



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:17 am BST

PDB ID : 6FKL
Title : Tubulin-TUB015 complex
Authors : Prota, A.E.; Steinmetz, M.O.; Priego, E.-M.
Deposited on : 2018-01-24
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

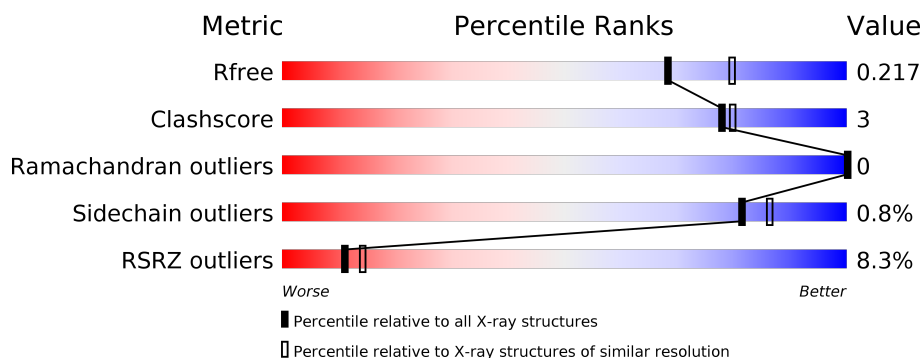
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	C	451	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
2	B	445	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
2	D	445	<div> <div>8%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
3	E	143	<div> <div>9%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>
4	F	384	<div> <div>26%</div> <div>82%</div> <div>9%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DLK	B	507	X	-	-	-
11	DLK	D	503	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18310 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
1	A	439	Total	C	N	O	S	0	8	0
			3463	2196	583	660	24			
1	C	439	Total	C	N	O	S	0	14	0
			3496	2216	592	666	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	4	0
			3363	2114	573	649	27			
2	D	422	Total	C	N	O	S	0	2	0
			3317	2085	563	643	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	3	0
			1022	632	184	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	cloning artifact	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	1	0
			2852	1827	488	523	14			

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		

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

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

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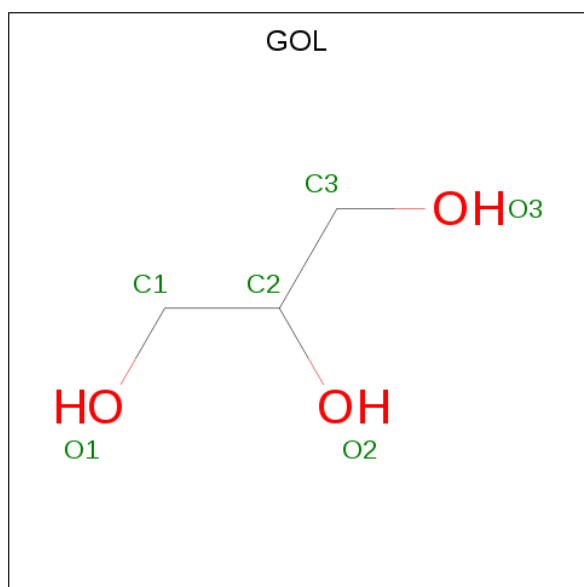
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

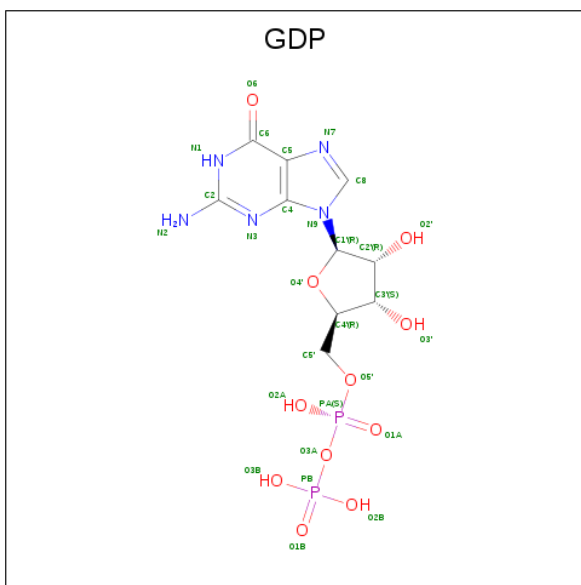
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



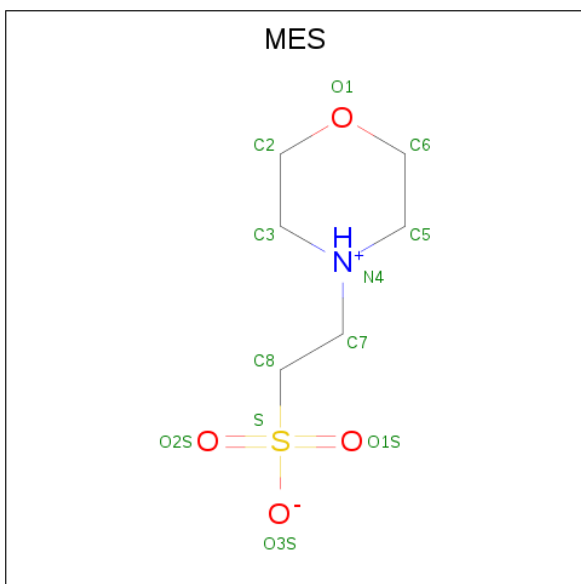
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



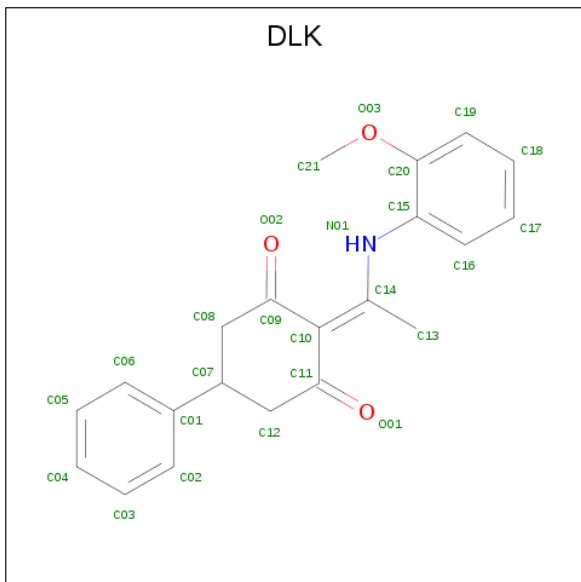
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



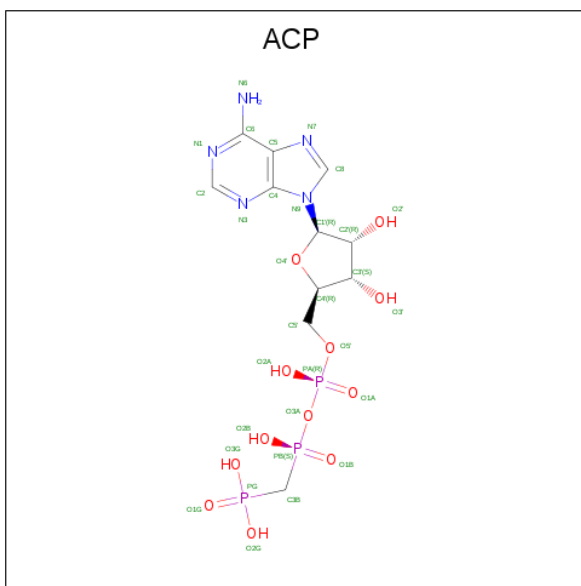
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-{1-[(2-Methoxyphenyl)amino]ethylidene}-5-phenyl-1,3-cyclohexanedione (three-letter code: DLK) (formula: $C_{21}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			25	21	1	3		
11	D	1	Total	C	N	O	0	0
			25	21	1	3		

- 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
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

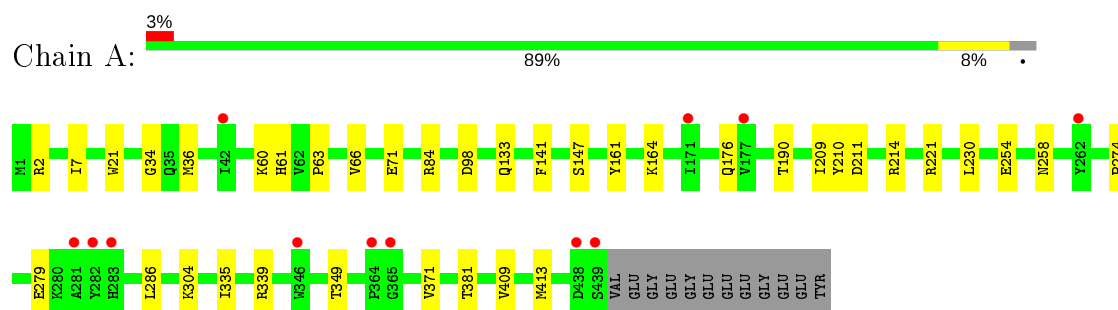
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	125	Total	O	0	0
			125	125		
13	B	120	Total	O	0	0
			120	120		
13	C	212	Total	O	0	0
			212	212		
13	D	53	Total	O	0	0
			53	53		
13	E	20	Total	O	0	0
			20	20		
13	F	32	Total	O	0	0
			32	32		

