Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2024 – 07:39 PM EST

PDB ID	:	5S4L
Title	:	Tubulin-Z1891773393-complex
Authors	:	Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on	:	2020-11-08
Resolution	:	2.30 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:

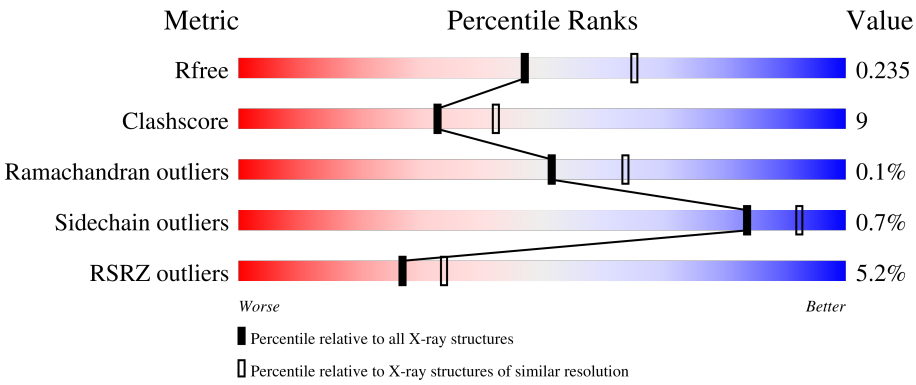
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	451	3% 76% 20% • •
1	C	451	% 80% 18% •
2	B	445	4% 75% 21% •
2	D	445	4% 76% 20% •
3	E	143	6% 74% 12% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	14% 73% 18% 8%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18067 atoms, of which 16 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3424	2167	582	653	22	0	0	0
1	C	440	3443	2178	585	657	23	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3359	2109	577	646	27	1	1	0
2	D	431	3368	2113	575	653	27	5	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1014	625	183	201	5	0	0	0

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	-	expression tag	UNP P63043

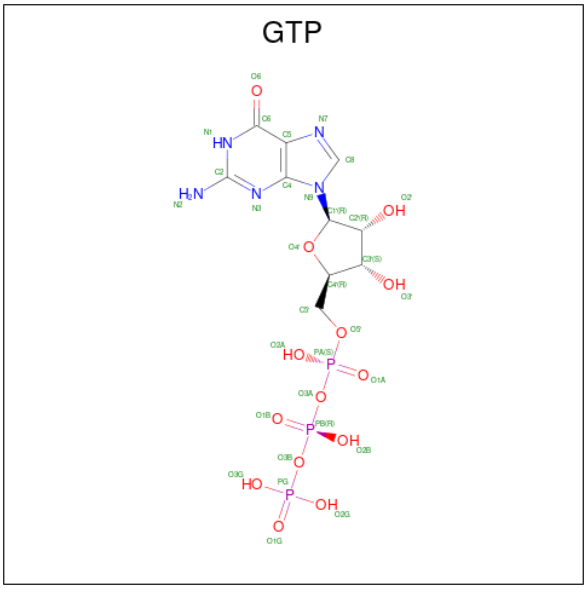
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	352	2877	1843	495	525	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	10	5	14	3	0	0
			Total	C	N	O	P		
5	C	1	32	10	5	14	3	0	0

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

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

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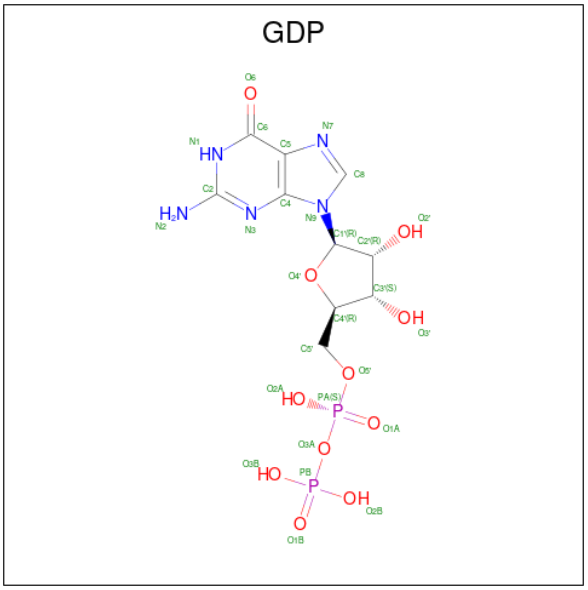
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

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

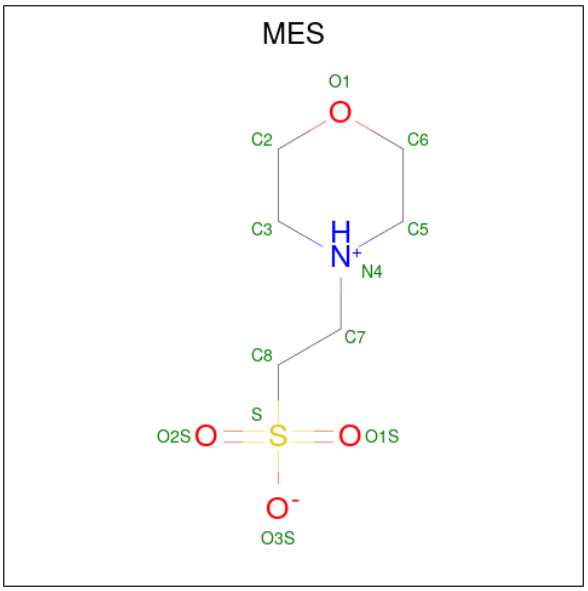
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	2	2	2	0	0
			Total	Ca		
7	B	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0

