64	119.49	112.73
1	R	142	GLY	N-CA-C	5.62	119.96	112.77
1	R	160	ASP	CA-CB-CG	5.46	118.06	112.60
2	S	64	ARG	N-CA-C	-5.22	103.42	110.68
2	B	31	ASP	CA-CB-CG	5.20	117.80	112.60
1	R	9	VAL	N-CA-C	5.17	115.41	108.17
3	T	93	ARG	CA-C-N	5.16	127.46	120.65
3	T	93	ARG	C-N-CA	5.16	127.46	120.65
2	S	59	ASN	CA-CB-CG	5.16	117.76	112.60
4	V	381	GLY	CA-C-N	5.15	127.14	120.44
4	V	381	GLY	C-N-CA	5.15	127.14	120.44
2	S	197	ASN	N-CA-C	5.14	119.65	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	136	ASP	CA-C-N	5.10	127.37	120.38
3	T	136	ASP	C-N-CA	5.10	127.37	120.38
2	B	197	ASN	N-CA-C	5.08	119.57	113.17
1	A	59	GLY	N-CA-C	5.05	122.67	114.90
2	S	31	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3380	0	3289	27	0
1	R	3396	0	3309	25	0
2	B	3367	0	3239	35	0
2	S	3389	0	3266	35	0
3	C	1633	0	1683	18	0
3	D	1011	0	882	5	0
3	T	1655	0	1717	17	0
3	U	837	0	618	7	0
4	P	369	0	329	11	0
4	V	320	0	287	5	0
5	A	32	12	12	0	0
5	R	32	12	12	0	0
6	A	1	0	0	0	0
6	R	1	0	0	0	0
7	A	5	0	0	0	0
7	R	5	0	0	0	0
8	B	28	12	12	0	0
8	S	28	12	12	0	0
9	B	24	13	26	1	0
9	S	24	13	26	5	0
10	D	13	5	5	0	0
11	A	226	0	0	2	0
11	B	108	0	0	2	0
11	C	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	6	0	0	0	0
11	P	5	0	0	0	0
11	R	225	0	0	0	0
11	S	62	0	0	0	0
11	T	36	0	0	0	0
11	U	2	0	0	0	0
11	V	5	0	0	0	0
All	All	20262	79	18724	165	0

