Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 08:09 PM EST

PDB ID	:	6N47
Title	:	The structure of SB-2-204-tubulin complex
Authors	:	Arnst, K.; Banerjee, S.; Wang, Y.; Li, W.; Miller, D.; Li, W.
Deposited on	:	2018-11-17
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

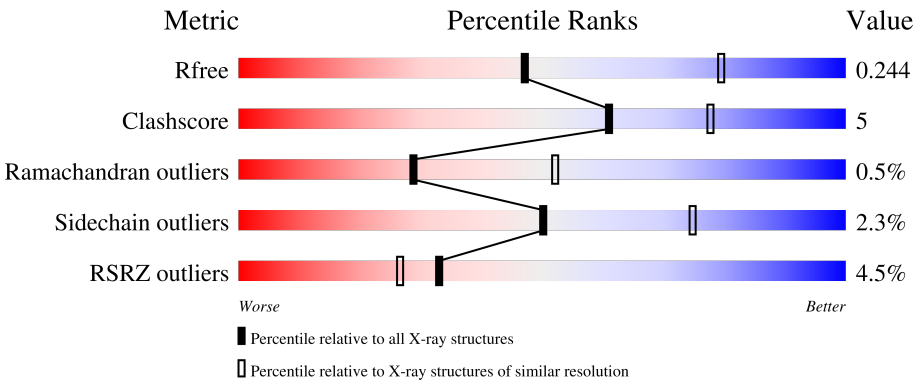
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	450	% 87% 10% •
1	C	450	86% 12% •
2	B	445	2% 84% 11% •
2	D	445	4% 80% 15% 5%
3	E	143	6% 76% 10% • 13%

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Mol	Chain	Length	Quality of chain
4	F	384	16% 81% 10% • 9%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 17917 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3416	2163	581	650	22	0	0	0
1	C	441	3446	2180	585	659	22	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	3372	2117	577	651	27	0	1	0
2	D	421	3309	2080	562	640	27	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	124	1036	641	187	202	6	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

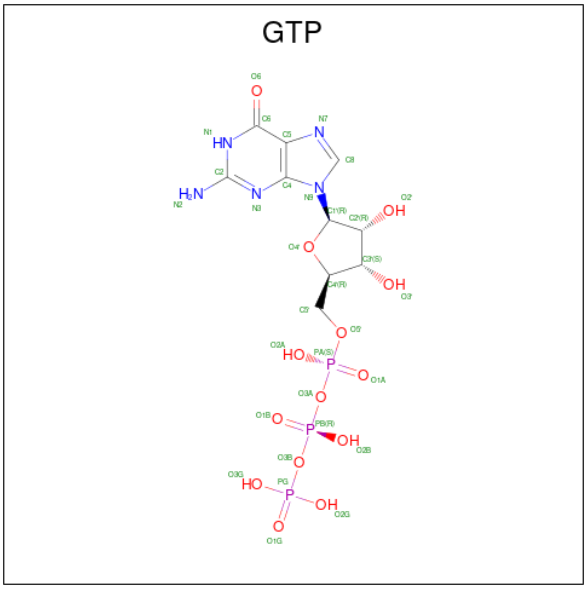
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	350	2873	1839	496	524	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total Ca 1 1	0	0

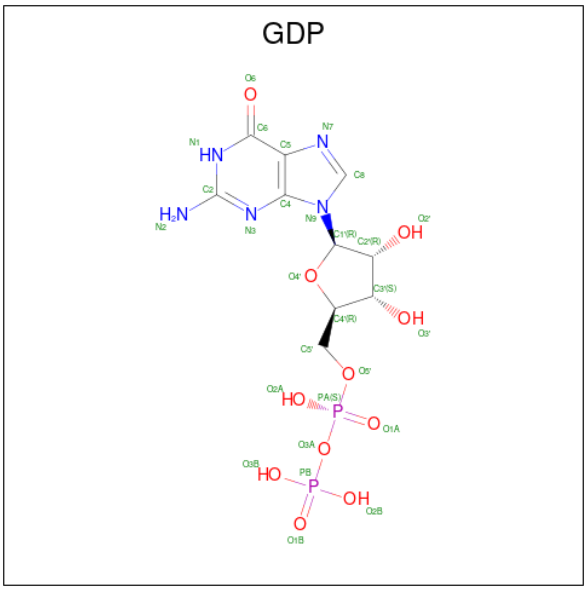
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

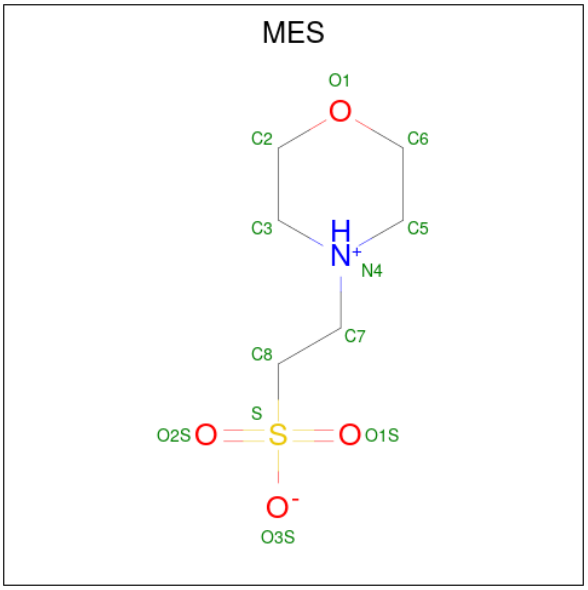
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0
8	B	1	Total Mg 1 1	0	0
8	C	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



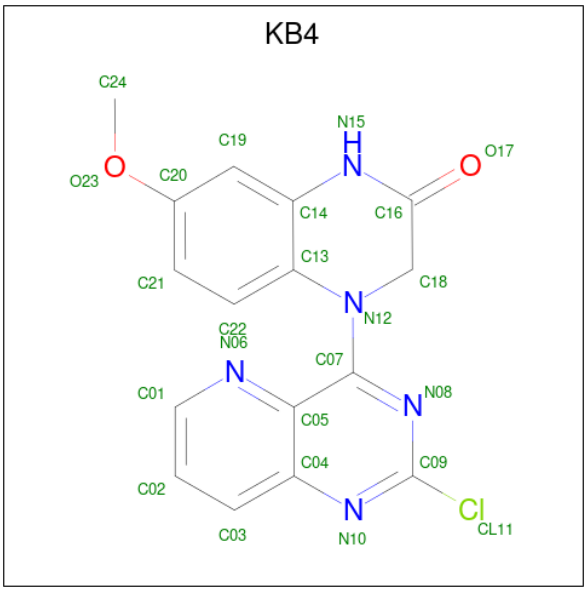
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	28	10	5	11	2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



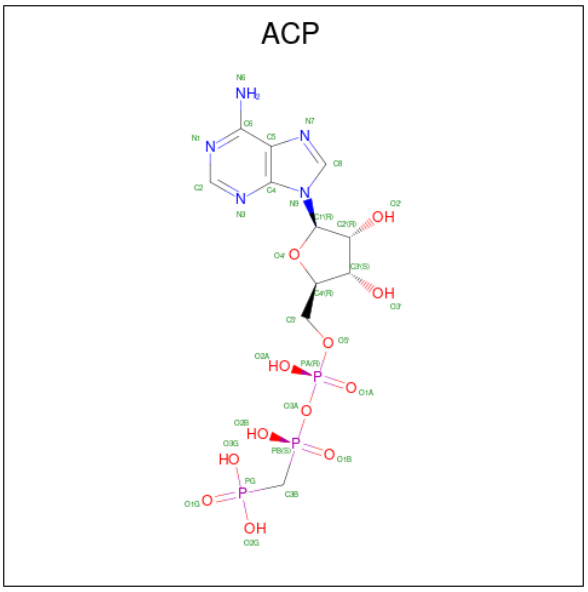
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is 4-(2-chloropyrido[3,2-d]pyrimidin-4-yl)-7-methoxy-3,4-dihydroquinoxalin-2(1 H)-one (three-letter code: KB4) (formula: $C_{16}H_{12}ClN_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
11	B	1	24	16	1	5	2	0	0
			Total	C	Cl	N	O		
11	D	1	24	16	1	5	2	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

- Molecule 13 is water.

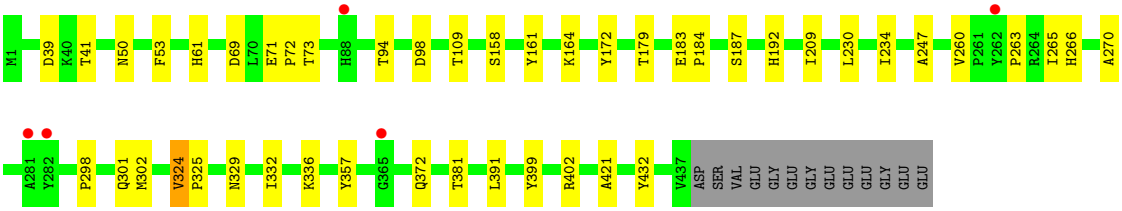
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	52	52	52	0	0
			Total	O		
13	B	46	46	46	0	0
			Total	O		
13	C	94	94	94	0	0
			Total	O		
13	D	15	15	15	0	0
			Total	O		
13	E	11	11	11	0	0
			Total	O		
13	F	11	11	11	0	0

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.

