Full wwPDB X-ray Structure Validation Report (i)

Apr 12, 2022 – 01:17 pm BST

PDB ID	:	7Q1F
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 (i) symbol.

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

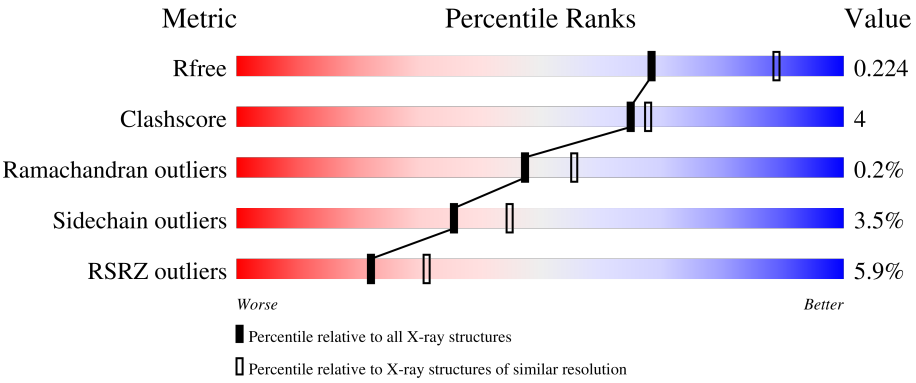
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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	85% 9%
1	R	451	85% 10%
2	B	445	84% 12%
2	S	445	5% 84% 13%
3	C	232	2% 80% 13% 6%

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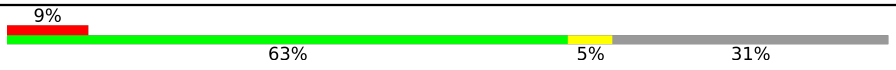
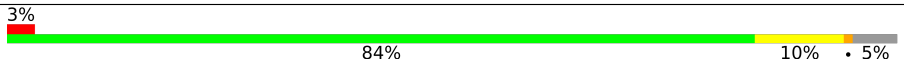
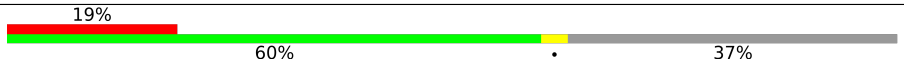
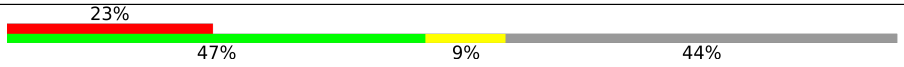
Mol	Chain	Length	Quality of chain
3	D	232	
3	T	232	
3	U	232	
4	P	75	
4	V	75	

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			

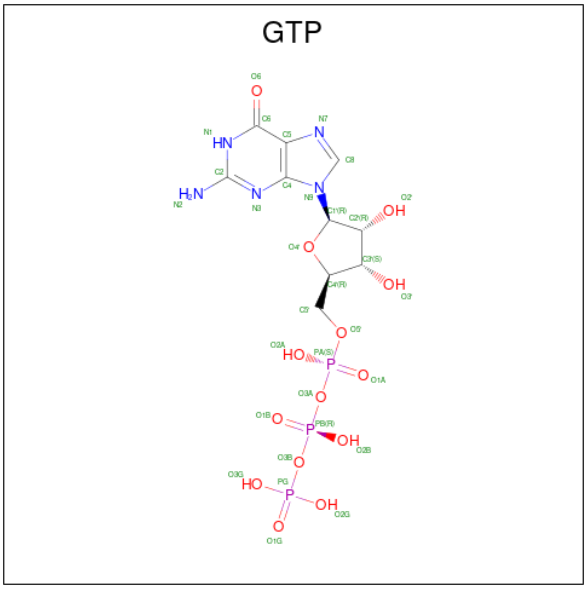
- Molecule 3 is a protein called IE5 ALPHAREP.

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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

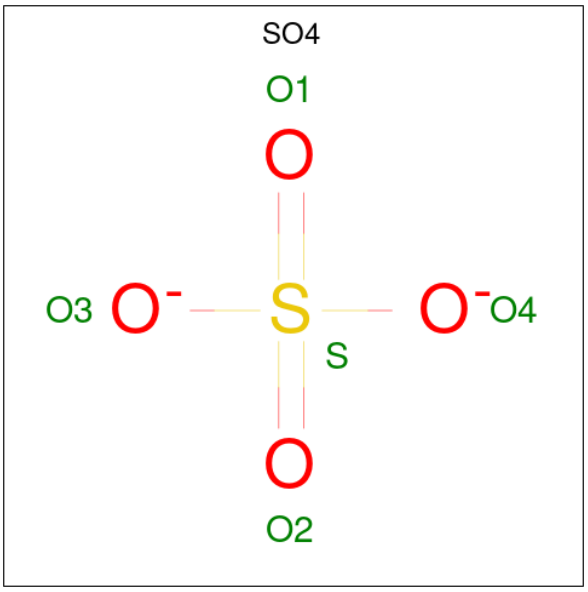


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
5	R	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

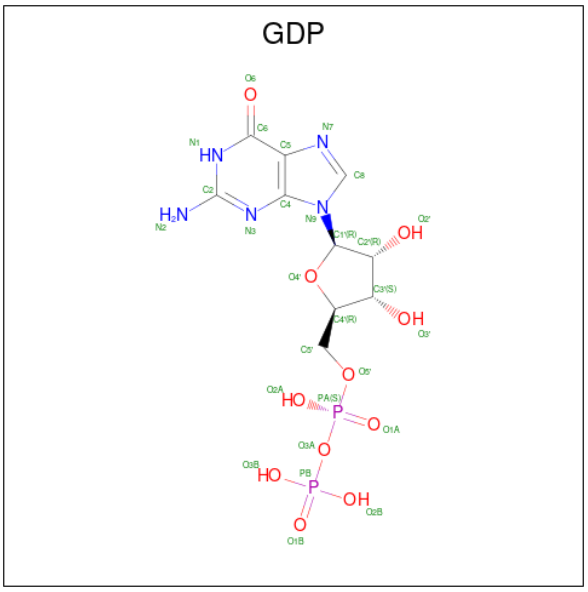
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	R	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