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



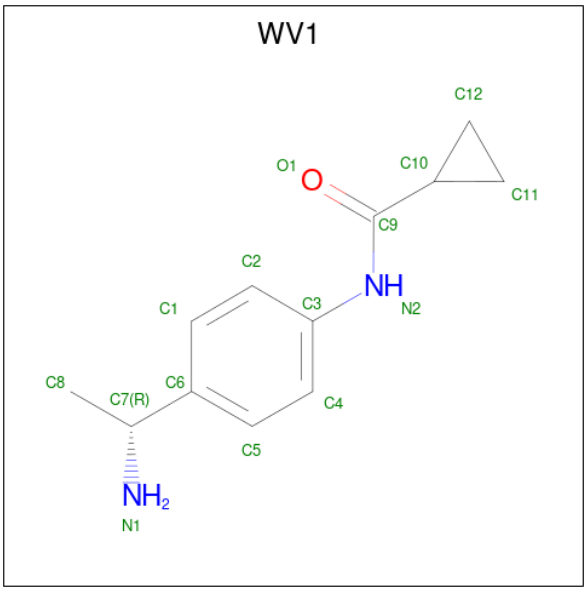
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
8	D	1	28	10	5	11	2	0	0

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



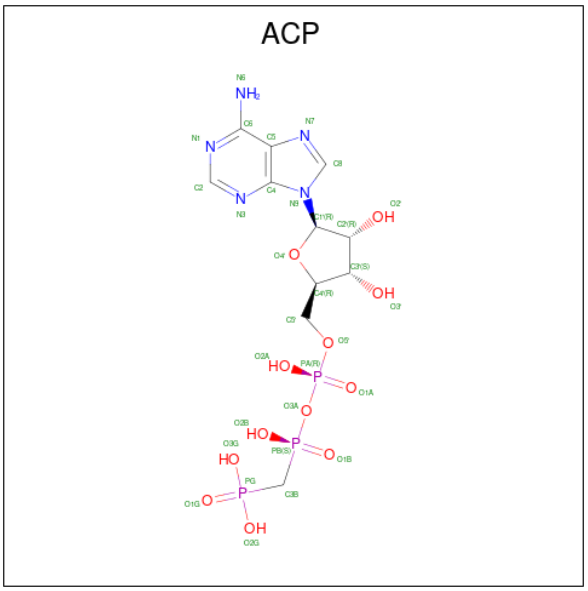
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is N-{4-[(1R)-1-aminoethyl]phenyl}cyclopropanecarboxamide (three-letter code: WV1) (formula: $C_{12}H_{16}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
10	D	1	31	12	16	2	1	0	0

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

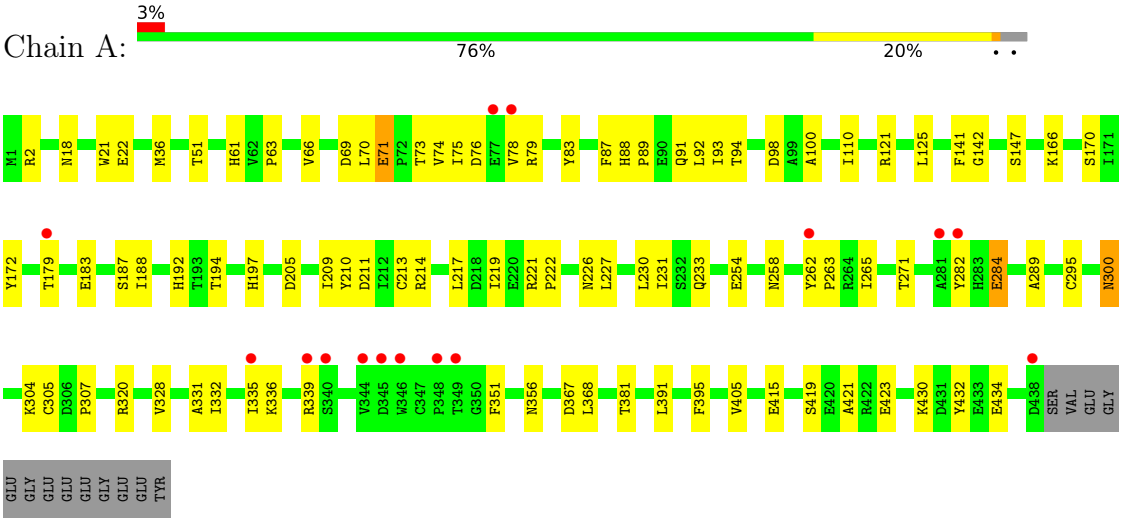
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	61	61	61	0	0
12	B	83	83	83	0	0
12	C	185	185	185	0	0
12	D	28	28	28	0	0
12	E	9	9	9	0	0
12	F	13	13	13	0	0

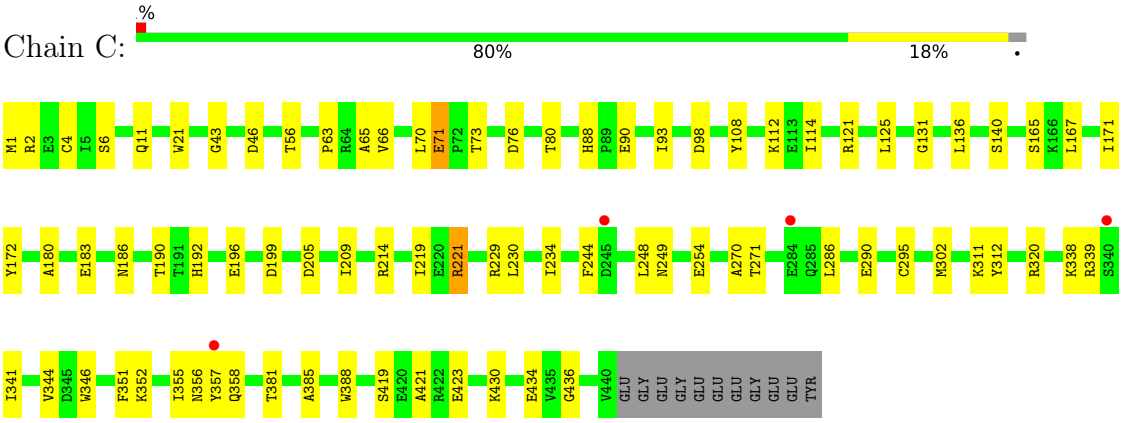
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

