Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 01:00 AM EST

PDB ID	:	6O61
Title	:	Tubulin-RB3_SLD-TTL in complex with compound ABI-231
Authors	:	Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on	:	2019-03-05
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:

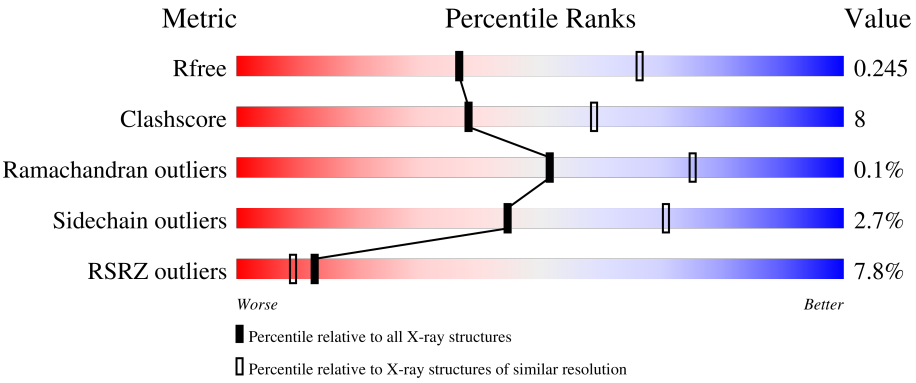
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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	2% 83% 14%
1	C	450	84% 14%
2	B	445	3% 79% 16%
2	D	445	12% 70% 24% 5%
3	E	143	5% 67% 16% 15%

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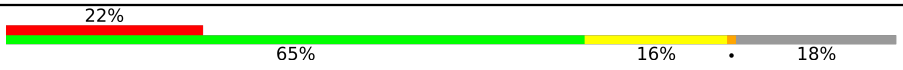
Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17165 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	437	Total	C	N	O	S	0	0	0
			3403	2156	579	646	22			
1	C	440	Total	C	N	O	S	0	0	0
			3427	2169	581	655	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3336	2098	570	642	26			
2	D	421	Total	C	N	O	S	0	0	0
			3156	1975	534	622	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			983	605	178	195	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

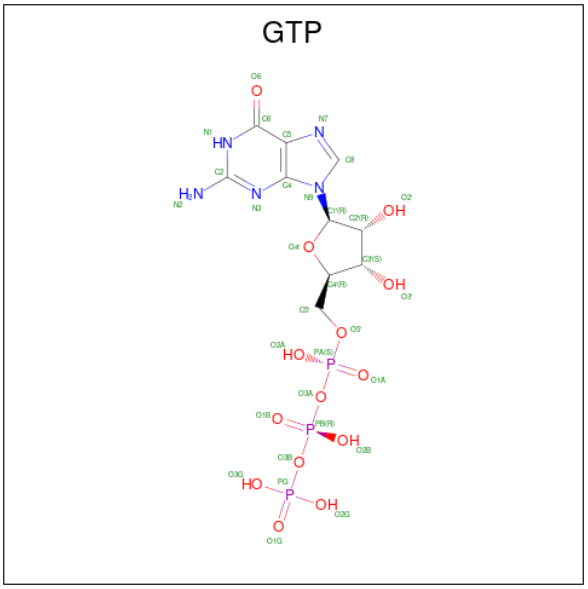
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	316	Total	C	N	O	S	0	0	0
			2390	1537	404	438	11			

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		

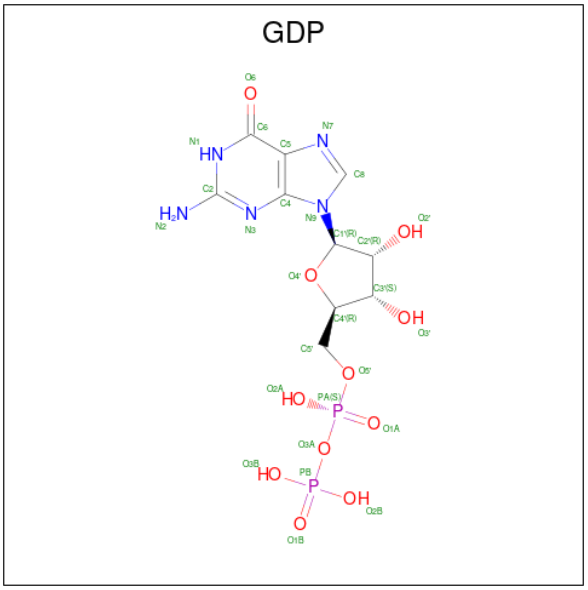
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

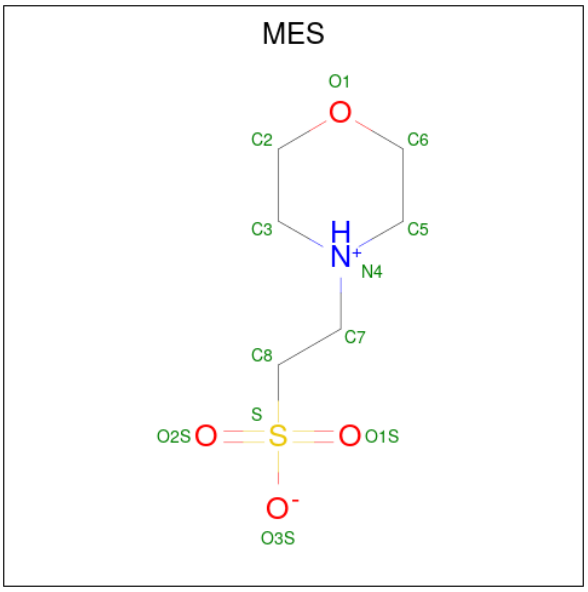
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



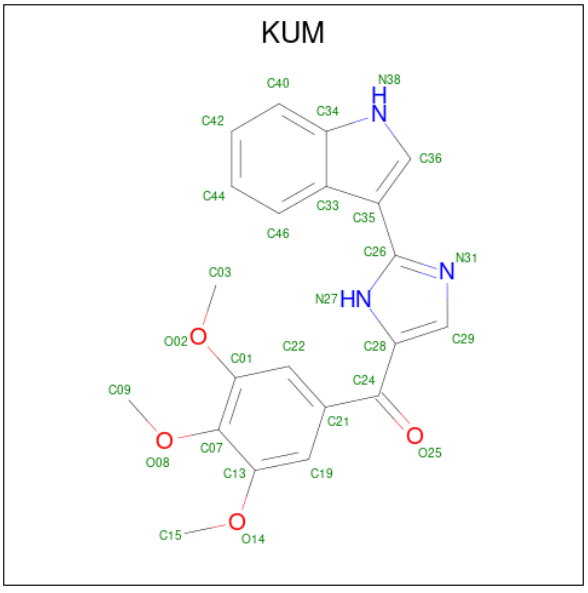
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- 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	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is [2-(1H-indol-3-yl)-1H-imidazol-5-yl](3,4,5-trimethoxyphenyl)methanone (three-letter code: KUM) (formula: $C_{21}H_{19}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			28	21	3	4		

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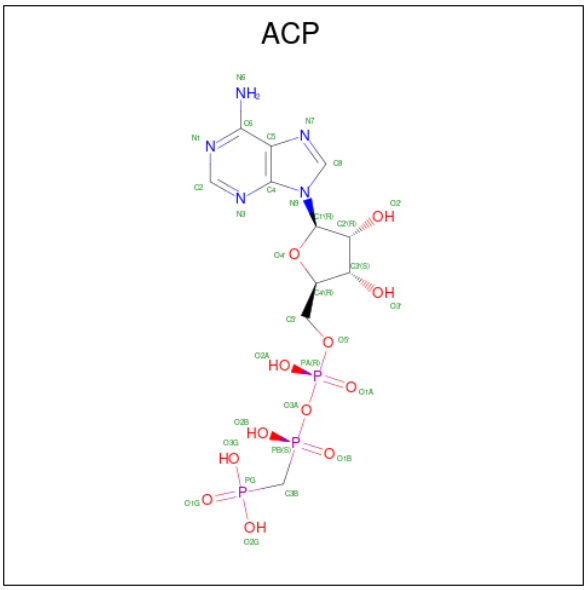
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			28	21	3	4		

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

- Molecule 12 is water.

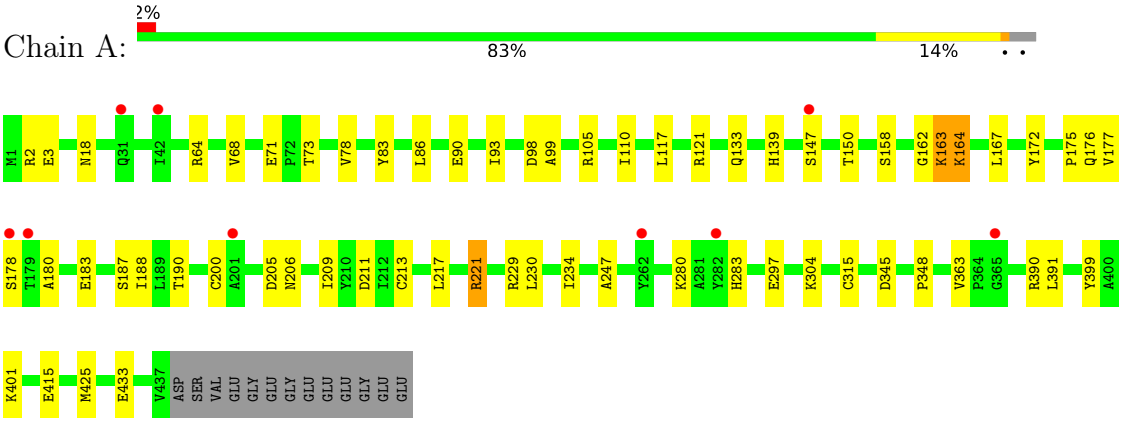
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	64	Total	O	0	0
			64	64		
12	B	38	Total	O	0	0
			38	38		
12	C	96	Total	O	0	0
			96	96		
12	D	13	Total	O	0	0
			13	13		
12	E	9	Total	O	0	0
			9	9		
12	F	14	Total	O	0	0
			14	14		

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.