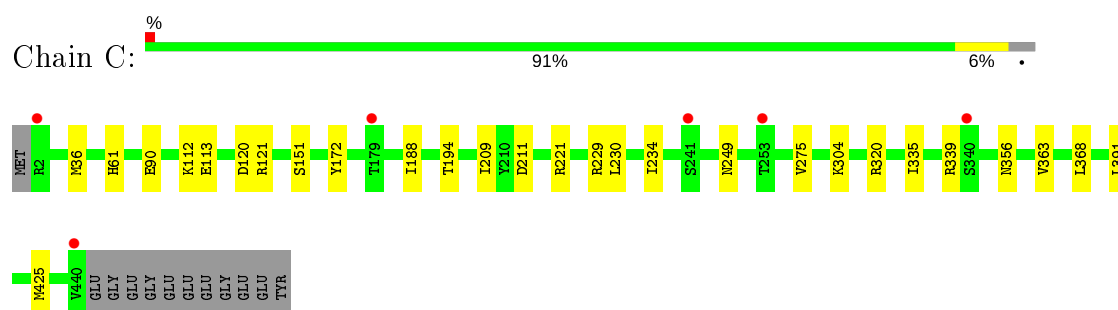
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

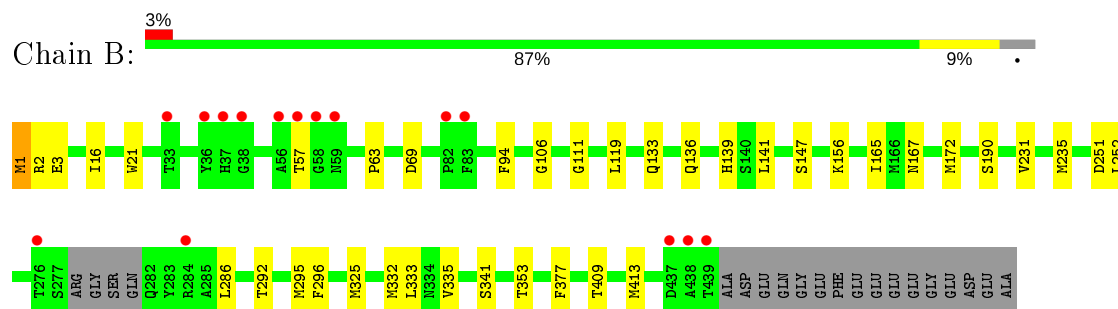
- Molecule 1: Tubulin alpha-1B chain



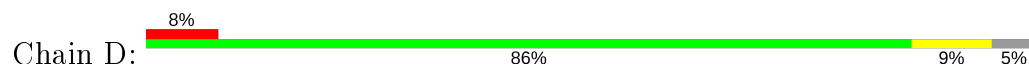
- Molecule 1: Tubulin alpha-1B chain

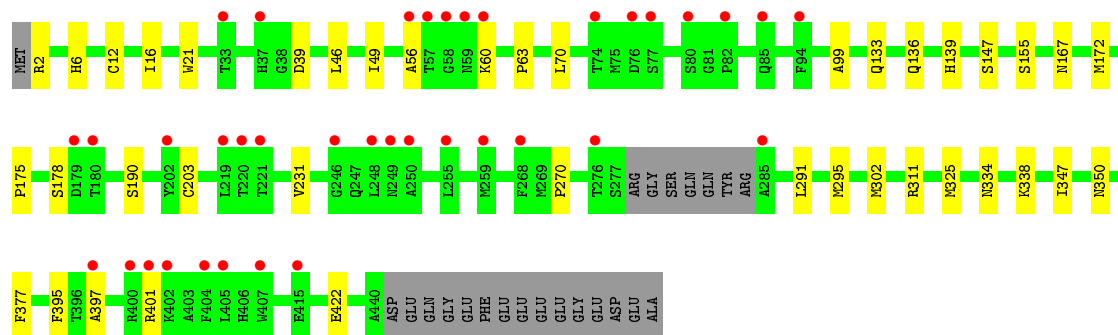


- Molecule 2: Tubulin beta-2B chain

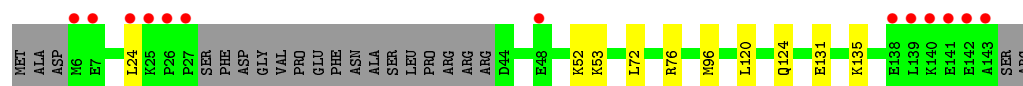
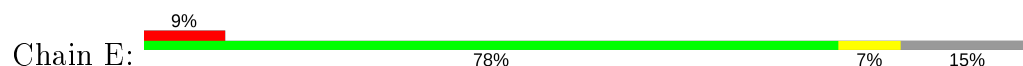


- Molecule 2: Tubulin beta-2B chain

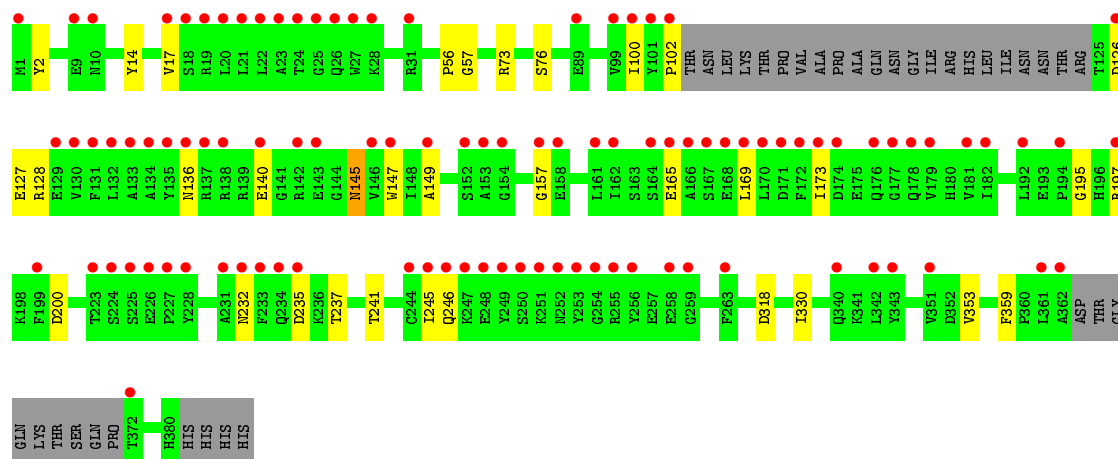
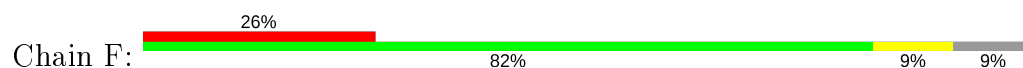




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.75Å 157.76Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 2.10 49.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.44-2.10) 98.4 (49.44-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, R_{free}	0.178 , 0.217 0.178 , 0.217	Depositor DCC
R_{free} test set	8575 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18310	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, DLK, CA, GTP, ACP, 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	0.27	0/3565	0.45	0/4840
1	C	0.29	0/3616	0.46	0/4911
2	B	0.27	0/3449	0.45	0/4670
2	D	0.26	0/3396	0.44	0/4601
3	E	0.25	0/1040	0.37	0/1381
4	F	0.25	0/2920	0.42	0/3944
All	All	0.27	0/17986	0.44	0/24347

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	3463	0	3393	20	0
1	C	3496	0	3436	18	0
2	B	3363	0	3255	20	0
2	D	3317	0	3200	23	0
3	E	1022	0	1043	5	0
4	F	2852	0	2821	21	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
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	12	0	12	0	0
11	B	25	0	0	0	0
11	D	25	0	0	0	0
12	F	31	0	14	2	0
13	A	125	0	0	0	0
13	B	120	0	0	0	0
13	C	212	0	0	1	0
13	D	53	0	0	1	0
13	E	20	0	0	0	0
13	F	32	0	0	1	0
All	All	18310	0	17238	101	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 3.