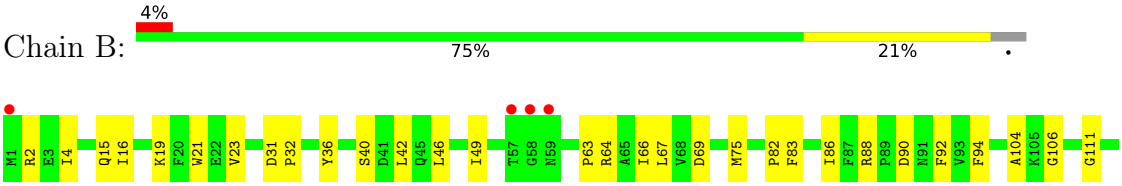
• Molecule 1: Tubulin alpha-1B chain

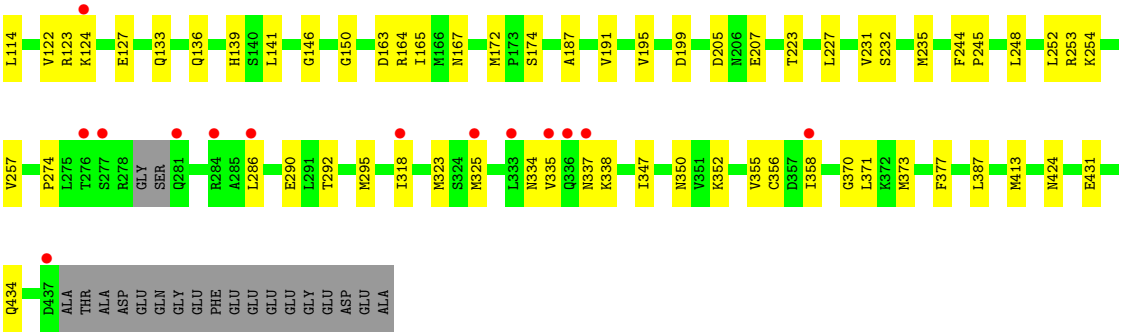


• Molecule 1: Tubulin alpha-1B chain



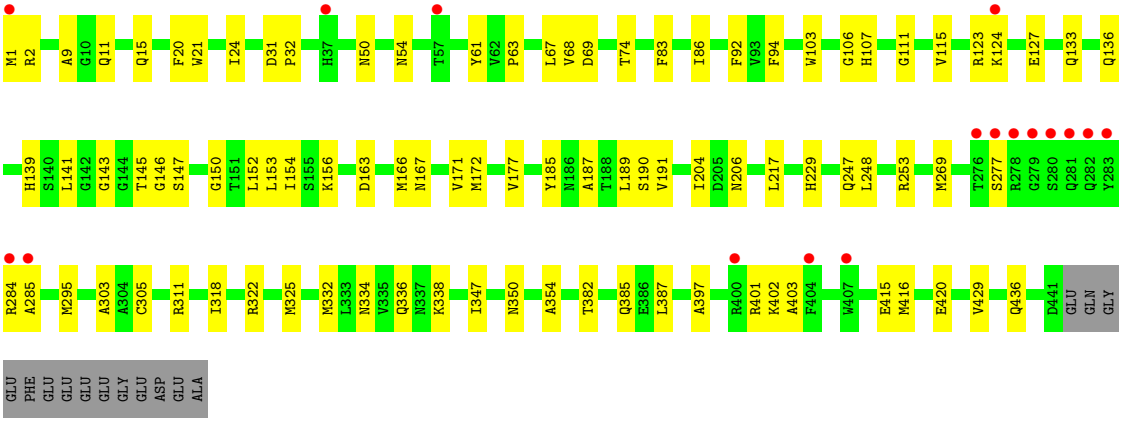
• Molecule 2: Tubulin beta-2B chain





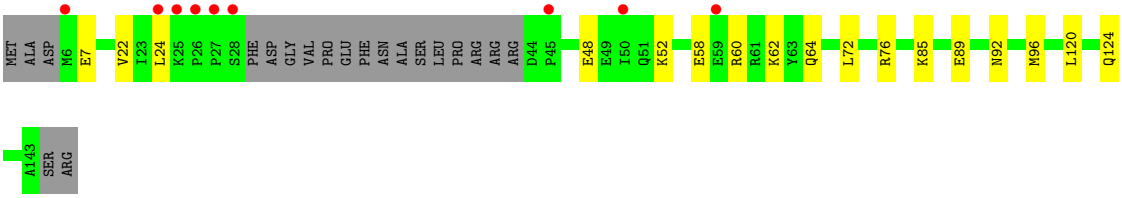
- Molecule 2: Tubulin beta-2B chain

Chain D:



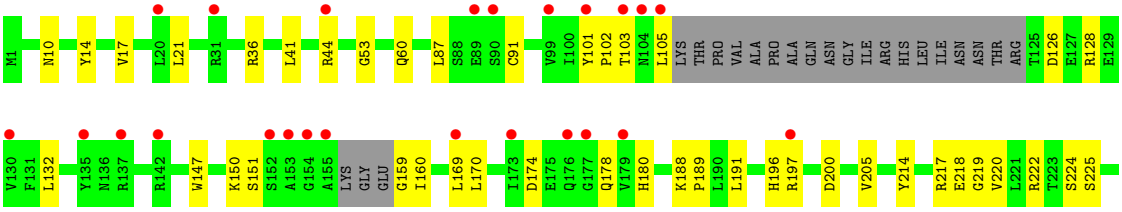
- Molecule 3: Stathmin-4

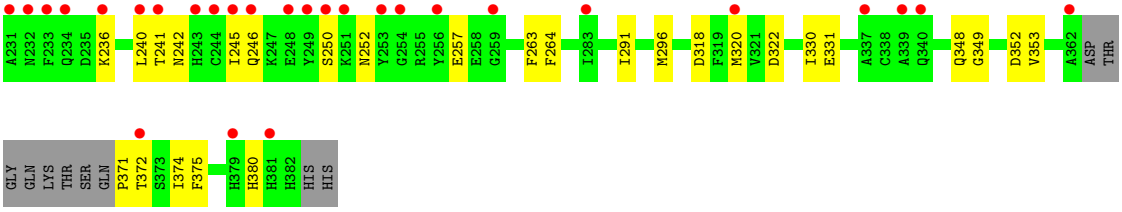
Chain E:



- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:




A231
N232
F233
Q234
D235
K236
L240
T241
N242
H243
C244
I245
Q246
K247
E248
Y249
S250
K251
N252
Y253
G254
R255
Y256
E257
E258
G259
F263
F264
I283
I291
M296
D318
F319
M320
V321
D322
I330
E331
A337
C338
A339
Q340
Q348
G349
D352
V353
A362
ASP
THR

GLY
GLN
LYS
THR
SER
GLN
P371
T372
S373
I374
F375
H379
H380
H381
H382
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	105.37Å 159.78Å 178.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.66 – 2.30 90.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (63.66-2.30) 99.6 (90.80-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.202 , 0.235 0.203 , 0.235	Depositor DCC
R_{free} test set	6627 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18067	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MES, GTP, MG, ACP, WV1, GDP

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	0.26	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.25	0/3433	0.41	0/4647
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.39	0/3978
All	All	0.25	0/17864	0.41	0/24179

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	3424	0	3335	70	0
1	C	3443	0	3352	52	0
2	B	3359	0	3235	69	0
2	D	3368	0	3236	59	0
3	E	1014	0	1029	11	0
4	F	2877	0	2839	50	0
5	A	32	0	12	1	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	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	12	0	12	4	0
10	D	15	16	0	0	0
11	F	31	0	14	6	0
12	A	61	0	0	2	0
12	B	83	0	0	1	0
12	C	185	0	0	3	0
12	D	28	0	0	0	0
12	E	9	0	0	0	0
12	F	13	0	0	1	0
All	All	18051	16	17100	303	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 9.