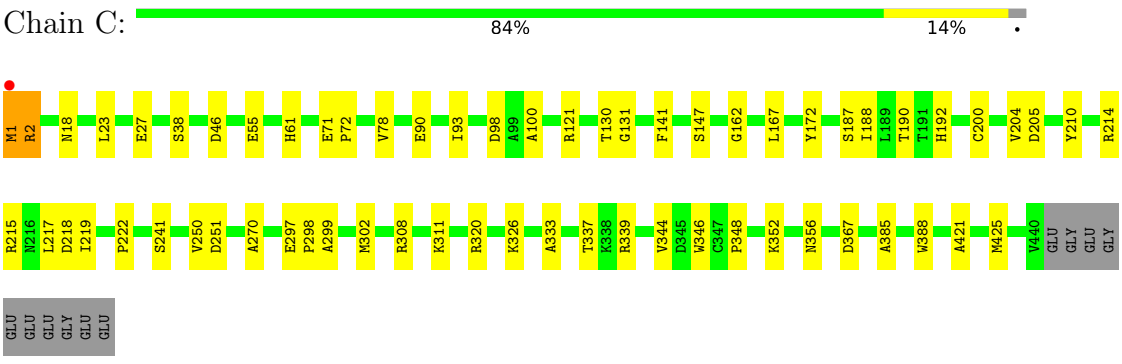
• Molecule 1: Tubulin alpha-1B chain

Chain A:



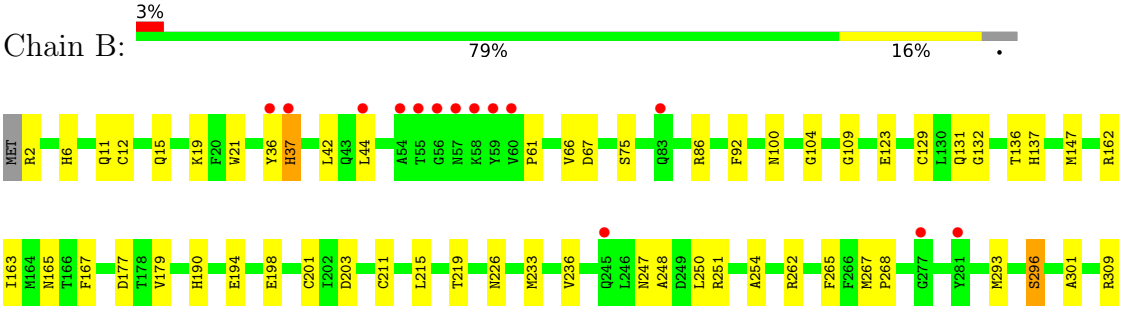
• Molecule 1: Tubulin alpha-1B chain

Chain C:



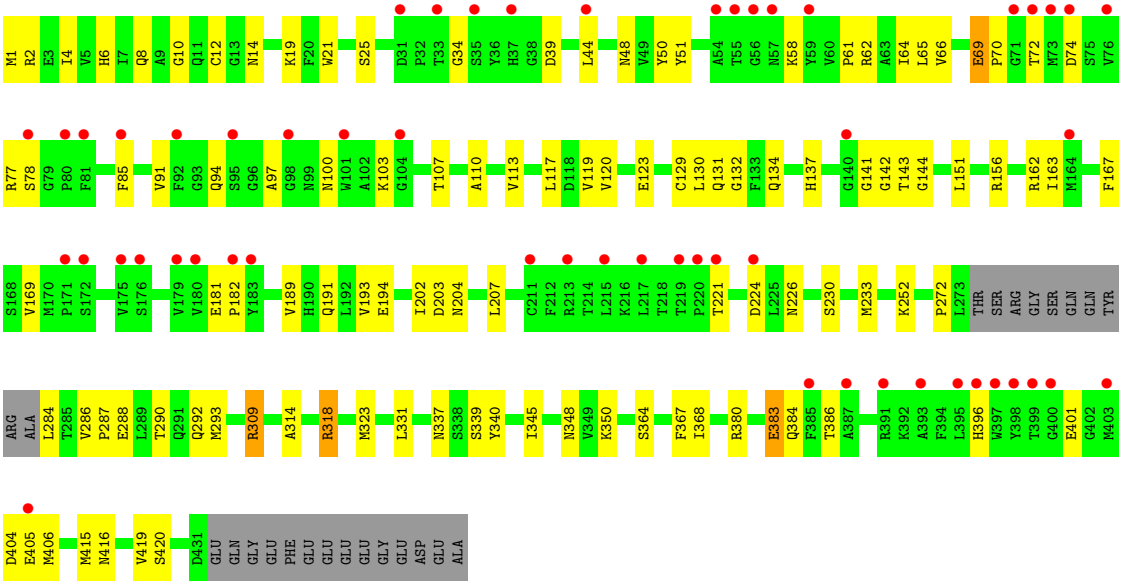
• Molecule 2: Tubulin beta-2B chain

Chain B:



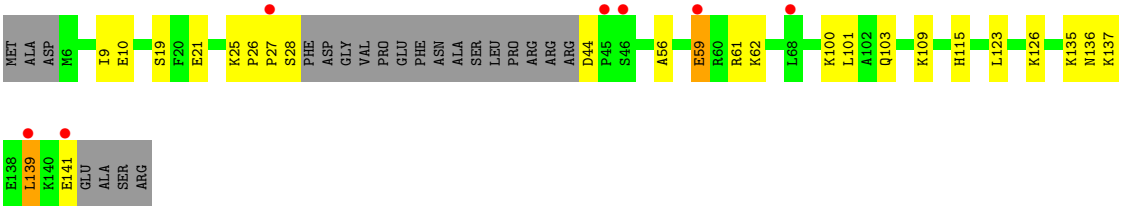
• Molecule 2: Tubulin beta-2B chain

Chain D:



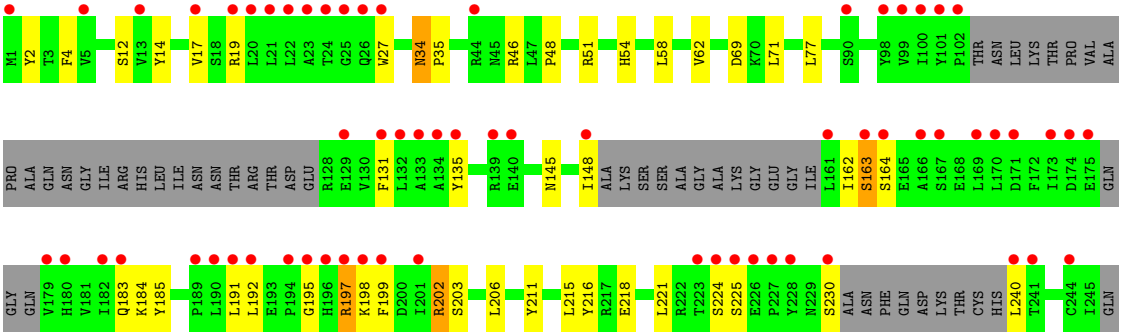
• Molecule 3: Stathmin-4

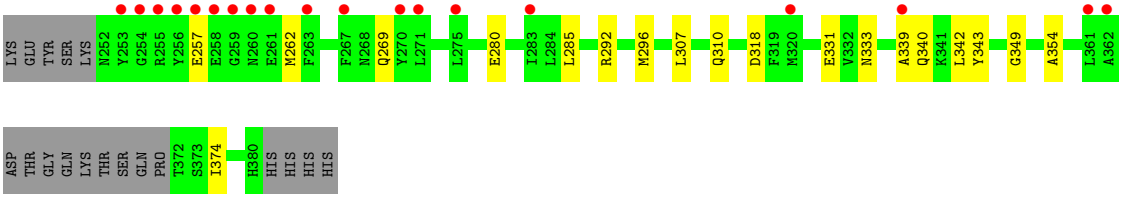
Chain E:



• Molecule 4: Tubulin Tyrosine Ligase

Chain F:




LYS GLU TYR SER LYS N252 Y253 G254 R255 Y256 E257 E258 G259 N260 E261 M262 F263 F267 N268 Q269 Y270 L271 L275 E280 I283 L284 L285 R292 M296 L307 Q310 D318 F319 M320 E331 V332 N333 A339 Q340 K341 L342 Y343 G349 A354 L361 A362
ASP THR GLY GLN LYS THR SER GLN PRO T372 S373 I374 H380 HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.26Å 157.09Å 184.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.60 48.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.16-2.60) 98.1 (48.16-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.204 , 0.243 0.205 , 0.245	Depositor DCC
R_{free} test set	4625 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.4	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	17165	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: CA, GDP, GTP, MG, ACP, MES, KUM

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	0.29	0/3480	0.49	0/4725
1	C	0.28	0/3505	0.49	0/4759
2	B	0.31	1/3411 (0.0%)	0.49	1/4622 (0.0%)
2	D	0.31	0/3224	0.58	5/4389 (0.1%)
3	E	0.30	0/995	0.45	1/1327 (0.1%)
4	F	0.26	0/2442	0.45	0/3322
All	All	0.29	1/17057 (0.0%)	0.50	7/23144 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	GLU	CG-CD	-6.15	1.42	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	44	LEU	CB-CG-CD2	9.94	127.89	111.00
2	D	48	ASN	CB-CA-C	-7.61	95.19	110.40
2	B	194	GLU	CA-CB-CG	-6.61	98.86	113.40
2	D	383	GLU	CA-CB-CG	6.41	127.51	113.40
2	D	331	LEU	CA-CB-CG	5.62	128.21	115.30
3	E	139	LEU	CA-CB-CG	5.11	127.06	115.30
2	D	69	GLU	CA-CB-CG	5.06	124.53	113.40

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	3403	0	3318	40	0
1	C	3427	0	3325	36	0
2	B	3336	0	3196	52	0
2	D	3156	0	2893	73	0
3	E	983	0	966	19	0
4	F	2390	0	2188	44	0
5	A	32	0	12	1	0
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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	4	0
8	D	28	0	12	6	0
9	B	24	0	24	3	0
10	B	28	0	0	3	0
10	D	28	0	0	1	0
11	F	31	0	13	3	0
12	A	64	0	0	0	0
12	B	38	0	0	0	0
12	C	96	0	0	1	0
12	D	13	0	0	0	0
12	E	9	0	0	0	0
12	F	14	0	0	1	0
All	All	17165	0	15971	250	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 8.