All (101) 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:D:147[A]:SER:HG	2:D:190:SER:HG	1.39	0.69
1:C:120[B]:ASP:OD2	1:C:121[B]:ARG:NH2	2.24	0.68
2:B:332:MET:HG3	2:B:353:THR:HG21	1.80	0.63
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.80	0.63
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.29	0.62
4:F:145:ASN:HD22	4:F:147:TRP:HE1	1.48	0.61
4:F:318:ASP:OD2	12:F:402:ACP:O3G	2.18	0.60
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.71	0.56
1:A:176:GLN:HG2	4:F:56:PRO:HB3	1.87	0.55
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.71	0.55
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.89	0.54
4:F:232:ASN:ND2	4:F:235:ASP:OD1	2.40	0.54
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.89	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.53
2:B:133:GLN:HG3	2:B:251:ASP:HB2	1.91	0.52
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.91	0.52
4:F:241:THR:OG1	12:F:402:ACP:O3'	2.21	0.52
2:D:147[A]:SER:OG	2:D:190:SER:OG	2.17	0.51
2:D:311:ARG:NH1	13:D:601:HOH:O	2.42	0.51
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.51
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.33	0.51
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.93	0.51
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.45	0.50
4:F:145:ASN:ND2	4:F:147:TRP:HE1	2.09	0.50
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.45	0.50
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.46	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.50
2:D:16:ILE:HD13	2:D:231:VAL:HG11	1.94	0.50
1:C:230:LEU:O	1:C:234:ILE:HD12	2.12	0.50
1:A:349:THR:HG22	3:E:24:LEU:HD12	1.94	0.49
1:C:221:ARG:HG2	2:D:325:MET:HG2	1.94	0.49
2:B:69:ASP:O	2:B:94:PHE:HA	2.12	0.49
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.93	0.48
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.96	0.48
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.94	0.48
2:D:175:PRO:HA	2:D:178:SER:HB2	1.94	0.48
4:F:237:THR:O	4:F:246:GLN:NE2	2.44	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.48
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.49	0.48
4:F:169:LEU:O	4:F:173:ILE:HG12	2.14	0.47
2:B:1:MET:N	2:B:3:GLU:OE1	2.32	0.47
4:F:100:ILE:HG23	4:F:128:ARG:HG3	1.97	0.47
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.79	0.47
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.96	0.47
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.97	0.46
2:D:39:ASP:N	2:D:39:ASP:OD1	2.48	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.46
1:C:221:ARG:HG2	2:D:325:MET:CG	2.45	0.46
2:D:2:ARG:HB3	2:D:133:GLN:NE2	2.31	0.46
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356[B]:ASN:ND2	13:C:605:HOH:O	2.49	0.45
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.51	0.45
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.98	0.45
4:F:157:GLY:HA3	4:F:245:ILE:HD11	1.98	0.45
4:F:149:ALA:HB1	4:F:173:ILE:HD11	1.99	0.45
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG23	2.00	0.44
2:D:397:ALA:O	2:D:401:ARG:HD3	2.17	0.44
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.53	0.44
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.44
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.00	0.44
4:F:14:TYR:HA	4:F:17:VAL:HB	1.99	0.44
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.43
2:D:46:LEU:HA	2:D:49:ILE:HB	2.00	0.43
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.36	0.43
2:B:296:PHE:CG	2:B:335:VAL:HG11	2.54	0.43
2:B:136:GLN:HA	2:B:167:ASN:O	2.17	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.43
2:B:235:MET:HE2	2:B:235:MET:HB3	1.87	0.43
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.43
1:A:221:ARG:HG2	2:B:325:MET:HG2	2.01	0.43
2:D:172:MET:HE2	2:D:203:CYS:HA	2.01	0.42
2:B:119:LEU:HD11	2:B:156:LYS:HB3	2.00	0.42
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.42
1:A:274:PRO:HG2	1:A:371:VAL:HG11	2.02	0.42
2:D:56:ALA:HB3	2:D:60:LYS:HB2	2.01	0.42
4:F:126:ASP:OD1	4:F:127:GLU:N	2.53	0.42
2:B:141:LEU:HD12	2:B:172:MET:SD	2.60	0.42
2:D:295:MET:CG	2:D:377:PHE:HB2	2.49	0.42
2:D:395:PHE:CE1	2:D:422:GLU:HB2	2.54	0.42
2:B:295:MET:CG	2:B:377:PHE:HB2	2.50	0.42
4:F:136:ASN:O	4:F:140:GLU:HG3	2.20	0.42
1:C:90:GLU:O	1:C:121[B]:ARG:HG2	2.20	0.42
3:E:131:GLU:O	3:E:135:LYS:HG2	2.19	0.42
3:E:52:LYS:HG2	3:E:53:LYS:NZ	2.35	0.42
1:C:229:ARG:NE	1:C:363:VAL:HG21	2.35	0.42
4:F:102:PRO:O	13:F:501:HOH:O	2.22	0.41
4:F:330:ILE:HA	4:F:330:ILE:HD13	1.91	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.41
4:F:73:ARG:HB2	4:F:76:SER:OG	2.21	0.41
2:B:409:THR:HA	2:B:413:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.57	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.40
4:F:195:GLY:HA3	4:F:197:ARG:HD3	2.01	0.40
3:E:120:LEU:O	3:E:124:GLN:HG3	2.22	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.03	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	445/451 (99%)	439 (99%)	6 (1%)	0	100	100
1	C	450/451 (100%)	439 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	420/445 (94%)	413 (98%)	7 (2%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	333 (97%)	11 (3%)	0	100	100
All	All	2205/2319 (95%)	2161 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	378/379 (100%)	375 (99%)	3 (1%)	81	86
1	C	384/379 (101%)	384 (100%)	0	100	100
2	B	372/383 (97%)	366 (98%)	6 (2%)	62	69
2	D	366/383 (96%)	362 (99%)	4 (1%)	73	79
3	E	112/127 (88%)	111 (99%)	1 (1%)	78	84
4	F	312/342 (91%)	309 (99%)	3 (1%)	76	82
All	All	1924/1993 (96%)	1907 (99%)	17 (1%)	81	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	279	GLU
1	A	381	THR
2	B	1	MET
2	B	2	ARG
2	B	57	THR
2	B	139	HIS
2	B	286	LEU
2	B	341	SER
2	D	139	HIS
2	D	155[A]	SER
2	D	155[B]	SER
2	D	291	LEU
3	E	96	MET
4	F	145	ASN
4	F	165	GLU
4	F	353	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
2	D	294	GLN
4	F	145	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	DLK	B	507	-	27,27,27	1.60	4 (14%)	37,37,37	1.97	10 (27%)
8	GOL	A	505	-	5,5,5	0.88	0	5,5,5	1.04	0
9	GDP	D	501	6	24,30,30	1.21	2 (8%)	31,47,47	1.91	7 (22%)
9	GDP	B	501	6	24,30,30	1.16	2 (8%)	31,47,47	1.93	7 (22%)
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.71	6 (18%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.71	7 (21%)
10	MES	B	506	-	12,12,12	2.23	1 (8%)	14,16,16	2.11	7 (50%)
12	ACP	F	402	6	27,33,33	1.68	6 (22%)	32,52,52	1.32	4 (12%)
8	GOL	B	505	-	5,5,5	1.04	0	5,5,5	0.87	0
11	DLK	D	503	-	27,27,27	1.66	4 (14%)	37,37,37	2.03	11 (29%)