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

All (165) 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)
3:C:121:THR:HG22	3:C:125:ARG:HE	1.28	0.98
2:S:2:ARG:HE	2:S:48:ASN:HB3	1.40	0.84
1:A:245:ASP:HB2	11:A:729:HOH:O	1.79	0.81
1:A:175:PRO:HA	1:A:178:SER:HB2	1.67	0.76
1:A:209:ILE:HD11	1:A:302:MET:HE3	1.68	0.75
1:A:209:ILE:HD11	1:A:302:MET:CE	2.17	0.74
1:R:209:ILE:HD11	1:R:302:MET:CE	2.19	0.72
1:R:209:ILE:HD11	1:R:302:MET:HE3	1.70	0.72
2:S:2:ARG:NE	2:S:48:ASN:HB3	2.08	0.68
2:B:179:ASP:HA	4:P:330:ALA:HB2	1.75	0.68
1:R:263:PRO:HG2	3:T:28:THR:HG22	1.77	0.66
2:S:119:LEU:HA	2:S:122:VAL:HG22	1.77	0.66
1:A:263:PRO:HG2	3:C:28:THR:HG22	1.78	0.64
1:R:311:LYS:NZ	1:R:438:ASP:HA	2.12	0.64
1:A:311:LYS:NZ	1:A:438:ASP:HA	2.13	0.63
2:S:180:THR:HB	2:S:183:GLU:HG3	1.82	0.61
3:C:121:THR:CG2	3:C:125:ARG:HE	2.07	0.61
2:S:158:ARG:HG3	9:S:502:MES:H62	1.83	0.61
1:A:176:GLN:H	1:A:176:GLN:HE21	1.49	0.60
2:B:108:TYR:CE2	4:P:373:GLN:HG2	2.36	0.60
1:R:176:GLN:HE21	1:R:176:GLN:H	1.49	0.59
2:S:165:ILE:HG21	2:S:252:LEU:HB3	1.85	0.59
1:R:209:ILE:HG23	1:R:230:LEU:HD23	1.85	0.59
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.86	0.58
2:S:248:LEU:HD23	2:S:354:ALA:HB2	1.86	0.58
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HZ1	1:A:438:ASP:HA	1.68	0.57
1:R:56:THR:HG22	1:R:58:ALA:H	1.67	0.57
3:U:46:ALA:HA	3:U:49:PRO:HD2	1.86	0.56
3:T:201:VAL:O	3:T:205:MET:HG2	2.07	0.55
2:B:12:CYS:HB3	2:B:140:SER:HB3	1.89	0.55
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.88	0.54
2:S:108:TYR:CE2	4:V:373:GLN:HG2	2.43	0.54
1:R:311:LYS:HZ1	1:R:438:ASP:HA	1.71	0.54
2:B:335:VAL:HG22	9:B:503:MES:H22	1.90	0.54
2:S:97:SER:OG	2:S:110:GLU:HG2	2.08	0.53
1:R:93:ILE:HD11	1:R:121:ARG:HG3	1.90	0.53
1:A:263:PRO:CG	3:C:28:THR:HG22	2.39	0.53
2:B:274:PRO:HB3	2:B:286:LEU:HD11	1.89	0.53
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.90	0.53
2:B:430:SER:O	2:B:434:GLN:HG3	2.10	0.52
2:S:253:ARG:NH1	9:S:502:MES:O2S	2.42	0.52
2:B:420:GLU:HG3	4:P:375:PHE:HE2	1.74	0.52
1:R:263:PRO:CG	3:T:28:THR:HG22	2.40	0.52
4:P:379:GLY:HA2	4:P:382:LEU:HD13	1.93	0.51
2:S:253:ARG:NH1	9:S:502:MES:O1S	2.44	0.51
2:S:269:MET:HG3	2:S:303:ALA:HB3	1.92	0.51
1:R:308:ARG:HG2	1:R:340:SER:HB2	1.91	0.51
2:S:335:VAL:HG22	9:S:503:MES:H22	1.92	0.51
2:S:12:CYS:HB3	2:S:140:SER:HB3	1.93	0.51
3:T:136:ASP:OD2	3:T:138:ARG:HD3	2.11	0.50
2:S:79:ARG:HD3	3:U:30:VAL:HG22	1.93	0.50
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.93	0.50
2:B:123:ARG:HD3	2:B:160:GLU:OE1	2.12	0.49
2:B:15:GLN:HG2	4:P:325:ARG:HH21	1.77	0.49
1:A:23:LEU:O	1:A:27:GLU:HG3	2.13	0.49
3:C:136:ASP:OD2	3:C:138:ARG:HD3	2.12	0.49
3:C:121:THR:HG22	3:C:125:ARG:NE	2.11	0.49
2:S:123:ARG:HD3	2:S:160:GLU:OE1	2.11	0.49
1:R:23:LEU:O	1:R:27:GLU:HG3	2.12	0.48
2:S:180:THR:HB	2:S:183:GLU:CG	2.43	0.48
1:R:163:LYS:HZ2	3:T:88:GLU:CD	2.21	0.48
4:V:379:GLY:HA2	4:V:382:LEU:HD13	1.94	0.48
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.94	0.48
3:C:201:VAL:O	3:C:205:MET:HG2	2.12	0.48
1:R:270:ALA:O	1:R:302:MET:HG2	2.13	0.48
2:S:181:VAL:HB	4:V:345:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.48	0.48
1:A:270:ALA:O	1:A:302:MET:HG2	2.13	0.48
2:B:311:ARG:HD3	11:B:687:HOH:O	2.13	0.48
2:S:347:ILE:HG22	2:S:350:ASN:HB3	1.96	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.47
2:S:83:PHE:O	2:S:86:ILE:HG12	2.14	0.47
1:R:210:TYR:CE1	1:R:214:ARG:HD2	2.50	0.47
1:A:271:THR:HG21	1:A:295:CYS:O	2.15	0.47
2:B:83:PHE:O	2:B:86:ILE:HG12	2.15	0.46
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.97	0.46
3:D:63:ALA:O	3:D:95:ARG:HG2	2.16	0.46
3:T:63:ALA:O	3:T:95:ARG:HG2	2.15	0.46
2:B:158:ARG:HD2	4:P:384:ARG:CZ	2.45	0.46
3:U:16:VAL:HG11	3:U:45:ARG:HD3	1.97	0.46
3:U:46:ALA:C	3:U:49:PRO:HD2	2.41	0.46
1:R:271:THR:HG21	1:R:295:CYS:O	2.16	0.46
2:S:171:VAL:HA	2:S:204:ILE:O	2.16	0.46
2:S:253:ARG:NH1	9:S:502:MES:S	2.90	0.46
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.96	0.45
2:S:420:GLU:OE2	4:V:378:ARG:HG3	2.16	0.45
1:A:304:LYS:NZ	11:A:606:HOH:O	2.49	0.45
1:A:49:PHE:HE1	1:A:61:HIS:CD2	2.34	0.45
2:B:346:TRP:HB3	2:B:440:ALA:HB2	1.99	0.45
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.99	0.45
1:A:308:ARG:HG2	1:A:340:SER:HB2	1.98	0.45
2:B:182:VAL:HA	2:B:398:MET:HE1	1.99	0.44
3:C:63:ALA:O	3:C:95:ARG:HG2	2.16	0.44
2:S:334:ASN:OD1	2:S:338:LYS:HE2	2.16	0.44
2:B:264:ARG:HD2	4:P:382:LEU:HD11	1.98	0.44
2:S:182:VAL:HA	2:S:398:MET:HE1	1.98	0.44
2:B:180:THR:HB	2:B:183:GLU:HG3	1.97	0.44
2:B:334:ASN:OD1	2:B:338:LYS:HE2	2.18	0.44
3:T:135:GLY:HA2	3:T:165:ILE:HG12	2.00	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.44
2:B:48:ASN:O	2:B:64:ARG:NH2	2.46	0.44
1:R:192:HIS:CG	1:R:421:ALA:HA	2.52	0.44
2:B:2:ARG:HD2	2:B:48:ASN:ND2	2.32	0.44
1:R:56:THR:HB	1:R:60:LYS:HB3	2.00	0.44
2:S:360:PRO:HG2	2:S:371:LEU:HD12	2.00	0.44
2:B:15:GLN:HG3	11:B:650:HOH:O	2.18	0.43
3:T:94:TYR:CE1	3:T:126:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:170:ALA:C	3:T:173:PRO:HD2	2.42	0.43
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.36	0.43
2:B:420:GLU:HG3	4:P:375:PHE:CE2	2.53	0.43
2:B:12:CYS:CB	2:B:140:SER:HB3	2.48	0.43
2:B:27:GLU:OE2	2:B:243:ARG:NH2	2.34	0.43
3:T:166:GLY:HA2	3:T:196:ILE:HG12	2.00	0.43
2:B:108:TYR:CD2	4:P:373:GLN:HG2	2.54	0.43
3:T:162:LEU:HD22	3:T:170:ALA:HB2	2.01	0.43
2:S:106:GLY:O	2:S:111:GLY:HA3	2.19	0.43
1:A:84:ARG:HH22	1:R:84:ARG:HG3	1.83	0.43
1:R:209:ILE:HG22	1:R:227:LEU:HD22	2.00	0.43
2:B:179:ASP:O	4:P:341:TYR:OH	2.27	0.42
3:C:87:ASP:O	3:C:93:ARG:HD3	2.19	0.42
1:R:109:THR:O	1:R:113:GLU:OE1	2.36	0.42
2:S:312:TYR:CE2	2:S:377:PHE:HZ	2.37	0.42
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.42
1:R:7:ILE:HG21	1:R:153:LEU:HD21	2.00	0.42
3:T:100:LEU:HD22	3:T:108:ALA:HB2	2.01	0.42
3:D:69:LEU:HD22	3:D:77:ALA:HB2	2.02	0.42
3:U:77:ALA:C	3:U:80:PRO:HD2	2.45	0.42
2:B:360:PRO:HG2	2:B:371:LEU:HD12	2.02	0.42
4:P:373:GLN:HA	4:P:374:PRO:HD3	1.94	0.42
3:T:77:ALA:C	3:T:80:PRO:HD2	2.45	0.42
3:D:77:ALA:C	3:D:80:PRO:HD2	2.45	0.42
2:S:295:MET:HE1	2:S:317:ALA:HB1	2.01	0.42
3:C:162:LEU:HD22	3:C:170:ALA:HB2	2.02	0.41
3:U:73:GLY:HA2	3:U:103:ILE:HG12	2.02	0.41
1:R:16:ILE:HD11	1:R:171:ILE:HD11	2.02	0.41
3:C:135:GLY:HA2	3:C:165:ILE:HG12	2.02	0.41
3:D:100:LEU:HD22	3:D:108:ALA:HB2	2.02	0.41
3:T:104:GLY:HA2	3:T:134:ILE:HG12	2.02	0.41
3:C:100:LEU:HD22	3:C:108:ALA:HB2	2.01	0.41
2:S:70:LEU:O	2:S:97:SER:O	2.38	0.41
2:S:315:VAL:HB	2:S:351:VAL:HG22	2.01	0.41
2:B:315:VAL:HB	2:B:351:VAL:HG22	2.02	0.41
3:D:73:GLY:HA2	3:D:103:ILE:HG12	2.01	0.41
2:S:12:CYS:CB	2:S:140:SER:HB3	2.51	0.41
2:S:78:VAL:HG23	2:S:92:PHE:HE1	1.86	0.41
2:S:420:GLU:HG3	4:V:375:PHE:HE2	1.84	0.41
1:R:71:GLU:OE1	1:R:73:THR:HB	2.21	0.41
3:T:73:GLY:HA2	3:T:103:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:94:TYR:HE1	3:T:126:ILE:HG12	1.85	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
3:C:166:GLY:HA2	3:C:196:ILE:HG12	2.03	0.41
1:R:328:VAL:HG11	1:R:353:VAL:HG11	2.02	0.41
3:T:16:VAL:HG22	3:T:41:ILE:HG21	2.03	0.41
3:U:170:ALA:C	3:U:173:PRO:HD2	2.45	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.41
2:B:295:MET:HE1	2:B:317:ALA:HB1	2.03	0.41
3:C:73:GLY:HA2	3:C:103:ILE:HG12	2.03	0.40
1:A:147:SER:HB2	1:A:190:THR:HB	2.04	0.40
3:C:77:ALA:C	3:C:80:PRO:HD2	2.46	0.40
3:C:170:ALA:C	3:C:173:PRO:HD2	2.47	0.40
2:S:6:HIS:CD2	2:S:21:TRP:HE1	2.39	0.40
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.03	0.40
3:C:69:LEU:HD22	3:C:77:ALA:HB2	2.04	0.40
3:C:104:GLY:HA2	3:C:134:ILE:HG12	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	428/451 (95%)	416 (97%)	12 (3%)	0	100	100
1	R	430/451 (95%)	420 (98%)	10 (2%)	0	100	100
2	B	426/445 (96%)	416 (98%)	10 (2%)	0	100	100
2	S	429/445 (96%)	415 (97%)	12 (3%)	2 (0%)	24	26
3	C	215/232 (93%)	214 (100%)	1 (0%)	0	100	100
3	D	150/232 (65%)	147 (98%)	3 (2%)	0	100	100
3	T	218/232 (94%)	216 (99%)	1 (0%)	1 (0%)	24	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	U	137/232 (59%)	137 (100%)	0	0	100	100
4	P	46/75 (61%)	39 (85%)	5 (11%)	2 (4%)	2	0
4	V	36/75 (48%)	35 (97%)	1 (3%)	0	100	100
All	All	2515/2870 (88%)	2455 (98%)	55 (2%)	5 (0%)	43	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	333	GLU
2	S	278	ARG
2	S	285	ALA
4	P	338	PHE
3	T	230	LEU