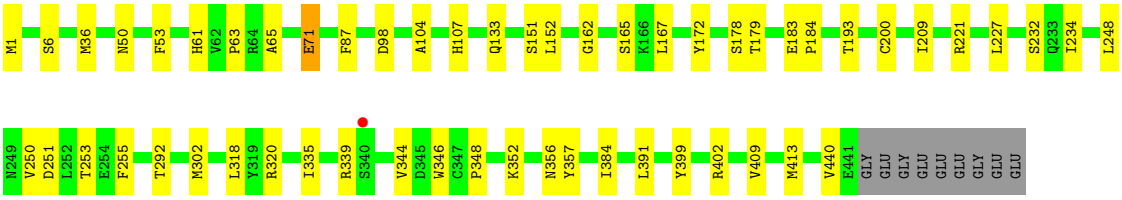
• Molecule 1: Tubulin alpha-1B chain

Chain A:



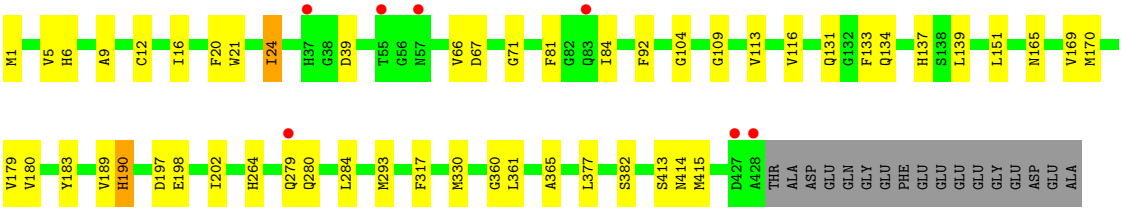
• Molecule 1: Tubulin alpha-1B chain

Chain C:



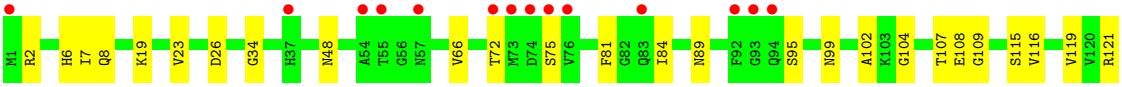
• Molecule 2: Tubulin beta-2B chain

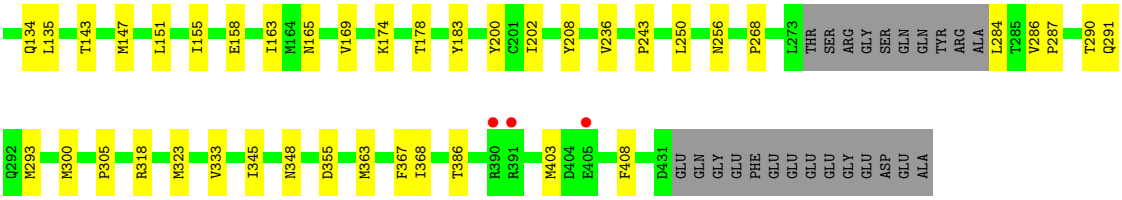
Chain B:



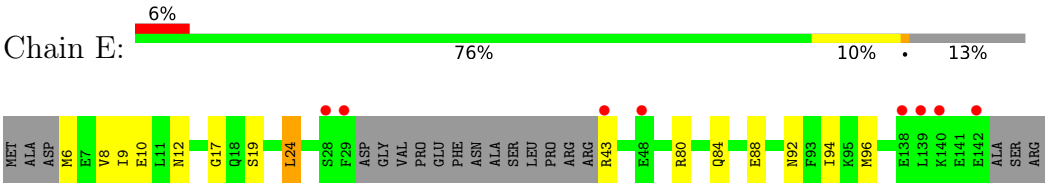
• Molecule 2: Tubulin beta-2B chain

Chain D:

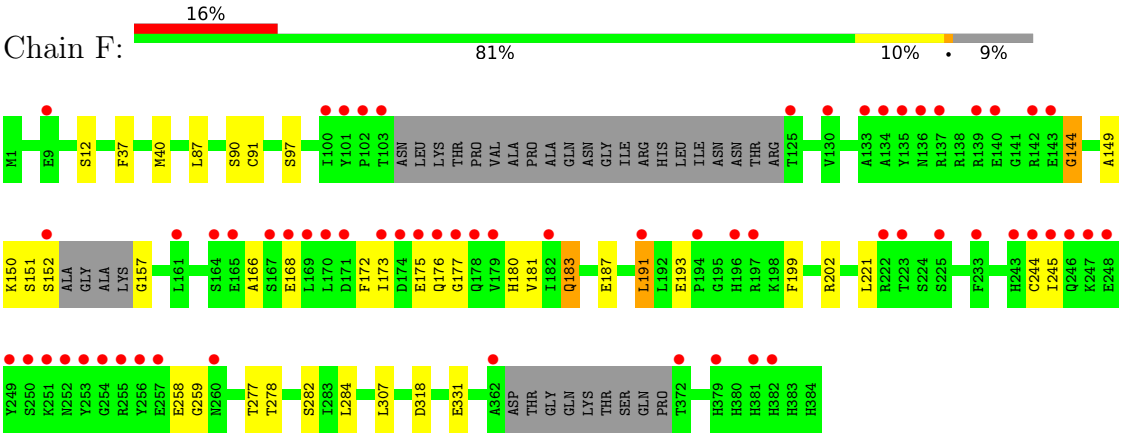




• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.30Å 157.84Å 182.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.16 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.60) 98.9 (48.16-2.58)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.201 , 0.246 0.205 , 0.244	Depositor DCC
R_{free} test set	4728 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17917	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CA, GDP, MG, KB4, ACP, CL, 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	0.66	0/3494	0.83	0/4743
1	C	0.68	0/3524	0.85	0/4784
2	B	0.69	0/3450	0.82	0/4672
2	D	0.68	0/3382	0.80	0/4581
3	E	0.67	0/1048	0.80	0/1389
4	F	0.68	0/2941	0.79	0/3973
All	All	0.68	0/17839	0.82	0/24142

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 (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	3416	0	3331	31	0
1	C	3446	0	3353	31	0
2	B	3372	0	3255	38	0
2	D	3309	0	3189	36	0
3	E	1036	0	1055	13	0
4	F	2873	0	2824	18	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	0	12	0	0
10	B	24	0	26	2	0
11	B	24	0	0	0	0
11	D	24	0	0	2	0
12	F	31	0	14	2	0
13	A	52	0	0	0	0
13	B	46	0	0	0	0
13	C	94	0	0	0	0
13	D	15	0	0	0	0
13	E	11	0	0	0	0
13	F	11	0	0	0	0
All	All	17917	0	17095	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 5.