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	DLK	B	507	-	1/1/5/6	4/14/30/30	0/3/3/3
8	GOL	A	505	-	-	4/4/4/4	-
9	GDP	D	501	6	-	5/12/32/32	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
10	MES	B	506	-	-	1/6/14/14	0/1/1/1
12	ACP	F	402	6	-	5/15/38/38	0/3/3/3
8	GOL	B	505	-	-	2/4/4/4	-
11	DLK	D	503	-	1/1/5/6	6/14/30/30	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	506	MES	C8-S	-7.43	1.66	1.77
11	D	503	DLK	O02-C09	6.34	1.35	1.23
11	B	507	DLK	O02-C09	6.05	1.35	1.23
9	D	501	GDP	C6-C5	4.25	1.48	1.41
12	F	402	ACP	PB-O1B	4.10	1.61	1.51
9	B	501	GDP	C6-C5	3.97	1.48	1.41
12	F	402	ACP	PB-O2B	-3.30	1.48	1.56
11	D	503	DLK	C10-C14	3.29	1.48	1.42
5	C	501	GTP	C6-N1	3.23	1.38	1.33
11	B	507	DLK	C10-C09	-3.18	1.38	1.46
11	D	503	DLK	C10-C09	-3.18	1.38	1.46
12	F	402	ACP	PB-O3A	3.16	1.61	1.58
5	A	501	GTP	C6-N1	3.07	1.38	1.33
11	B	507	DLK	C10-C14	3.05	1.48	1.42
12	F	402	ACP	PG-O2G	2.91	1.61	1.54
12	F	402	ACP	PG-O3G	2.76	1.61	1.54
12	F	402	ACP	C5-C4	2.57	1.47	1.40
9	D	501	GDP	C5-C4	2.41	1.47	1.40
9	B	501	GDP	C5-C4	2.15	1.46	1.40
11	B	507	DLK	C14-N01	-2.15	1.29	1.34
11	D	503	DLK	C14-N01	-2.06	1.29	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	503	DLK	C09-C10-C14	7.02	123.72	120.55
11	B	507	DLK	C09-C10-C14	6.41	123.44	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.29	120.17	127.22
5	A	501	GTP	N3-C2-N1	-5.23	120.24	127.22
9	B	501	GDP	C2-N3-C4	4.95	121.02	115.36
9	D	501	GDP	C2-N3-C4	4.91	120.96	115.36
9	B	501	GDP	C6-C5-C4	-4.50	116.51	120.80
11	D	503	DLK	C20-C15-N01	4.38	124.51	116.66
11	D	503	DLK	O03-C20-C15	4.11	119.84	114.80
9	B	501	GDP	C6-N1-C2	4.11	122.45	115.93
9	D	501	GDP	C6-N1-C2	4.10	122.45	115.93
9	D	501	GDP	C5-C6-N1	-4.08	117.86	123.43
10	B	506	MES	C5-N4-C3	3.91	117.64	108.83
5	A	501	GTP	C2-N3-C4	3.91	119.83	115.36
11	B	507	DLK	C20-C15-N01	3.88	123.62	116.66
5	C	501	GTP	C2-N3-C4	3.82	119.72	115.36
9	D	501	GDP	C6-C5-C4	-3.78	117.19	120.80
11	D	503	DLK	C08-C09-C10	3.75	123.83	116.36
11	B	507	DLK	C08-C09-C10	3.72	123.76	116.36
9	B	501	GDP	C5-C6-N1	-3.71	118.35	123.43
9	B	501	GDP	N3-C2-N1	-3.71	122.27	127.22
11	B	507	DLK	O03-C20-C15	3.52	119.11	114.80
9	D	501	GDP	N3-C2-N1	-3.32	122.80	127.22
12	F	402	ACP	PA-O3A-PB	-3.30	122.11	132.56
5	C	501	GTP	C5-C6-N1	-3.25	118.99	123.43
5	A	501	GTP	C5-C6-N1	-3.20	119.06	123.43
12	F	402	ACP	C3'-C2'-C1'	3.11	105.66	100.98
11	D	503	DLK	C11-C10-C14	-3.07	119.16	120.55
11	B	507	DLK	C07-C08-C09	-3.05	106.77	114.14
12	F	402	ACP	N3-C2-N1	-3.04	123.93	128.68
11	B	507	DLK	C11-C10-C14	-3.00	119.19	120.55
9	D	501	GDP	C4-C5-N7	-2.97	106.30	109.40
10	B	506	MES	O2S-S-C8	2.90	110.41	106.92
5	C	501	GTP	C6-N1-C2	2.88	120.50	115.93
5	A	501	GTP	PA-O3A-PB	-2.82	123.14	132.83
9	D	501	GDP	PA-O3A-PB	-2.82	123.15	132.83
11	D	503	DLK	O03-C20-C19	-2.76	119.64	124.37
10	B	506	MES	C7-N4-C5	2.73	118.22	111.23
5	A	501	GTP	C6-N1-C2	2.73	120.27	115.93
10	B	506	MES	C7-N4-C3	2.71	118.16	111.23
12	F	402	ACP	C4-C5-N7	-2.67	106.61	109.40
11	B	507	DLK	O03-C20-C19	-2.66	119.81	124.37
11	B	507	DLK	C07-C12-C11	-2.65	107.72	114.14
5	C	501	GTP	PA-O3A-PB	-2.63	123.79	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	PB-O3B-PG	-2.60	123.89	132.83
5	A	501	GTP	PB-O3B-PG	-2.51	124.20	132.83
9	B	501	GDP	C4-C5-N7	-2.47	106.83	109.40
11	B	507	DLK	O02-C09-C08	-2.45	111.19	120.77
11	D	503	DLK	O02-C09-C08	-2.39	111.40	120.77
10	B	506	MES	O3S-S-C8	2.26	109.43	105.77
10	B	506	MES	C2-C3-N4	-2.24	106.70	110.10
9	B	501	GDP	PA-O3A-PB	-2.14	125.47	132.83
11	D	503	DLK	C07-C08-C09	-2.12	109.00	114.14
11	D	503	DLK	C12-C11-C10	2.12	120.57	116.36
5	A	501	GTP	N2-C2-N1	2.11	120.54	117.25
11	D	503	DLK	C13-C14-C10	-2.06	119.65	122.56
11	B	507	DLK	C13-C14-C10	-2.06	119.66	122.56
10	B	506	MES	C6-O1-C2	2.05	116.75	109.89
11	D	503	DLK	C16-C15-N01	-2.05	117.04	121.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	B	507	DLK	C10
11	D	503	DLK	C10

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	505	GOL	O1-C1-C2-C3
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
11	D	503	DLK	C09-C10-C14-C13
11	D	503	DLK	C09-C10-C14-N01
11	D	503	DLK	C11-C10-C14-N01
11	D	503	DLK	C11-C10-C14-C13
8	A	505	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	B	505	GOL	C1-C2-C3-O3
8	A	505	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O1G
8	B	505	GOL	O2-C2-C3-O3
8	A	505	GOL	O2-C2-C3-O3
9	D	501	GDP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
11	B	507	DLK	C09-C10-C14-C13
10	B	506	MES	C8-C7-N4-C3
11	D	503	DLK	C06-C01-C07-C12
12	F	402	ACP	PG-C3B-PB-O1B
5	A	501	GTP	PB-O3A-PA-O2A
11	B	507	DLK	C06-C01-C07-C12
11	B	507	DLK	C09-C10-C14-N01
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3B-PG-O2G
11	D	503	DLK	C02-C01-C07-C12
12	F	402	ACP	PB-O3A-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
9	D	501	GDP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A
11	B	507	DLK	C02-C01-C07-C12
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA

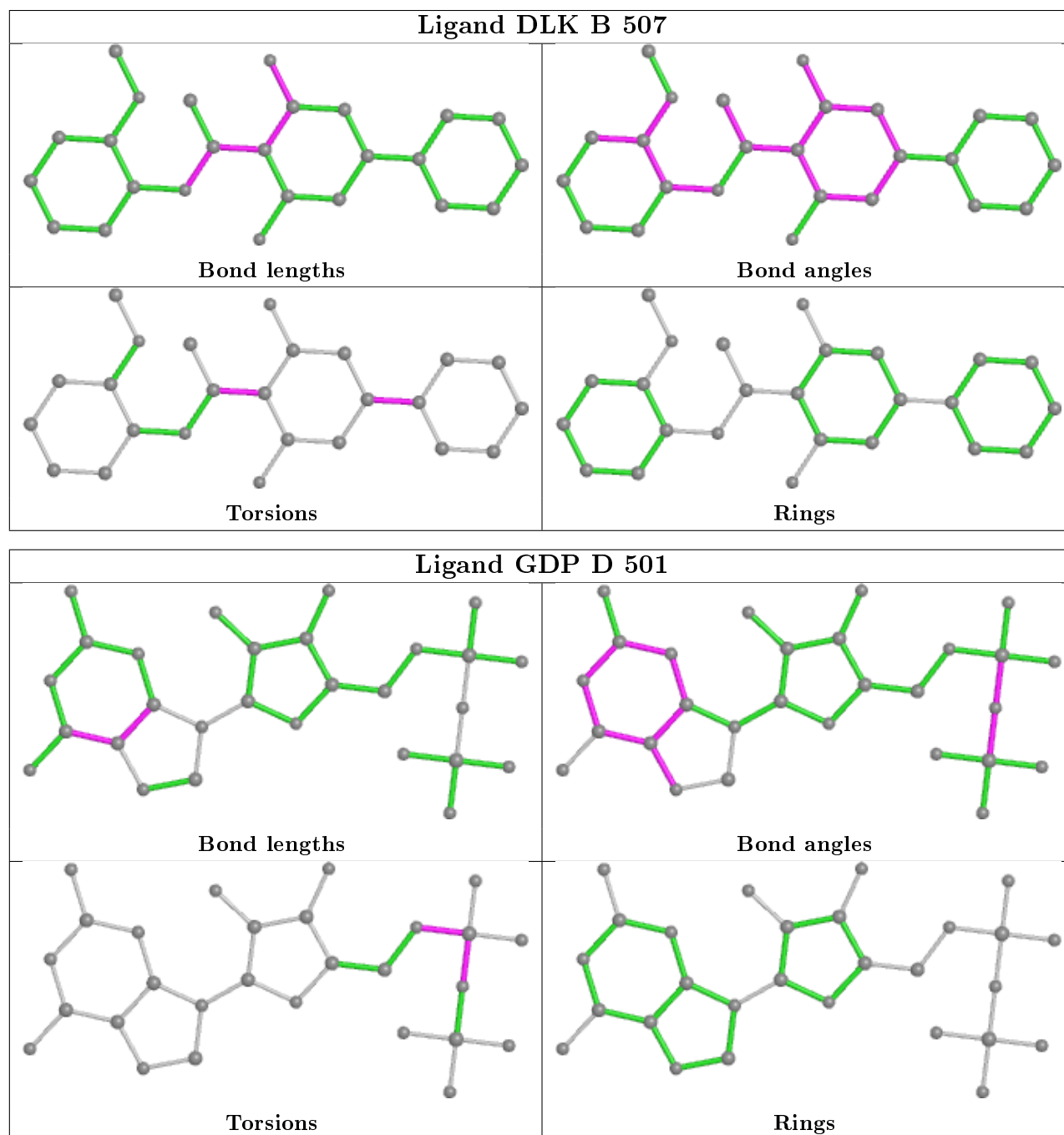
There are no ring outliers.