All (303) 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)
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.38	1.02
2:D:217:LEU:HA	2:D:277:SER:HB3	1.43	0.99
4:F:318:ASP:OD2	11:F:401:ACP:O2G	1.93	0.86
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.60	0.84
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.44	0.83
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.61	0.82
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.63	0.81
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.00	0.79
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.17	0.77
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.69	0.75
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.21	0.74
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.04	0.74
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.71	0.73
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.73
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.53	0.72
2:B:83:PHE:O	2:B:86:ILE:HG22	1.90	0.71
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.40	0.70
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.74	0.69
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.74	0.69
1:C:271:THR:HG21	1:C:295:CYS:O	1.94	0.68
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.74	0.68
1:C:76:ASP:O	1:C:80:THR:HG22	1.93	0.68
1:C:270:ALA:O	1:C:302:MET:HG2	1.93	0.68
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.27	0.68
4:F:371:PRO:HA	4:F:372:THR:O	1.94	0.67
1:A:179:THR:HA	2:B:352:LYS:HD2	1.76	0.67
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.10	0.67
2:B:424:ASN:HB3	12:B:610:HOH:O	1.95	0.66
2:D:83:PHE:O	2:D:86:ILE:HG22	1.95	0.65
4:F:91:CYS:HA	12:F:511:HOH:O	1.95	0.65
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.77	0.65
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.78	0.65
3:E:85:LYS:O	3:E:89:GLU:HG3	1.96	0.65
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.13	0.64
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.12	0.63
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.33	0.63
2:B:136:GLN:HA	2:B:167:ASN:O	1.97	0.63
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.80	0.63
1:A:166:LYS:HE2	1:A:197:HIS:O	1.99	0.62
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.32	0.62
1:C:419:SER:O	1:C:423:GLU:HG3	1.99	0.62
1:C:320:ARG:HA	1:C:356:ASN:O	2.00	0.62
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.64	0.61
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.14	0.61
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.82	0.60
1:A:74:VAL:HB	12:A:603:HOH:O	2.01	0.60
2:D:152:LEU:O	2:D:156:LYS:HG2	2.01	0.60
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.84	0.60
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.32	0.60
4:F:371:PRO:HA	4:F:372:THR:C	2.21	0.60
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.01	0.60
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.41	0.60
2:D:147:SER:HB2	2:D:190:SER:OG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:159:GLY:C	4:F:160:ILE:HD12	2.23	0.59
2:D:332:MET:O	2:D:336:GLN:HG3	2.03	0.59
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.85	0.59
1:C:1:MET:O	12:C:601:HOH:O	2.16	0.59
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.85	0.59
1:C:209:ILE:HD11	1:C:302:MET:CE	2.30	0.59
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.84	0.59
2:D:69:ASP:O	2:D:94:PHE:HA	2.04	0.58
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.39	0.58
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.84	0.58
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.38	0.58
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.86	0.57
4:F:296:MET:SD	4:F:380:HIS:HB2	2.45	0.57
4:F:320:MET:CG	4:F:330:ILE:HD11	2.35	0.57
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.57
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.70	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.57
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.41	0.56
1:A:300:ASN:HB3	12:A:601:HOH:O	2.04	0.56
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.87	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.06	0.56
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.87	0.56
4:F:371:PRO:CA	4:F:372:THR:HB	2.36	0.56
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.88	0.55
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.06	0.55
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.69	0.55
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.41	0.55
1:A:141:PHE:HB3	1:A:187:SER:OG	2.07	0.55
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.35	0.55
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.88	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.55
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.39	0.55
2:B:106:GLY:O	2:B:111:GLY:HA3	2.06	0.55
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.89	0.54
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.89	0.54
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.43	0.54
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.08	0.54
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.42	0.54
2:B:141:LEU:HD12	2:B:172:MET:SD	2.47	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.54
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:371:PRO:HA	4:F:372:THR:HB	1.89	0.53
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.73	0.53
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.91	0.53
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.91	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.53
2:B:199:ASP:OD1	9:B:504:MES:H62	2.08	0.53
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.73	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.45	0.52
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.74	0.52
1:A:179:THR:HG21	2:B:248:LEU:CB	2.38	0.52
2:B:205:ASP:OD1	2:B:207:GLU:N	2.39	0.52
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.92	0.52
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.35	0.52
2:B:223:THR:O	2:B:227:LEU:HD13	2.10	0.52
2:B:370:GLY:O	2:B:371:LEU:HD23	2.10	0.52
1:A:69:ASP:O	1:A:94:THR:HA	2.10	0.52
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.92	0.52
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.45	0.52
1:C:165:SER:HA	1:C:199:ASP:OD2	2.10	0.51
2:D:397:ALA:O	2:D:401:ARG:NH1	2.43	0.51
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.45	0.51
1:A:284:GLU:CD	1:A:284:GLU:H	2.14	0.51
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.45	0.51
2:D:124:LYS:C	2:D:124:LYS:HD3	2.30	0.51
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.91	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.91	0.51
2:D:106:GLY:O	2:D:111:GLY:HA3	2.11	0.51
3:E:92:ASN:O	3:E:96:MET:HG2	2.10	0.50
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.11	0.50
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.94	0.50
2:B:295:MET:CG	2:B:377:PHE:HB2	2.42	0.50
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.47	0.50
3:E:72:LEU:O	3:E:76:ARG:HG2	2.11	0.50
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.46	0.50
1:C:108:TYR:O	1:C:112:LYS:HG2	2.12	0.50
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.11	0.50
3:E:120:LEU:O	3:E:124:GLN:HG3	2.12	0.50
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.12	0.50
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.27	0.50
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.42	0.50
4:F:246:GLN:O	4:F:250:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:O	1:A:423:GLU:HG3	2.12	0.50
2:B:174:SER:OG	2:B:207:GLU:HB2	2.12	0.50
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.94	0.50
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.93	0.50
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.93	0.49
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.49
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.42	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.49
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.43	0.49
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.42	0.49