All (250) 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:226:ASN:HD21	8:D:501:GDP:HN1	1.04	0.98
4:F:280:GLU:O	4:F:285:LEU:HD13	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:GLU:HG2	2:D:72:THR:HG23	1.58	0.84
2:D:226:ASN:ND2	8:D:501:GDP:HN1	1.79	0.77
2:B:226:ASN:HD21	8:B:501:GDP:HN1	1.32	0.76
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.67	0.76
2:D:70:PRO:HG3	2:D:94:GLN:HA	1.70	0.74
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.70	0.74
1:A:206:ASN:HD21	5:A:501:GTP:HN22	1.34	0.73
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.23	0.71
2:B:66:VAL:CG1	2:B:147:MET:CE	2.69	0.71
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.72	0.71
2:B:226:ASN:OD1	8:B:501:GDP:N2	2.21	0.70
2:D:309:ARG:HD2	2:D:339:SER:O	1.91	0.70
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.73	0.70
4:F:202:ARG:HH22	4:F:333:ASN:HD22	1.40	0.69
2:D:204:ASN:HA	2:D:207:LEU:HD12	1.73	0.69
3:E:61:ARG:HH12	3:E:62:LYS:HG3	1.58	0.68
2:B:177:ASP:O	1:C:352:LYS:NZ	2.24	0.68
2:D:284:LEU:HD21	2:D:292:GLN:HE22	1.59	0.67
2:D:21:TRP:O	2:D:25:SER:OG	2.10	0.66
1:A:230:LEU:O	1:A:234:ILE:HD12	1.96	0.66
1:A:163:LYS:HG2	1:A:164:LYS:HD2	1.76	0.66
1:A:221:ARG:NH1	2:B:327:ASP:OD1	2.30	0.65
4:F:292:ARG:HG2	4:F:296:MET:SD	2.37	0.65
4:F:191:LEU:H	4:F:191:LEU:HD12	1.62	0.64
2:B:165:ASN:HD22	2:B:198:GLU:HB2	1.63	0.64
1:A:2:ARG:O	1:A:133:GLN:NE2	2.29	0.64
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.62	0.64
2:D:383:GLU:HA	2:D:386:THR:HG22	1.81	0.63
2:D:404:ASP:OD1	2:D:405:GLU:N	2.32	0.63
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.81	0.62
2:D:286:VAL:HG22	2:D:287:PRO:HD3	1.82	0.61
2:D:191:GLN:HE22	3:E:126:LYS:HE2	1.65	0.61
1:A:163:LYS:H	1:A:163:LYS:HD3	1.66	0.61
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.83	0.60
2:B:226:ASN:ND2	8:B:501:GDP:HN1	1.99	0.60
4:F:199:PHE:HD1	4:F:221:LEU:HD11	1.66	0.60
1:A:401:LYS:HD2	2:B:344:TRP:CD2	2.37	0.60
4:F:202:ARG:HH21	4:F:318:ASP:CG	2.05	0.60
1:C:2:ARG:NH1	1:C:131:GLY:O	2.34	0.60
1:C:1:MET:HG2	1:C:130:THR:OG1	2.01	0.60
4:F:34:ASN:HD22	4:F:35:PRO:HD2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.33	0.59
2:D:181:GLU:OE1	8:D:501:GDP:O3'	2.16	0.59
3:E:44:ASP:N	3:E:44:ASP:OD2	2.35	0.59
2:B:66:VAL:HG12	2:B:147:MET:CE	2.32	0.59
2:D:10:GLY:O	2:D:14:ASN:ND2	2.22	0.58
2:D:117:LEU:HA	2:D:120:VAL:HG22	1.85	0.58
2:D:314:ALA:HB3	2:D:368:ILE:HG12	1.85	0.57
1:A:433:GLU:OE1	4:F:46:ARG:NH1	2.37	0.57
1:A:345:ASP:O	3:E:28:SER:N	2.37	0.57
2:D:97:ALA:HB2	2:D:143:THR:HG22	1.87	0.57
2:D:182:PRO:HG3	2:D:384:GLN:HE21	1.70	0.56
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.86	0.56
4:F:148:ILE:HD12	4:F:162:ILE:HG12	1.87	0.56
2:D:6:HIS:NE2	2:D:8:GLN:HG2	2.20	0.56
2:B:236:VAL:HG22	2:B:368:ILE:HD11	1.88	0.56
4:F:14:TYR:HA	4:F:17:VAL:HB	1.88	0.56
1:C:147:SER:HB2	1:C:190:THR:OG1	2.05	0.56
2:D:19:LYS:HE3	2:D:230:SER:OG	2.06	0.56
2:B:386:THR:O	2:B:390:ARG:HG2	2.05	0.56
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.87	0.55
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.88	0.55
2:D:226:ASN:O	2:D:230:SER:OG	2.23	0.55
4:F:148:ILE:N	4:F:183:GLN:O	2.37	0.54
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.89	0.54
4:F:199:PHE:CD1	4:F:221:LEU:HD11	2.42	0.54
2:D:293:MET:CG	2:D:367:PHE:HB2	2.38	0.54
1:C:1:MET:CG	1:C:130:THR:OG1	2.56	0.54
4:F:135:TYR:O	4:F:145:ASN:ND2	2.28	0.54
2:B:66:VAL:HG11	2:B:147:MET:CE	2.38	0.54
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.91	0.53
2:D:318:ARG:HG3	2:D:364:SER:HB3	1.90	0.53
1:C:214:ARG:HG2	1:C:219:ILE:O	2.09	0.52
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.91	0.52
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.45	0.52
2:B:262:ARG:NH2	2:B:421:GLU:OE1	2.43	0.52
2:D:66:VAL:HA	2:D:91:VAL:O	2.10	0.52
2:D:51:TYR:HE1	2:D:61:PRO:HG3	1.74	0.52
2:D:74:ASP:HA	2:D:77:ARG:HB2	1.93	0.51
3:E:61:ARG:NH1	3:E:62:LYS:HG3	2.24	0.51
2:D:97:ALA:HB2	2:D:143:THR:CG2	2.41	0.51
1:C:46:ASP:OD1	1:C:46:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.51
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.46	0.50
2:B:2:ARG:HA	2:B:129:CYS:O	2.11	0.50
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.93	0.50
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.94	0.50
2:B:86:ARG:NH1	2:B:123:GLU:OE2	2.45	0.50
1:A:180:ALA:O	1:A:183:GLU:HG3	2.12	0.50
2:D:193:VAL:HG13	2:D:194:GLU:HG2	1.94	0.50
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.94	0.50
2:B:350:LYS:HB2	10:B:505:KUM:C34	2.42	0.49
4:F:48:PRO:HB2	4:F:51:ARG:HG3	1.93	0.49
4:F:203:SER:HB3	4:F:215:LEU:HD11	1.94	0.49
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.93	0.49
2:B:248:ALA:HB1	10:B:505:KUM:C19	2.43	0.49
2:D:50:TYR:OH	2:D:134:GLN:OE1	2.14	0.49
2:B:251:ARG:NH1	9:B:503:MES:O1S	2.45	0.49
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.48	0.49
3:E:10:GLU:O	3:E:10:GLU:HG2	2.13	0.49
4:F:34:ASN:HD22	4:F:35:PRO:CD	2.26	0.49
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.94	0.49
2:D:64:ILE:HD12	2:D:119:VAL:HG12	1.95	0.49
4:F:197:ARG:HB3	4:F:224:SER:O	2.13	0.48
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.93	0.48
2:D:39:ASP:OD1	2:D:39:ASP:N	2.41	0.48
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.95	0.48
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.48	0.48
2:B:36:TYR:CD1	2:B:44:LEU:HD21	2.48	0.48
2:B:350:LYS:HD3	10:B:505:KUM:C36	2.42	0.48
2:D:132:GLY:HA3	2:D:163:ILE:O	2.13	0.48
12:C:603:HOH:O	3:E:115[B]:HIS:HE1	1.96	0.48
2:B:136:THR:HG22	2:B:167:PHE:HB2	1.95	0.48
2:D:65:LEU:HD11	2:D:85:PHE:CD1	2.49	0.48
2:B:296:SER:N	9:B:504:MES:O3S	2.30	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.48
2:B:392:LYS:HB3	2:B:395:LEU:HD12	1.96	0.48
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.29	0.47
4:F:184:LYS:O	11:F:401:ACP:N6	2.47	0.47
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.95	0.47
4:F:163:SER:OG	4:F:164:SER:N	2.47	0.47
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.97	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.50	0.47
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.97	0.47
4:F:221:LEU:HD12	4:F:221:LEU:HA	1.57	0.47
1:A:105:ARG:HG3	1:A:110:ILE:HG13	1.97	0.46
2:D:110:ALA:O	2:D:113:VAL:HG12	2.14	0.46
1:A:175:PRO:HA	1:A:178:SER:HB2	1.96	0.46
2:B:11:GLN:O	2:B:15:GLN:HG3	2.13	0.46
2:D:191:GLN:HE22	3:E:126:LYS:CE	2.27	0.46
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.97	0.46
4:F:202:ARG:HH22	4:F:333:ASN:ND2	2.08	0.46
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.46
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.45	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.51	0.46
2:D:103:LYS:HA	2:D:107:THR:OG1	2.16	0.46
1:A:117:LEU:HD11	1:A:121:ARG:NH1	2.30	0.46
2:B:198:GLU:OE1	2:B:254:ALA:HB2	2.16	0.46
2:B:332:ASN:O	2:B:336:LYS:HG3	2.15	0.46
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.98	0.45
4:F:4:PHE:HB3	4:F:27:TRP:CZ3	2.50	0.45
1:A:280:LYS:HD3	1:A:283:HIS:HB2	1.98	0.45
2:D:143:THR:N	8:D:501:GDP:O1B	2.47	0.45
4:F:195:GLY:C	4:F:197:ARG:HG3	2.37	0.45
4:F:185:TYR:HA	11:F:401:ACP:N6	2.31	0.45
1:A:247:ALA:HB3	3:E:19:SER:OG	2.17	0.45
3:E:56:ALA:O	3:E:59:GLU:HG3	2.16	0.45
1:C:270:ALA:HB3	1:C:302:MET:HE3	1.99	0.45
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.29	0.45
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.81	0.45
1:A:147:SER:OG	1:A:190:THR:HB	2.17	0.45
1:A:213:CYS:O	1:A:217:LEU:HB2	2.16	0.45
1:C:100:ALA:HA	2:D:252:LYS:HE2	1.98	0.45
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.51	0.45
4:F:192:LEU:HB3	4:F:197:ARG:O	2.17	0.45
2:B:211:CYS:HA	2:B:215:LEU:HD12	1.98	0.45
2:D:2:ARG:HA	2:D:129:CYS:O	2.17	0.45
2:D:151:LEU:HD13	2:D:151:LEU:C	2.37	0.44
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.18	0.44
4:F:71:LEU:HD12	4:F:77:LEU:HD23	1.99	0.44
4:F:198:LYS:HZ3	4:F:240:LEU:N	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:NE	1:A:363:VAL:HG21	2.32	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
2:D:141:GLY:HA3	8:D:501:GDP:O3A	2.17	0.44
4:F:280:GLU:O	4:F:285:LEU:CD1	2.52	0.44
2:B:36:TYR:C	2:B:37:HIS:HD1	2.20	0.44
9:B:504:MES:H51	9:B:504:MES:H81	1.51	0.44
2:B:219:THR:HG21	1:C:326:LYS:HA	1.98	0.44
2:D:286:VAL:O	2:D:290:THR:HG23	2.18	0.44
3:E:136:ASN:HA	3:E:139:LEU:HB2	1.99	0.44
1:A:211:ASP:OD1	1:A:304:LYS:NZ	2.34	0.44
1:C:333:ALA:O	1:C:337:THR:HG23	2.18	0.44
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.53	0.44
2:D:221:THR:HG23	2:D:224:ASP:H	1.82	0.44
2:D:350:LYS:HB2	10:D:502:KUM:C34	2.48	0.44
1:C:217:LEU:HD13	1:C:367:ASP:HB2	2.00	0.43
1:A:401:LYS:HE3	2:B:428:ALA:HB1	2.00	0.43
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.54	0.43
4:F:331:GLU:OE1	4:F:333:ASN:ND2	2.48	0.43
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.58	0.43
1:A:90:GLU:HB3	1:A:121:ARG:NE	2.33	0.43
2:B:66:VAL:CG1	2:B:147:MET:HE3	2.45	0.43
11:F:401:ACP:H5'2	11:F:401:ACP:O1B	2.18	0.43
2:B:309:ARG:NH1	2:B:343:GLU:OE1	2.47	0.43
2:D:143:THR:OG1	2:D:144:GLY:N	2.52	0.43
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.53	0.43
3:E:136:ASN:HA	3:E:139:LEU:CB	2.49	0.43
4:F:202:ARG:NH2	4:F:333:ASN:HD22	2.13	0.43
1:A:177:VAL:O	1:A:177:VAL:HG22	2.19	0.43
1:C:90:GLU:HB3	1:C:121:ARG:HD2	2.00	0.43
1:C:141:PHE:HB3	1:C:187:SER:OG	2.19	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.53	0.42
2:D:2:ARG:NH2	2:D:131:GLN:HB3	2.34	0.42
3:E:137:LYS:HE2	3:E:137:LYS:HB3	1.77	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
2:B:66:VAL:HG12	2:B:147:MET:HE1	1.99	0.42
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.42
2:D:74:ASP:O	2:D:78:SER:N	2.44	0.42
1:A:68:VAL:HA	1:A:93:ILE:O	2.19	0.42
2:D:189:VAL:HG11	2:D:415:MET:HG3	2.02	0.42
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.84	0.42
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HB3	2:B:19:LYS:HE3	1.87	0.42
2:B:132:GLY:HA3	2:B:163:ILE:O	2.20	0.42
2:D:288:GLU:O	2:D:292:GLN:HB2	2.20	0.42
3:E:135:LYS:O	3:E:139:LEU:HB2	2.19	0.42
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.55	0.42
4:F:221:LEU:HB3	4:F:262:MET:HB3	2.01	0.42
4:F:198:LYS:O	4:F:224:SER:HB3	2.18	0.42
1:A:83:TYR:CD1	1:A:86:LEU:HD22	2.55	0.41
2:D:19:LYS:HD2	2:D:19:LYS:HA	1.89	0.41
2:D:203:ASP:OD2	2:D:380:ARG:NH1	2.38	0.41
1:C:297:GLU:CD	1:C:339:ARG:HH22	2.24	0.41
2:D:34:GLY:O	2:D:58:LYS:HA	2.20	0.41
2:B:12:CYS:HB2	8:B:501:GDP:C4	2.55	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.41
2:D:290:THR:HA	2:D:293:MET:HE2	2.03	0.41
1:A:187:SER:CB	1:A:391:LEU:HD21	2.50	0.41
2:B:391:ARG:HD2	2:B:391:ARG:HA	1.89	0.41
2:D:1:MET:O	2:D:129:CYS:HB3	2.20	0.41
2:D:130:LEU:HD23	2:D:162:ARG:HH11	1.85	0.41
4:F:62:VAL:HG12	4:F:310:GLN:O	2.20	0.41
2:B:104:GLY:O	2:B:109:GLY:HA3	2.20	0.41
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.03	0.41
1:A:99:ALA:HA	1:A:105:ARG:HG2	2.03	0.41
1:A:399:TYR:OH	1:A:415:GLU:HG2	2.21	0.41
2:D:4:ILE:HG12	2:D:131:GLN:HG3	2.03	0.41
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.56	0.41
2:B:67:ASP:O	2:B:92:PHE:HA	2.21	0.41
2:D:401:GLU:HA	3:E:137:LYS:HG3	2.03	0.41
2:D:416:ASN:HA	2:D:419:VAL:HG22	2.02	0.41
1:C:71:GLU:CB	1:C:98:ASP:HB3	2.48	0.41
2:D:416:ASN:HA	2:D:416:ASN:HD22	1.72	0.41
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.56	0.40
2:B:203:ASP:OD1	2:B:380:ARG:NH1	2.41	0.40
3:E:25:LYS:HA	3:E:26:PRO:HD3	1.85	0.40
1:A:297:GLU:HG3	12:F:507:HOH:O	2.21	0.40
2:B:203:ASP:CG	2:B:380:ARG:HH22	2.23	0.40
2:D:151:LEU:HD13	2:D:151:LEU:O	2.21	0.40
2:D:337:ASN:HB3	2:D:340:TYR:HD2	1.86	0.40
4:F:339:ALA:HB3	4:F:342:LEU:HD12	2.04	0.40
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.03	0.40
2:D:97:ALA:HB1	2:D:142:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.04	0.40
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.87	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%)	427 (98%)	7 (2%)	1 (0%)	47 71
1	C	438/450 (97%)	429 (98%)	8 (2%)	1 (0%)	47 71
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100 100
2	D	417/445 (94%)	410 (98%)	7 (2%)	0	100 100
3	E	118/143 (82%)	117 (99%)	1 (1%)	0	100 100
4	F	302/384 (79%)	291 (96%)	11 (4%)	0	100 100
All	All	2135/2317 (92%)	2092 (98%)	41 (2%)	2 (0%)	51 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
1	C	162	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	365/378 (97%)	359 (98%)	6 (2%)	62	82
1	C	368/378 (97%)	361 (98%)	7 (2%)	57	79
2	B	362/383 (94%)	353 (98%)	9 (2%)	47	73
2	D	326/383 (85%)	318 (98%)	8 (2%)	47	73
3	E	104/127 (82%)	98 (94%)	6 (6%)	20	40
4	F	234/342 (68%)	222 (95%)	12 (5%)	24	46
All	All	1759/1991 (88%)	1711 (97%)	48 (3%)	44	71