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)
2:B:20:PHE:CE1	2:B:24:ILE:CD1	2.69	0.76
2:D:134:GLN:HA	2:D:165:ASN:O	1.88	0.74
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.70	0.72
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.71	0.72
2:B:20:PHE:CE1	2:B:24:ILE:HD12	2.24	0.72
1:C:234:ILE:HD13	1:C:302:MET:SD	2.29	0.71
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.55	0.71
2:B:197:ASP:OD1	10:B:504:MES:H32	1.93	0.69
2:B:165:ASN:HD22	2:B:198:GLU:HG3	1.58	0.68
2:B:139:LEU:HD12	2:B:170:MET:SD	2.34	0.67
1:A:69:ASP:O	1:A:94:THR:HA	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:ALA:HB2	2:D:403:MET:HE3	1.79	0.65
4:F:168:GLU:O	4:F:172:PHE:N	2.30	0.64
2:B:189:VAL:HB	2:B:415:MET:HE3	1.81	0.63
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.80	0.63
2:B:134:GLN:HA	2:B:165:ASN:O	1.99	0.62
2:B:116:VAL:HG11	2:B:151:LEU:HD21	1.82	0.62
2:D:200:TYR:CZ	2:D:236:VAL:CG1	2.82	0.62
1:C:107:HIS:O	1:C:152:LEU:HD22	1.98	0.61
1:A:336:LYS:NZ	3:E:6:MET:SD	2.74	0.61
1:A:247:ALA:CB	3:E:12:ASN:HD22	2.14	0.60
2:B:279:GLN:NE2	2:B:280:GLN:O	2.34	0.59
1:A:247:ALA:HB1	3:E:12:ASN:HD22	1.66	0.59
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.38	0.59
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.86	0.57
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.05	0.57
2:D:200:TYR:CZ	2:D:236:VAL:HG13	2.41	0.56
2:D:169:VAL:HA	2:D:202:ILE:O	2.05	0.56
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.87	0.56
1:A:234:ILE:HD13	1:A:302:MET:SD	2.45	0.55
2:B:104:GLY:O	2:B:109:GLY:HA3	2.06	0.55
3:E:80:ARG:O	3:E:84:GLN:HG3	2.07	0.55
2:B:197:ASP:OD2	10:B:504:MES:H52	2.06	0.55
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.89	0.54
1:A:332:ILE:HG22	1:A:336:LYS:CE	2.37	0.54
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.42	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
2:D:102:ALA:HB2	2:D:403:MET:CE	2.37	0.54
2:B:165:ASN:ND2	2:B:198:GLU:HG3	2.21	0.54
2:B:189:VAL:HB	2:B:415:MET:CE	2.38	0.53
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.44	0.53
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.91	0.53
2:B:113:VAL:HG23	2:B:151:LEU:HD12	1.91	0.52
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.44	0.52
4:F:278:THR:O	4:F:282:SER:OG	2.21	0.52
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.92	0.52
2:D:7:ILE:O	2:D:135:LEU:HA	2.11	0.51
1:A:324:VAL:HG22	1:A:325:PRO:HD2	1.92	0.51
2:B:165:ASN:HD22	2:B:198:GLU:CG	2.24	0.51
4:F:173:ILE:HG23	4:F:176:GLN:HB2	1.92	0.51
1:A:329:ASN:ND2	3:E:8:VAL:HG21	2.25	0.51
1:C:6:SER:O	1:C:65:ALA:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:SER:HB3	1:C:193:THR:HG21	1.93	0.50
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.46	0.50
2:B:169:VAL:HA	2:B:202:ILE:O	2.11	0.50
1:A:332:ILE:HG22	1:A:336:LYS:HE3	1.94	0.49
2:B:81:PHE:O	2:B:84:ILE:HG22	2.11	0.49
2:B:317:PHE:HZ	2:B:330:MET:HE2	1.77	0.49
2:D:200:TYR:CZ	2:D:236:VAL:HG11	2.47	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.49
2:D:72:THR:O	2:D:75:SER:OG	2.26	0.49
2:D:174:LYS:HD3	2:D:208:TYR:CD2	2.48	0.49
2:B:67:ASP:O	2:B:92:PHE:HA	2.13	0.49
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.48
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.48	0.48
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.96	0.48
2:B:20:PHE:CZ	2:B:24:ILE:CD1	2.96	0.48
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.95	0.48
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.78	0.48
2:D:151:LEU:O	2:D:155:ILE:HG13	2.14	0.48
1:C:234:ILE:CD1	1:C:302:MET:SD	3.02	0.48
1:A:263:PRO:O	1:A:266:HIS:HD2	1.97	0.48
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.48	0.48
3:E:43:ARG:O	3:E:43:ARG:HG3	2.14	0.48
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.95	0.48
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.49	0.48
2:D:256:ASN:HB3	11:D:503:KB4:C19	2.45	0.47
4:F:173:ILE:HD13	4:F:180:HIS:CE1	2.49	0.47
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.97	0.47
1:C:133:GLN:HE21	1:C:253:THR:HG21	1.80	0.47
2:D:104:GLY:O	2:D:109:GLY:HA3	2.15	0.47
2:D:256:ASN:HB3	11:D:503:KB4:C20	2.44	0.47
2:D:89:ASN:HA	2:D:119:VAL:HG21	1.96	0.47
2:D:318:ARG:O	2:D:363:MET:HA	2.14	0.47
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.96	0.47
4:F:331:GLU:OE2	12:F:401:ACP:O1G	2.33	0.47
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.98	0.46
4:F:97:SER:OG	4:F:183:GLN:OE1	2.32	0.46
4:F:149:ALA:HA	4:F:181:VAL:O	2.16	0.46
1:C:399:TYR:O	1:C:402:ARG:NH2	2.48	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.56	0.46
4:F:150:LYS:NZ	12:F:401:ACP:O5'	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PRO:HA	1:A:301:GLN:CD	2.36	0.46
4:F:173:ILE:HG21	4:F:180:HIS:NE2	2.31	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.45
4:F:191:LEU:O	4:F:191:LEU:HD12	2.16	0.45
1:A:183:GLU:N	1:A:184:PRO:CD	2.79	0.45
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.62	0.45
2:D:200:TYR:OH	2:D:236:VAL:HG13	2.16	0.45
1:A:332:ILE:HG22	1:A:336:LYS:NZ	2.32	0.45
1:C:133:GLN:HE21	1:C:253:THR:CG2	2.30	0.45
2:B:189:VAL:CB	2:B:415:MET:CE	2.95	0.44
2:D:34:GLY:HA2	2:D:84:ILE:HD11	1.99	0.44
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.98	0.44
2:D:293:MET:CG	2:D:367:PHE:HB2	2.48	0.44
2:D:121:ARG:NE	2:D:158:GLU:OE2	2.34	0.44
2:D:268:PRO:HG2	2:D:300:MET:HB2	1.98	0.44
1:C:167:LEU:HA	1:C:200:CYS:O	2.17	0.43
1:C:440:VAL:O	1:C:440:VAL:HG23	2.18	0.43
2:D:81:PHE:O	2:D:84:ILE:HG22	2.18	0.43
3:E:92:ASN:O	3:E:96:MET:HG2	2.18	0.43
2:B:9:ALA:HA	2:B:66:VAL:O	2.18	0.43
1:C:183:GLU:N	1:C:184:PRO:CD	2.81	0.43
2:D:116:VAL:O	2:D:119:VAL:HG12	2.19	0.43
2:D:183:TYR:CD1	2:D:408:PHE:HE2	2.36	0.43
2:B:12:CYS:SG	2:B:16:ILE:HD12	2.58	0.43
4:F:157:GLY:CA	4:F:245:ILE:HD11	2.49	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.43
2:D:66:VAL:HG12	2:D:147:MET:HE1	2.01	0.43
1:A:71:GLU:OE1	1:A:73:THR:CB	2.66	0.43
1:A:399:TYR:O	1:A:402:ARG:NH1	2.50	0.43
2:D:236:VAL:HG22	2:D:368:ILE:HG12	2.01	0.43
1:A:50:ASN:HA	1:A:53:PHE:O	2.18	0.42
1:C:50:ASN:HA	1:C:53:PHE:O	2.18	0.42
2:D:19:LYS:O	2:D:23:VAL:HG23	2.19	0.42
2:B:197:ASP:O	2:B:264:HIS:HB2	2.20	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.42
2:B:317:PHE:HZ	2:B:330:MET:CE	2.32	0.42
1:A:329:ASN:O	3:E:6:MET:HE1	2.20	0.42
2:B:360:GLY:C	2:B:361:LEU:HD12	2.40	0.42
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.00	0.42
3:E:88:GLU:HA	3:E:88:GLU:OE1	2.20	0.42
2:B:179:VAL:HG12	1:C:348:PRO:CG	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:202:ARG:NE	4:F:318:ASP:OD1	2.43	0.42
1:C:1:MET:C	1:C:1:MET:SD	2.98	0.41
1:A:270:ALA:HB3	1:A:302:MET:CG	2.50	0.41
2:D:107:THR:OG1	2:D:108:GLU:N	2.52	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HG2	2.02	0.41
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.02	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.02	0.41
2:B:1:MET:SD	2:B:131:GLN:HA	2.61	0.41
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.20	0.41
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.02	0.41
2:B:180:VAL:O	2:B:183:TYR:HB2	2.21	0.41
2:B:293:MET:CE	2:B:365:ALA:HB1	2.50	0.41
2:B:317:PHE:CZ	2:B:330:MET:CE	3.03	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.41
1:C:409:VAL:HA	1:C:413:MET:O	2.20	0.41
2:D:66:VAL:HG12	2:D:147:MET:CE	2.51	0.41
3:E:9:ILE:HD12	3:E:10:GLU:HG3	2.02	0.41
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.91	0.41
1:A:263:PRO:O	1:A:266:HIS:CD2	2.73	0.41
2:D:165:ASN:HB2	2:D:250:LEU:HD22	2.02	0.40
4:F:258:GLU:HA	4:F:259:GLY:HA2	1.81	0.40
1:A:192:HIS:CG	1:A:421:ALA:HA	2.57	0.40
2:B:5:VAL:O	2:B:133:PHE:HA	2.21	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	435/450 (97%)	416 (96%)	18 (4%)	1 (0%)	47 71
1	C	439/450 (98%)	422 (96%)	16 (4%)	1 (0%)	47 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	427/445 (96%)	408 (96%)	17 (4%)	2 (0%)	29	52
2	D	417/445 (94%)	389 (93%)	27 (6%)	1 (0%)	47	71
3	E	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
4	F	342/384 (89%)	320 (94%)	17 (5%)	5 (2%)	10	21
All	All	2181/2317 (94%)	2070 (95%)	101 (5%)	10 (0%)	29	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	71	GLY
1	C	178	SER
2	D	243	PRO
4	F	144	GLY
4	F	166	ALA
4	F	175	GLU
1	A	109	THR
4	F	91	CYS
2	B	39	ASP
4	F	177	GLY

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	368/378 (97%)	361 (98%)	7 (2%)	57	79
1	C	372/378 (98%)	365 (98%)	7 (2%)	57	79
2	B	371/383 (97%)	365 (98%)	6 (2%)	62	82
2	D	364/383 (95%)	352 (97%)	12 (3%)	38	64
3	E	113/127 (89%)	111 (98%)	2 (2%)	59	80
4	F	315/342 (92%)	305 (97%)	10 (3%)	39	65
All	All	1903/1991 (96%)	1859 (98%)	44 (2%)	50	75

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	158	SER
1	A	172	TYR
1	A	179	THR
1	A	324	VAL
1	A	372	GLN
1	A	381	THR
2	B	24	ILE
2	B	137	HIS
2	B	190	HIS
2	B	284	LEU
2	B	382	SER
2	B	413	SER
1	C	71	GLU
1	C	165	SER
1	C	179	THR
1	C	221	ARG
1	C	232	SER
1	C	251	ASP
1	C	384	ILE
2	D	2	ARG
2	D	26	ASP
2	D	48	ASN
2	D	95	SER
2	D	115	SER
2	D	143	THR
2	D	284	LEU
2	D	291	GLN
2	D	305	PRO
2	D	323	MET
2	D	355	ASP
2	D	386	THR
3	E	19	SER
3	E	24	LEU
4	F	12	SER
4	F	87	LEU
4	F	90	SER
4	F	152	SER
4	F	183	GLN
4	F	191	LEU
4	F	193	GLU
4	F	244	CYS