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.95	0.49
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.45	0.49
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.93	0.49
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.43	0.49
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.13	0.49
2:B:187:ALA:O	2:B:191:VAL:HG23	2.13	0.48
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.48	0.48
1:A:254:GLU:HG2	1:A:258:ASN:HD21	1.79	0.48
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.48
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.96	0.47
2:B:123:ARG:O	2:B:127:GLU:HG3	2.14	0.47
2:B:42:LEU:H	2:B:42:LEU:HD12	1.79	0.47
1:C:196:GLU:HG2	12:C:660:HOH:O	2.14	0.47
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.97	0.47
4:F:349:GLY:O	4:F:353:VAL:HG22	2.14	0.47
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.80	0.47
1:A:271:THR:HG23	1:A:300:ASN:HD22	1.79	0.47
2:B:318:ILE:N	2:B:318:ILE:HD12	2.29	0.47
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.50	0.47
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.97	0.46
1:C:234:ILE:HD12	1:C:234:ILE:H	1.80	0.46
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.50	0.46
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.97	0.46
2:D:284:ARG:O	2:D:285:ALA:HB3	2.16	0.46
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.15	0.46
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.51	0.46
2:B:164:ARG:O	9:B:504:MES:H31	2.14	0.46
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.97	0.46
2:B:124:LYS:HD3	2:B:124:LYS:C	2.36	0.46
2:D:1:MET:CE	2:D:50:ASN:HB2	2.44	0.46
1:A:289:ALA:HA	1:A:331:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:ARG:NH1	2:D:436:GLN:O	2.49	0.45
1:A:227:LEU:O	1:A:231:ILE:HG13	2.15	0.45
1:C:311:LYS:HD2	1:C:436:GLY:O	2.16	0.45
1:A:213:CYS:O	1:A:217:LEU:HB2	2.16	0.45
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.97	0.45
1:C:229:ARG:NH1	12:C:610:HOH:O	2.49	0.45
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.45
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.52	0.45
4:F:222:ARG:O	4:F:241:THR:HB	2.17	0.45
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.99	0.45
2:B:46:LEU:HA	2:B:49:ILE:HB	1.98	0.45
1:C:11:GLN:HE22	2:D:247:GLN:CD	2.21	0.45
1:A:187:SER:CB	1:A:391:LEU:HD21	2.47	0.45
2:D:11:GLN:HA	2:D:74:THR:HG21	1.98	0.45
2:D:163:ASP:O	2:D:253:ARG:NH2	2.45	0.45
1:A:271:THR:CG2	1:A:300:ASN:HD22	2.30	0.45
3:E:60:ARG:O	3:E:64:GLN:HG3	2.17	0.45
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.44
1:A:405:VAL:HG11	1:A:415:GLU:HG3	1.99	0.44
2:B:114:LEU:O	2:B:114:LEU:HG	2.16	0.44
2:B:231:VAL:O	2:B:235:MET:HG3	2.18	0.44
1:C:6:SER:O	1:C:65:ALA:HA	2.16	0.44
4:F:150:LYS:HZ3	11:F:401:ACP:C8	2.31	0.44
2:D:9:ALA:HA	2:D:68:VAL:O	2.18	0.44
4:F:197:ARG:HB2	4:F:224:SER:O	2.18	0.44
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.53	0.44
2:B:323:MET:HE2	2:B:373:MET:HB2	1.99	0.44
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.33	0.44
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.51	0.44
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.33	0.44
2:B:253[B]:ARG:O	2:B:257:VAL:HG23	2.18	0.44
2:B:253[A]:ARG:O	2:B:257:VAL:HG23	2.18	0.44
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.45	0.43
2:D:187:ALA:O	2:D:191:VAL:HG23	2.18	0.43
4:F:178:GLN:HE21	4:F:180:HIS:HE1	1.66	0.43
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.36	0.43
4:F:101:TYR:N	4:F:126:ASP:OD1	2.40	0.43
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.49	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.43
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.53	0.43
1:C:248:LEU:HD13	1:C:355:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.43
1:A:328:VAL:O	1:A:332:ILE:HG13	2.18	0.43
2:B:19:LYS:O	2:B:23:VAL:HG23	2.19	0.43
1:A:100:ALA:HB1	2:B:253[B]:ARG:HG2	2.01	0.43
2:D:217:LEU:HA	2:D:277:SER:CB	2.32	0.43
2:D:382:THR:O	2:D:385:GLN:HG2	2.19	0.43
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.42
2:B:191:VAL:O	2:B:195:VAL:HG23	2.18	0.42
2:D:123:ARG:O	2:D:127:GLU:HG3	2.18	0.42
3:E:7:GLU:O	3:E:22:VAL:HA	2.17	0.42
3:E:58:GLU:HG2	3:E:62:LYS:HE3	2.01	0.42
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.53	0.42
2:D:115:VAL:HG23	2:D:153:LEU:HD23	2.00	0.42
4:F:17:VAL:O	4:F:21:LEU:HG	2.19	0.42
1:A:320:ARG:HA	1:A:356:ASN:O	2.20	0.42
2:B:67:LEU:N	2:B:67:LEU:HD12	2.34	0.42
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.02	0.42
2:B:325:MET:HE2	2:B:355:VAL:HG21	2.02	0.42
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.42
4:F:53:GLY:N	4:F:60:GLN:OE1	2.41	0.42
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.19	0.42
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.52	0.42
9:B:504:MES:H81	9:B:504:MES:H51	1.78	0.42
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.55	0.42
1:A:271:THR:HG21	1:A:295:CYS:O	2.19	0.42
2:D:146:GLY:O	2:D:150:GLY:HA3	2.20	0.42
1:A:100:ALA:CB	2:B:253[B]:ARG:HG2	2.50	0.42
1:A:305:CYS:O	1:A:307:PRO:HD3	2.20	0.42
2:B:104:ALA:HB2	2:B:413:MET:SD	2.59	0.42
2:B:355:VAL:HG12	2:B:356:CYS:N	2.35	0.42
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.02	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:D:322:ARG:NH1	2:D:322:ARG:HB3	2.34	0.42
2:D:107:HIS:O	2:D:152:LEU:HD22	2.20	0.42
2:D:141:LEU:HD12	2:D:172:MET:SD	2.60	0.42
4:F:87:LEU:O	4:F:91:CYS:HB2	2.20	0.42
1:A:66:VAL:HG23	1:A:125:LEU:HD12	2.00	0.41
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.35	0.41
1:A:214:ARG:HG2	1:A:219:ILE:O	2.20	0.41
2:B:40:SER:OG	2:B:42:LEU:HD13	2.20	0.41
1:C:43:GLY:HA2	1:C:56:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.41
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.01	0.41
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.01	0.41
2:B:146:GLY:O	2:B:150:GLY:HA3	2.20	0.41
2:B:431:GLU:O	2:B:434:GLN:HG2	2.21	0.41
1:C:46:ASP:OD1	1:C:46:ASP:N	2.52	0.41
2:D:295:MET:HE3	2:D:295:MET:HB2	1.74	0.41
2:B:323:MET:HB3	2:B:373:MET:CE	2.51	0.41
2:D:11:GLN:O	2:D:15:GLN:HG2	2.20	0.41
2:D:416:MET:O	2:D:420:GLU:HG3	2.20	0.41
1:C:234:ILE:HG12	1:C:302:MET:HE2	2.02	0.41
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.56	0.41
2:B:235:MET:HE2	2:B:235:MET:HB3	1.89	0.41
2:D:185:TYR:HE2	2:D:403:ALA:O	2.04	0.41
4:F:225:SER:HB2	4:F:252:ASN:O	2.20	0.41
4:F:371:PRO:HA	4:F:372:THR:CB	2.49	0.41
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.39	0.41
1:A:2:ARG:O	1:A:51:THR:HG22	2.20	0.41
2:B:4:ILE:O	2:B:64:ARG:HD2	2.20	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.41
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.41
1:A:75:ILE:HB	1:A:94:THR:HG21	2.02	0.41
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.95	0.41
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.85	0.41
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.02	0.41
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.21	0.41
1:C:234:ILE:HD12	1:C:234:ILE:N	2.35	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.56	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.40
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.87	0.40
1:C:286:LEU:HA	1:C:286:LEU:HD23	1.93	0.40
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.40
2:D:145:THR:HB	8:D:501:GDP:O2B	2.21	0.40
2:D:303:ALA:O	2:D:305:CYS:N	2.49	0.40
4:F:189:PRO:HA	4:F:322:ASP:HA	2.04	0.40
1:A:87:PHE:HA	1:A:91:GLN:OE1	2.22	0.40
1:C:186:ASN:O	1:C:190:THR:HG22	2.21	0.40
2:D:54:ASN:O	2:D:61:TYR:HA	2.21	0.40
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.56	0.40
1:A:194:THR:O	1:A:194:THR:HG22	2.20	0.40
1:A:430:LYS:O	1:A:434:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HB2	1:C:98:ASP:HA	2.02	0.40
1:C:180:ALA:O	1:C:183:GLU:HG3	2.21	0.40
4:F:188:LYS:O	4:F:322:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	429 (98%)	7 (2%)	0	100	100
1	C	439/451 (97%)	429 (98%)	9 (2%)	1 (0%)	47	58
2	B	422/445 (95%)	409 (97%)	12 (3%)	1 (0%)	47	58
2	D	429/445 (96%)	417 (97%)	12 (3%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	334 (97%)	10 (3%)	0	100	100
All	All	2189/2319 (94%)	2136 (98%)	51 (2%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	LYS
2	B	82	PRO