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	364/379 (96%)	345 (95%)	19 (5%)	21	25
1	R	367/379 (97%)	351 (96%)	16 (4%)	25	33
2	B	369/383 (96%)	356 (96%)	13 (4%)	32	41
2	S	372/383 (97%)	360 (97%)	12 (3%)	34	44
3	C	160/176 (91%)	154 (96%)	6 (4%)	29	38
3	D	70/176 (40%)	64 (91%)	6 (9%)	10	10
3	T	163/176 (93%)	160 (98%)	3 (2%)	51	64
3	U	39/176 (22%)	39 (100%)	0	100	100
4	P	32/62 (52%)	31 (97%)	1 (3%)	35	45
4	V	29/62 (47%)	28 (97%)	1 (3%)	32	42
All	All	1965/2352 (84%)	1888 (96%)	77 (4%)	28	37

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	50	ASN
1	A	71	GLU
1	A	84	ARG
1	A	97	GLU
1	A	176	GLN
1	A	178	SER
1	A	220	GLU
1	A	232	SER
1	A	256	GLN
1	A	286	LEU
1	A	324	VAL
1	A	335	ILE
1	A	342	GLN
1	A	352	LYS
1	A	378	LEU
1	A	414	GLU
1	A	437	VAL
1	A	438	ASP
2	B	15	GLN
2	B	30	ILE
2	B	48	ASN
2	B	53	GLU
2	B	57	THR
2	B	167	ASN
2	B	181	VAL
2	B	291	LEU
2	B	293	GLN
2	B	298	SER
2	B	344	VAL
2	B	345	GLU
2	B	409	THR
3	C	17	GLU
3	C	94	TYR
3	C	95	ARG
3	C	191	GLN
3	C	202	ARG
3	C	218	LYS
3	D	24	GLN
3	D	45	ARG
3	D	52	LYS
3	D	95	ARG
3	D	119	GLU

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Mol	Chain	Res	Type
3	D	120	ASP
4	P	345	GLN
1	R	2	ARG
1	R	38	SER
1	R	56	THR
1	R	97	GLU
1	R	176	GLN
1	R	220	GLU
1	R	256	GLN
1	R	324	VAL
1	R	335	ILE
1	R	342	GLN
1	R	352	LYS
1	R	378	LEU
1	R	413	MET
1	R	414	GLU
1	R	437	VAL
1	R	438	ASP
2	S	15	GLN
2	S	30	ILE
2	S	167	ASN
2	S	282	GLN
2	S	286	LEU
2	S	298	SER
2	S	344	VAL
2	S	345	GLU
2	S	372	LYS
2	S	377	PHE
2	S	409	THR
2	S	434	GLN
3	T	71	GLN
3	T	95	ARG
3	T	230	LEU
4	V	346	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	50	ASN
1	A	85	GLN
1	A	256	GLN

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Mol	Chain	Res	Type
1	A	356	ASN
1	A	358	GLN
1	A	393	HIS
2	B	11	GLN
2	B	91	ASN
2	B	101	ASN
2	B	247	GLN
2	B	337	ASN
1	R	11	GLN
1	R	15	GLN
1	R	101	ASN
1	R	256	GLN
1	R	393	HIS
2	S	59	ASN
2	S	247	GLN
2	S	282	GLN
2	S	331	GLN
2	S	337	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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	MES	S	502	-	12,12,12	0.73	0	15,16,16	0.39	0
9	MES	B	503	-	12,12,12	0.59	0	15,16,16	0.33	0
5	GTP	A	501	6	33,34,34	0.45	0	50,54,54	0.57	1 (2%)
8	GDP	B	501	-	29,30,30	0.41	0	45,47,47	0.69	2 (4%)
5	GTP	R	501	6	33,34,34	0.47	0	50,54,54	0.58	1 (2%)
7	SO4	R	503	-	4,4,4	0.30	0	6,6,6	0.16	0
9	MES	S	503	-	12,12,12	0.60	0	15,16,16	0.32	0
9	MES	B	502	-	12,12,12	0.78	0	15,16,16	0.38	0
10	FLC	D	501	-	12,12,12	1.07	0	17,17,17	1.38	2 (11%)
8	GDP	S	501	-	29,30,30	0.39	0	45,47,47	0.78	3 (6%)
7	SO4	A	503	-	4,4,4	0.35	0	6,6,6	0.30	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
9	MES	S	502	-	-	0/6/14/14	0/1/1/1
9	MES	B	503	-	-	5/6/14/14	0/1/1/1
8	GDP	B	501	-	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
5	GTP	R	501	6	-	8/22/38/38	0/3/3/3
9	MES	S	503	-	-	5/6/14/14	0/1/1/1
9	MES	B	502	-	-	0/6/14/14	0/1/1/1
10	FLC	D	501	-	-	2/16/16/16	-
8	GDP	S	501	-	-	4/16/32/32	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	501	FLC	OB1-CBC-CB	-2.83	116.60	122.09
8	S	501	GDP	O2B-PB-O3A	2.74	113.83	104.64
8	B	501	GDP	O5'-PA-O1A	-2.55	98.84	108.94
10	D	501	FLC	OB2-CBC-CB	2.44	117.82	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	501	GTP	O2B-PB-O3B	2.25	113.36	107.27
8	B	501	GDP	O2A-PA-O5'	2.20	117.53	107.57
8	S	501	GDP	O5'-PA-O1A	2.19	117.60	108.94
8	S	501	GDP	O2A-PA-O5'	-2.04	98.32	107.57
5	A	501	GTP	O2B-PB-O3B	2.03	112.75	107.27