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Mol	Chain	Res	Type
4	F	277	THR
4	F	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	35	GLN
1	A	61	HIS
1	A	266	HIS
1	A	285	GLN
2	B	165	ASN
1	C	133	GLN
1	C	309	HIS
2	D	99	ASN
2	D	134	GLN
2	D	137	HIS
2	D	347	ASN
3	E	12	ASN
4	F	242	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
11	KB4	B	506	-	26,27,27	2.56	7 (26%)	32,39,39	2.16	7 (21%)
5	GTP	D	501	8	26,34,34	0.92	1 (3%)	32,54,54	0.82	0
12	ACP	F	401	-	27,33,33	2.14	8 (29%)	32,52,52	1.49	5 (15%)
11	KB4	D	503	-	26,27,27	2.47	9 (34%)	32,39,39	2.12	7 (21%)
5	GTP	A	501	8	26,34,34	0.93	1 (3%)	32,54,54	0.85	0
9	GDP	B	501	8	24,30,30	1.32	3 (12%)	30,47,47	1.29	4 (13%)
10	MES	B	504	-	12,12,12	0.79	0	14,16,16	0.82	0
5	GTP	C	501	8	26,34,34	0.95	1 (3%)	32,54,54	0.80	1 (3%)
10	MES	B	505	-	12,12,12	0.69	0	14,16,16	0.61	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
11	KB4	B	506	-	-	2/5/18/18	0/4/4/4
5	GTP	D	501	8	-	7/18/38/38	0/3/3/3
12	ACP	F	401	-	-	3/15/38/38	0/3/3/3
11	KB4	D	503	-	-	2/5/18/18	0/4/4/4
5	GTP	A	501	8	-	6/18/38/38	0/3/3/3
9	GDP	B	501	8	-	3/12/32/32	0/3/3/3
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
5	GTP	C	501	8	-	6/18/38/38	0/3/3/3
10	MES	B	505	-	-	0/6/14/14	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	KB4	C16-N15	8.01	1.44	1.35
11	B	506	KB4	C16-N15	7.52	1.43	1.35
12	F	401	ACP	PG-O1G	5.89	1.62	1.50
12	F	401	ACP	PB-O1B	4.73	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	506	KB4	C14-N15	4.70	1.47	1.39
11	B	506	KB4	C05-C04	-4.69	1.35	1.42
11	D	503	KB4	C14-N15	3.89	1.46	1.39
11	B	506	KB4	C14-C13	-3.87	1.36	1.40
11	B	506	KB4	C18-N12	-3.78	1.42	1.46
12	F	401	ACP	PB-O3A	3.71	1.62	1.58
12	F	401	ACP	PB-O2B	-3.56	1.48	1.56
11	D	503	KB4	C18-N12	-3.49	1.42	1.46
9	B	501	GDP	O4'-C1'	3.48	1.45	1.41
11	D	503	KB4	C13-N12	3.46	1.46	1.40
11	D	503	KB4	C18-C16	3.46	1.55	1.51
11	D	503	KB4	C05-C04	-3.32	1.37	1.42
11	B	506	KB4	C18-C16	3.12	1.55	1.51
12	F	401	ACP	PG-O3G	2.85	1.61	1.54
11	D	503	KB4	O17-C16	-2.79	1.17	1.23
12	F	401	ACP	C5-C4	2.76	1.48	1.40
9	B	501	GDP	C6-N1	-2.69	1.33	1.37
5	A	501	GTP	C5-C6	-2.60	1.42	1.47
11	B	506	KB4	O17-C16	-2.58	1.18	1.23
5	D	501	GTP	C5-C6	-2.55	1.42	1.47
9	B	501	GDP	C2'-C1'	-2.48	1.50	1.53
11	D	503	KB4	C14-C13	-2.46	1.37	1.40
5	C	501	GTP	C5-C6	-2.43	1.42	1.47
12	F	401	ACP	PG-O2G	-2.32	1.49	1.54
11	D	503	KB4	C07-N12	2.26	1.44	1.39
12	F	401	ACP	C2-N3	2.19	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	506	KB4	N10-C09-N08	-7.86	122.70	130.62
11	D	503	KB4	N10-C09-N08	-6.79	123.78	130.62
11	B	506	KB4	CL11-C09-N10	5.72	120.58	115.70
11	D	503	KB4	CL11-C09-N10	4.30	119.37	115.70
11	D	503	KB4	C14-N15-C16	-4.04	119.50	124.49
11	D	503	KB4	C09-N08-C07	3.71	122.05	111.04
12	F	401	ACP	C3'-C2'-C1'	3.67	106.50	100.98
11	D	503	KB4	C05-C07-N08	-3.61	117.81	120.81
12	F	401	ACP	N3-C2-N1	-3.33	123.47	128.68
9	B	501	GDP	O6-C6-C5	-3.19	118.15	124.37
9	B	501	GDP	O6-C6-N1	3.11	124.32	120.65
11	B	506	KB4	C14-N15-C16	-3.10	120.66	124.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	506	KB4	C09-N08-C07	3.09	120.20	111.04
11	D	503	KB4	C02-C03-C04	-2.79	116.07	120.08
12	F	401	ACP	O1G-PG-C3B	-2.74	105.34	111.24
12	F	401	ACP	PB-O3A-PA	-2.50	124.65	132.56
11	B	506	KB4	C01-N06-C05	2.47	120.38	117.30
11	B	506	KB4	C18-C16-N15	-2.37	113.18	116.13
9	B	501	GDP	PA-O3A-PB	-2.36	124.73	132.83
11	B	506	KB4	O17-C16-N15	2.28	123.44	121.43
5	C	501	GTP	O6-C6-C5	2.23	128.72	124.37
11	D	503	KB4	C01-N06-C05	2.12	119.94	117.30
12	F	401	ACP	C4-C5-N7	-2.04	107.28	109.40
9	B	501	GDP	C5-C6-N1	2.02	117.51	113.95

There are no chirality outliers.

All (30) 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	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
10	B	504	MES	C8-C7-N4-C5
11	D	503	KB4	C05-C07-N12-C18
11	B	506	KB4	C05-C07-N12-C18
5	D	501	GTP	PB-O3B-PG-O1G
11	B	506	KB4	N08-C07-N12-C18
12	F	401	ACP	C3'-C4'-C5'-O5'
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
11	D	503	KB4	N08-C07-N12-C18
12	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
12	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	D	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PG-O3B-PB-O2B

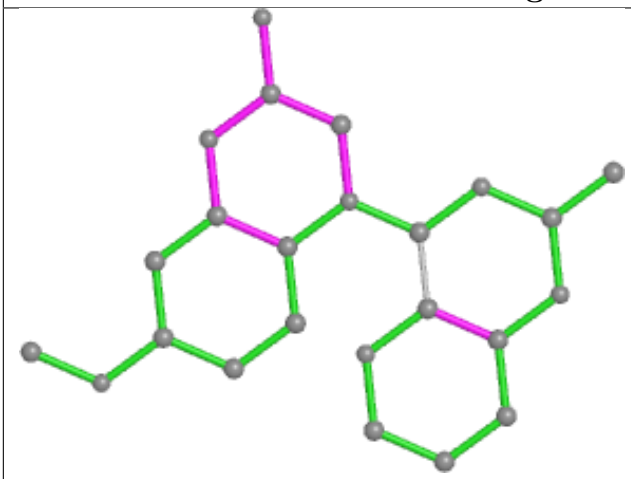
There are no ring outliers.

3 monomers are involved in 6 short contacts:

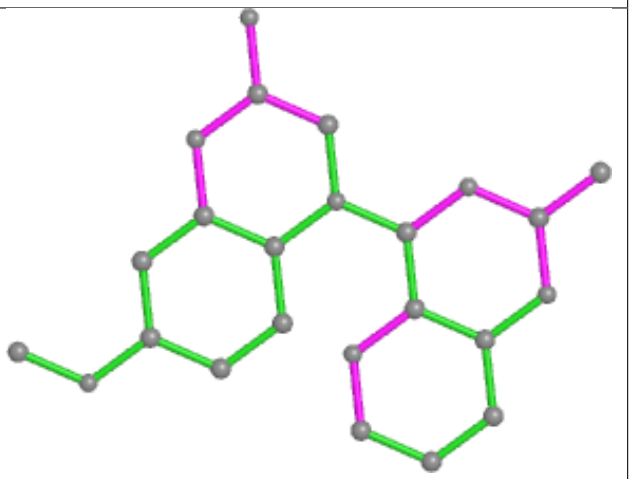
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	2	0
11	D	503	KB4	2	0
10	B	504	MES	2	0

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.