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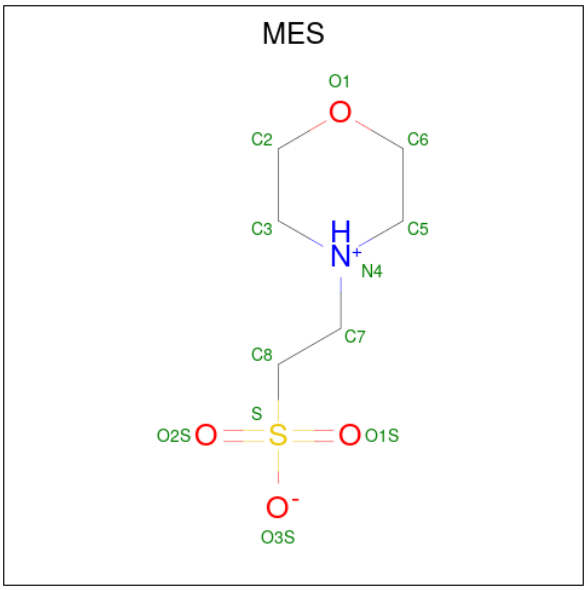
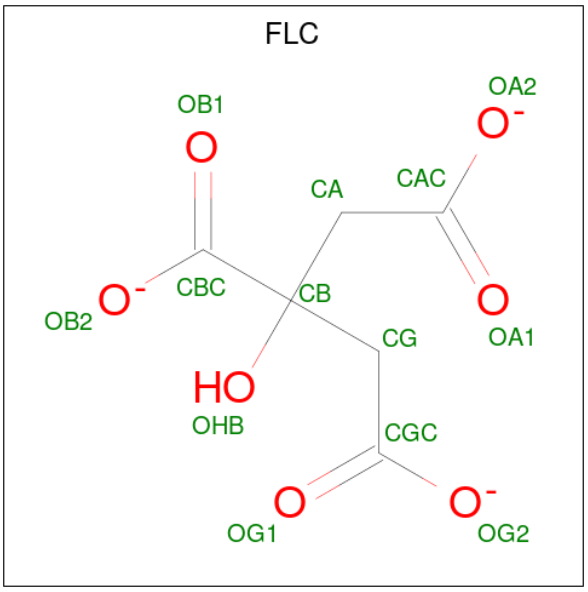
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	S	1	Total C H N O P 40 10 12 5 11 2	0	0

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



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

- Molecule 10 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

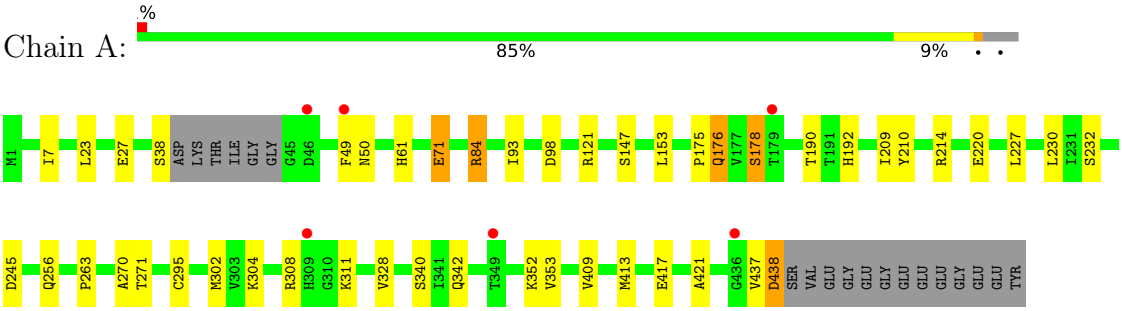
- Molecule 11 is water.

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

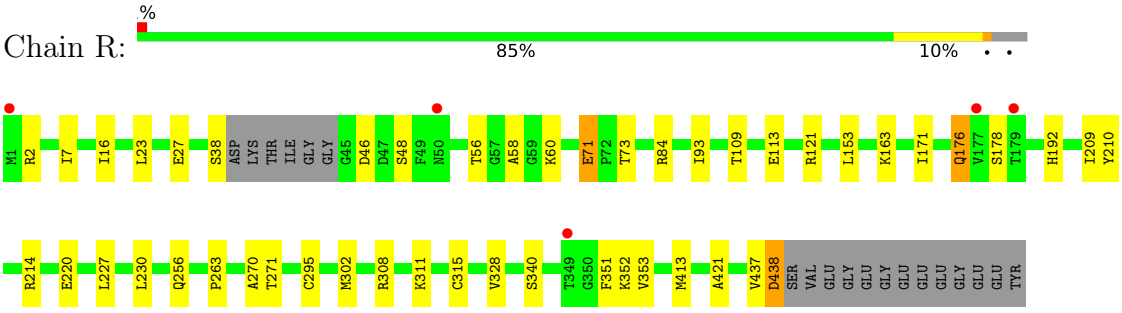
3 Residue-property plots (i)

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.