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	SER
1	A	163	LYS
1	A	164	LYS
1	A	176	GLN
1	A	221	ARG
1	A	315	CYS
2	B	37	HIS
2	B	42	LEU
2	B	75	SER
2	B	100	ASN
2	B	137	HIS
2	B	162	ARG
2	B	247	ASN
2	B	268	PRO
2	B	296	SER
1	C	1	MET
1	C	2	ARG
1	C	38	SER
1	C	218	ASP
1	C	241	SER
1	C	251	ASP
1	C	311	LYS
2	D	100	ASN
2	D	137	HIS
2	D	309	ARG
2	D	318	ARG
2	D	323	MET
2	D	396	HIS
2	D	406	MET
2	D	420	SER

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Mol	Chain	Res	Type
3	E	59	GLU
3	E	100	LYS
3	E	101	LEU
3	E	103	GLN
3	E	109	LYS
3	E	141	GLU
4	F	12	SER
4	F	19	ARG
4	F	34	ASN
4	F	69	ASP
4	F	131	PHE
4	F	163	SER
4	F	197	ARG
4	F	202	ARG
4	F	211	TYR
4	F	225	SER
4	F	230	SER
4	F	269	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	186	ASN
1	A	206	ASN
1	A	301	GLN
1	A	358	GLN
1	A	406	HIS
2	B	100	ASN
2	B	165	ASN
2	B	247	ASN
2	B	292	GLN
2	B	414	ASN
1	C	372	GLN
1	C	380	ASN
2	D	99	ASN
2	D	100	ASN
2	D	226	ASN
2	D	292	GLN
2	D	384	GLN
2	D	396	HIS
2	D	416	ASN

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Mol	Chain	Res	Type
4	F	34	ASN
4	F	269	GLN
4	F	333	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 14 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.17	1 (3%)	32,54,54	1.47	5 (15%)
11	ACP	F	401	-	27,33,33	4.68	10 (37%)	32,52,52	2.25	5 (15%)
10	KUM	B	505	-	30,31,31	1.33	6 (20%)	35,44,44	1.34	7 (20%)
9	MES	B	504	-	12,12,12	2.29	1 (8%)	14,16,16	1.94	6 (42%)
8	GDP	B	501	6	24,30,30	1.85	3 (12%)	30,47,47	3.57	8 (26%)
9	MES	B	503	-	12,12,12	2.18	1 (8%)	14,16,16	1.89	6 (42%)
5	GTP	C	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.43	6 (18%)
8	GDP	D	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.23	3 (10%)
10	KUM	D	502	-	30,31,31	1.32	6 (20%)	35,44,44	1.39	8 (22%)

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
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
11	ACP	F	401	-	-	4/15/38/38	0/3/3/3
10	KUM	B	505	-	-	3/10/18/18	0/4/4/4
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	GDP	D	501	-	-	4/12/32/32	0/3/3/3
10	KUM	D	502	-	-	4/10/18/18	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	O4'-C1'	15.11	1.62	1.41
11	F	401	ACP	C2'-C1'	-14.81	1.31	1.53
9	B	504	MES	C8-S	-7.66	1.66	1.77
9	B	503	MES	C8-S	-7.28	1.67	1.77
8	B	501	GDP	O6-C6	-6.91	1.09	1.23
11	F	401	ACP	PB-O3A	6.45	1.65	1.58
11	F	401	ACP	O4'-C4'	-6.39	1.30	1.45
5	A	501	GTP	C5-C6	-4.09	1.39	1.47
5	C	501	GTP	C5-C6	-4.00	1.39	1.47
10	B	505	KUM	C29-N31	-3.31	1.31	1.36
8	B	501	GDP	C2-N3	3.29	1.41	1.33
10	D	502	KUM	C29-N31	-3.26	1.31	1.36
11	F	401	ACP	C6-N6	3.14	1.45	1.34
8	B	501	GDP	C8-N7	3.02	1.40	1.35
11	F	401	ACP	O2'-C2'	3.01	1.50	1.43
11	F	401	ACP	O3'-C3'	-2.84	1.36	1.43
11	F	401	ACP	C5-C4	-2.63	1.34	1.40
8	D	501	GDP	C6-N1	-2.52	1.34	1.37
11	F	401	ACP	C2-N3	2.32	1.35	1.32
11	F	401	ACP	PB-O2B	-2.28	1.51	1.56
10	B	505	KUM	O25-C24	-2.26	1.18	1.22
10	D	502	KUM	O02-C01	2.26	1.40	1.37
10	B	505	KUM	O02-C01	2.24	1.40	1.37
10	D	502	KUM	C33-C34	-2.24	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	KUM	C33-C34	-2.19	1.36	1.42
10	B	505	KUM	O14-C13	2.17	1.40	1.37
10	D	502	KUM	C21-C24	2.16	1.53	1.49
10	D	502	KUM	O25-C24	-2.15	1.18	1.22
10	D	502	KUM	O14-C13	2.10	1.40	1.37
10	B	505	KUM	C21-C24	2.03	1.52	1.49
5	C	501	GTP	C2-N3	2.03	1.38	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	GDP	O6-C6-N1	-13.28	104.97	120.65
8	B	501	GDP	C5-C6-N1	9.54	130.79	113.95
8	B	501	GDP	C2-N1-C6	-8.49	109.46	125.10
11	F	401	ACP	C5-C6-N6	8.13	132.71	120.35
11	F	401	ACP	N3-C2-N1	-5.47	120.13	128.68
11	F	401	ACP	N6-C6-N1	-5.42	107.32	118.57
11	F	401	ACP	C3'-C2'-C1'	3.89	106.84	100.98
9	B	504	MES	C5-N4-C3	3.83	117.45	108.83
9	B	503	MES	C5-N4-C3	3.58	116.89	108.83
5	A	501	GTP	C5-C6-N1	3.30	119.78	113.95
10	B	505	KUM	O14-C13-C07	3.28	120.92	115.16
5	C	501	GTP	C5-C6-N1	3.20	119.59	113.95
5	A	501	GTP	PA-O3A-PB	-3.09	122.21	132.83
10	D	502	KUM	C35-C26-N27	3.04	127.55	123.67
5	A	501	GTP	C8-N7-C5	3.04	108.77	102.99
5	C	501	GTP	PB-O3B-PG	-3.03	122.44	132.83
5	C	501	GTP	C8-N7-C5	3.01	108.73	102.99
9	B	504	MES	C6-C5-N4	-3.01	105.53	110.10
10	D	502	KUM	O14-C13-C07	2.98	120.41	115.16
10	D	502	KUM	O02-C01-C07	2.86	120.20	115.16
5	A	501	GTP	C2-N1-C6	-2.75	120.03	125.10
5	C	501	GTP	C2-N1-C6	-2.74	120.06	125.10
8	D	501	GDP	PA-O3A-PB	-2.72	123.49	132.83
8	B	501	GDP	PA-O3A-PB	-2.70	123.55	132.83
8	B	501	GDP	C8-N7-C5	2.69	108.11	102.99
9	B	503	MES	C6-C5-N4	-2.65	106.08	110.10
10	D	502	KUM	O14-C13-C19	-2.64	119.57	124.12
8	B	501	GDP	N2-C2-N1	-2.63	111.11	116.71
5	C	501	GTP	PA-O3A-PB	-2.63	123.80	132.83
5	A	501	GTP	PB-O3B-PG	-2.62	123.84	132.83
9	B	503	MES	C7-N4-C5	2.60	117.88	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	505	KUM	O14-C13-C19	-2.59	119.66	124.12
10	D	502	KUM	C15-O14-C13	-2.55	113.68	117.53
9	B	503	MES	O3S-S-C8	2.54	109.87	105.77
10	D	502	KUM	O02-C01-C22	-2.51	119.80	124.12
10	B	505	KUM	C15-O14-C13	-2.47	113.80	117.53
10	B	505	KUM	O02-C01-C07	2.47	119.50	115.16
10	D	502	KUM	C46-C33-C35	-2.46	132.12	135.63
8	D	501	GDP	C2'-C3'-C4'	2.44	107.38	102.64
10	B	505	KUM	C35-C26-N27	2.42	126.77	123.67
9	B	504	MES	O1S-S-C8	2.33	109.73	106.92
8	B	501	GDP	C3'-C2'-C1'	2.33	104.48	100.98
9	B	503	MES	O2S-S-C8	2.31	109.70	106.92
8	B	501	GDP	N2-C2-N3	2.26	124.14	119.74
9	B	503	MES	O1S-S-C8	2.26	109.64	106.92
9	B	504	MES	O2S-S-C8	2.25	109.63	106.92
11	F	401	ACP	PB-O3A-PA	-2.23	125.50	132.56
9	B	504	MES	C7-N4-C5	2.20	116.86	111.23
10	B	505	KUM	C46-C33-C35	-2.18	132.52	135.63
9	B	504	MES	O3S-S-C8	2.17	109.28	105.77
8	D	501	GDP	C8-N7-C5	2.16	107.10	102.99
10	D	502	KUM	C03-O02-C01	-2.12	114.33	117.53
10	B	505	KUM	O02-C01-C22	-2.03	120.63	124.12
5	C	501	GTP	O6-C6-C5	-2.02	120.42	124.37