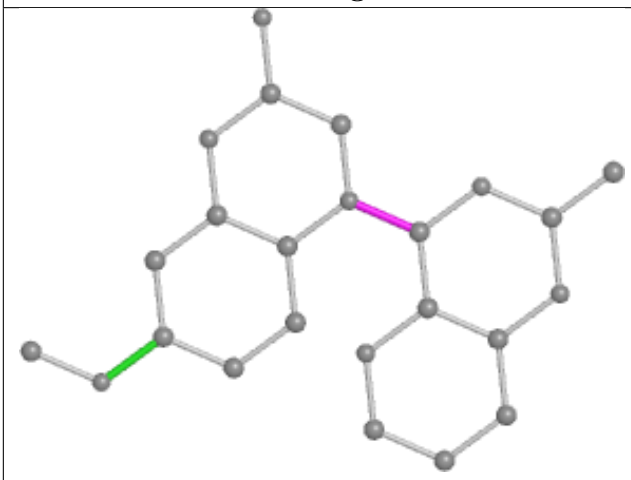
Ligand KB4 B 506



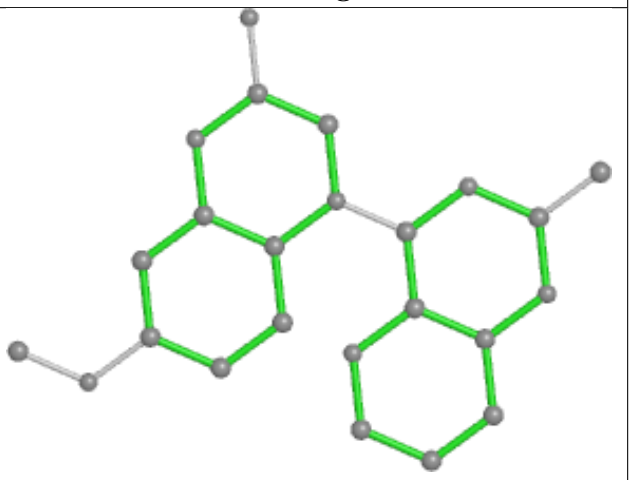
Bond lengths



Bond angles

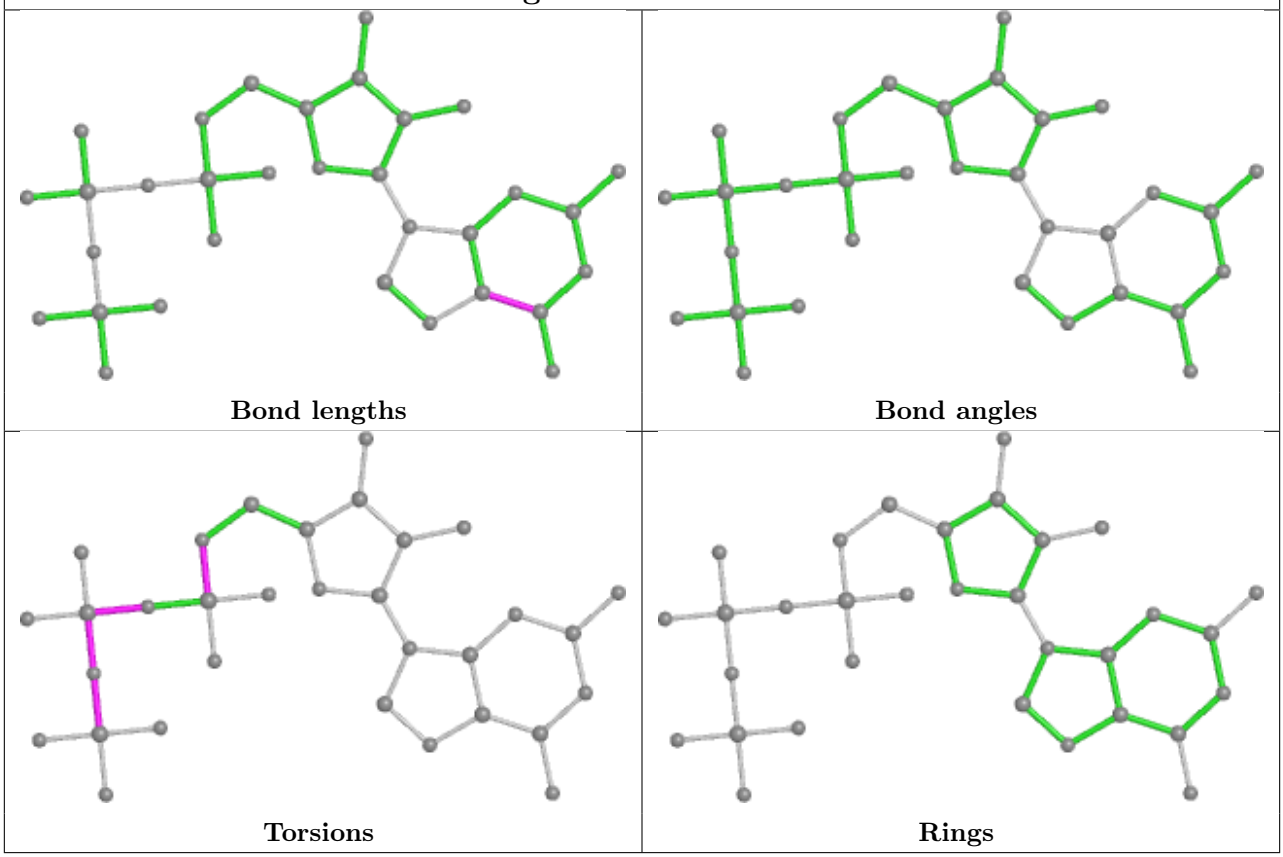


Torsions

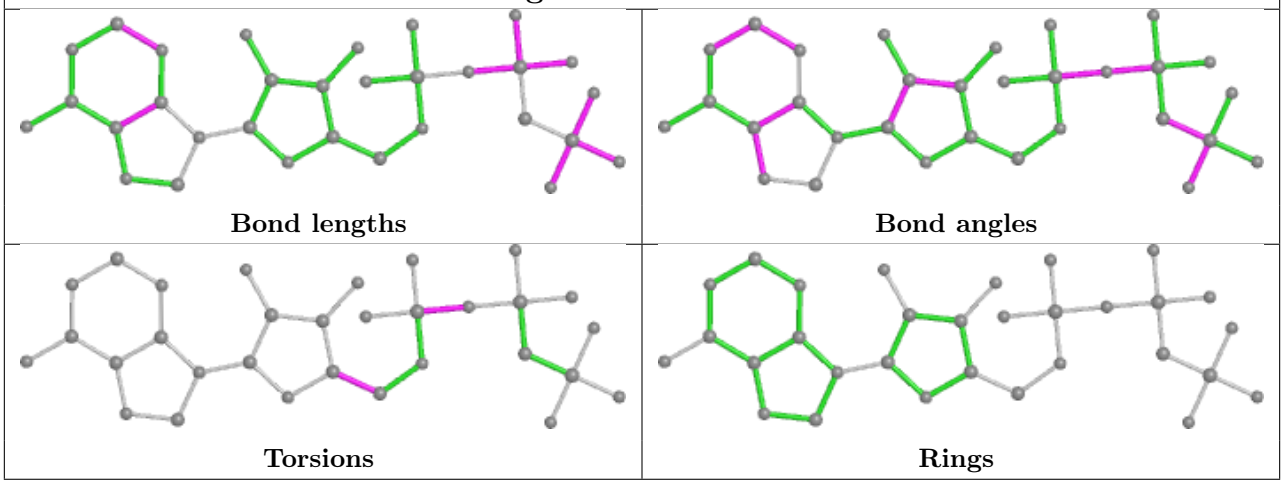


Rings

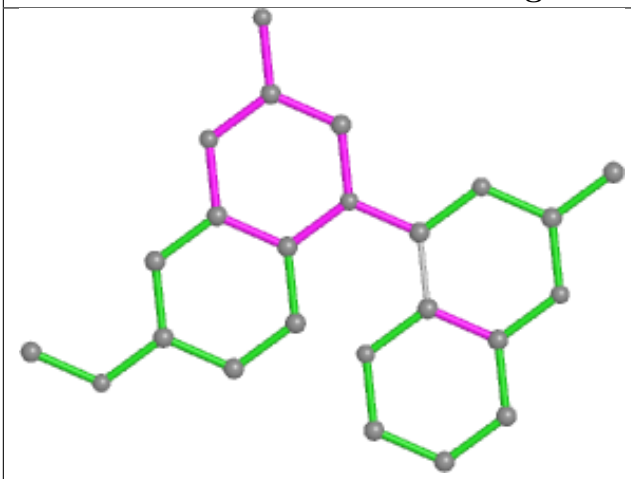
Ligand GTP D 501



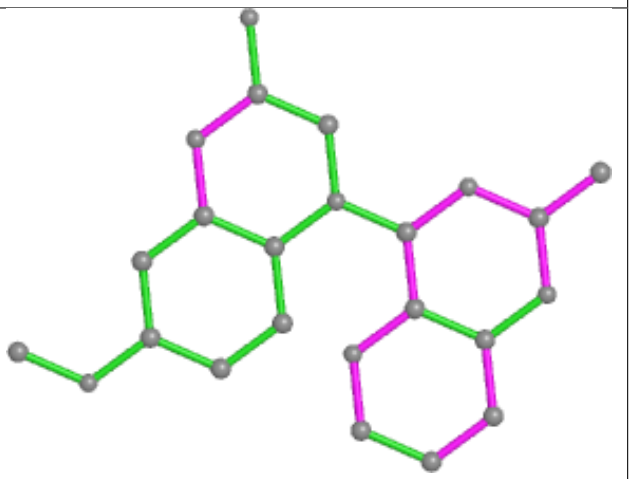
Ligand ACP F 401



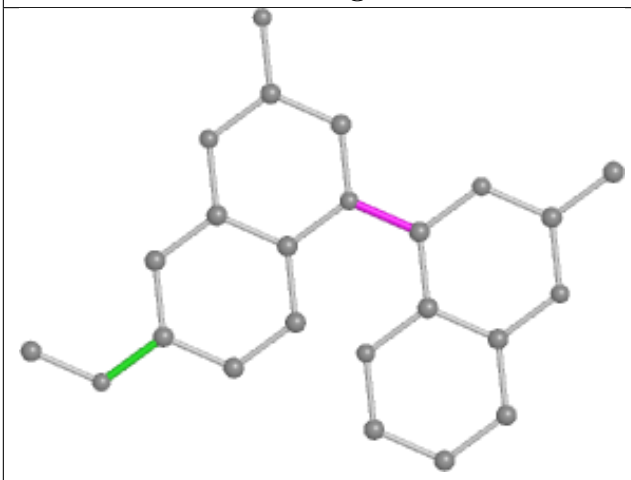
Ligand KB4 D 503



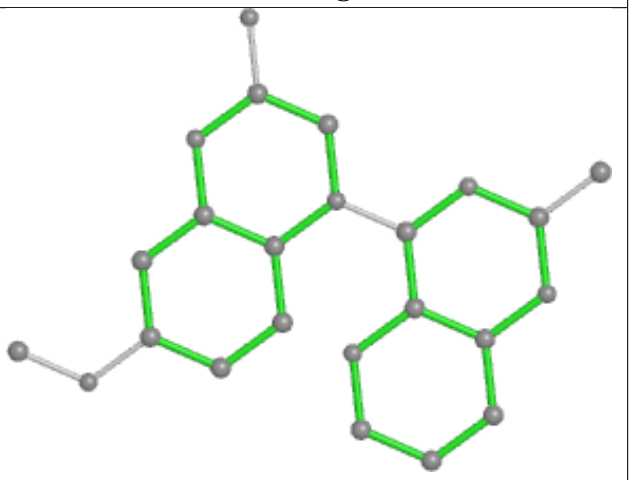
Bond lengths



Bond angles

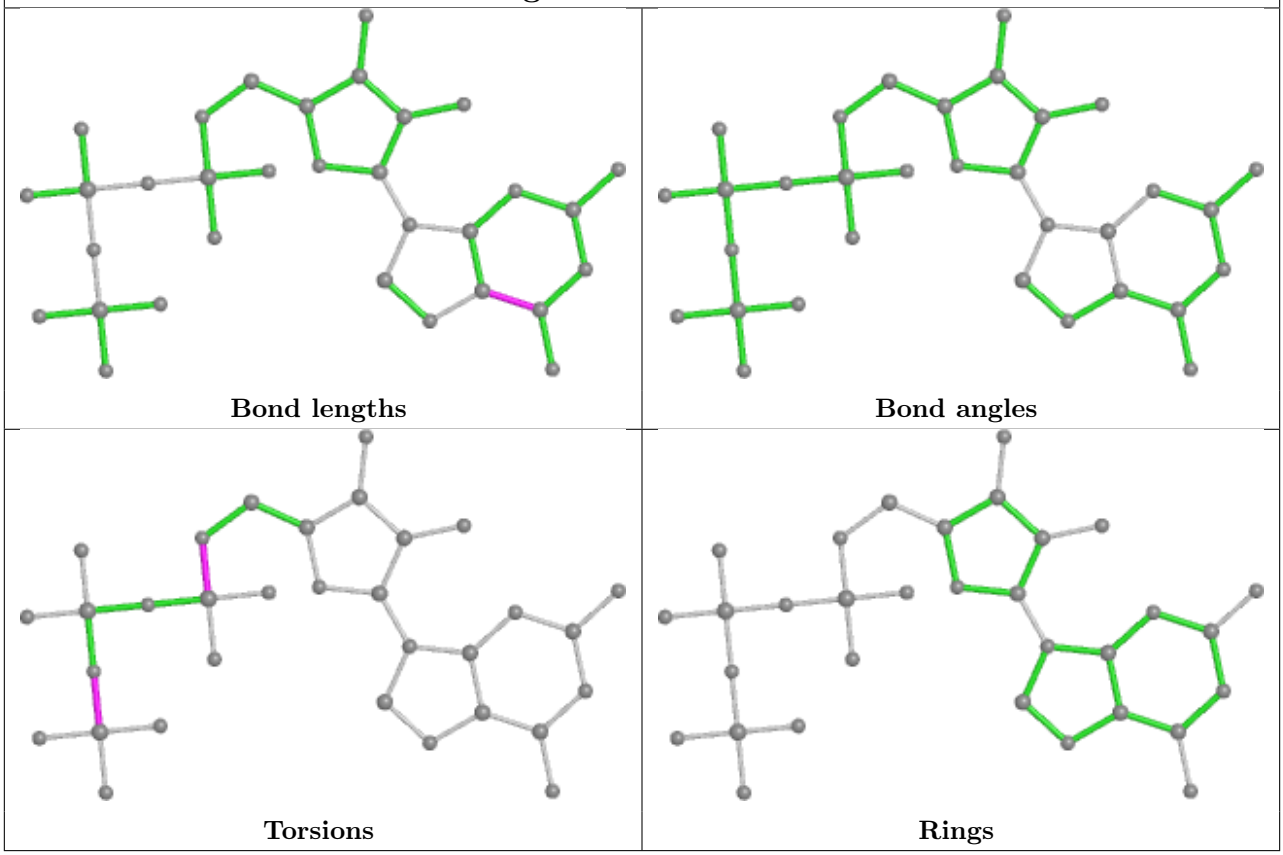


Torsions

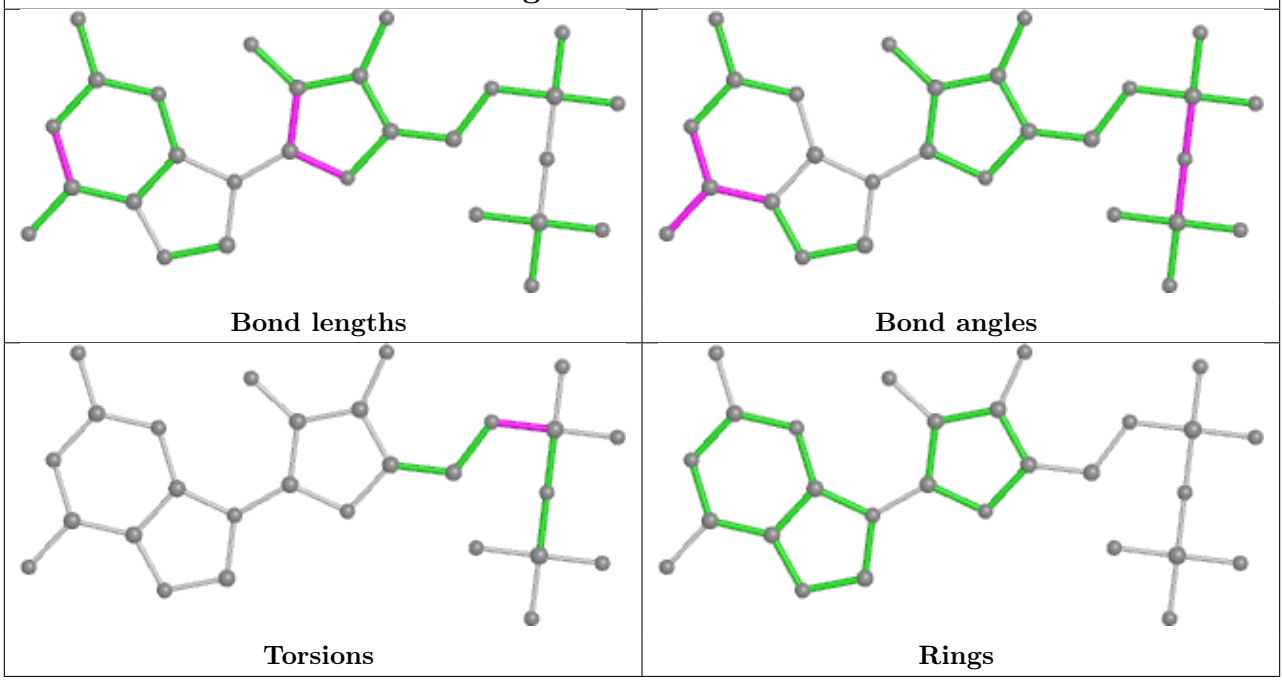


Rings

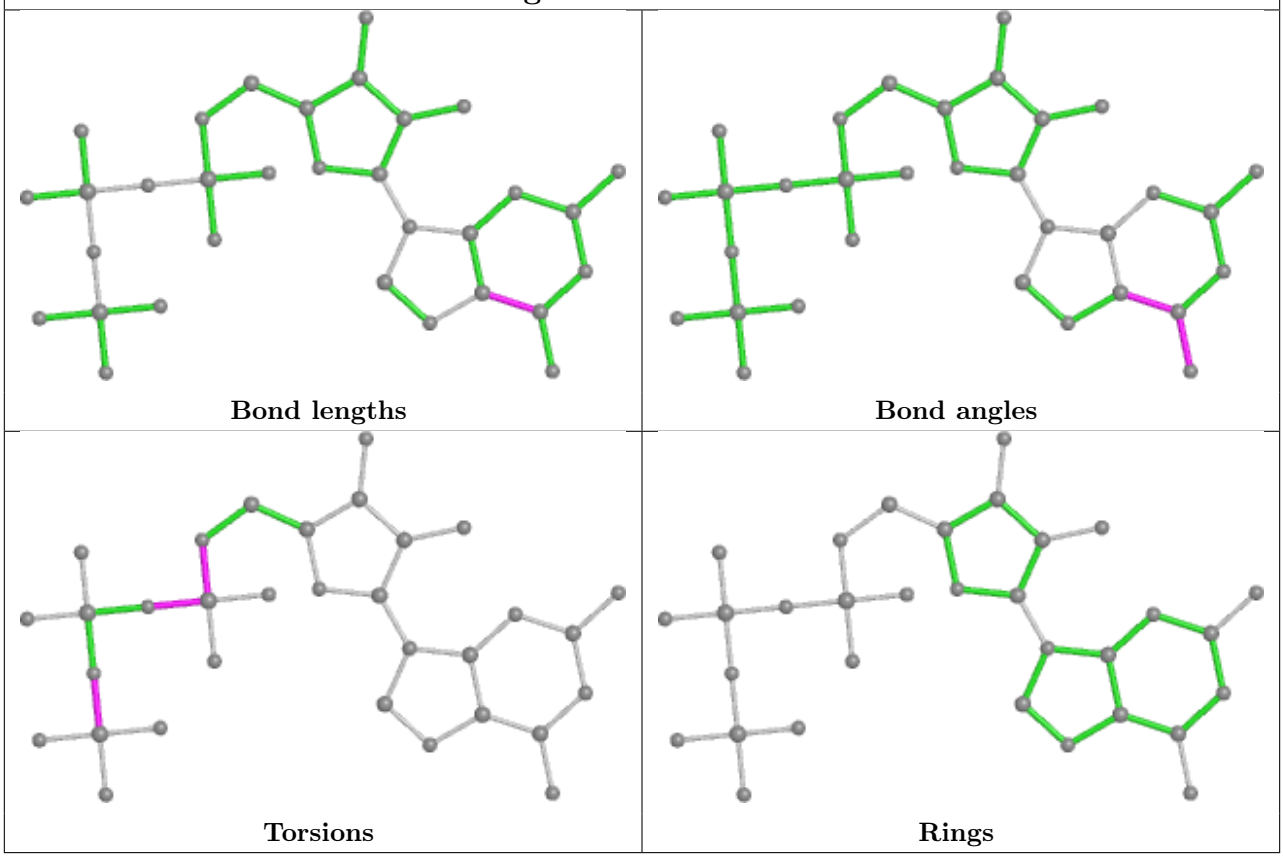
Ligand GTP A 501



Ligand GDP B 501



Ligand GTP C 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	437/450 (97%)	-0.18	5 (1%)	80	78	17, 38, 66, 92	0
1	C	441/450 (98%)	-0.41	1 (0%)	95	95	14, 28, 54, 99	1 (0%)
2	B	428/445 (96%)	-0.17	7 (1%)	72	68	17, 35, 76, 106	2 (0%)
2	D	421/445 (94%)	0.19	17 (4%)	38	31	24, 55, 94, 125	3 (0%)
3	E	124/143 (86%)	0.25	8 (6%)	18	14	28, 53, 99, 120	0
4	F	350/384 (91%)	0.73	62 (17%)	1	0	28, 66, 133, 170	0
All	All	2201/2317 (94%)	0.02	100 (4%)	33	26	14, 43, 97, 170	6 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	251	LYS	10.1
4	F	244	CYS	6.1
4	F	101	TYR	5.7
4	F	142	ARG	5.5
4	F	177	GLY	5.4
4	F	372	THR	5.4
4	F	225	SER	5.3
4	F	178	GLN	5.1
4	F	175	GLU	5.1
4	F	167	SER	5.0
4	F	253	TYR	4.7