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	R	501	GTP	C5'-O5'-PA-O3A
5	R	501	GTP	C5'-O5'-PA-O1A
5	R	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	O4'-C4'-C5'-O5'
8	S	501	GDP	O4'-C4'-C5'-O5'
9	B	503	MES	C7-C8-S-O3S
9	S	503	MES	C7-C8-S-O3S
8	B	501	GDP	C3'-C4'-C5'-O5'
8	S	501	GDP	C3'-C4'-C5'-O5'
9	B	503	MES	C8-C7-N4-C3
9	S	503	MES	C8-C7-N4-C3
5	A	501	GTP	PG-O3B-PB-O1B
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	S	503	MES	C7-C8-S-O1S
9	S	503	MES	C7-C8-S-O2S
10	D	501	FLC	CA-CB-CG-CGC
5	R	501	GTP	PG-O3B-PB-O1B
10	D	501	FLC	OHB-CB-CG-CGC
8	S	501	GDP	C5'-O5'-PA-O1A
9	B	503	MES	C8-C7-N4-C5
9	S	503	MES	C8-C7-N4-C5
5	A	501	GTP	PG-O3B-PB-O2B
5	A	501	GTP	PB-O3A-PA-O2A
5	R	501	GTP	PG-O3B-PB-O2B
5	R	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	C4'-C5'-O5'-PA
8	S	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA

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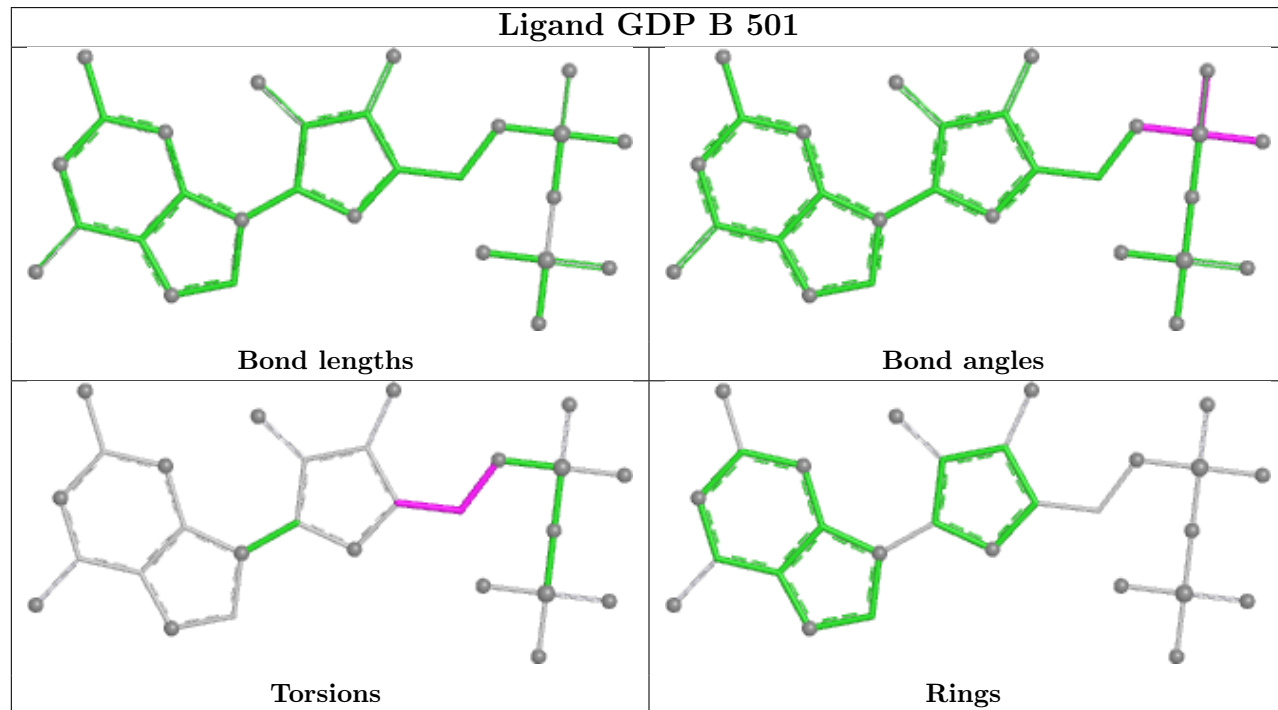
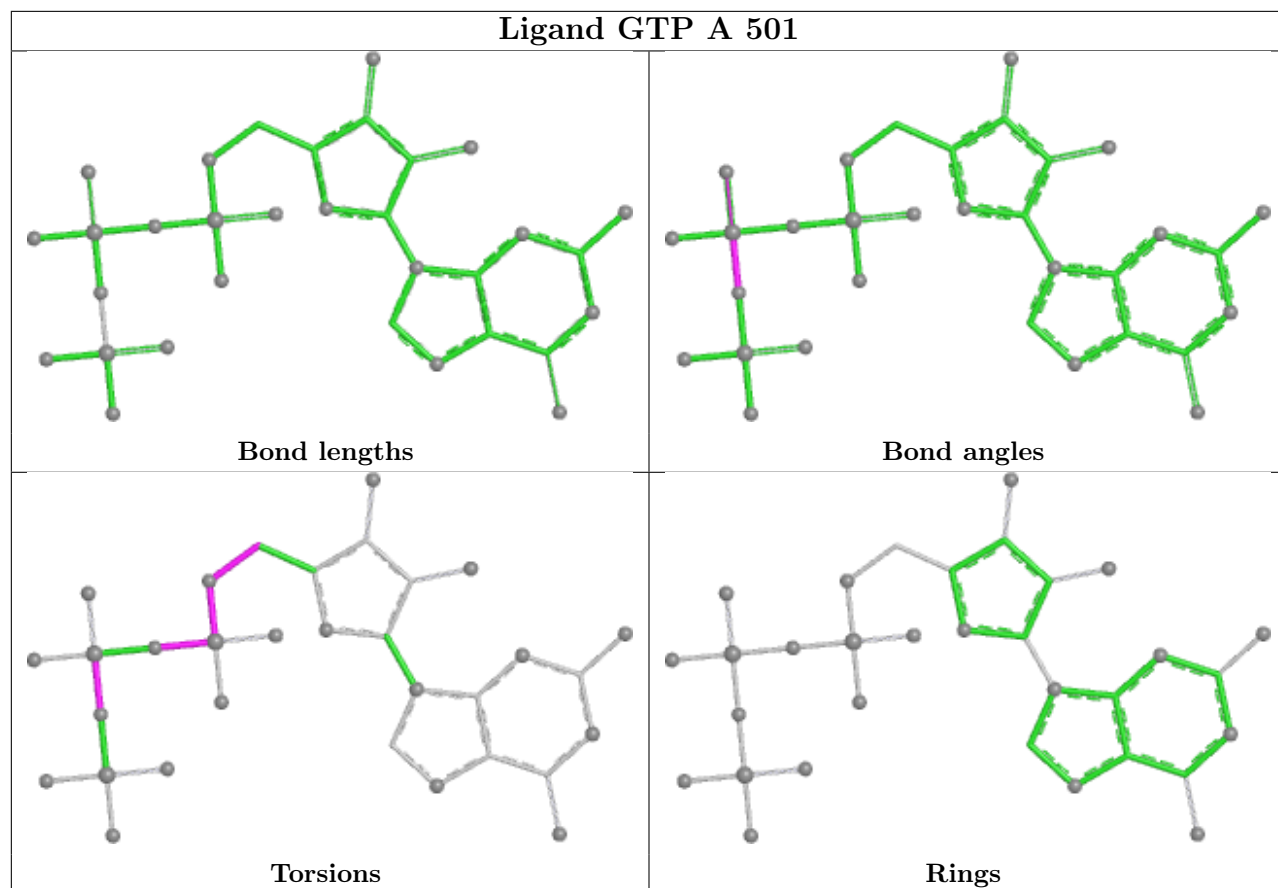
Mol	Chain	Res	Type	Atoms
5	R	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A
5	R	501	GTP	PB-O3A-PA-O2A