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
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
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
10	D	502	KUM	C07-C13-O14-C15
11	F	401	ACP	C3'-C4'-C5'-O5'
10	D	502	KUM	C19-C13-O14-C15
10	D	502	KUM	C07-C01-O02-C03
10	B	505	KUM	C07-C13-O14-C15
10	D	502	KUM	C22-C01-O02-C03
9	B	504	MES	C7-C8-S-O3S
8	D	501	GDP	PA-O3A-PB-O1B
10	B	505	KUM	C19-C13-O14-C15
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
9	B	503	MES	C7-C8-S-O2S
10	B	505	KUM	C07-C01-O02-C03
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

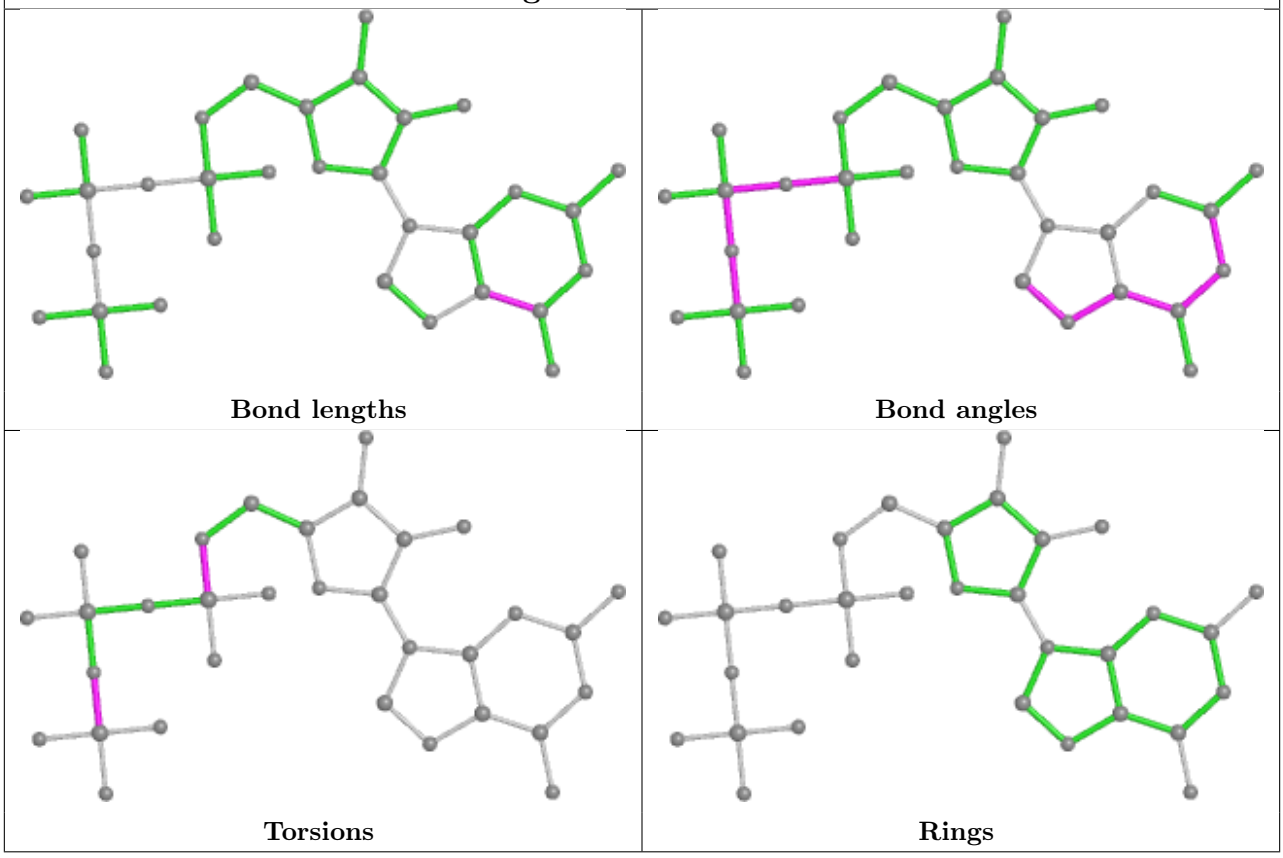
8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
11	F	401	ACP	3	0
10	B	505	KUM	3	0
9	B	504	MES	2	0
8	B	501	GDP	4	0
9	B	503	MES	1	0
8	D	501	GDP	6	0
10	D	502	KUM	1	0

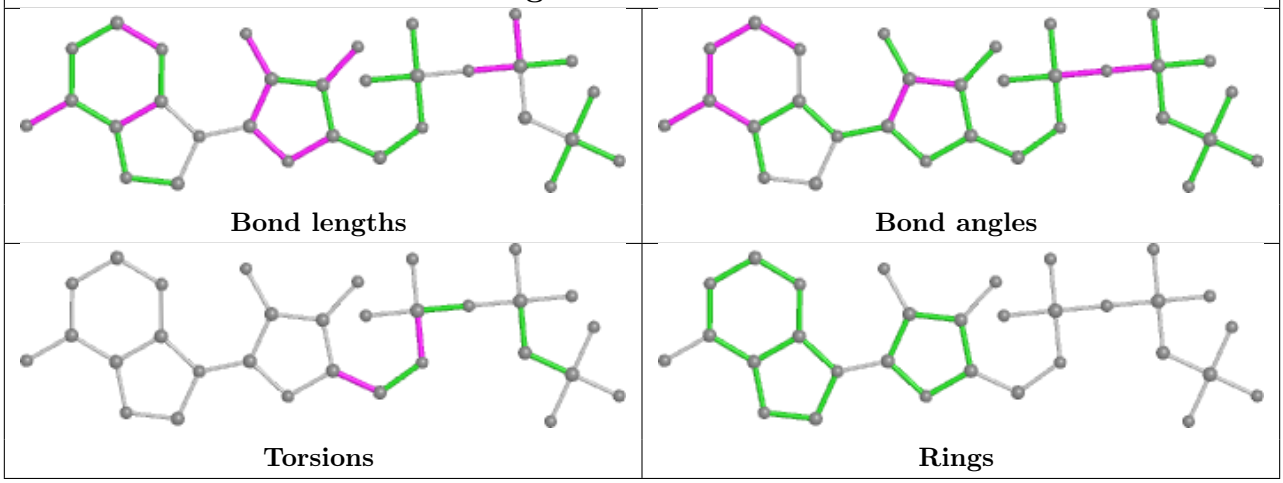
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