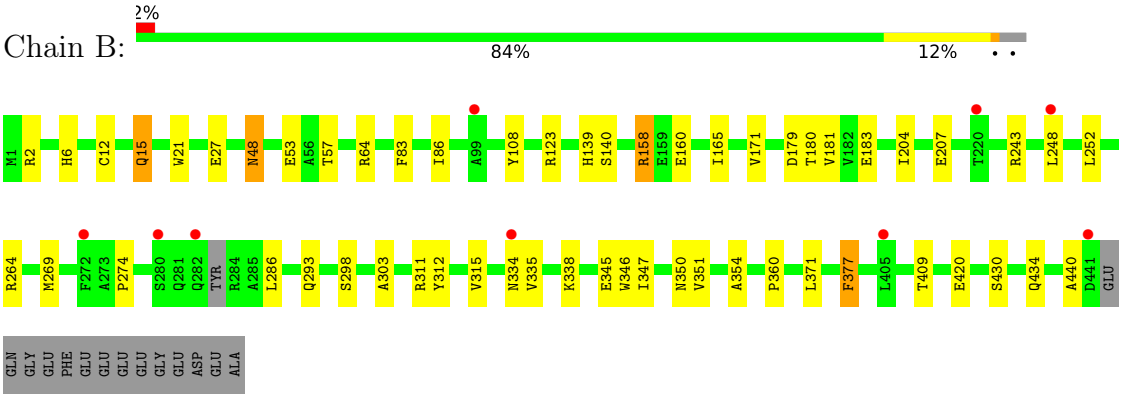
• Molecule 1: Tubulin alpha chain



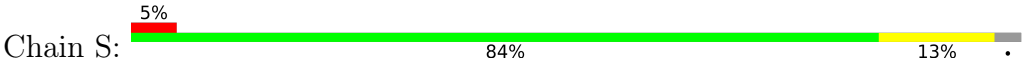
• Molecule 1: Tubulin alpha chain

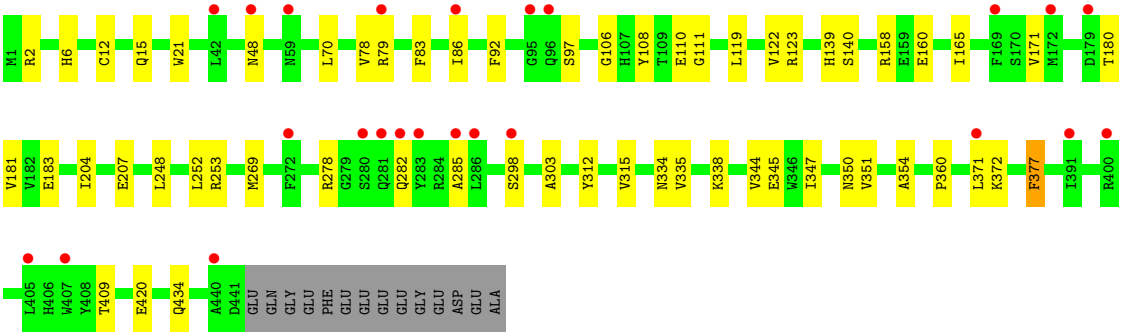


• Molecule 2: Tubulin beta chain



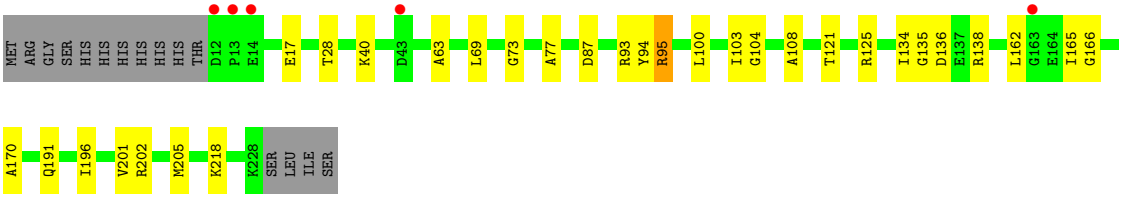
• Molecule 2: Tubulin beta chain





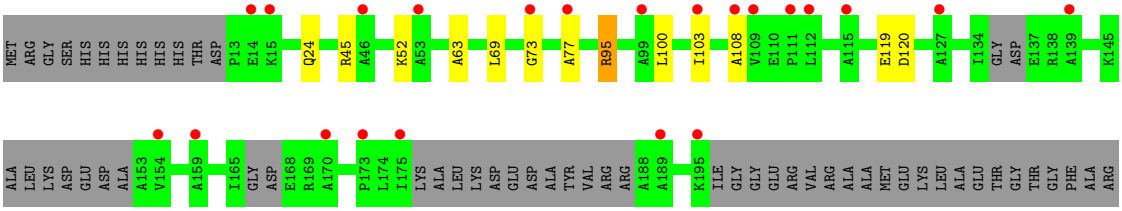
• Molecule 3: IE5 ALPHAREP

Chain C:



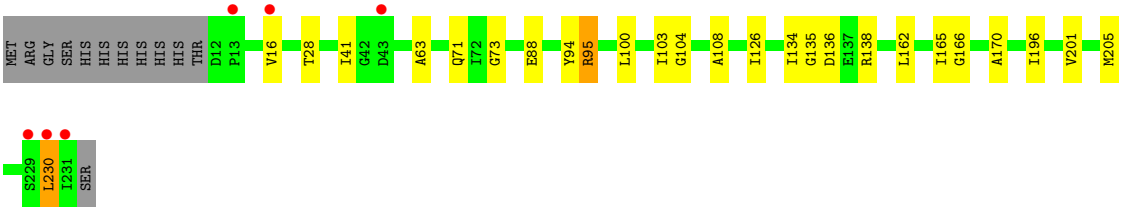
• Molecule 3: IE5 ALPHAREP

Chain D:



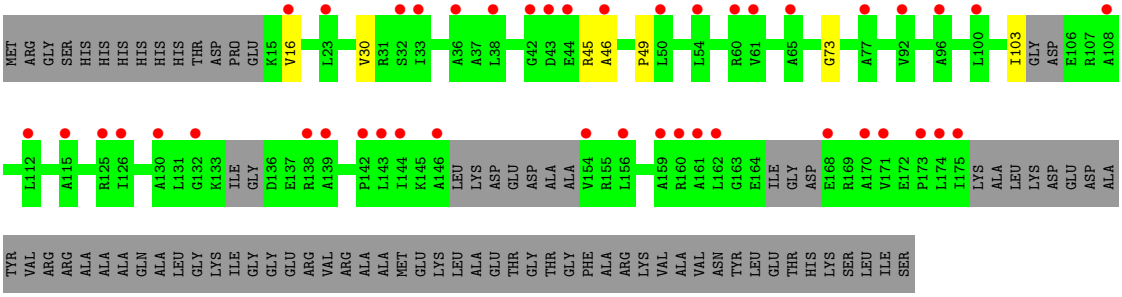
• Molecule 3: IE5 ALPHAREP

Chain T:

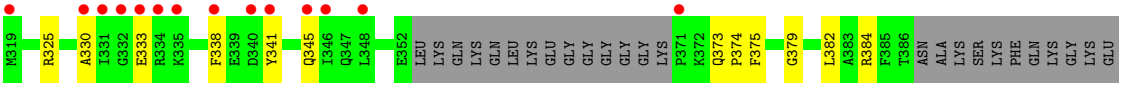


• Molecule 3: IE5 ALPHAREP

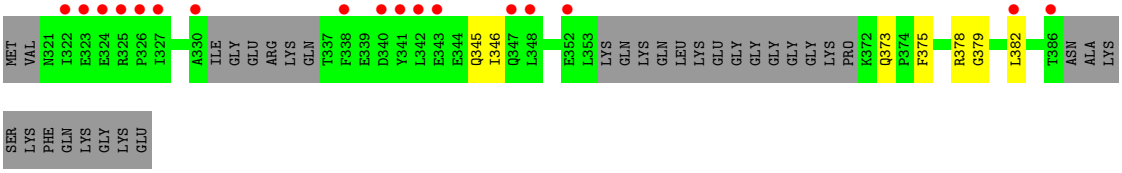
Chain U:



• Molecule 4: Centromere protein J



• Molecule 4: Centromere protein J



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, SO4, FLC, GTP, MES

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	0.47	0/3457	0.62	0/4693
1	R	0.47	0/3479	0.62	0/4723
2	B	0.44	0/3440	0.60	0/4659
2	S	0.40	0/3464	0.59	0/4692
3	C	0.41	0/1645	0.53	0/2215
3	D	0.34	0/1014	0.47	0/1383
3	T	0.40	0/1667	0.53	0/2244
3	U	0.33	0/838	0.46	0/1153
4	P	0.44	0/373	0.62	0/502
4	V	0.38	0/322	0.54	0/431
All	All	0.43	0/19699	0.58	0/26695

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	28	0
2	B	3367	0	3239	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	3389	0	3266	33	0
3	C	1633	0	1683	16	0
3	D	1011	0	882	4	0
3	T	1655	0	1717	16	0
3	U	837	0	618	5	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
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	157	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 (157) 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:209:ILE:HD11	1:A:302:MET:HE3	1.64	0.79
1:R:209:ILE:HD11	1:R:302:MET:HE3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PRO:HA	1:A:178:SER:HB2	1.67	0.76
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
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
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
1:A:311:LYS:HZ2	1:A:438:ASP:HA	1.71	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
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:311:LYS:HZ1	1:R:438:ASP:HA	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:413:MET:HE3	1:A:417:GLU:HB3	1.94	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:R:163:LYS:HZ2	3:T:88:GLU:CB	2.30	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:U:46:ALA:C	3:U:49:PRO:HD2	2.41	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
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
1:R:311:LYS:HZ2	1:R:438:ASP:HA	1.85	0.41
3:C:166:GLY:HA2	3:C:196:ILE:HG12	2.03	0.41
1:R:315:CYS:HG	1:R:351:PHE:HD1	1.67	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
1:A:409:VAL:HA	1:A:413:MET:O	2.21	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
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
1:R:163:LYS:HZ2	3:T:88:GLU:CD	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	29 31
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%)	29 31
3	U	137/232 (59%)	137 (100%)	0	0	100 100
4	P	46/75 (61%)	39 (85%)	5 (11%)	2 (4%)	2 1
4	V	36/75 (48%)	35 (97%)	1 (3%)	0	100 100
All	All	2515/2870 (88%)	2455 (98%)	55 (2%)	5 (0%)	47 55