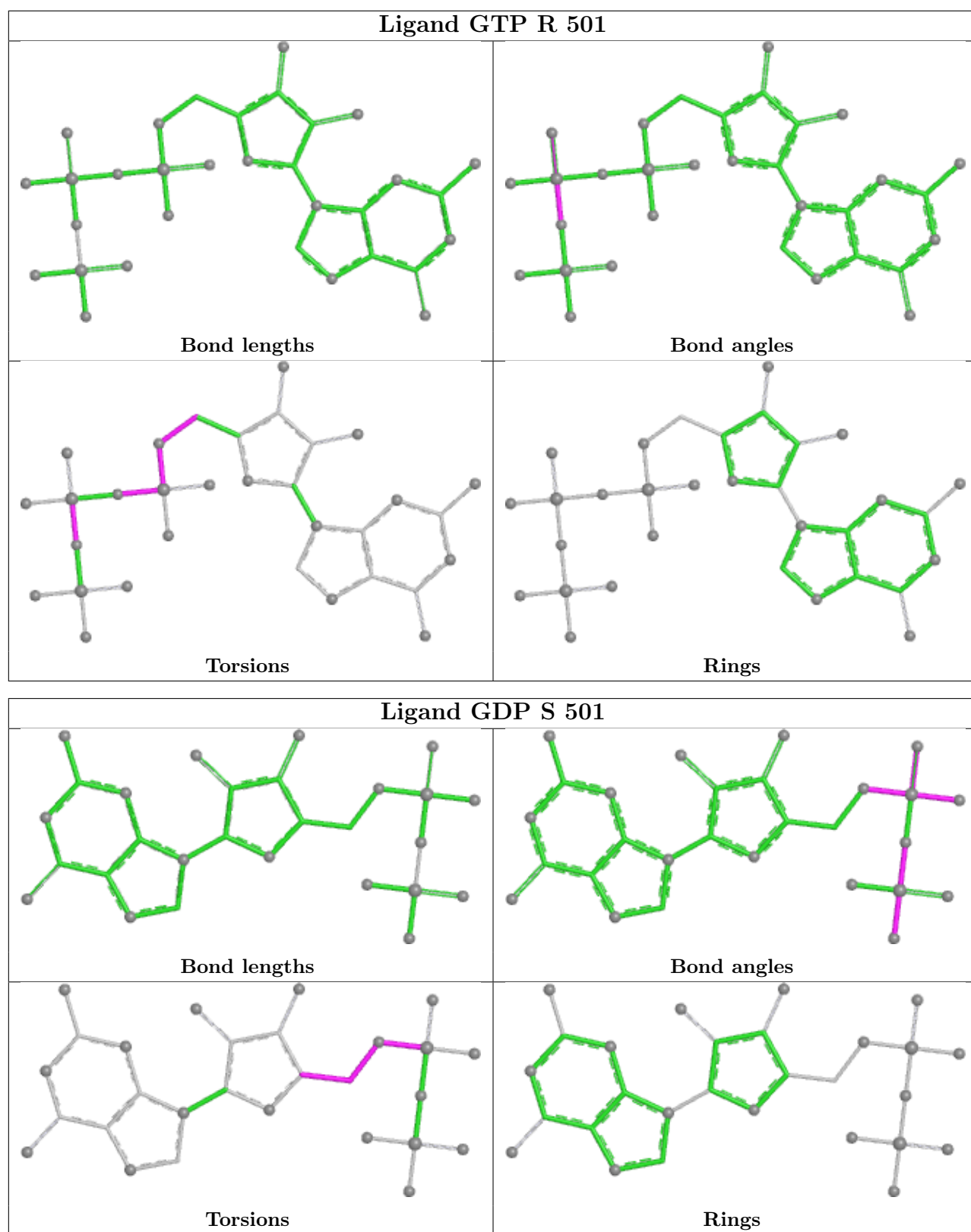
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	S	502	MES	4	0
9	B	503	MES	1	0
9	S	503	MES	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	432/451 (95%)	-0.04	9 (2%) 63 68	31, 43, 69, 90	1 (0%)
1	R	432/451 (95%)	-0.04	7 (1%) 70 75	22, 44, 69, 90	3 (0%)
2	B	430/445 (96%)	0.25	9 (2%) 63 68	34, 54, 77, 112	0
2	S	431/445 (96%)	0.56	21 (4%) 35 41	37, 66, 95, 131	0
3	C	217/232 (93%)	0.64	6 (2%) 55 61	50, 71, 99, 117	0
3	D	160/232 (68%)	2.12	69 (43%) 0 0	62, 105, 210, 234	0
3	T	220/232 (94%)	0.80	11 (5%) 34 40	51, 73, 103, 122	0
3	U	147/232 (63%)	2.61	94 (63%) 0 0	90, 122, 170, 257	0
4	P	50/75 (66%)	1.99	25 (50%) 0 0	51, 103, 136, 138	0
4	V	42/75 (56%)	1.96	21 (50%) 0 0	58, 123, 131, 136	0
All	All	2561/2870 (89%)	0.60	272 (10%) 11 13	22, 60, 129, 257	4 (0%)