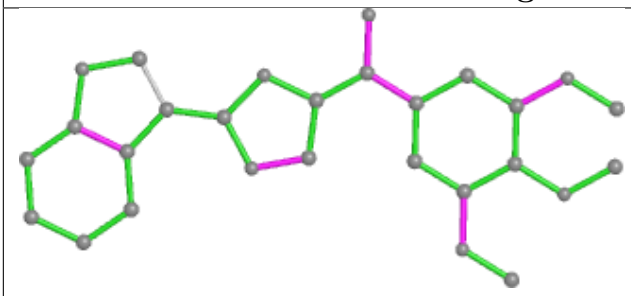
Ligand GTP A 501



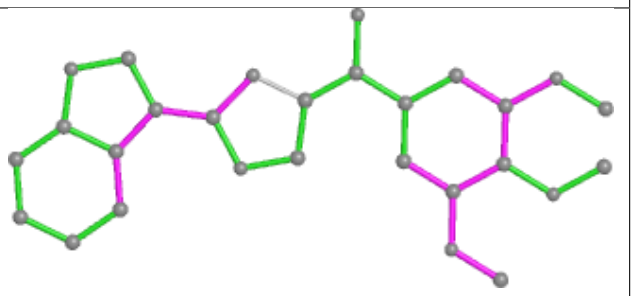
Ligand ACP F 401



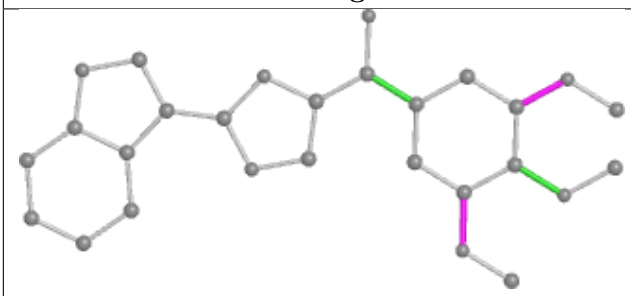
Ligand KUM B 505



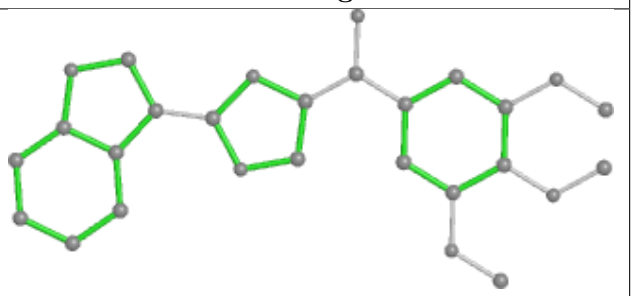
Bond lengths



Bond angles

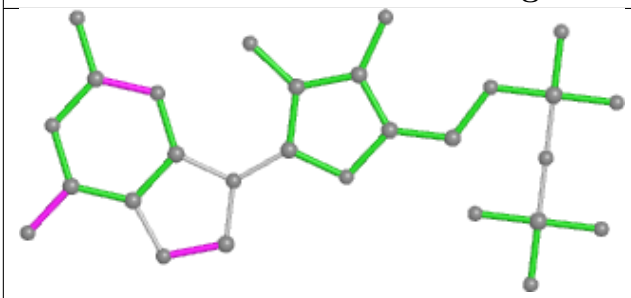


Torsions

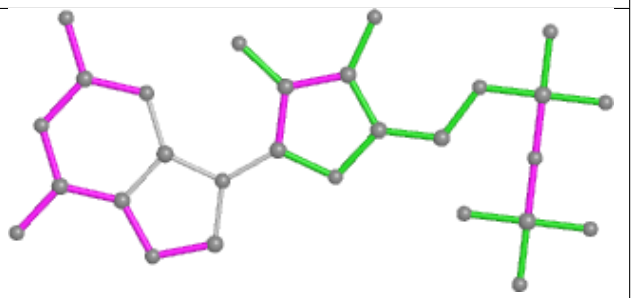


Rings

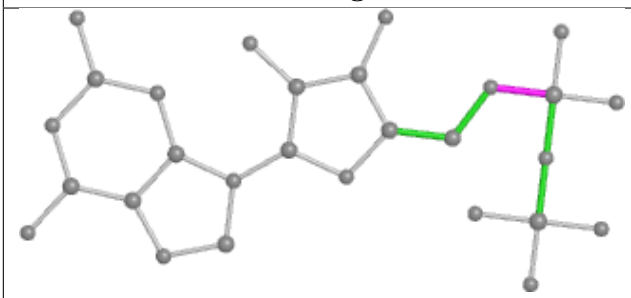
Ligand GDP B 501



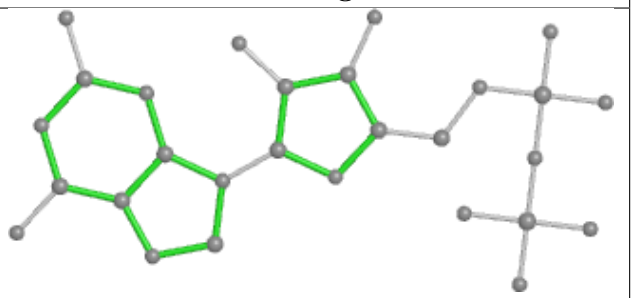
Bond lengths



Bond angles

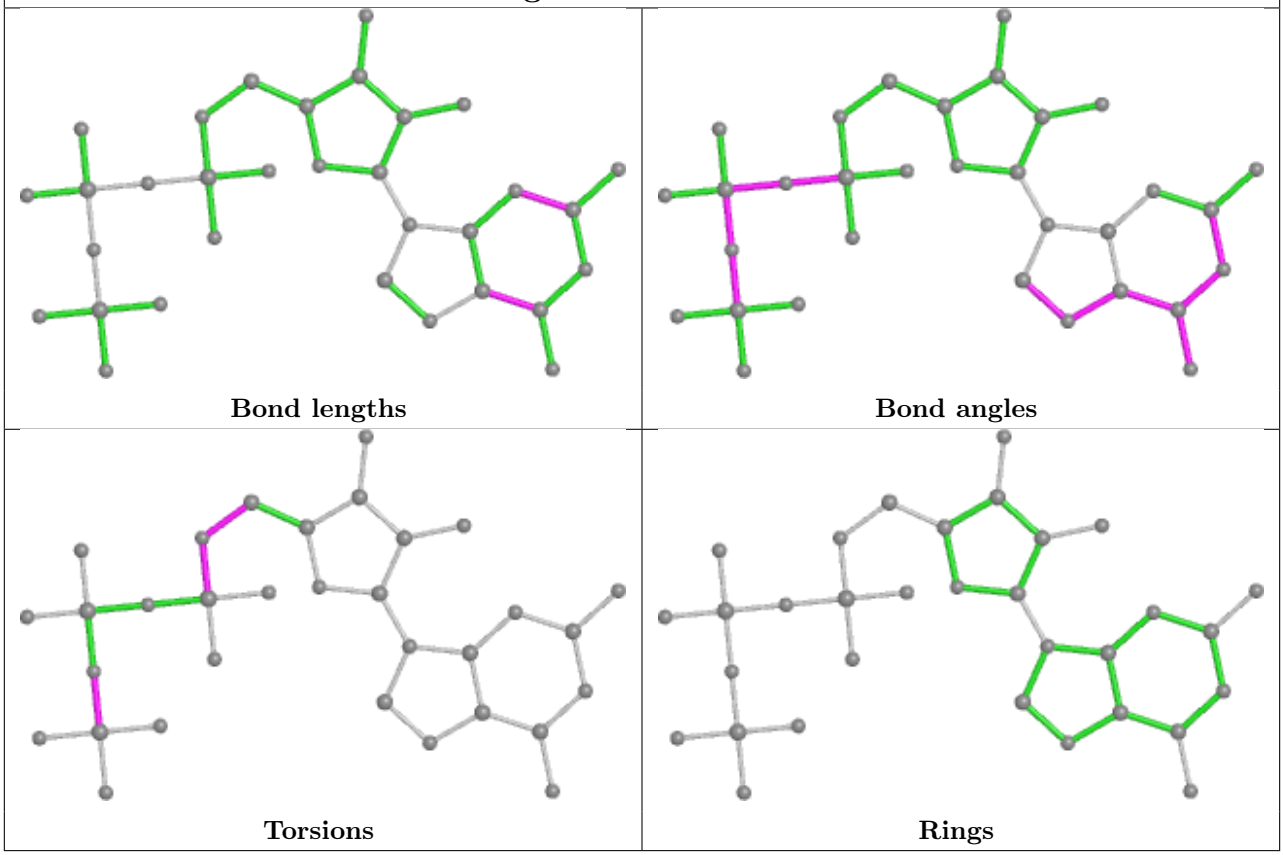


Torsions

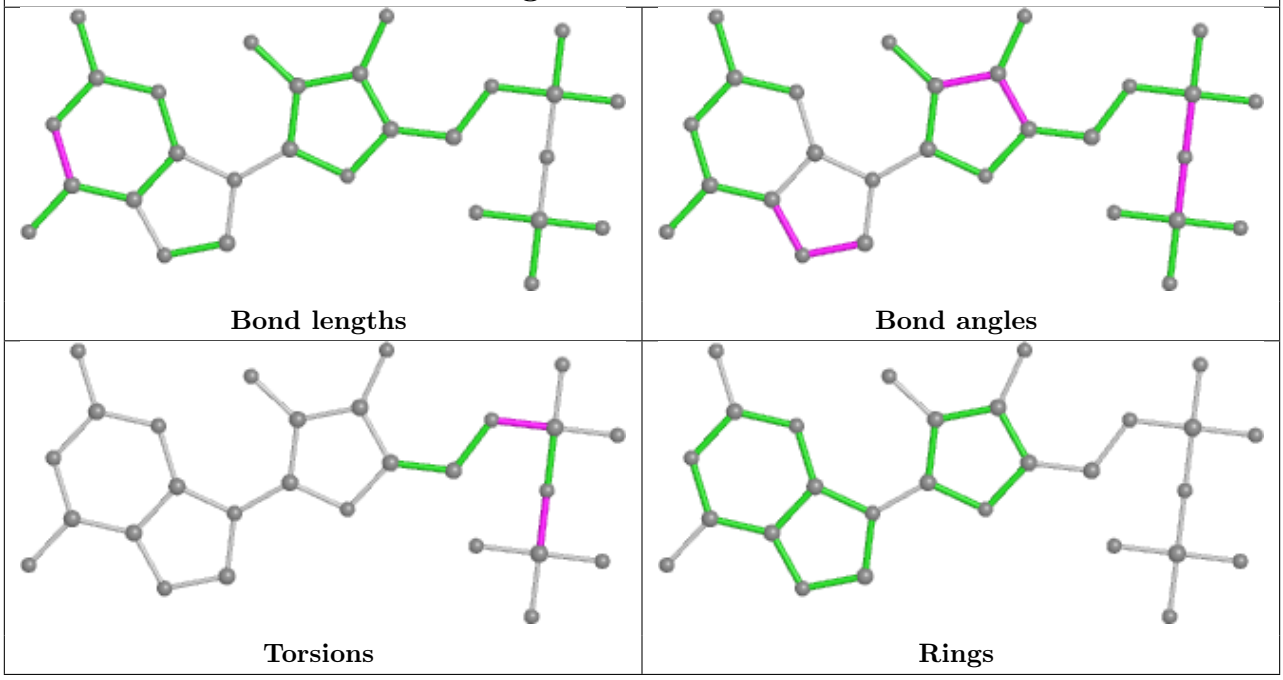


Rings

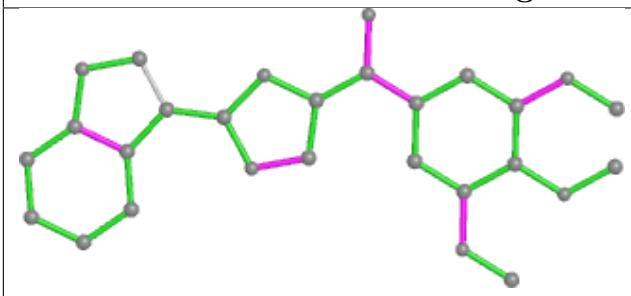
Ligand GTP C 501



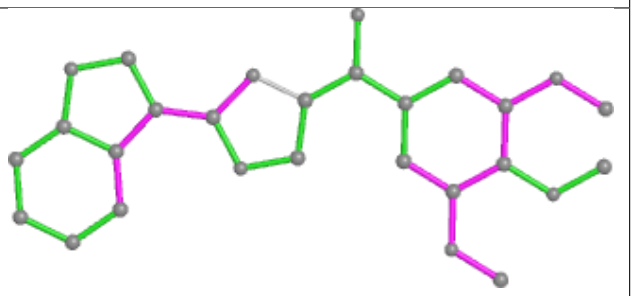
Ligand GDP D 501



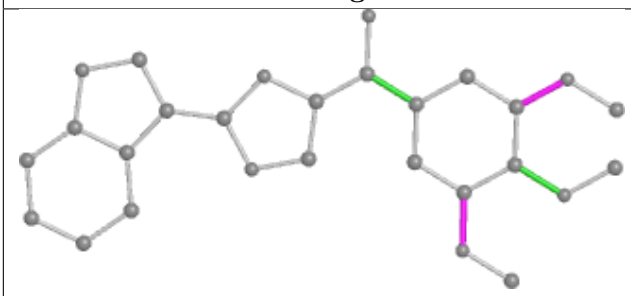
Ligand KUM D 502



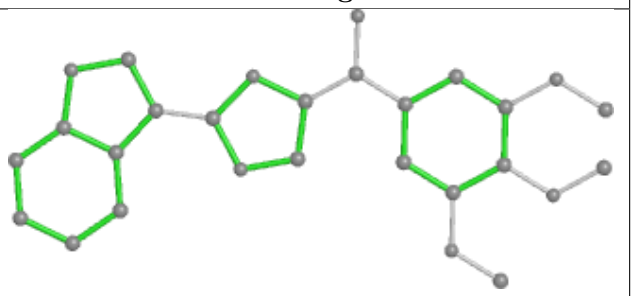
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	437/450 (97%)	0.11	9 (2%) 63 58	28, 46, 75, 95	0
1	C	440/450 (97%)	-0.04	1 (0%) 95 95	22, 34, 60, 86	0
2	B	427/445 (95%)	0.12	14 (3%) 46 39	20, 40, 79, 133	0
2	D	421/445 (94%)	0.73	54 (12%) 3 2	34, 71, 109, 137	0
3	E	121/143 (84%)	0.43	7 (5%) 23 17	30, 60, 102, 117	0
4	F	316/384 (82%)	1.23	84 (26%) 0 0	31, 75, 131, 152	0
All	All	2162/2317 (93%)	0.39	169 (7%) 13 9	20, 51, 106, 152	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	256	TYR	7.9
4	F	133	ALA	7.2
4	F	134	ALA	6.5
2	D	396	HIS	6.3
4	F	167	SER	6.0
4	F	224	SER	5.8
4	F	166	ALA	5.3
2	D	72	THR	5.2
4	F	24	THR	5.2
4	F	191	LEU	5.2
4	F	259	GLY	5.1
4	F	223	THR	4.9
2	D	180	VAL	4.8
4	F	258	GLU	4.8
4	F	225	SER	4.8
4	F	254	GLY	4.6
2	D	76	VAL	4.6
2	B	54	ALA	4.6
4	F	21	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	4.6
4	F	244	CYS	4.5
2	D	85	PHE	4.5
4	F	179	VAL	4.5
4	F	148	ILE	4.4
3	E	27	PRO	4.4
2	D	395	LEU	4.3
2	B	55	THR	4.2
2	D	98	GLY	4.2
2	D	55	THR	4.2
4	F	25	GLY	4.2
2	D	397	TRP	4.1
4	F	227	PRO	4.1
2	D	81	PHE	4.1
4	F	362	ALA	4.0
4	F	201	ILE	4.0
4	F	241	THR	4.0
4	F	20	LEU	4.0
4	F	180	HIS	4.0
2	D	44	LEU	4.0
4	F	100	ILE	4.0
4	F	173	ILE	4.0
2	B	56	GLY	3.9
4	F	196	HIS	3.9
4	F	161	LEU	3.9
4	F	182	ILE	3.9
2	D	54	ALA	3.8
2	D	80	PRO	3.8
4	F	253	TYR	3.7
2	D	35	SER	3.7
2	D	57	ASN	3.7
4	F	1	MET	3.7
4	F	140	GLU	3.7
1	A	262	TYR	3.6
4	F	198	LYS	3.6
4	F	230	SER	3.5
2	B	57	ASN	3.5
2	D	211	CYS	3.5
3	E	139	LEU	3.5
4	F	169	LEU	3.5
4	F	255	ARG	3.5
4	F	170	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	90	SER	3.4
2	D	92	PHE	3.4
4	F	270	TYR	3.4
4	F	361	LEU	3.3
4	F	132	LEU	3.3
4	F	257	GLU	3.3
2	D	59	TYR	3.2
1	A	178	SER	3.2