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 (i)

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%)	351 (96%)	13 (4%)	35 44
1	R	367/379 (97%)	354 (96%)	13 (4%)	36 45
2	B	369/383 (96%)	356 (96%)	13 (4%)	36 45
2	S	372/383 (97%)	361 (97%)	11 (3%)	41 50
3	C	160/176 (91%)	153 (96%)	7 (4%)	28 35
3	D	70/176 (40%)	64 (91%)	6 (9%)	10 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	T	163/176 (93%)	160 (98%)	3 (2%)	59 70
3	U	39/176 (22%)	39 (100%)	0	100 100
4	P	32/62 (52%)	31 (97%)	1 (3%)	40 49
4	V	29/62 (47%)	28 (97%)	1 (3%)	37 46
All	All	1965/2352 (84%)	1897 (96%)	68 (4%)	36 45

All (68) 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	176	GLN
1	A	178	SER
1	A	220	GLU
1	A	232	SER
1	A	256	GLN
1	A	342	GLN
1	A	352	LYS
1	A	437	VAL
1	A	438	ASP
2	B	15	GLN
2	B	48	ASN
2	B	53	GLU
2	B	57	THR
2	B	139	HIS
2	B	158	ARG
2	B	181	VAL
2	B	207	GLU
2	B	293	GLN
2	B	298	SER
2	B	345	GLU
2	B	377	PHE
2	B	409	THR
3	C	17	GLU
3	C	40	LYS
3	C	94	TYR
3	C	95	ARG
3	C	191	GLN
3	C	202	ARG

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Mol	Chain	Res	Type
3	C	218	LYS
3	D	24	GLN
3	D	45	ARG
3	D	52	LYS
3	D	95	ARG
3	D	119	GLU
3	D	120	ASP
4	P	345	GLN
1	R	2	ARG
1	R	38	SER
1	R	46	ASP
1	R	48	SER
1	R	71	GLU
1	R	176	GLN
1	R	178	SER
1	R	220	GLU
1	R	256	GLN
1	R	352	LYS
1	R	413	MET
1	R	437	VAL
1	R	438	ASP
2	S	15	GLN
2	S	139	HIS
2	S	207	GLU
2	S	282	GLN
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. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
10	FLC	D	501	-	3,12,12	0.31	0	3,17,17	1.64	1 (33%)
7	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.28	0
7	SO4	R	503	-	4,4,4	0.18	0	6,6,6	0.18	0
9	MES	B	503	-	12,12,12	0.60	0	14,16,16	0.37	0
8	GDP	S	501	-	24,30,30	0.93	1 (4%)	31,47,47	2.21	8 (25%)
9	MES	S	503	-	12,12,12	0.61	0	14,16,16	0.37	0
5	GTP	R	501	6	26,34,34	0.94	1 (3%)	33,54,54	1.99	5 (15%)
5	GTP	A	501	6	26,34,34	1.02	2 (7%)	33,54,54	2.00	5 (15%)
9	MES	B	502	-	12,12,12	0.77	0	14,16,16	0.40	0
8	GDP	B	501	-	24,30,30	0.90	1 (4%)	31,47,47	2.16	7 (22%)
9	MES	S	502	-	12,12,12	0.73	0	14,16,16	0.44	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
10	FLC	D	501	-	-	3/6/16/16	-
9	MES	B	503	-	-	5/6/14/14	0/1/1/1
8	GDP	S	501	-	-	4/12/32/32	0/3/3/3
9	MES	S	503	-	-	5/6/14/14	0/1/1/1
5	GTP	R	501	6	-	7/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
9	MES	B	502	-	-	0/6/14/14	0/1/1/1
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
9	MES	S	502	-	-	0/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	501	GDP	C6-N1	3.22	1.38	1.33
5	A	501	GTP	C6-N1	3.18	1.38	1.33
8	B	501	GDP	C6-N1	3.06	1.38	1.33
5	R	501	GTP	C6-N1	2.99	1.38	1.33
5	A	501	GTP	C5-C6	2.11	1.45	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	501	GTP	C5-C6-N1	-8.35	112.01	123.43
5	A	501	GTP	C5-C6-N1	-8.32	112.05	123.43
8	S	501	GDP	C5-C6-N1	-8.23	112.17	123.43
8	B	501	GDP	C5-C6-N1	-8.16	112.27	123.43
8	S	501	GDP	C2-N1-C6	5.95	125.38	115.93
8	B	501	GDP	C2-N1-C6	5.95	125.38	115.93
5	R	501	GTP	C2-N1-C6	5.87	125.25	115.93
5	A	501	GTP	C2-N1-C6	5.80	125.15	115.93
8	S	501	GDP	N3-C2-N1	-2.95	123.28	127.22
8	B	501	GDP	N3-C2-N1	-2.92	123.33	127.22
5	R	501	GTP	N3-C2-N1	-2.91	123.34	127.22
5	A	501	GTP	N3-C2-N1	-2.80	123.48	127.22
8	S	501	GDP	O2B-PB-O3A	2.74	113.83	104.64
8	S	501	GDP	C4-C5-C6	-2.73	118.19	120.80
8	B	501	GDP	C4-C5-C6	-2.64	118.28	120.80
8	B	501	GDP	O5'-PA-O1A	-2.62	98.84	109.07
5	A	501	GTP	C4-C5-C6	-2.55	118.37	120.80
10	D	501	FLC	CB-CG-CGC	2.54	119.05	114.98
8	B	501	GDP	C2-N3-C4	-2.45	112.56	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	501	GTP	C4-C5-C6	-2.30	118.60	120.80
8	S	501	GDP	C2-N3-C4	-2.26	112.78	115.36
8	S	501	GDP	O5'-PA-O1A	2.18	117.60	109.07
5	A	501	GTP	C2-N3-C4	-2.14	112.92	115.36
8	B	501	GDP	O2A-PA-O5'	2.11	117.53	107.75
5	R	501	GTP	C2-N3-C4	-2.05	113.02	115.36
8	S	501	GDP	O2A-PA-O5'	-2.03	98.32	107.75

There are no chirality outliers.