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	171	VAL	7.7
3	U	159	ALA	7.2
3	D	159	ALA	6.1
3	U	175	ILE	6.0
3	D	189	ALA	5.9
3	U	19	TYR	5.8
3	D	174	LEU	5.8
3	U	115	ALA	5.7
3	D	190	ALA	5.7
4	P	331	ILE	5.6
3	D	175	ILE	5.6
2	B	282	GLN	5.5
3	D	188	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
3	D	192	ALA	5.1
3	D	171	VAL	5.0
3	D	134	ILE	5.0
3	D	162	LEU	5.0
2	S	283	TYR	4.9
4	V	322	ILE	4.9
3	D	173	PRO	4.9
3	D	169	ARG	4.9
3	U	122	THR	4.8
3	U	81	LEU	4.7
3	U	126	ILE	4.6
3	U	154	VAL	4.6
3	U	100	LEU	4.6
3	U	170	ALA	4.5
3	D	195	LYS	4.5
3	U	174	LEU	4.4
3	U	120	ASP	4.4
3	T	231	ILE	4.4
3	D	123	VAL	4.3
2	S	285	ALA	4.3
3	U	65	ALA	4.3
4	P	338	PHE	4.3
3	U	38	LEU	4.3
3	U	43	ASP	4.3
3	D	127	ALA	4.3
3	U	96	ALA	4.3
3	U	139	ALA	4.2
3	U	112	LEU	4.2
3	U	60	ARG	4.2
3	D	170	ALA	4.2
3	D	121	THR	4.2
3	U	136	ASP	4.1
3	D	143	LEU	4.0
4	V	382	LEU	4.0
3	U	94	TYR	4.0
3	D	191	GLN	4.0
3	U	61	VAL	4.0
3	U	109	VAL	4.0
4	P	329	ALA	4.0
3	U	50	LEU	4.0
3	U	173	PRO	3.9
4	P	386	THR	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	157	THR	3.8
3	D	193	LEU	3.8
3	U	169	ARG	3.8
3	U	155	ARG	3.8
3	U	54	LEU	3.8
4	V	353	LEU	3.8
3	U	108	ALA	3.7
3	U	146	ALA	3.7
3	T	230	LEU	3.7
4	P	320	VAL	3.7
3	U	168	GLU	3.7
4	V	329	ALA	3.7
3	U	123	VAL	3.7
3	D	165	ILE	3.6
3	D	194	GLY	3.6
4	P	322	ILE	3.6
4	P	382	LEU	3.6
3	D	131	LEU	3.6
4	P	337	THR	3.6
3	U	77	ALA	3.6
4	V	323	GLU	3.6
3	D	126	ILE	3.5
4	V	386	THR	3.5
3	C	13	PRO	3.5
3	D	139	ALA	3.5
3	D	168	GLU	3.5
4	P	342	LEU	3.5
3	D	13	PRO	3.4
3	D	108	ALA	3.4
3	U	116	LEU	3.4
1	A	349	THR	3.4
2	B	241	CYS	3.4
3	U	48	GLU	3.3
3	U	46	ALA	3.3
4	P	330	ALA	3.3
4	P	333	GLU	3.3
3	D	105	ASP	3.2
3	U	156	LEU	3.2
3	D	144	ILE	3.2
3	U	144	ILE	3.2
3	D	153	ALA	3.2
3	U	125	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
3	U	106	GLU	3.2
1	A	38	SER	3.2
3	U	97	ALA	3.2
3	D	116	LEU	3.2
3	U	131	LEU	3.2
3	U	129	THR	3.2
3	U	85	LEU	3.1
4	V	325	ARG	3.1
4	V	330	ALA	3.1
4	P	335	LYS	3.1
4	P	339	GLU	3.1
3	D	15	LYS	3.0
4	V	341	TYR	3.0
3	U	20	ILE	3.0
3	D	24	GLN	3.0
3	U	58	ASP	3.0
3	U	172	GLU	3.0
3	T	208	LEU	3.0
3	D	124	ARG	3.0
3	D	14	GLU	3.0
3	D	142	PRO	3.0
2	S	42	LEU	2.9
3	U	143	LEU	2.9
4	V	348	LEU	2.9
3	U	138	ARG	2.9
3	U	23	LEU	2.9
3	U	29	LEU	2.9
2	B	216	THR	2.9
3	D	115	ALA	2.9
3	U	92	VAL	2.9
4	V	346	ILE	2.9
2	S	172	MET	2.9
3	D	36	ALA	2.9
3	D	130	ALA	2.8
2	S	78	VAL	2.8
3	C	163	GLY	2.8
3	U	130	ALA	2.8
3	U	161	ALA	2.8
1	R	179	THR	2.8
3	C	43	ASP	2.8
3	U	69	LEU	2.8
3	T	57	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	2.8
4	V	337	THR	2.7
3	U	98	GLU	2.7
3	U	37	ALA	2.7
3	D	113	ILE	2.7
3	D	73	GLY	2.7
1	R	38	SER	2.7
3	U	137	GLU	2.7
3	D	138	ARG	2.7
3	U	127	ALA	2.7
4	P	341	TYR	2.7
2	S	59	ASN	2.7
3	U	118	ASP	2.7
3	U	113	ILE	2.7
2	B	172	MET	2.7
3	U	124	ARG	2.7
3	D	112	LEU	2.7
2	S	440	ALA	2.7
3	U	82	ILE	2.6
4	P	325	ARG	2.6
4	P	336	GLN	2.6
3	D	160	ARG	2.6
2	S	391	ILE	2.6
3	U	55	LYS	2.6
3	D	158	ALA	2.6
3	U	84	ALA	2.6
3	D	155	ARG	2.6
3	U	93	ARG	2.6
4	P	385	PHE	2.6
3	U	160	ARG	2.6
3	U	22	ASN	2.6
1	R	177	VAL	2.6
3	U	91	SER	2.6
3	U	101	GLY	2.5
4	V	350	GLU	2.5
3	U	107	ARG	2.5
3	U	142	PRO	2.5
2	S	57	THR	2.5
2	S	220	THR	2.5
3	D	72	ILE	2.5
3	U	51	ILE	2.5
2	S	371	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	91	GLN	2.5
2	S	282	GLN	2.5
2	S	277	SER	2.5
3	U	157	THR	2.4
3	D	94	TYR	2.4
4	P	319	MET	2.4
4	V	338	PHE	2.4
1	A	1	MET	2.4
2	S	281	GLN	2.4
2	S	400	ARG	2.4
4	P	334	ARG	2.4
2	S	279	GLY	2.4
3	D	145	LYS	2.4
3	D	154	VAL	2.4
4	V	342	LEU	2.4
3	D	107	ARG	2.4
4	P	332	GLY	2.4
3	D	109	VAL	2.4
3	T	119	GLU	2.4
3	T	13	PRO	2.3
3	C	28	THR	2.3
3	T	229	SER	2.3
1	R	36	MET	2.3
2	S	276	THR	2.3
3	U	121	THR	2.3
2	S	272	PHE	2.3
3	U	44	GLU	2.3
3	D	43	ASP	2.3
4	V	372	LYS	2.3
1	A	350	GLY	2.3
1	R	1	MET	2.3
3	C	226	THR	2.3
3	D	172	GLU	2.3
3	D	118	ASP	2.3
3	U	119	GLU	2.3
2	S	169	PHE	2.2
3	D	140	VAL	2.3
3	U	26	ASP	2.2
3	U	80	PRO	2.2
3	D	93	ARG	2.2
3	T	211	THR	2.2
3	U	40	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	U	90	PRO	2.2
3	U	32	SER	2.2
3	U	72	ILE	2.2
1	A	177	VAL	2.2
3	U	78	VAL	2.2
3	U	111	PRO	2.2
4	V	326	PRO	2.2
2	B	98	GLY	2.2
3	U	110	GLU	2.2
4	P	349	GLU	2.2
2	B	280	SER	2.2
3	D	129	THR	2.2
3	T	226	THR	2.2
2	S	407	TRP	2.2
3	D	100	LEU	2.2
3	D	156	LEU	2.2
3	U	162	LEU	2.2
3	C	14	GLU	2.2
1	A	179	THR	2.2
3	U	53	ALA	2.2
4	V	383	ALA	2.2
3	D	85	LEU	2.1
3	U	103	ILE	2.1
3	U	18	MET	2.1
3	D	98	GLU	2.1
3	D	111	PRO	2.1
1	A	340	SER	2.1
3	T	204	ALA	2.1
4	P	348	LEU	2.1
4	V	328	LYS	2.1
3	U	164	GLU	2.1
1	A	176	GLN	2.1
2	B	410	GLY	2.1
2	S	286	LEU	2.1
3	D	74	ASP	2.1
3	D	82	ILE	2.1
1	R	437	VAL	2.1
3	D	77	ALA	2.0
2	B	286	LEU	2.0
3	T	74	ASP	2.0
4	V	321	ASN	2.0
4	P	327	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
4	V	374	PRO	2.0
3	U	31	ARG	2.0
4	P	384	ARG	2.0
2	B	272	PHE	2.0
3	D	91	SER	2.0
4	P	351	GLN	2.0
3	U	145	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.