4	F	17	VAL	3.1
2	D	393	ALA	3.1
4	F	13	VAL	3.1
4	F	194	PRO	3.0
4	F	171	ASP	3.0
2	D	183	TYR	3.0
4	F	22	LEU	3.0
4	F	26	GLN	3.0
4	F	199	PHE	3.0
2	D	400	GLY	3.0
2	D	74	ASP	3.0
2	D	179	VAL	3.0
2	D	217	LEU	3.0
4	F	139	ARG	3.0
4	F	101	TYR	2.9
4	F	102	PRO	2.9
2	D	78	SER	2.9
4	F	267	PHE	2.9
2	D	391	ARG	2.9
2	D	398	TYR	2.9
4	F	228	TYR	2.9
3	E	46	SER	2.9
4	F	174	ASP	2.9
2	D	175	VAL	2.9
1	A	42	ILE	2.9
2	B	37	HIS	2.9
1	A	31	GLN	2.9
2	D	399	THR	2.9
2	D	37	HIS	2.9
4	F	190	LEU	2.9
4	F	197	ARG	2.8
3	E	68	LEU	2.8
4	F	23	ALA	2.8
4	F	260	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	263	PHE	2.8
1	C	1	MET	2.8
2	D	213	ARG	2.7
4	F	240	LEU	2.7
2	B	277	GLY	2.7
2	B	59	TYR	2.7
4	F	226	GLU	2.7
2	D	405	GLU	2.7
2	D	171	PRO	2.7
2	D	172	SER	2.6
2	D	219	THR	2.6
2	D	182	PRO	2.6
4	F	261	GLU	2.6
2	D	71	GLY	2.6
2	D	140	GLY	2.6
2	B	36	TYR	2.6
2	D	220	PRO	2.5
4	F	195	GLY	2.5
4	F	175	GLU	2.5
4	F	183	GLN	2.5
4	F	27	TRP	2.5
4	F	135	TYR	2.5
2	D	101	TRP	2.5
2	D	95	SER	2.5
4	F	98	TYR	2.4
4	F	275	LEU	2.4
2	D	31	ASP	2.4
4	F	189	PRO	2.4
2	D	385	PHE	2.4
4	F	339	ALA	2.4
4	F	99	VAL	2.4
1	A	147	SER	2.4
2	D	56	GLY	2.3
2	D	104	GLY	2.3
1	A	179	THR	2.3
2	B	281	TYR	2.3
4	F	19	ARG	2.3
2	B	58	LYS	2.3
2	D	73	MET	2.3
1	A	365	GLY	2.2
4	F	44	ARG	2.2
3	E	59	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	129	GLU	2.2
2	D	221	THR	2.2
2	D	224	ASP	2.2
2	B	60	VAL	2.2
2	B	83	GLN	2.2
1	A	282	TYR	2.2
4	F	163	SER	2.2
4	F	271	LEU	2.2
2	D	403	MET	2.1
4	F	5	VAL	2.1
1	A	201	ALA	2.1
2	D	33	THR	2.1
3	E	141	GLU	2.1
4	F	283	ILE	2.1
2	D	215	LEU	2.1
4	F	164	SER	2.1
2	B	44	LEU	2.1
4	F	192	LEU	2.1
2	D	176	SER	2.1
2	B	245	GLN	2.1
2	D	164	MET	2.1
2	D	387	ALA	2.1
3	E	45	PRO	2.0
4	F	320	MET	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)

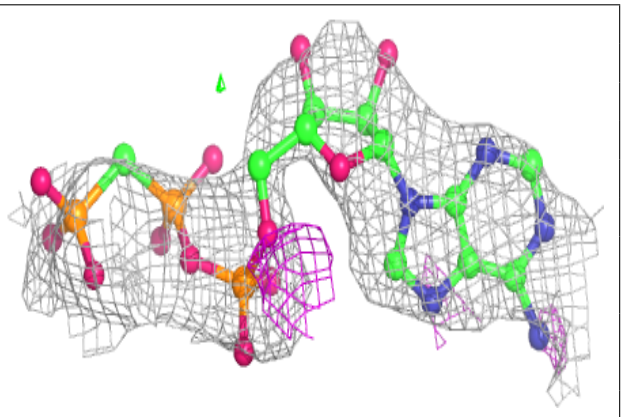
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

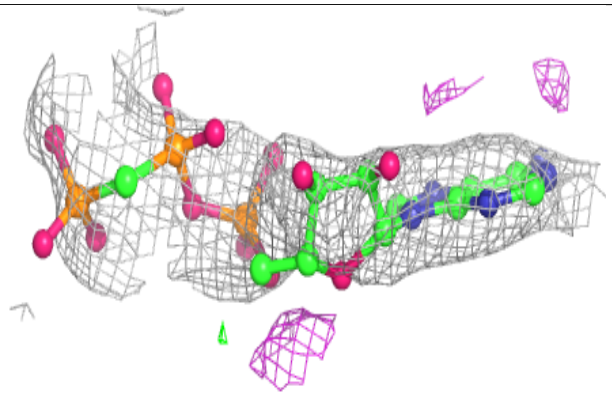
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	ACP	F	401	31/31	0.83	0.35	88,108,155,157	0
8	GDP	D	501	28/28	0.88	0.17	55,64,76,84	0
6	MG	B	502	1/1	0.88	0.29	39,39,39,39	0
9	MES	B	504	12/12	0.92	0.20	82,86,93,98	0
8	GDP	B	501	28/28	0.94	0.21	19,34,47,63	0
10	KUM	D	502	28/28	0.94	0.20	38,55,76,87	0
7	CA	C	503	1/1	0.94	0.07	55,55,55,55	0
7	CA	A	503	1/1	0.96	0.05	71,71,71,71	0
6	MG	C	502	1/1	0.96	0.16	39,39,39,39	0
9	MES	B	503	12/12	0.96	0.15	31,49,69,73	0
6	MG	A	502	1/1	0.97	0.18	43,43,43,43	0
10	KUM	B	505	28/28	0.97	0.19	25,38,53,58	0
5	GTP	A	501	32/32	0.98	0.20	26,29,38,42	0
5	GTP	C	501	32/32	0.98	0.17	27,28,33,35	0