All (34) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
8	S	501	GDP	C4'-C5'-O5'-PA
8	S	501	GDP	C5'-O5'-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
5	R	501	GTP	C4'-C5'-O5'-PA

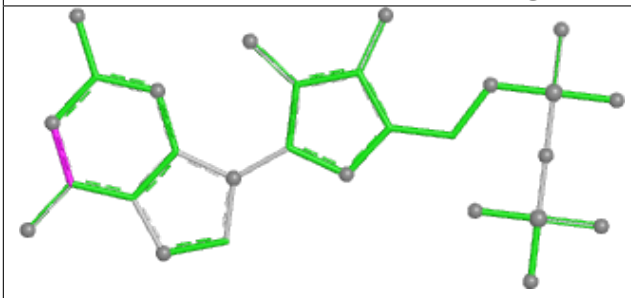
There are no ring outliers.

3 monomers are involved in 6 short contacts:

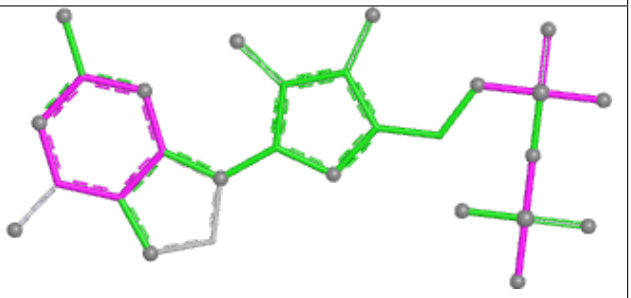
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	1	0
9	S	503	MES	1	0
9	S	502	MES	4	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