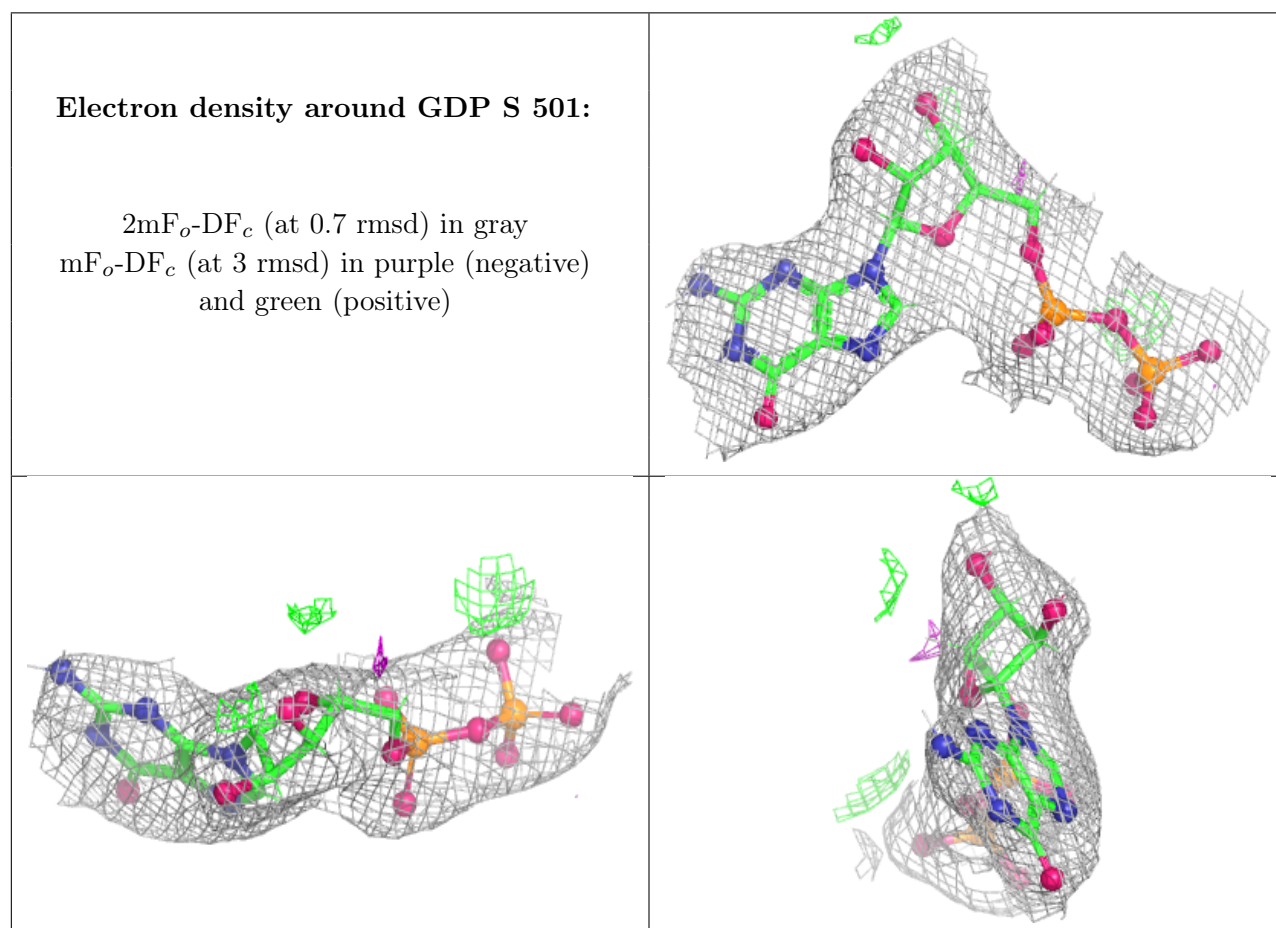
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
10	FLC	D	501	13/13	0.72	0.12	93,95,112,112	0
7	SO4	R	503	5/5	0.83	0.18	119,119,119,119	0
7	SO4	A	503	5/5	0.85	0.17	117,117,117,117	0
9	MES	S	502	12/12	0.89	0.14	64,65,66,66	0
9	MES	S	503	12/12	0.90	0.14	94,97,116,118	0
9	MES	B	503	12/12	0.91	0.13	87,90,113,114	0
8	GDP	S	501	28/28	0.94	0.08	71,73,99,100	0
9	MES	B	502	12/12	0.94	0.10	57,57,60,60	0
6	MG	A	502	1/1	0.97	0.04	42,42,42,42	0
8	GDP	B	501	28/28	0.97	0.06	48,49,62,62	0
5	GTP	R	501	32/32	0.98	0.05	34,37,39,41	0
5	GTP	A	501	32/32	0.98	0.05	34,37,38,40	0
6	MG	R	502	1/1	0.98	0.04	45,45,45,45	0