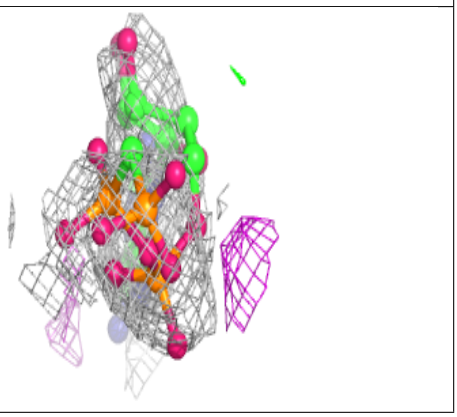
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

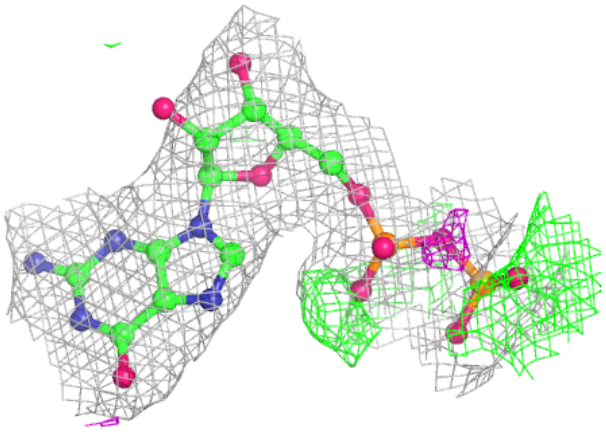


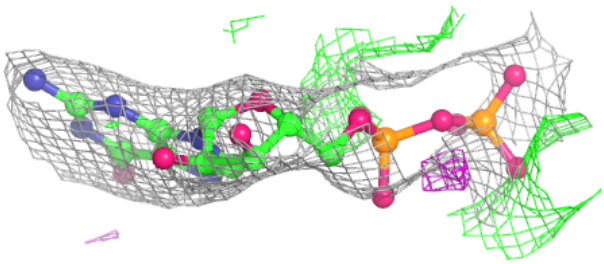


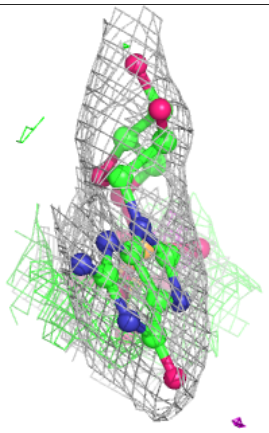


Electron density around GDP D 501:

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

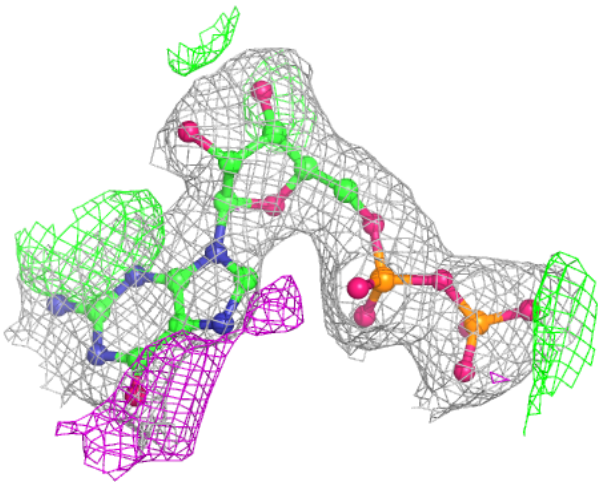


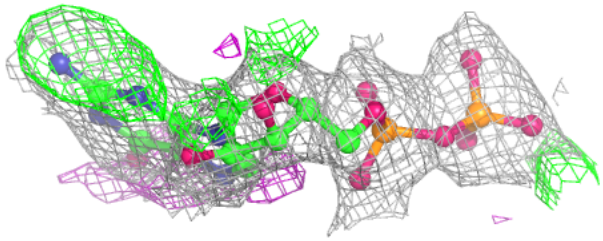


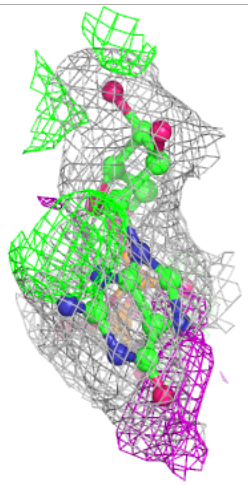


Electron density around GDP B 501:

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

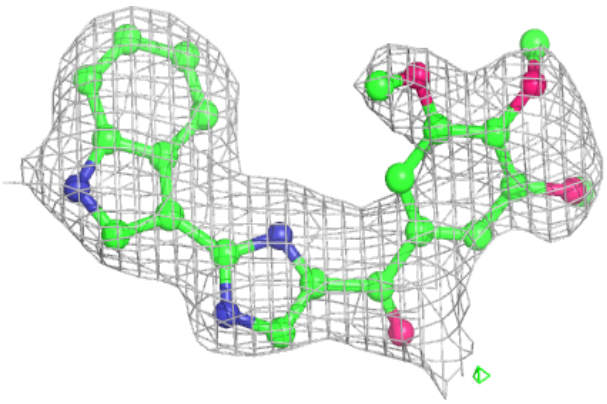


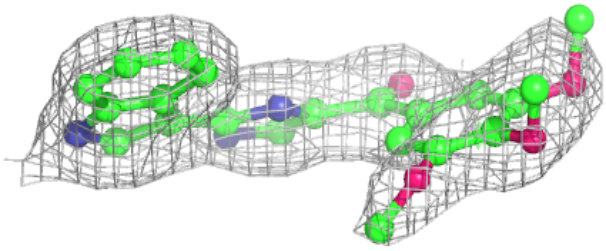


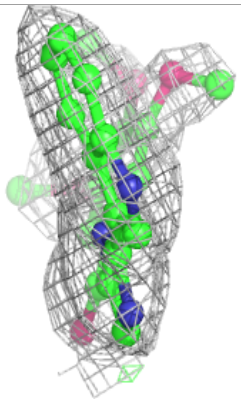


Electron density around KUM D 502:

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

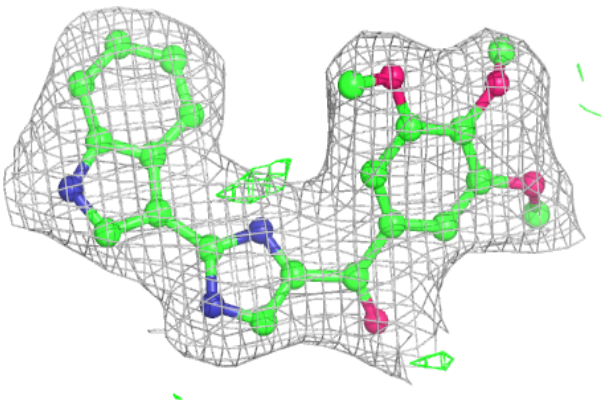


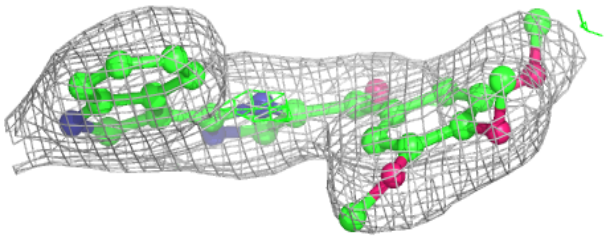


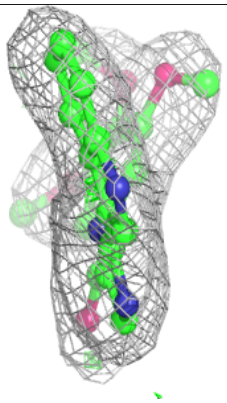


Electron density around KUM B 505:

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

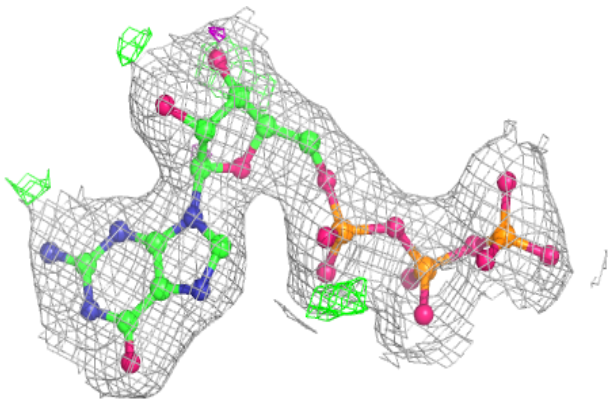


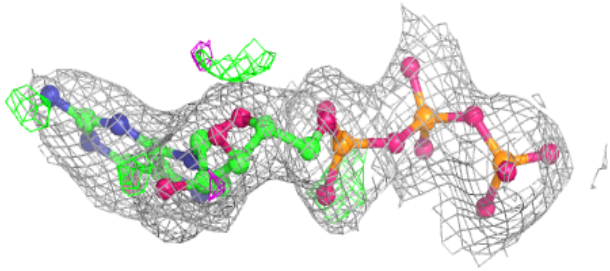


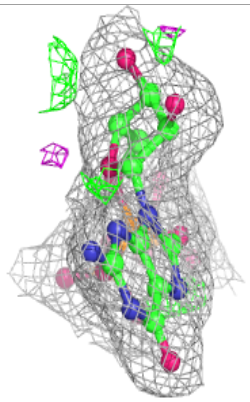


Electron density around GTP A 501:

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

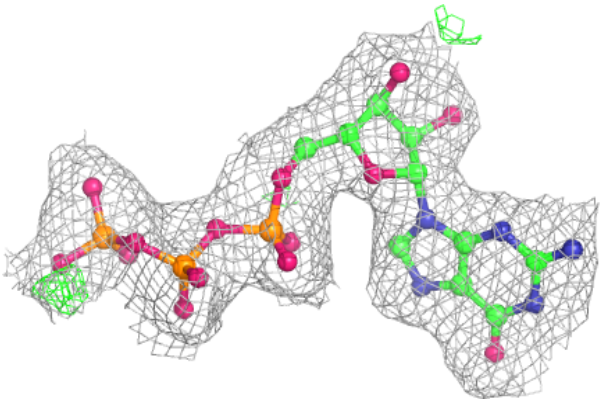


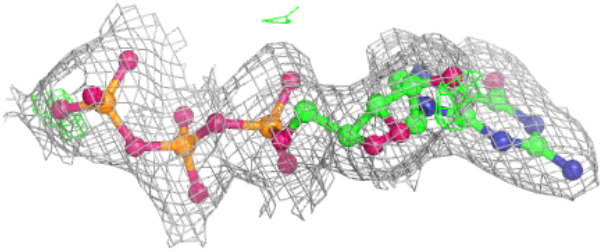


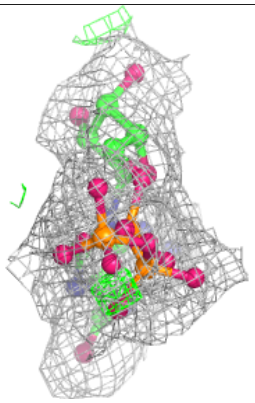


Electron density around GTP C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.