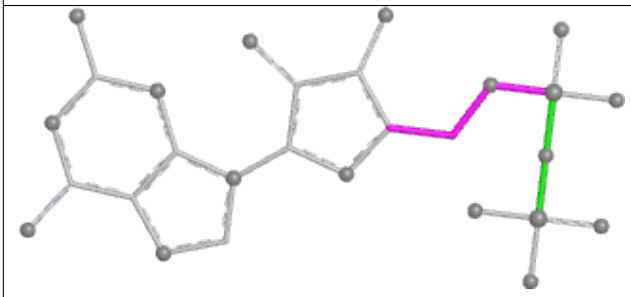
Ligand GDP S 501



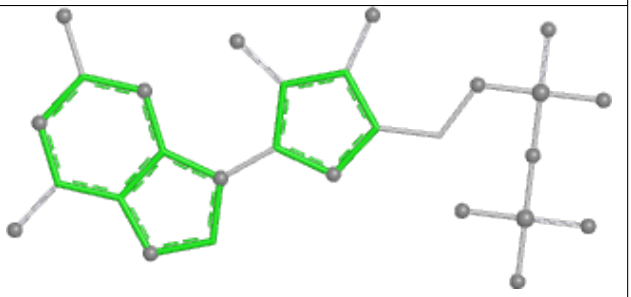
Bond lengths



Bond angles

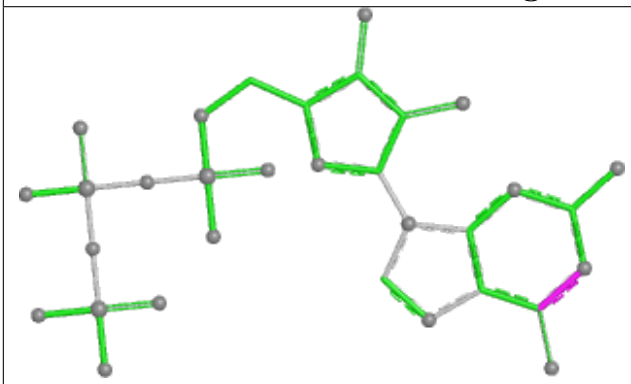


Torsions

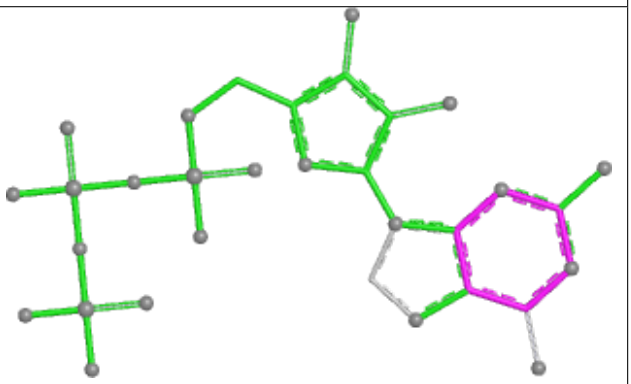


Rings

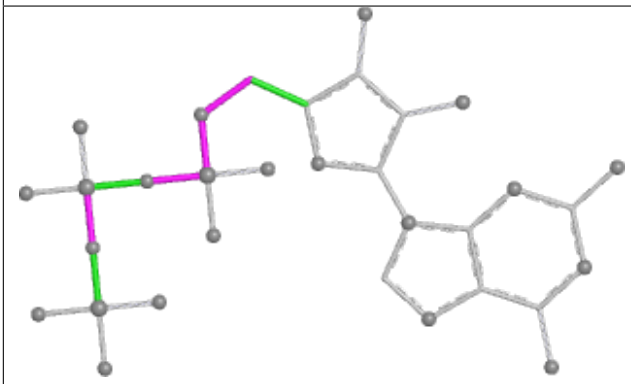
Ligand GTP R 501



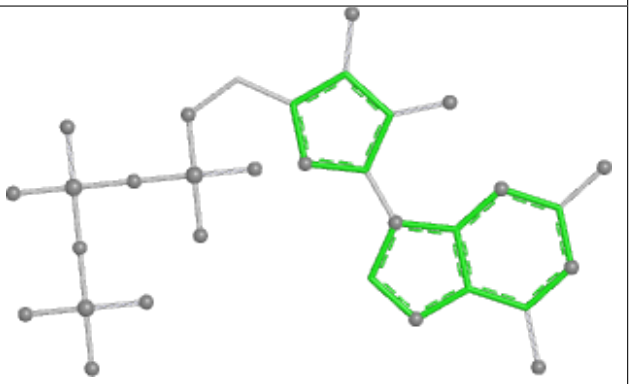
Bond lengths



Bond angles

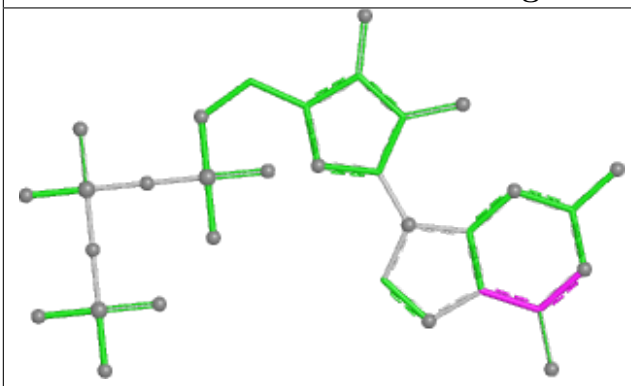


Torsions

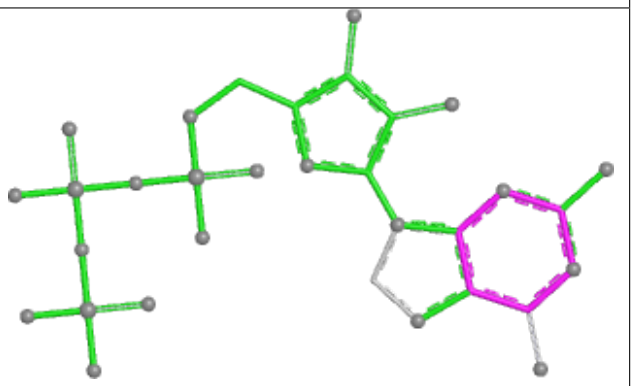


Rings

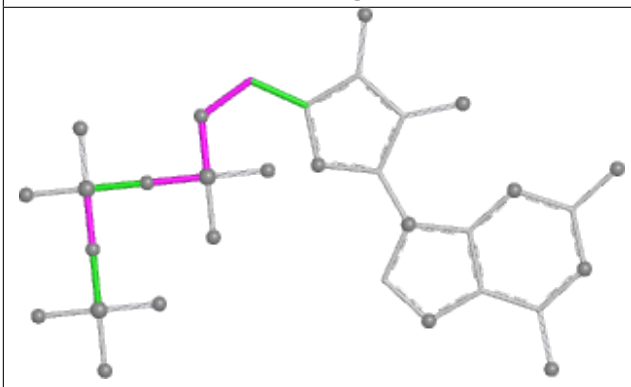
Ligand GTP A 501



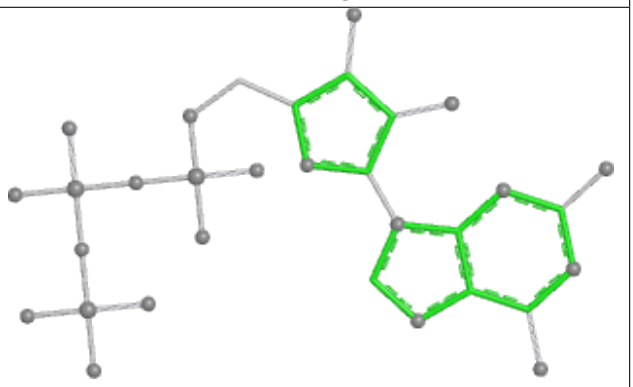
Bond lengths



Bond angles

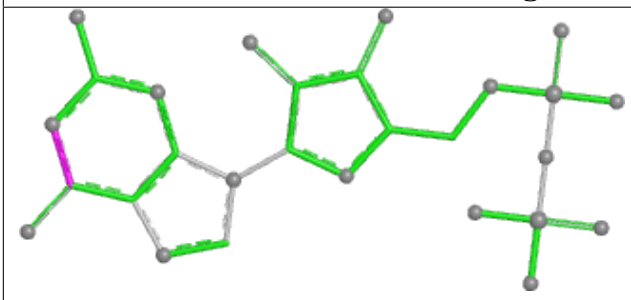


Torsions

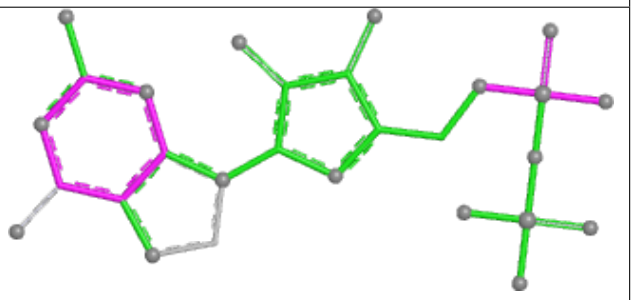


Rings

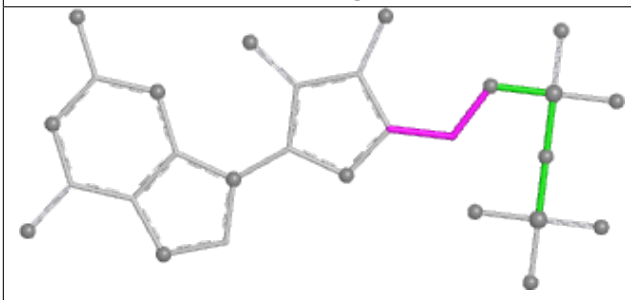
Ligand GDP B 501



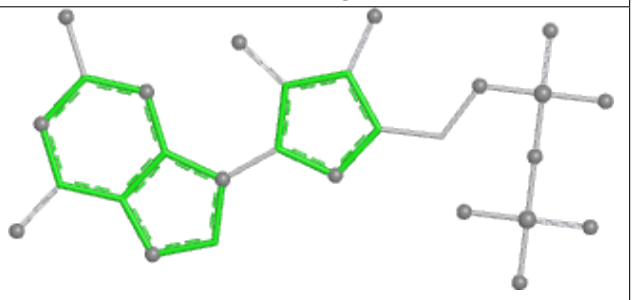
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.60	6 (1%) 75 82	31, 43, 69, 90	1 (0%)
1	R	432/451 (95%)	0.60	5 (1%) 79 85	32, 44, 70, 90	1 (0%)
2	B	430/445 (96%)	0.63	9 (2%) 63 73	34, 54, 77, 112	0
2	S	431/445 (96%)	0.73	24 (5%) 24 33	37, 66, 95, 131	0
3	C	217/232 (93%)	0.53	5 (2%) 60 69	50, 71, 99, 117	0
3	D	160/232 (68%)	0.94	22 (13%) 2 4	62, 105, 210, 234	0
3	T	220/232 (94%)	0.63	6 (2%) 54 64	51, 73, 103, 122	0
3	U	147/232 (63%)	1.55	44 (29%) 0 0	90, 122, 170, 257	0
4	P	50/75 (66%)	1.56	14 (28%) 0 0	51, 103, 136, 138	0
4	V	42/75 (56%)	1.69	17 (40%) 0 0	58, 123, 131, 136	0
All	All	2561/2870 (89%)	0.73	152 (5%) 22 31	31, 60, 129, 257	2 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	161	ALA	8.4
3	U	115	ALA	7.3
3	U	159	ALA	7.3
3	U	46	ALA	5.9
3	D	115	ALA	5.8
3	D	159	ALA	5.7
4	P	334	ARG	5.6
3	U	96	ALA	5.5
3	D	173	PRO	4.9
4	P	333	GLU	4.9
4	P	330	ALA	4.8
2	S	282	GLN	4.8
3	D	139	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
3	D	112	LEU	4.7
2	S	285	ALA	4.6
2	S	283	TYR	4.6
3	U	146	ALA	4.5
3	C	13	PRO	4.5
3	U	65	ALA	4.5
3	U	156	LEU	4.2
4	P	335	LYS	4.2
3	D	189	ALA	4.2
4	V	322	ILE	4.2
4	V	323	GLU	4.2
3	U	130	ALA	3.9
4	P	332	GLY	3.9
4	V	340	ASP	3.9
3	U	54	LEU	3.9
3	U	50	LEU	3.8
4	V	341	TYR	3.8
4	P	331	ILE	3.8
3	U	142	PRO	3.7
4	P	319	MET	3.7
3	T	229	SER	3.7
3	C	14	GLU	3.7
3	U	125	ARG	3.6
4	V	325	ARG	3.6
3	T	230	LEU	3.6
4	V	352	GLU	3.5
3	U	92	VAL	3.5
3	U	162	LEU	3.5
3	T	231	ILE	3.5
4	V	327	ILE	3.4
2	S	280	SER	3.4
3	D	111	PRO	3.4
3	D	175	ILE	3.4
3	U	43	ASP	3.4
3	U	42	GLY	3.4
3	D	170	ALA	3.4
3	U	100	LEU	3.4
3	D	127	ALA	3.3
3	D	108	ALA	3.3
3	U	170	ALA	3.3
3	U	168	GLU	3.2
4	V	348	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
4	V	386	THR	3.2
2	S	281	GLN	3.2
4	P	371	PRO	3.2
3	U	160	ARG	3.1