4	F	243	HIS	4.6
4	F	248	GLU	4.5
2	D	55	THR	4.5
4	F	174	ASP	4.3
4	F	102	PRO	4.3
4	F	194	PRO	4.3
2	D	73	MET	4.3
4	F	249	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
4	F	250	SER	4.1
2	D	391	ARG	4.1
3	E	142	GLU	4.1
4	F	252	ASN	3.9
3	E	43	ARG	3.8
4	F	103	THR	3.8
4	F	137	ARG	3.8
4	F	256	TYR	3.7
4	F	381	HIS	3.7
4	F	125	THR	3.7
2	B	428	ALA	3.6
2	D	37	HIS	3.6
4	F	173	ILE	3.6
4	F	143	GLU	3.5
3	E	139	LEU	3.4
4	F	152	SER	3.4
4	F	362	ALA	3.3
4	F	254	GLY	3.3
4	F	133	ALA	3.2
4	F	170	LEU	3.2
2	D	72	THR	3.2
2	D	390	ARG	3.2
4	F	139	ARG	3.2
4	F	100	ILE	3.1
4	F	140	GLU	3.1
2	D	93	GLY	3.0
2	B	279	GLN	3.0
2	B	37	HIS	3.0
2	D	92	PHE	3.0
4	F	169	LEU	3.0
4	F	260	ASN	2.9
4	F	247	LYS	2.9
4	F	255	ARG	2.9
4	F	179	VAL	2.9
4	F	164	SER	2.9
2	D	54	ALA	2.9
4	F	233	PHE	2.8
4	F	161	LEU	2.8
4	F	136	ASN	2.8
4	F	257	GLU	2.8
3	E	140	LYS	2.7
2	D	405	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	427	ASP	2.7
4	F	191	LEU	2.7
2	D	76	VAL	2.7
4	F	165	GLU	2.6
4	F	246	GLN	2.6
2	D	1	MET	2.5
4	F	176	GLN	2.5
3	E	29	PHE	2.5
2	B	57	ASN	2.5
4	F	171	ASP	2.5
4	F	135	TYR	2.5
3	E	28	SER	2.5
2	D	74	ASP	2.4
4	F	245	ILE	2.4
4	F	182	ILE	2.4
4	F	130	VAL	2.4
1	A	262	TYR	2.3
4	F	197	ARG	2.3
4	F	382	HIS	2.3
2	D	83	GLN	2.3
1	C	340	SER	2.3
1	A	282	TYR	2.2
2	D	94	GLN	2.2
4	F	379	HIS	2.2
3	E	138	GLU	2.2
4	F	134	ALA	2.2
2	B	55	THR	2.2
2	D	57	ASN	2.1
4	F	196	HIS	2.1
3	E	48	GLU	2.1
1	A	281	ALA	2.1