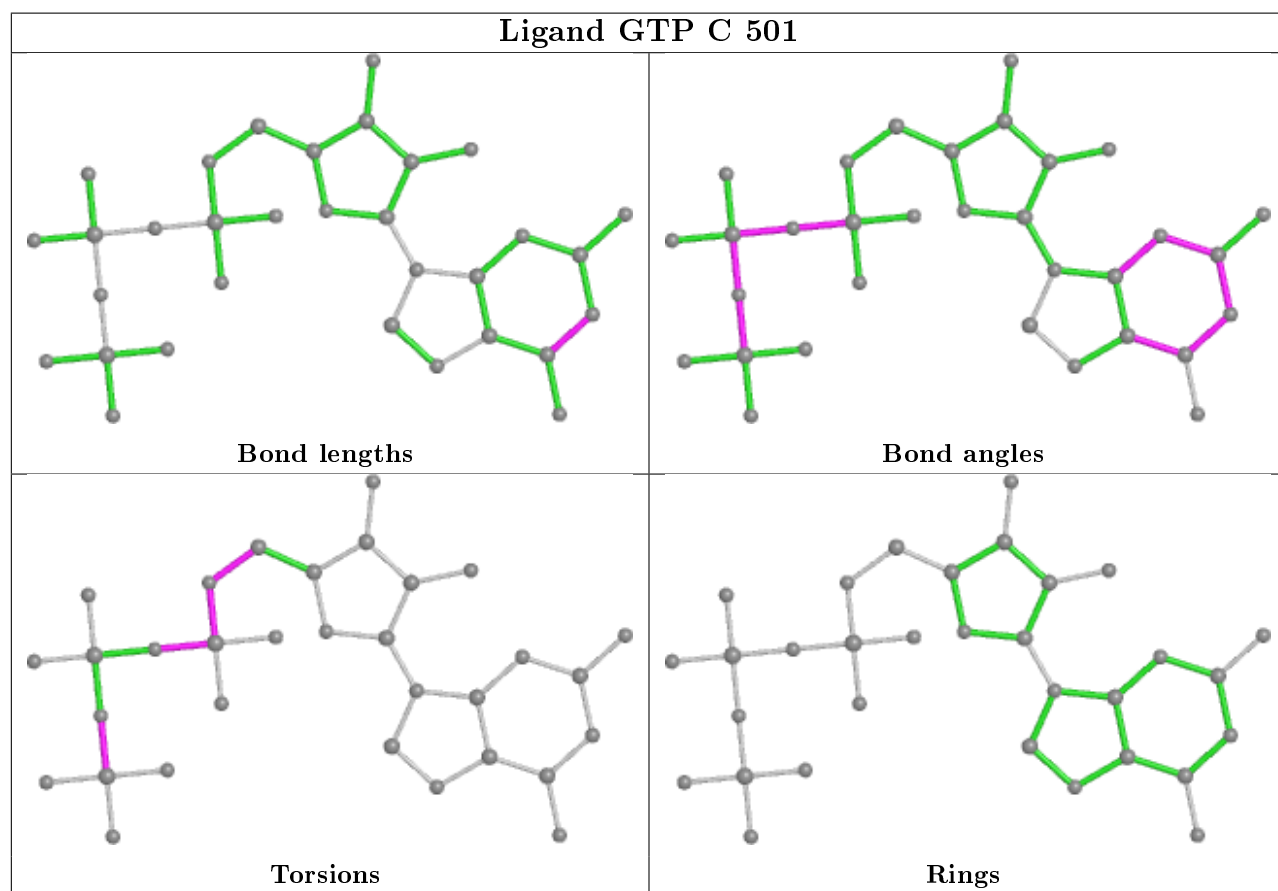
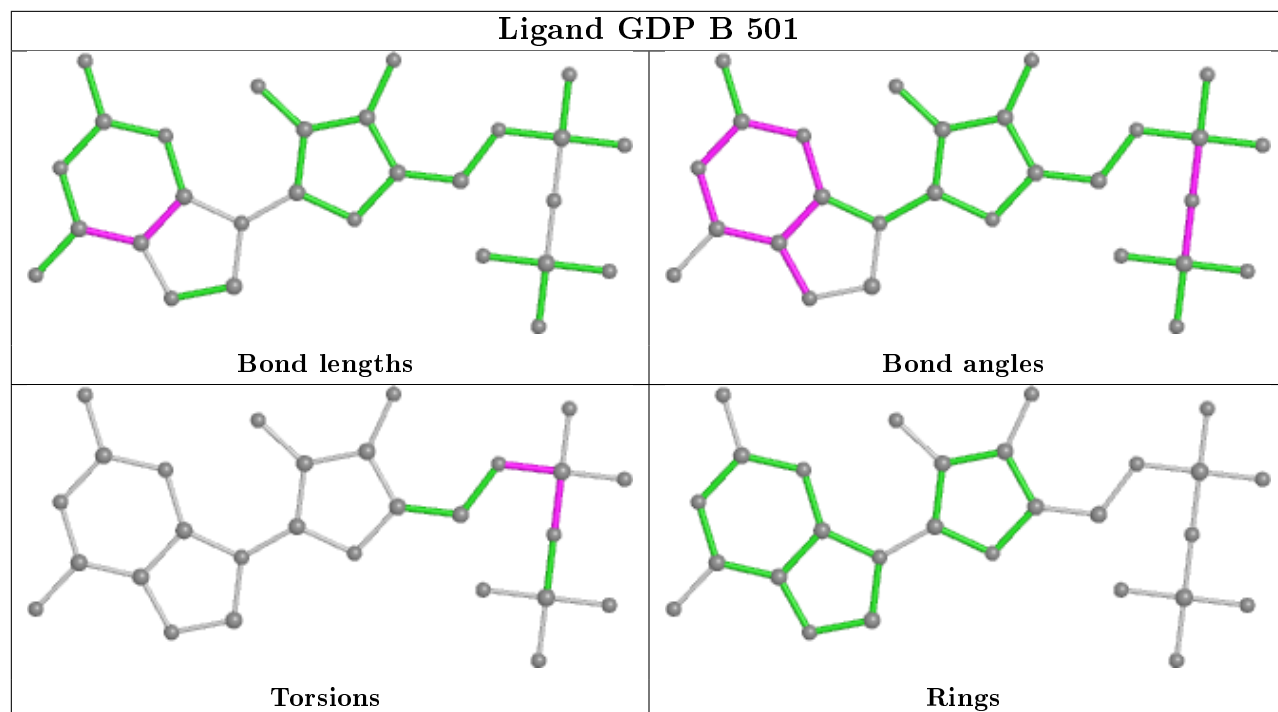
2 monomers are involved in 3 short contacts:

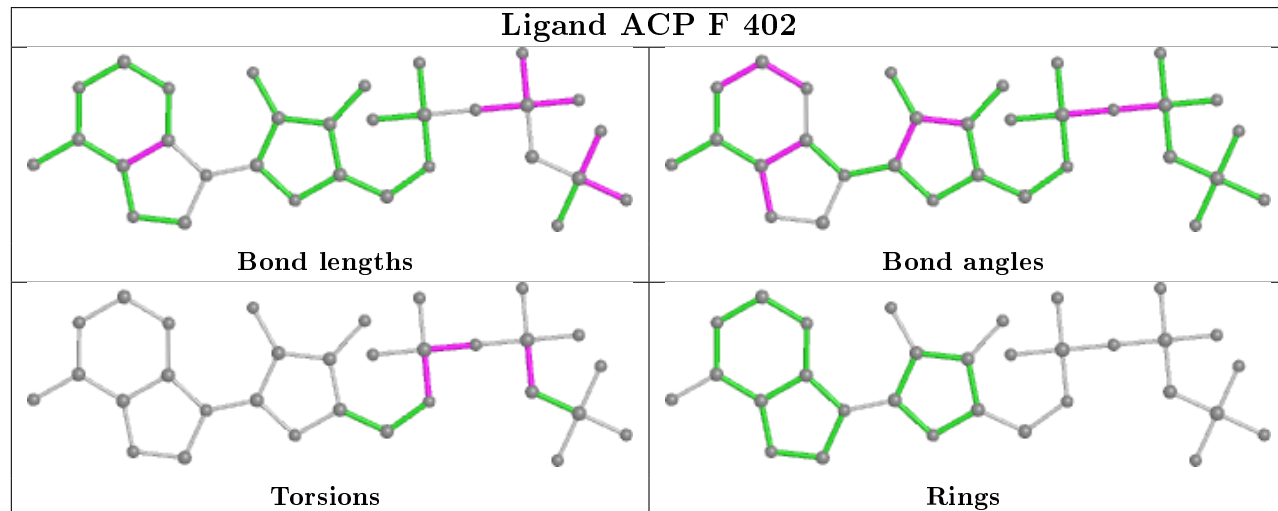
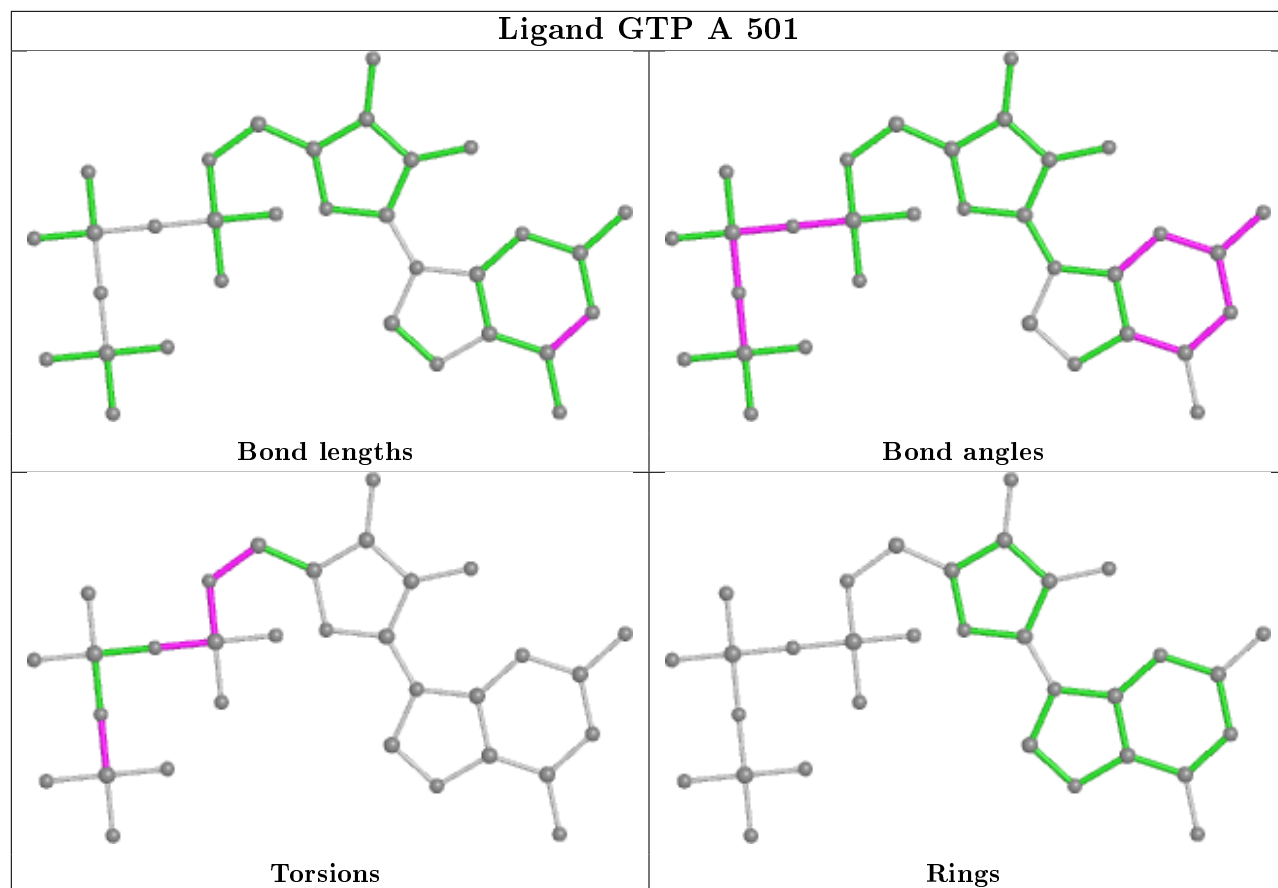
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
12	F	402	ACP	2	0

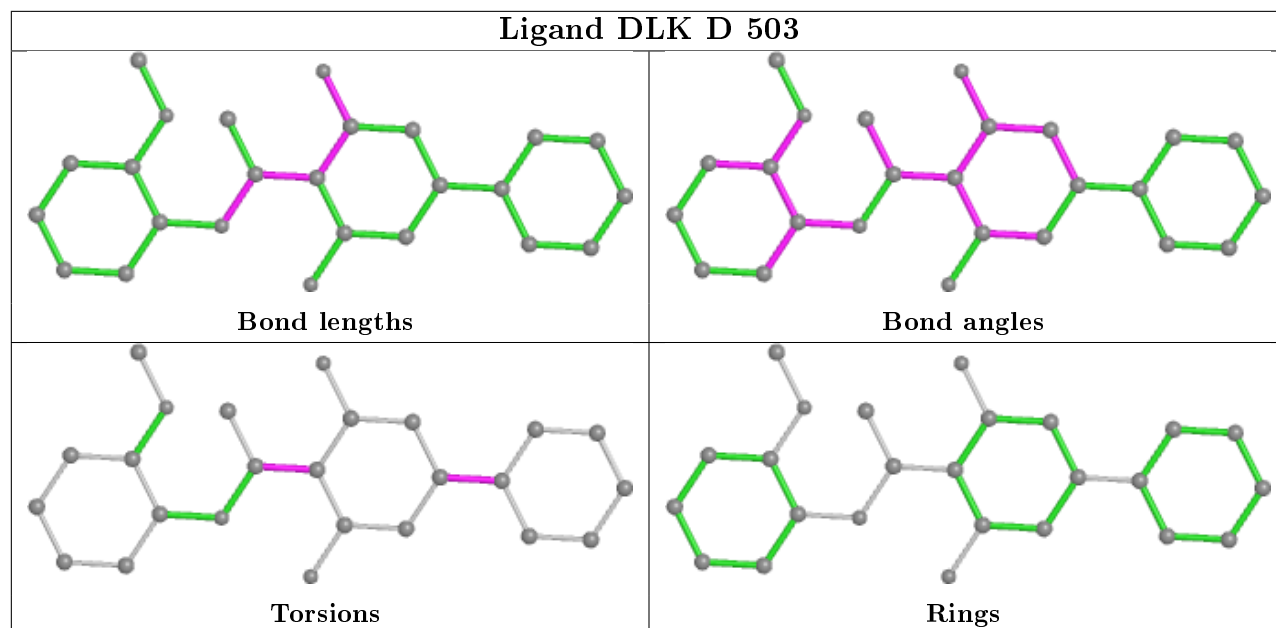
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 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	439/451 (97%)	0.28	12 (2%) 54 60	32, 49, 81, 138	0
1	C	439/451 (97%)	0.06	6 (1%) 75 78	26, 38, 65, 95	0
2	B	425/445 (95%)	0.26	15 (3%) 44 50	26, 45, 82, 115	0
2	D	422/445 (94%)	0.48	37 (8%) 10 12	34, 58, 89, 143	0
3	E	122/143 (85%)	0.46	13 (10%) 6 7	38, 64, 100, 122	0
4	F	349/384 (90%)	1.25	100 (28%) 0 0	39, 78, 143, 170	0
All	All	2196/2319 (94%)	0.44	183 (8%) 11 14	26, 51, 103, 170	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.5
2	D	57	THR	8.6
4	F	130	VAL	7.6
4	F	249	TYR	7.0
4	F	233	PHE	6.8
2	D	59	ASN	6.7
4	F	20	LEU	6.7
1	A	282	TYR	6.3
4	F	253	TYR	6.2
1	A	439	SER	6.1
4	F	177	GLY	6.1
4	F	132	LEU	6.1
4	F	231	ALA	5.8
4	F	250	SER	5.8
2	D	285	ALA	5.6
4	F	251	LYS	5.3
4	F	182	ILE	5.3
2	B	59	ASN	5.2
4	F	167	SER	5.2