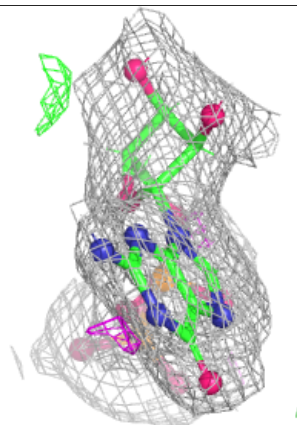
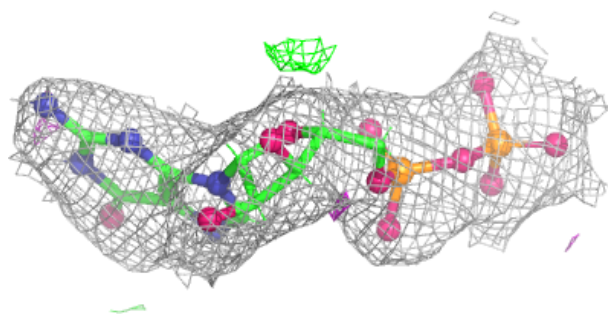
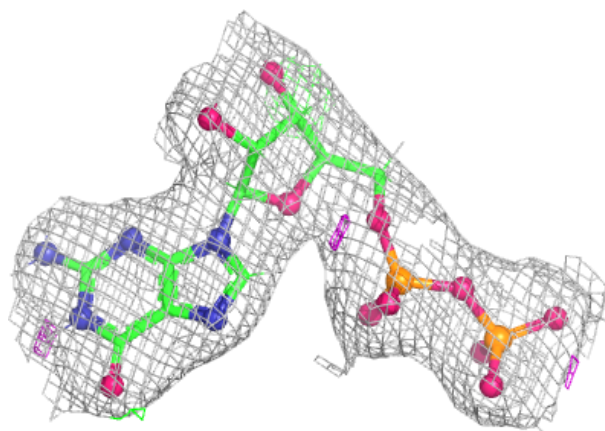
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

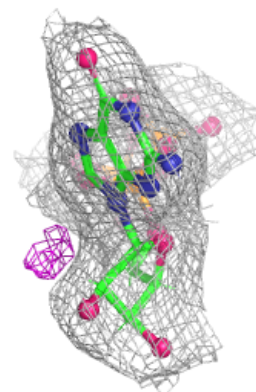
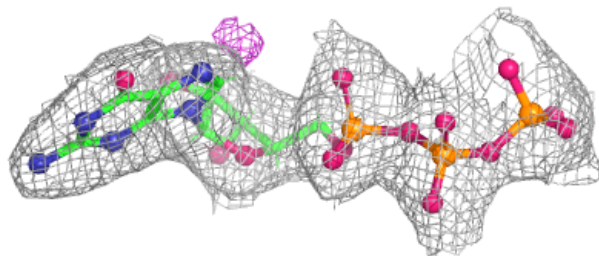
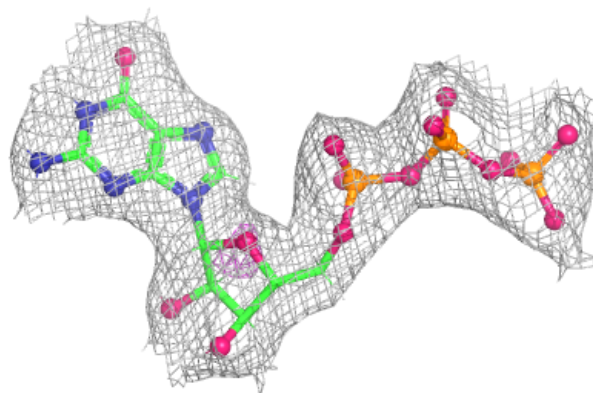


Electron density around GDP B 501:

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

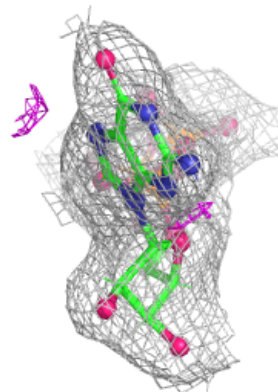
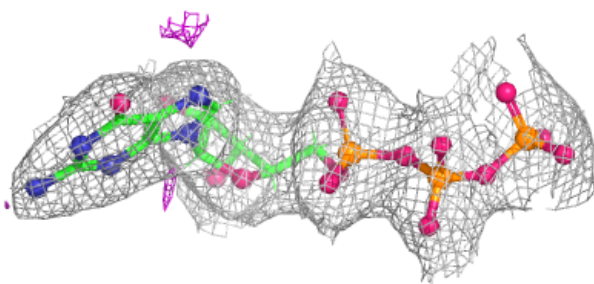
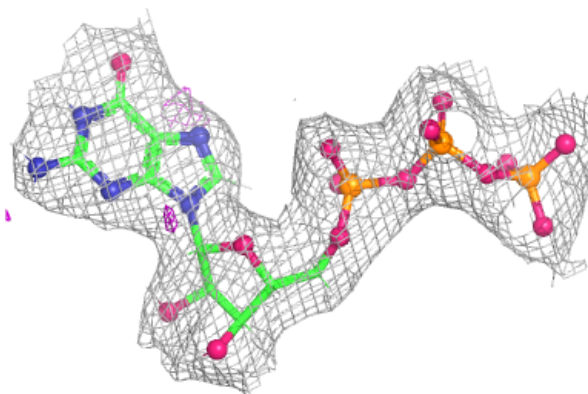
**Electron density around GTP R 501:**

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.