4	F	222	ARG	2.1
4	F	223	THR	2.1
2	D	75	SER	2.1
1	A	365	GLY	2.1
1	A	88	HIS	2.1
4	F	9	GLU	2.0
2	B	83	GLN	2.0
4	F	168	GLU	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)

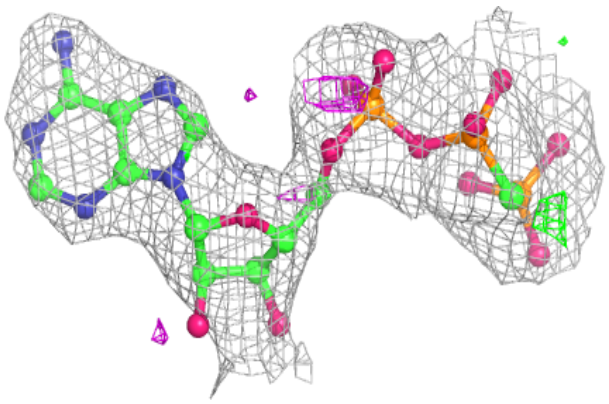
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

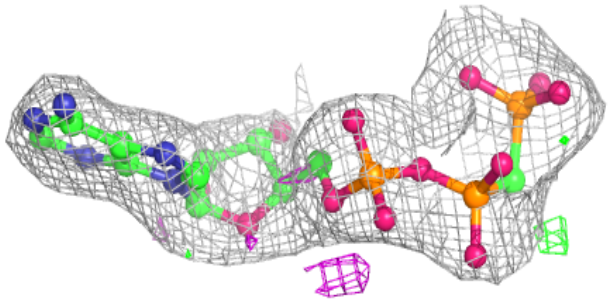
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CL	A	503	1/1	0.79	0.25	74,74,74,74	0
6	CA	E	201	1/1	0.81	0.13	73,73,73,73	0
8	MG	D	502	1/1	0.83	0.08	68,68,68,68	0
12	ACP	F	401	31/31	0.89	0.19	67,80,90,97	0
5	GTP	D	501	32/32	0.93	0.15	44,50,79,86	0
10	MES	B	505	12/12	0.94	0.18	60,67,71,74	0
6	CA	B	503	1/1	0.95	0.07	73,73,73,73	0
10	MES	B	504	12/12	0.95	0.15	43,51,56,59	0
11	KB4	D	503	24/24	0.96	0.16	30,36,50,50	0
8	MG	B	502	1/1	0.96	0.17	24,24,24,24	0
6	CA	A	502	1/1	0.97	0.04	55,55,55,55	0
11	KB4	B	506	24/24	0.98	0.13	24,28,33,35	0
6	CA	C	503	1/1	0.98	0.05	43,43,43,43	0
8	MG	A	504	1/1	0.98	0.07	29,29,29,29	0
8	MG	C	502	1/1	0.99	0.05	22,22,22,22	0
5	GTP	A	501	32/32	0.99	0.14	20,24,26,28	0
9	GDP	B	501	28/28	0.99	0.16	18,21,23,26	0
5	GTP	C	501	32/32	0.99	0.13	18,20,23,24	0

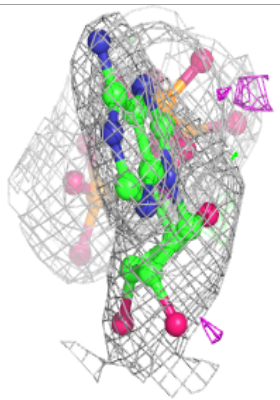
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

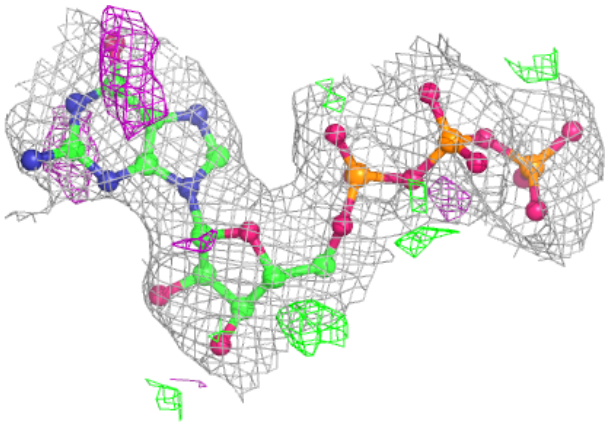


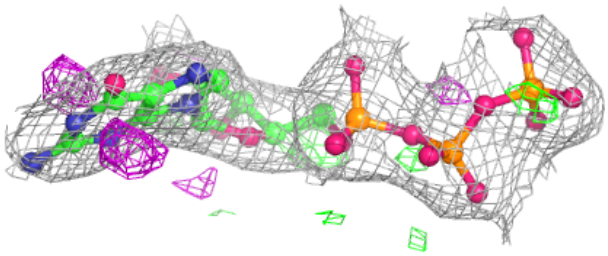


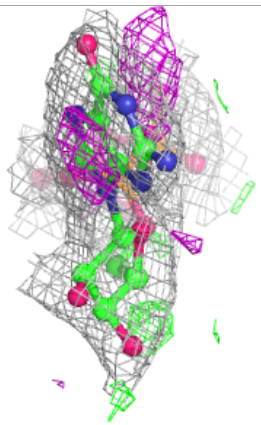


Electron density around GTP D 501:

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

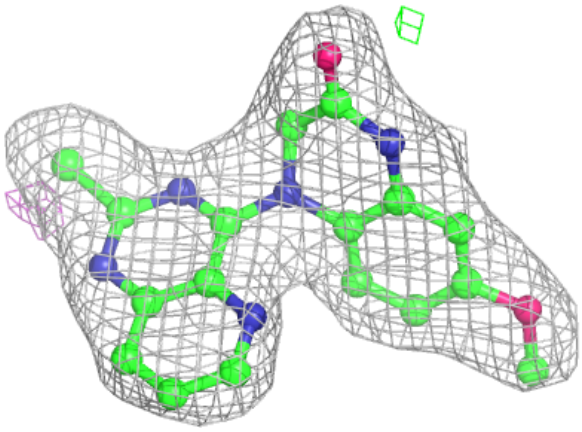


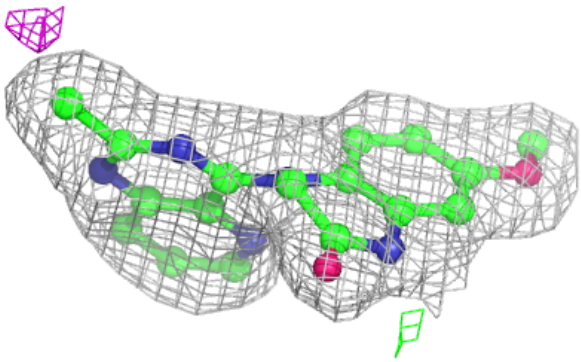


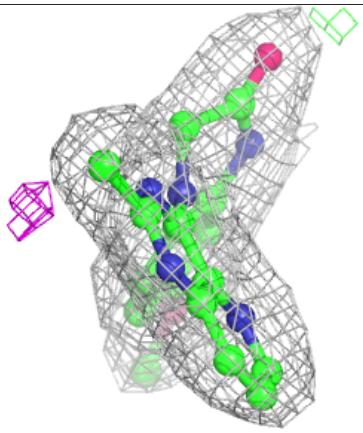


Electron density around KB4 D 503:

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

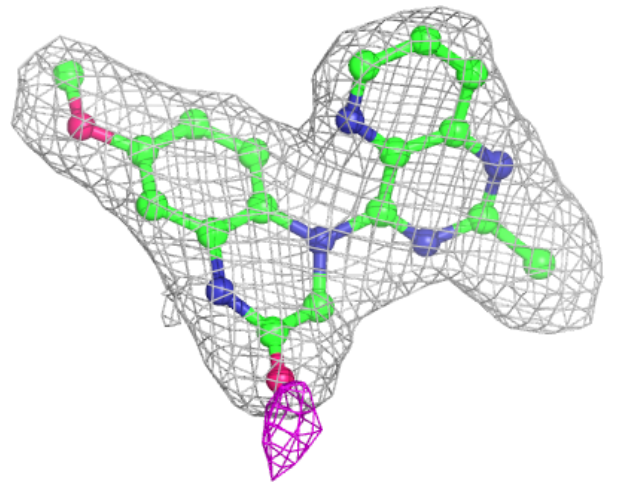


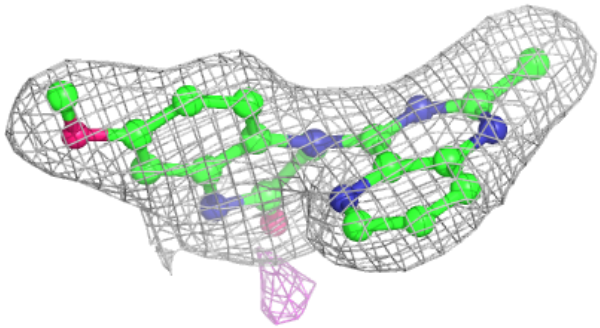


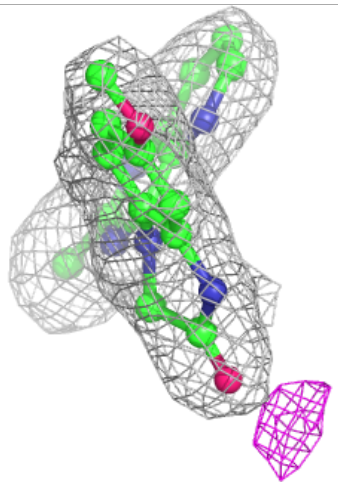


Electron density around KB4 B 506:

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

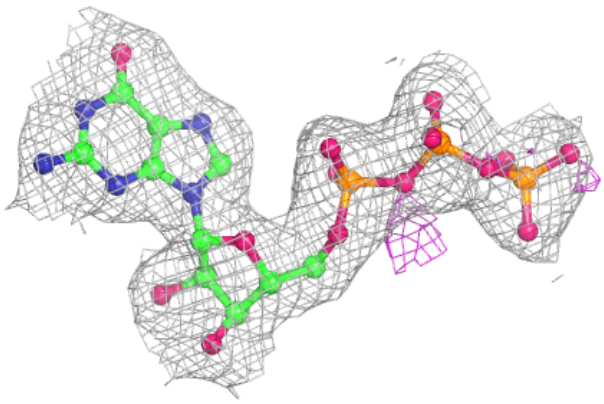


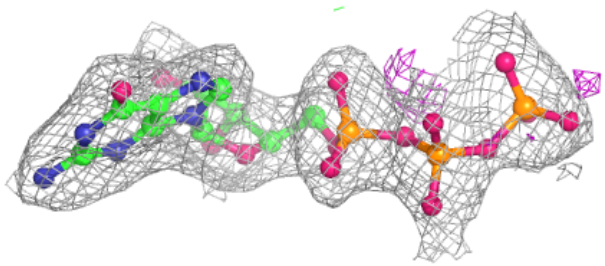


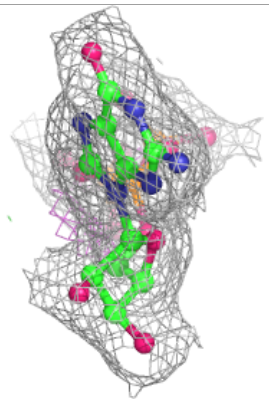


Electron density around GTP A 501:

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

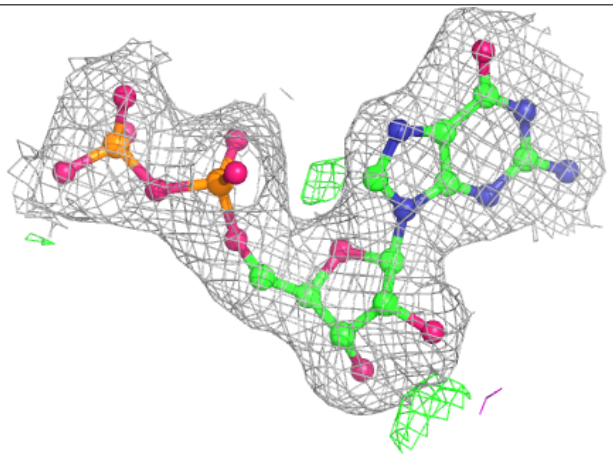


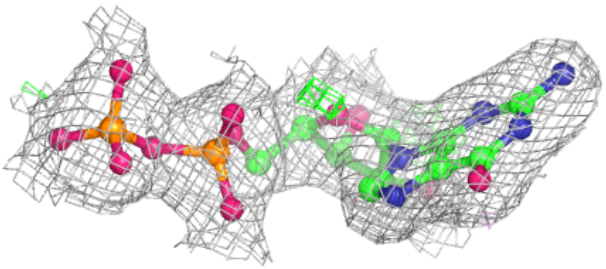


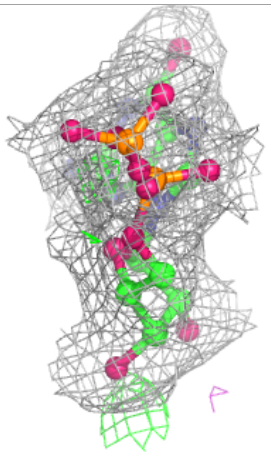


Electron density around GDP B 501:

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

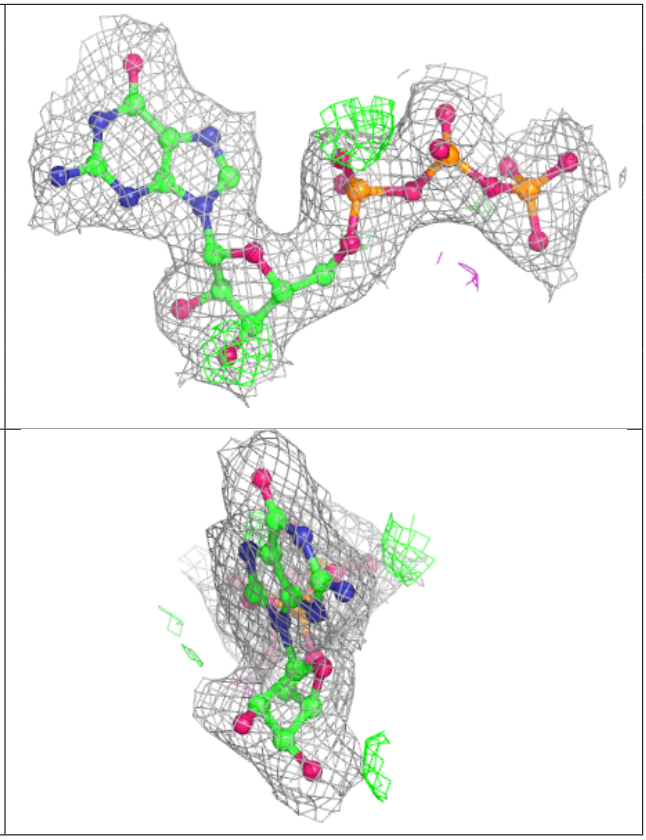






Electron density around GTP C 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.