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Mol	Chain	Res	Type	RSRZ
4	F	22	LEU	5.0
4	F	170	LEU	5.0
4	F	361	LEU	4.9
2	B	439	THR	4.9
3	E	139	LEU	4.9
4	F	99	VAL	4.8
4	F	21	LEU	4.8
4	F	131	PHE	4.8
4	F	161	LEU	4.8
4	F	169	LEU	4.8
2	B	58	GLY	4.7
3	E	27	PRO	4.6
4	F	174	ASP	4.5
1	A	281	ALA	4.5
2	B	57	THR	4.3
4	F	372	THR	4.3
2	B	438	ALA	4.3
4	F	179	VAL	4.3
4	F	172	PHE	4.3
4	F	362	ALA	4.3
1	C	2[A]	ARG	4.2
4	F	142	ARG	4.2
4	F	227	PRO	4.2
1	C	179	THR	4.0
4	F	137	ARG	4.0
4	F	101	TYR	4.0
4	F	259	GLY	4.0
4	F	133	ALA	4.0
3	E	26	PRO	3.9
4	F	24	THR	3.9
4	F	100	ILE	3.9
3	E	142	GLU	3.9
1	C	440	VAL	3.9
2	D	37	HIS	3.9
4	F	157	GLY	3.9
4	F	248	GLU	3.8
1	A	262	TYR	3.8
4	F	263	PHE	3.8
4	F	244	CYS	3.7
4	F	17	VAL	3.7
4	F	136	ASN	3.7
1	C	340	SER	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	252	ASN	3.6
2	B	284	ARG	3.6
4	F	232	ASN	3.6
4	F	18	SER	3.6
4	F	234	GLN	3.6
2	B	37	HIS	3.6
2	B	276	THR	3.6
4	F	256	TYR	3.5
3	E	24	LEU	3.5
2	D	56	ALA	3.4
4	F	135	TYR	3.4
4	F	168	GLU	3.4
2	B	56	ALA	3.3
2	D	246	GLY	3.3
4	F	23	ALA	3.3
4	F	176	GLN	3.2
4	F	194	PRO	3.2
4	F	245	ILE	3.2
4	F	178	GLN	3.2
4	F	166	ALA	3.2
2	D	276	THR	3.2
4	F	25	GLY	3.2
2	D	401	ARG	3.2
1	A	438	ASP	3.1
3	E	140	LYS	3.1
2	D	220	THR	3.1
4	F	126	ASP	3.1
2	D	94	PHE	3.0
4	F	134	ALA	3.0
4	F	171	ASP	3.0
4	F	138	ARG	3.0
4	F	143	GLU	3.0
3	E	6	MET	2.9
4	F	164	SER	2.9
2	D	404	PHE	2.9
4	F	255	ARG	2.9
2	D	400	ARG	2.9
4	F	89	GLU	2.8
3	E	7	GLU	2.8
2	D	82	PRO	2.8
3	E	143	ALA	2.7
1	A	346	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	2.7
2	D	249	ASN	2.7
4	F	129	GLU	2.7
2	D	250	ALA	2.7
4	F	153	ALA	2.6
2	D	221	THR	2.6
2	D	407	TRP	2.6
2	B	83	PHE	2.6
4	F	247	LYS	2.6
4	F	235	ASP	2.6
3	E	25	LYS	2.6
4	F	31	ARG	2.5
4	F	102	PRO	2.5
2	D	255	LEU	2.5
2	B	437	ASP	2.5
4	F	158	GLU	2.5
4	F	162	ILE	2.5
2	B	38	GLY	2.5
4	F	165	GLU	2.5
4	F	19	ARG	2.5
4	F	246	GLN	2.5
4	F	340	GLN	2.4
4	F	147	TRP	2.4
4	F	149	ALA	2.4
4	F	181	VAL	2.4
2	B	82	PRO	2.4
2	D	248	LEU	2.4
1	A	171	ILE	2.4
4	F	9	GLU	2.4
2	D	58	GLY	2.4
2	D	60	LYS	2.4
4	F	254	GLY	2.4
2	D	179	ASP	2.4
2	B	33	THR	2.3
4	F	1	MET	2.3
2	D	219	LEU	2.3
4	F	192	LEU	2.3
2	D	80	SER	2.3
1	A	364	PRO	2.3
4	F	228	TYR	2.3
4	F	27	TRP	2.3
4	F	140	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	258	GLU	2.2
2	D	77	SER	2.2
2	B	36	TYR	2.2
2	D	268	PHE	2.2
2	D	76	ASP	2.2
3	E	138	GLU	2.2
4	F	224	SER	2.2
4	F	197	ARG	2.2
2	D	33	THR	2.2
4	F	152	SER	2.2
2	D	405	LEU	2.1
1	A	177	VAL	2.1
2	D	85	GLN	2.1
3	E	48	GLU	2.1
3	E	141	GLU	2.1
4	F	351	VAL	2.1
2	D	397	ALA	2.1
2	D	415	GLU	2.1
4	F	226	GLU	2.1
4	F	146	VAL	2.1
1	C	253	THR	2.1
2	D	402	LYS	2.1
4	F	28	LYS	2.1
4	F	199	PHE	2.1
4	F	26	GLN	2.1
1	C	241	SER	2.1
2	D	74	THR	2.1
4	F	225	SER	2.0
4	F	10	ASN	2.0
2	D	180	THR	2.0
2	D	202	TYR	2.0
4	F	343	TYR	2.0
4	F	342	LEU	2.0
1	A	283	HIS	2.0
4	F	223	THR	2.0
2	D	259	MET	2.0
1	A	365	GLY	2.0
4	F	154	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

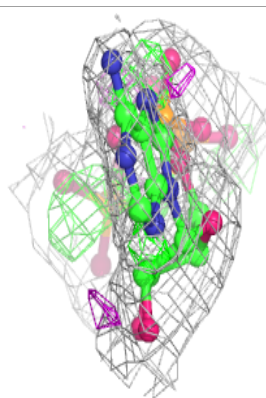
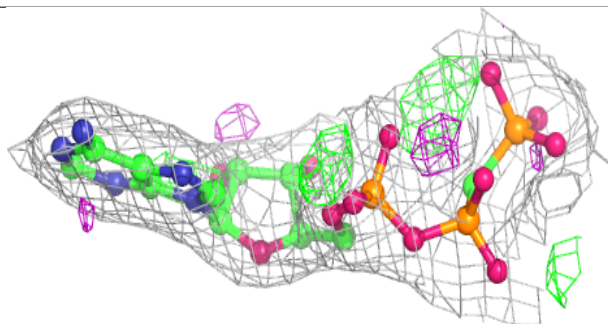
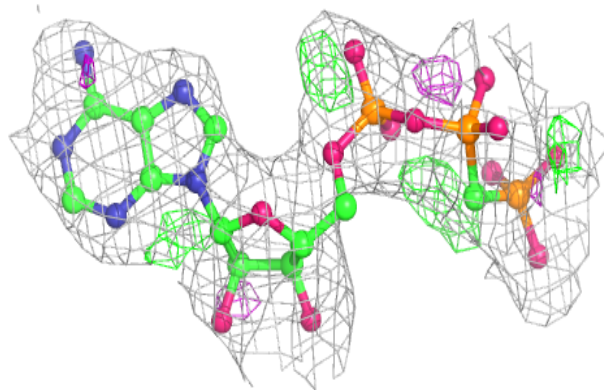
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	505	6/6	0.70	0.29	51,72,73,77	0
12	ACP	F	402	31/31	0.86	0.14	68,78,107,108	0
6	MG	F	401	1/1	0.86	0.06	76,76,76,76	0
11	DLK	D	503	25/25	0.87	0.26	48,69,77,79	0
6	MG	D	502	1/1	0.89	0.09	55,55,55,55	0
7	CA	A	504	1/1	0.91	0.08	101,101,101,101	0
8	GOL	A	505	6/6	0.91	0.19	59,68,72,76	0
7	CA	B	504	1/1	0.93	0.11	122,122,122,122	0
10	MES	B	506	12/12	0.95	0.15	41,51,77,89	0
7	CA	B	503	1/1	0.95	0.09	94,94,94,94	0
7	CA	A	503	1/1	0.97	0.04	63,63,63,63	0
11	DLK	B	507	25/25	0.97	0.14	30,36,43,47	0
9	GDP	D	501	28/28	0.97	0.11	44,51,56,62	0
5	GTP	A	501	32/32	0.98	0.18	24,33,40,42	0
6	MG	A	502	1/1	0.98	0.12	32,32,32,32	0
5	GTP	C	501	32/32	0.99	0.14	21,29,32,38	0
7	CA	C	503	1/1	0.99	0.04	49,49,49,49	0
6	MG	C	502	1/1	0.99	0.14	28,28,28,28	0
9	GDP	B	501	28/28	0.99	0.16	27,31,36,36	0
6	MG	B	502	1/1	1.00	0.21	24,24,24,24	0

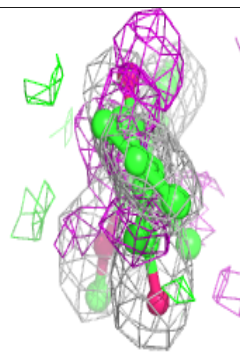
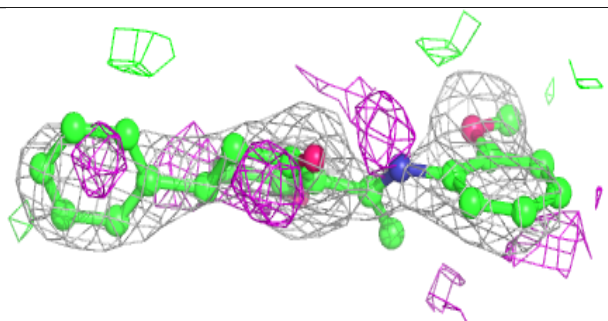
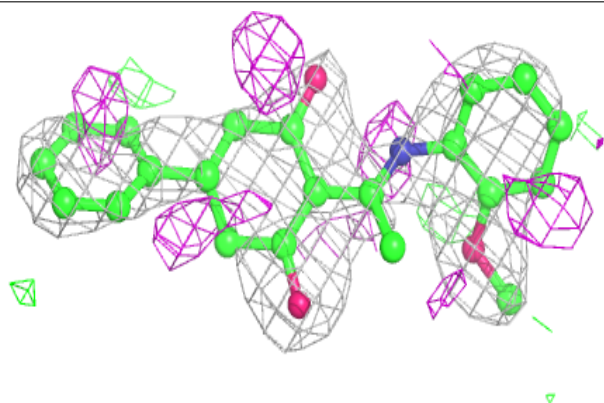
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