3	U	61	VAL	3.1
3	U	108	ALA	3.1
4	P	348	LEU	3.1
1	R	177	VAL	3.0
2	B	220	THR	3.0
3	U	36	ALA	3.0
3	U	139	ALA	3.0
2	S	440	ALA	2.9
3	U	171	VAL	2.9
4	P	340	ASP	2.9
4	V	382	LEU	2.9
4	P	341	TYR	2.9
3	C	12	ASP	2.9
2	S	95	GLY	2.9
2	B	272	PHE	2.9
4	V	330	ALA	2.9
2	B	280	SER	2.8
2	S	400	ARG	2.8
2	S	179	ASP	2.7
2	B	441	ASP	2.6
2	S	172	MET	2.6
3	U	138	ARG	2.6
3	D	109	VAL	2.6
3	D	103	ILE	2.6
3	U	154	VAL	2.6
2	S	59	ASN	2.6
4	V	326	PRO	2.5
3	U	174	LEU	2.5
3	D	15	LYS	2.5
1	R	50	ASN	2.5
2	S	371	LEU	2.5
3	D	77	ALA	2.5
3	U	77	ALA	2.5
3	U	60	ARG	2.5
1	R	179	THR	2.5
3	U	112	LEU	2.5
3	D	46	ALA	2.4
3	U	16	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	49	PHE	2.4
3	D	14	GLU	2.4
3	U	44	GLU	2.4
4	V	347	GLN	2.4
1	R	1	MET	2.4
4	V	324	GLU	2.4
1	A	436	GLY	2.4
2	S	79	ARG	2.4
3	D	154	VAL	2.4
3	U	126	ILE	2.3
2	B	99	ALA	2.3
3	U	143	LEU	2.3
3	U	173	PRO	2.3
4	V	338	PHE	2.3
2	B	282	GLN	2.3
3	U	144	ILE	2.3
1	A	349	THR	2.3
2	B	248	LEU	2.3
3	D	53	ALA	2.3
2	S	286	LEU	2.3
3	U	23	LEU	2.3
2	S	42	LEU	2.2
2	S	405	LEU	2.2
3	U	175	ILE	2.2
3	U	38	LEU	2.2
4	V	343	GLU	2.2
2	S	169	PHE	2.2
3	C	163	GLY	2.2
3	D	73	GLY	2.2
3	U	32	SER	2.2
3	U	33	ILE	2.1
3	D	195	LYS	2.1
1	A	309	HIS	2.1
2	B	405	LEU	2.1
3	U	132	GLY	2.1
3	D	99	ALA	2.1
2	B	334	ASN	2.1
2	S	48	ASN	2.1
2	S	86	ILE	2.1
3	T	13	PRO	2.1
4	V	342	LEU	2.1
3	C	43	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	P	338	PHE	2.1
2	S	96	GLN	2.1
3	T	16	VAL	2.1
2	S	298	SER	2.1
1	A	46	ASP	2.1
3	T	43	ASP	2.1
4	P	345	GLN	2.0
4	P	346	ILE	2.0
1	R	349	THR	2.0
1	A	179	THR	2.0
2	S	272	PHE	2.0
2	S	407	TRP	2.0
2	S	391	ILE	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 monosaccharides 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, 95^{th} 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	0.76	0.18	93,95,112,112	0
7	SO4	A	503	5/5	0.83	0.23	117,117,117,117	0
9	MES	S	503	12/12	0.87	0.23	94,97,116,118	0
7	SO4	R	503	5/5	0.87	0.22	119,119,119,119	0
9	MES	S	502	12/12	0.90	0.23	64,65,66,66	0
9	MES	B	503	12/12	0.92	0.17	87,90,113,114	0
9	MES	B	502	12/12	0.95	0.21	57,57,60,60	0
8	GDP	S	501	28/28	0.97	0.19	71,73,99,100	0
8	GDP	B	501	28/28	0.98	0.17	48,49,62,62	0
5	GTP	R	501	32/32	0.99	0.18	34,37,39,41	0

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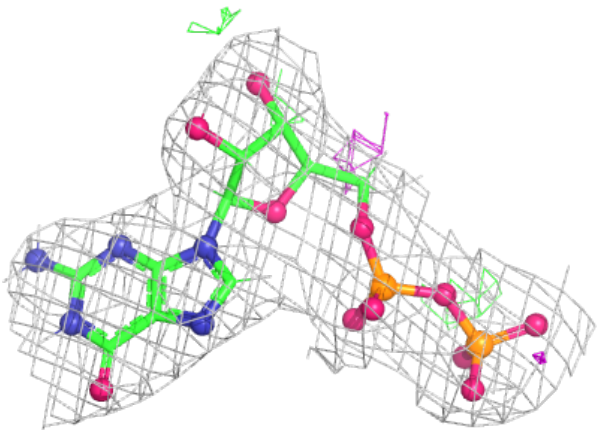
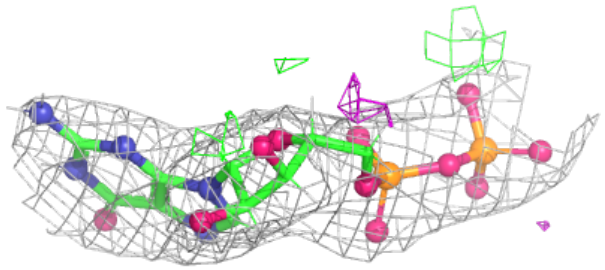
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	A	502	1/1	0.99	0.10	42,42,42,42	0
6	MG	R	502	1/1	0.99	0.09	45,45,45,45	0
5	GTP	A	501	32/32	0.99	0.17	34,37,38,40	0

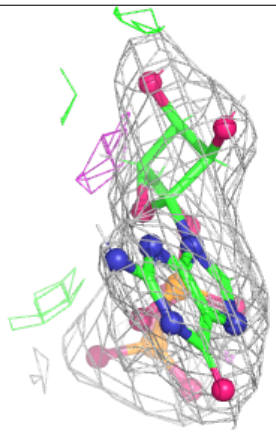
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP S 501:

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

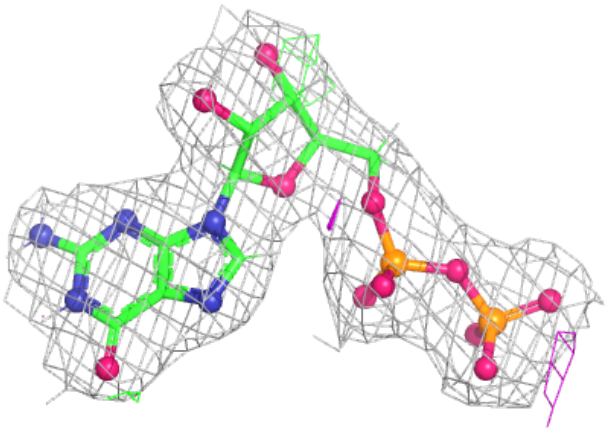


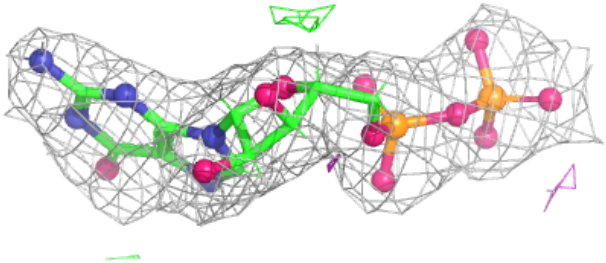


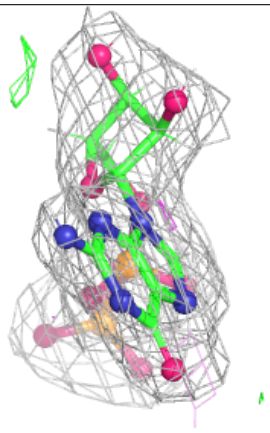


Electron density around GDP B 501:

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

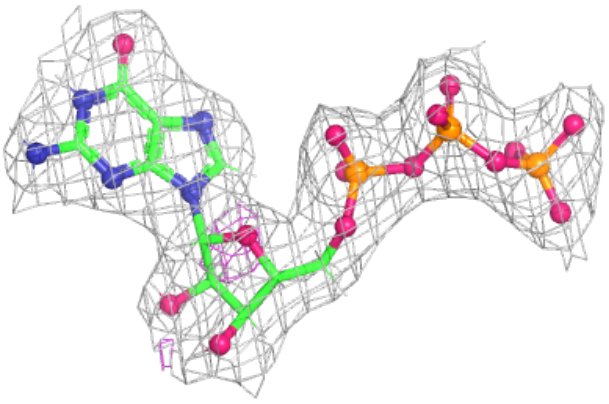


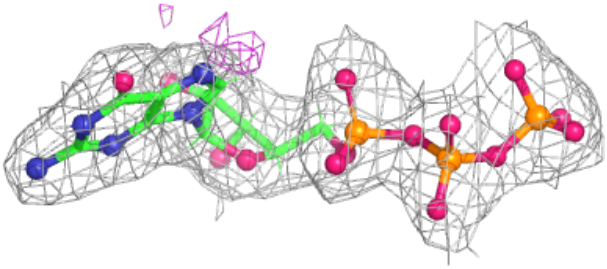


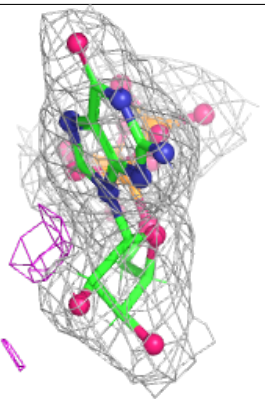


Electron density around GTP R 501:

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

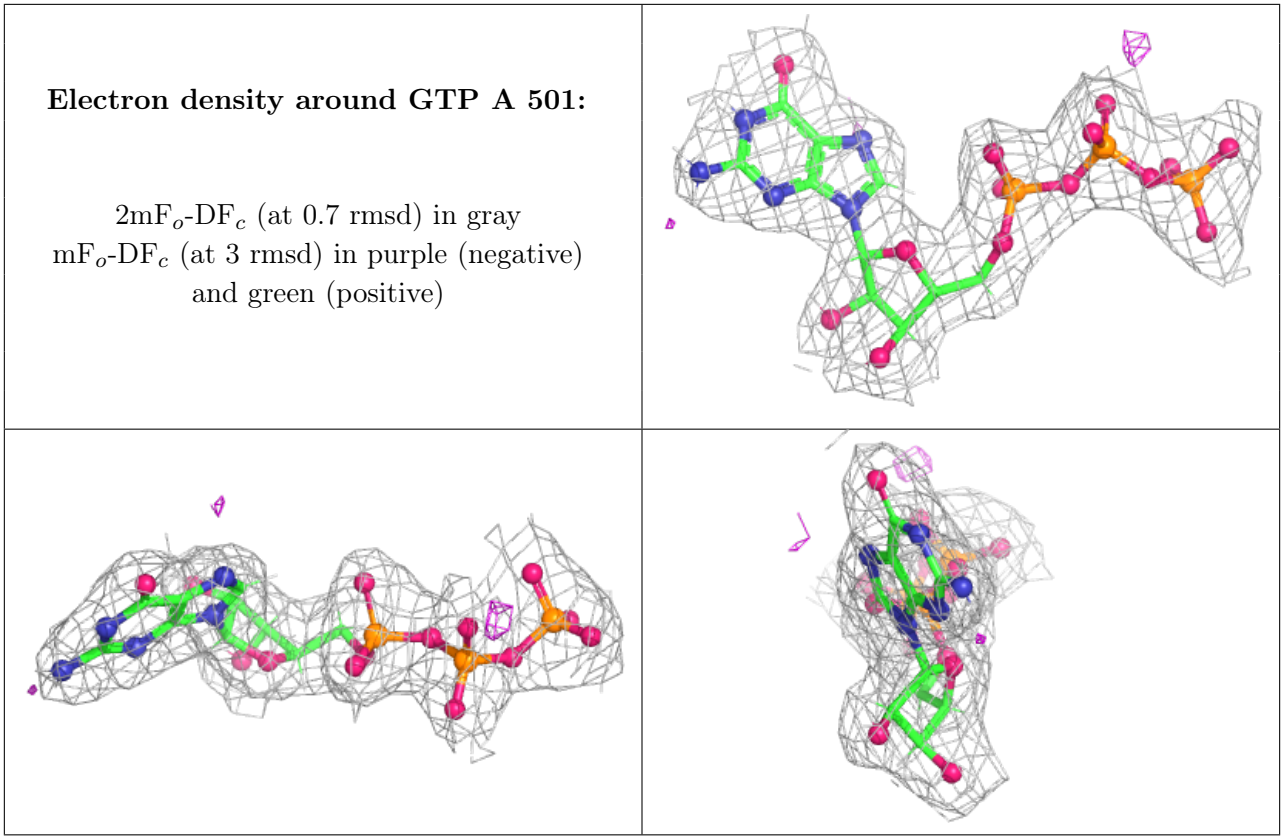






Electron density around GTP A 501:

$2mF_o$-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 (i)

There are no such residues in this entry.