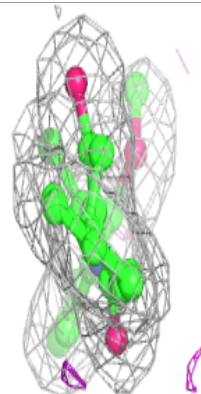
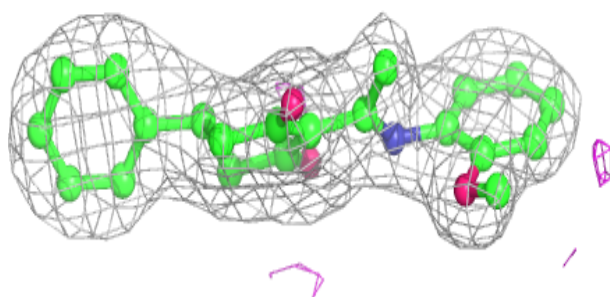
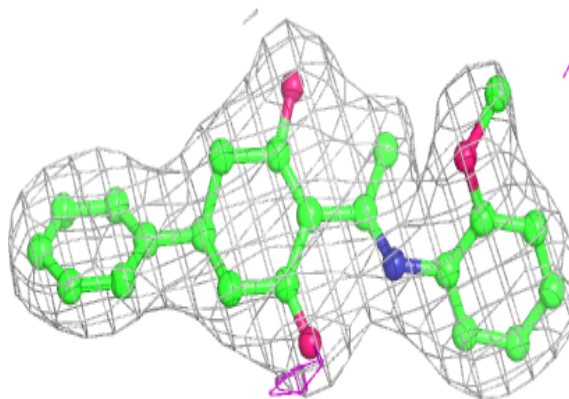
**Electron density around DLK D 503:**

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

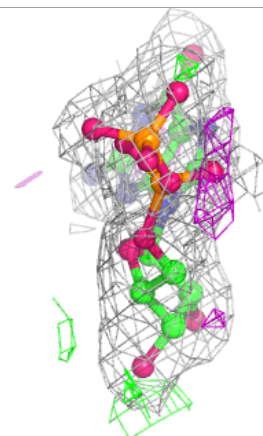
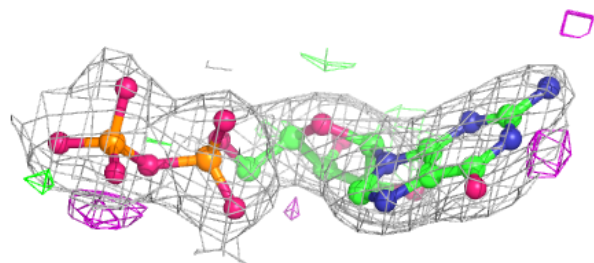
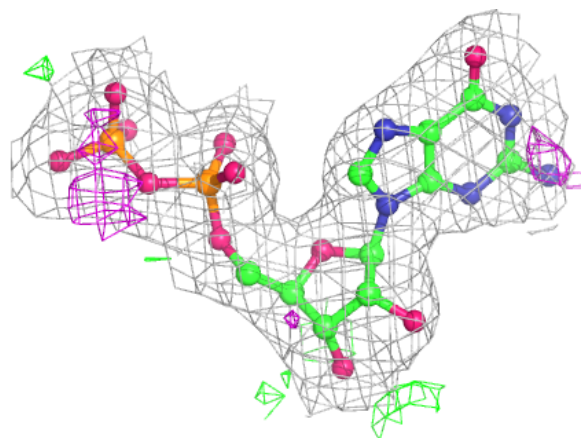


Electron density around DLK B 507:

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

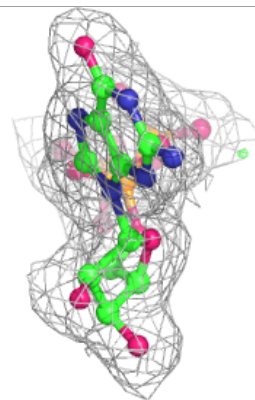
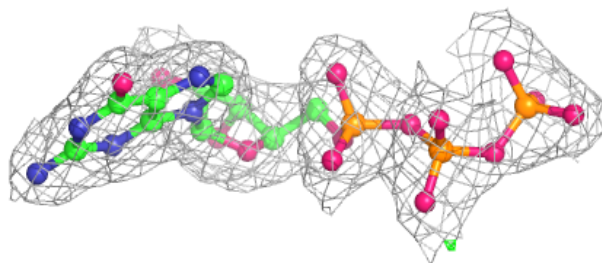
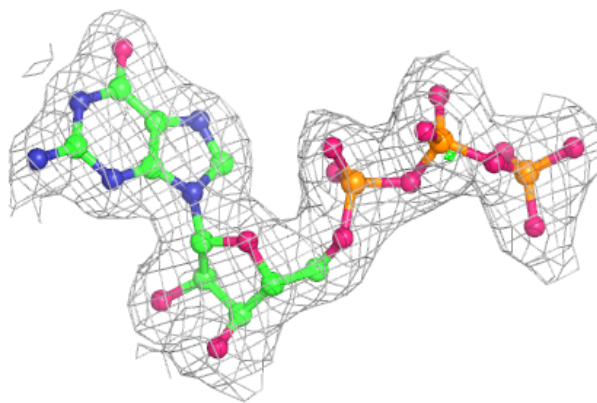
**Electron density around GDP D 501:**

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

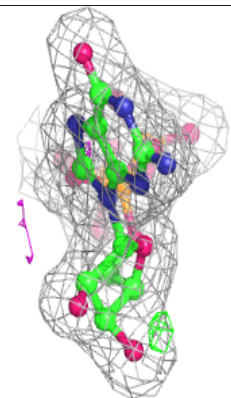
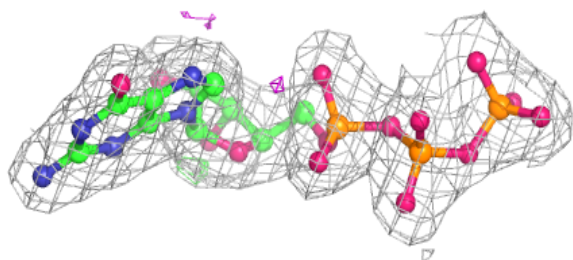
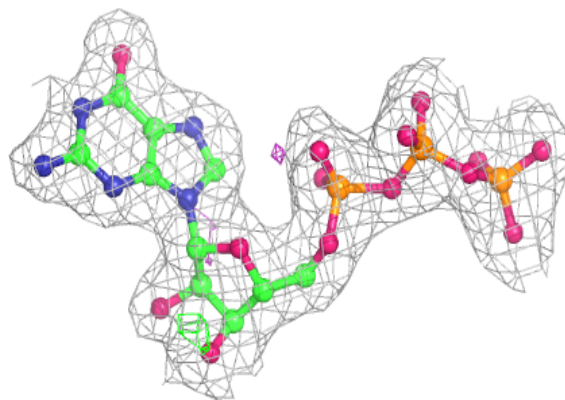


Electron density around GTP A 501:

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

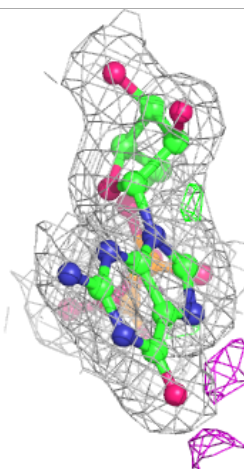
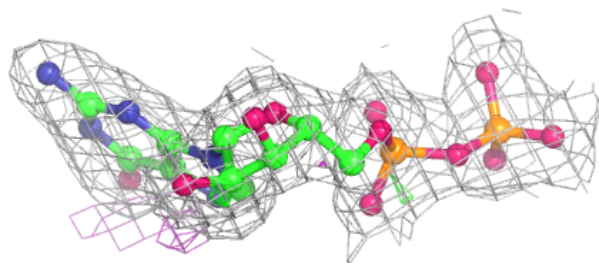
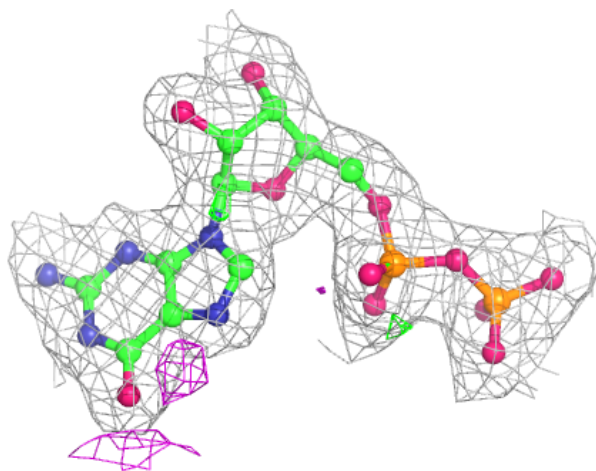
**Electron density around GTP C 501:**

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



Electron density around GDP B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.