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	369/379 (97%)	363 (98%)	6 (2%)	62	78
1	C	372/379 (98%)	367 (99%)	5 (1%)	69	82
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	97
2	D	368/383 (96%)	366 (100%)	2 (0%)	88	95
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1902/1993 (95%)	1888 (99%)	14 (1%)	84	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
1	A	381	THR
2	B	139	HIS
1	C	2	ARG
1	C	71	GLU
1	C	221	ARG
1	C	339	ARG
1	C	381	THR
2	D	139	HIS
2	D	229	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
2	B	15	GLN
2	B	294	GLN
1	C	11	GLN
2	D	294	GLN
4	F	180	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

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Mol	Chain	Res	Type
4	F	380	HIS

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 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
8	GDP	B	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)
10	WV1	D	503	-	15,16,16	0.94	2 (13%)	20,22,22	0.44	0
11	ACP	F	401	6	27,33,33	1.42	5 (18%)	32,52,52	1.44	4 (12%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.96	6 (42%)
5	GTP	A	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.39	6 (18%)
5	GTP	C	501	6	26,34,34	1.10	2 (7%)	32,54,54	1.32	5 (15%)
8	GDP	D	501	6	24,30,30	0.92	1 (4%)	30,47,47	1.09	3 (10%)

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
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
10	WV1	D	503	-	-	6/12/14/14	0/2/2/2
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.50	1.66	1.77
5	A	501	GTP	C5-C6	-3.94	1.39	1.47
5	C	501	GTP	C5-C6	-3.81	1.39	1.47
11	F	401	ACP	PG-O3G	3.01	1.61	1.54
11	F	401	ACP	PB-O3A	2.92	1.61	1.58
11	F	401	ACP	PG-O2G	2.87	1.61	1.54
10	D	503	WV1	C7-N1	-2.64	1.40	1.48
11	F	401	ACP	C5-C4	2.55	1.47	1.40
8	B	501	GDP	C6-N1	-2.39	1.34	1.37
10	D	503	WV1	C10-C9	-2.37	1.47	1.51
11	F	401	ACP	PB-O2B	2.28	1.61	1.56
8	D	501	GDP	C6-N1	-2.22	1.34	1.37
5	C	501	GTP	C2-N3	2.20	1.38	1.33
5	A	501	GTP	C2-N3	2.09	1.38	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F	401	ACP	PB-O3A-PA	-3.87	120.29	132.56
9	B	504	MES	C5-N4-C3	3.70	117.15	108.83
11	F	401	ACP	C3'-C2'-C1'	3.44	106.16	100.98
5	C	501	GTP	C8-N7-C5	3.17	109.04	102.99
11	F	401	ACP	N3-C2-N1	-3.11	123.82	128.68
5	A	501	GTP	PA-O3A-PB	-3.07	122.30	132.83
5	A	501	GTP	C5-C6-N1	3.06	119.35	113.95
5	A	501	GTP	C8-N7-C5	2.99	108.68	102.99
8	B	501	GDP	PA-O3A-PB	-2.97	122.63	132.83
5	C	501	GTP	PA-O3A-PB	-2.88	122.93	132.83
9	B	504	MES	C6-C5-N4	-2.83	105.81	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	501	GTP	C5-C6-N1	2.80	118.90	113.95
8	D	501	GDP	PA-O3A-PB	-2.73	123.45	132.83
5	A	501	GTP	C2-N1-C6	-2.73	120.07	125.10
11	F	401	ACP	C4-C5-N7	-2.58	106.71	109.40
5	C	501	GTP	C2-N1-C6	-2.54	120.41	125.10
5	A	501	GTP	PB-O3B-PG	-2.54	124.10	132.83
9	B	504	MES	O3S-S-C8	2.53	109.85	105.77
5	C	501	GTP	PB-O3B-PG	-2.51	124.23	132.83
8	B	501	GDP	C5-C6-N1	2.45	118.27	113.95
8	B	501	GDP	C8-N7-C5	2.43	107.62	102.99
9	B	504	MES	O1S-S-C8	2.41	109.82	106.92
8	D	501	GDP	C8-N7-C5	2.41	107.58	102.99
9	B	504	MES	C7-N4-C5	2.37	117.30	111.23
8	D	501	GDP	C5-C6-N1	2.27	117.96	113.95
5	A	501	GTP	O6-C6-C5	-2.09	120.28	124.37
9	B	504	MES	O2S-S-C8	2.07	109.41	106.92

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	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	PA-O3A-PB-O3B
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
10	D	503	WV1	C11-C10-C9-N2
10	D	503	WV1	C12-C10-C9-N2
10	D	503	WV1	C12-C10-C9-O1
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C3'-C4'-C5'-O5'
10	D	503	WV1	C10-C9-N2-C3
10	D	503	WV1	O1-C9-N2-C3
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
9	B	504	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
10	D	503	WV1	C11-C10-C9-O1
5	C	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

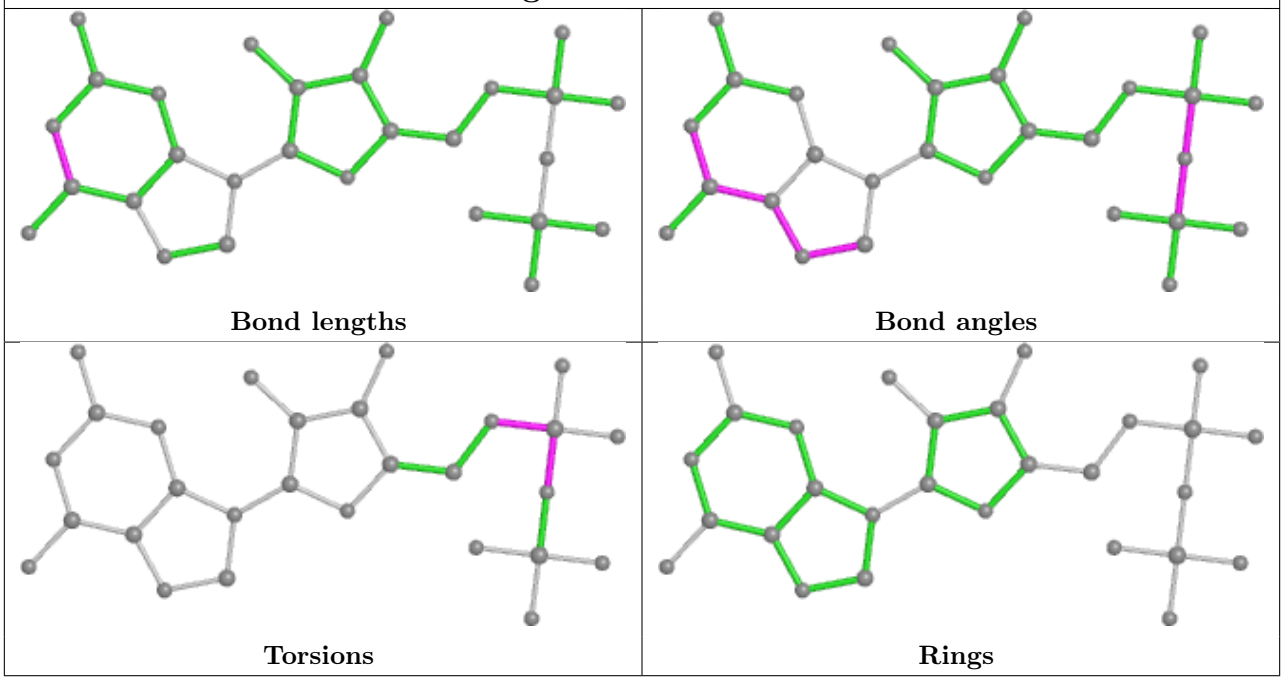
5 monomers are involved in 14 short contacts:

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

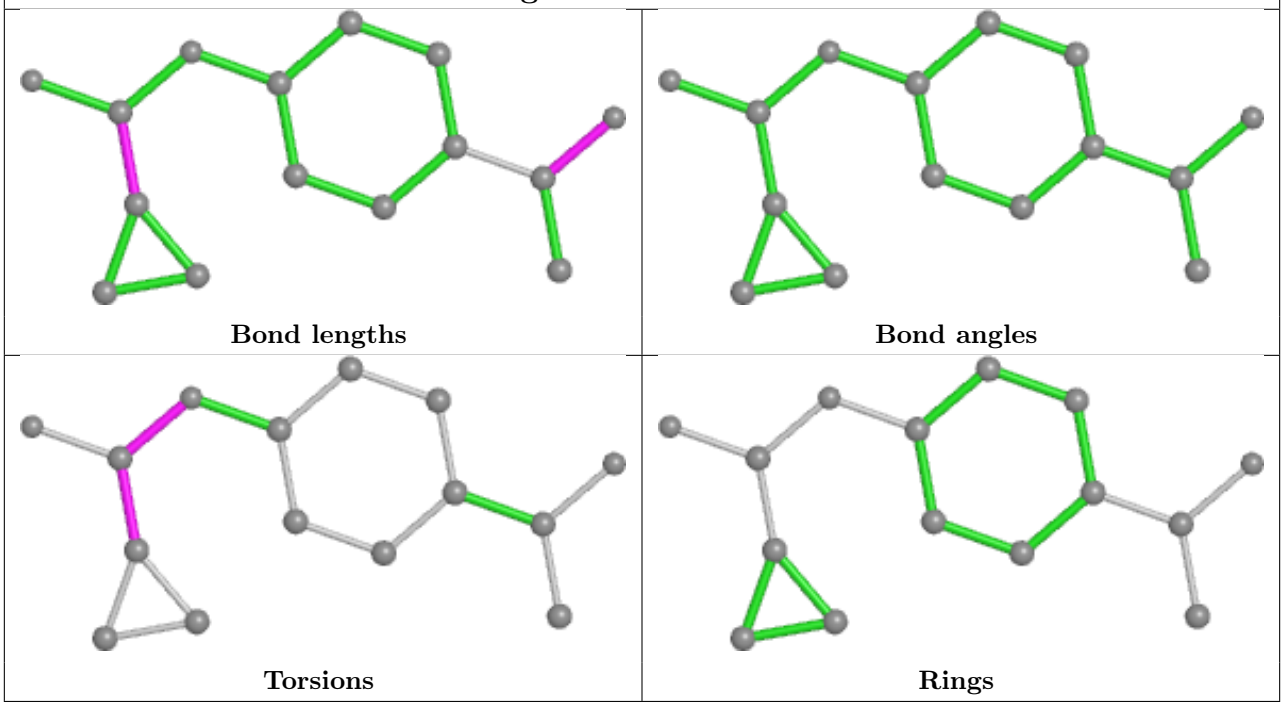
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

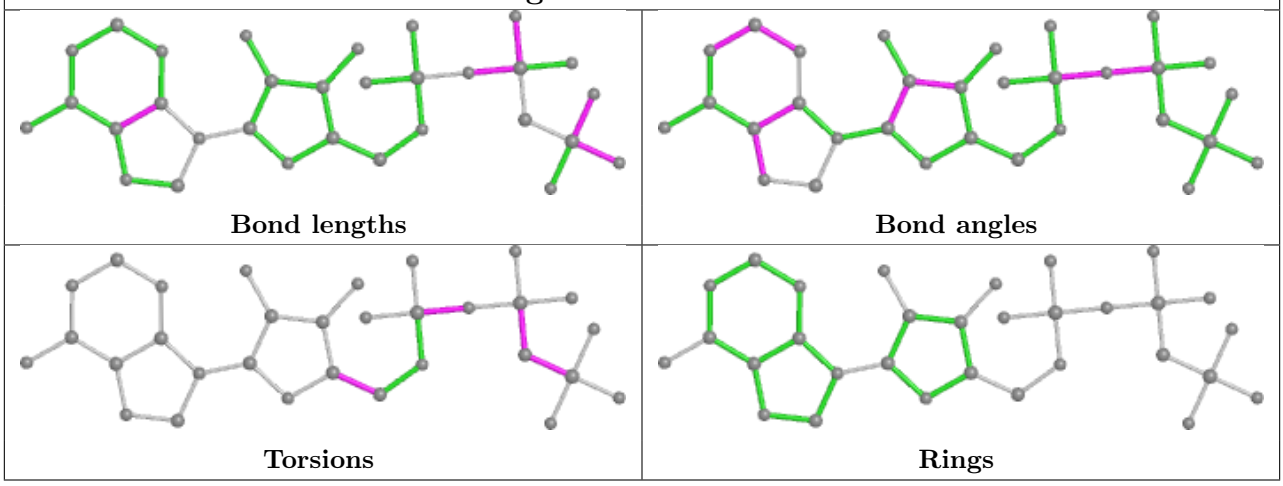
Ligand GDP B 501



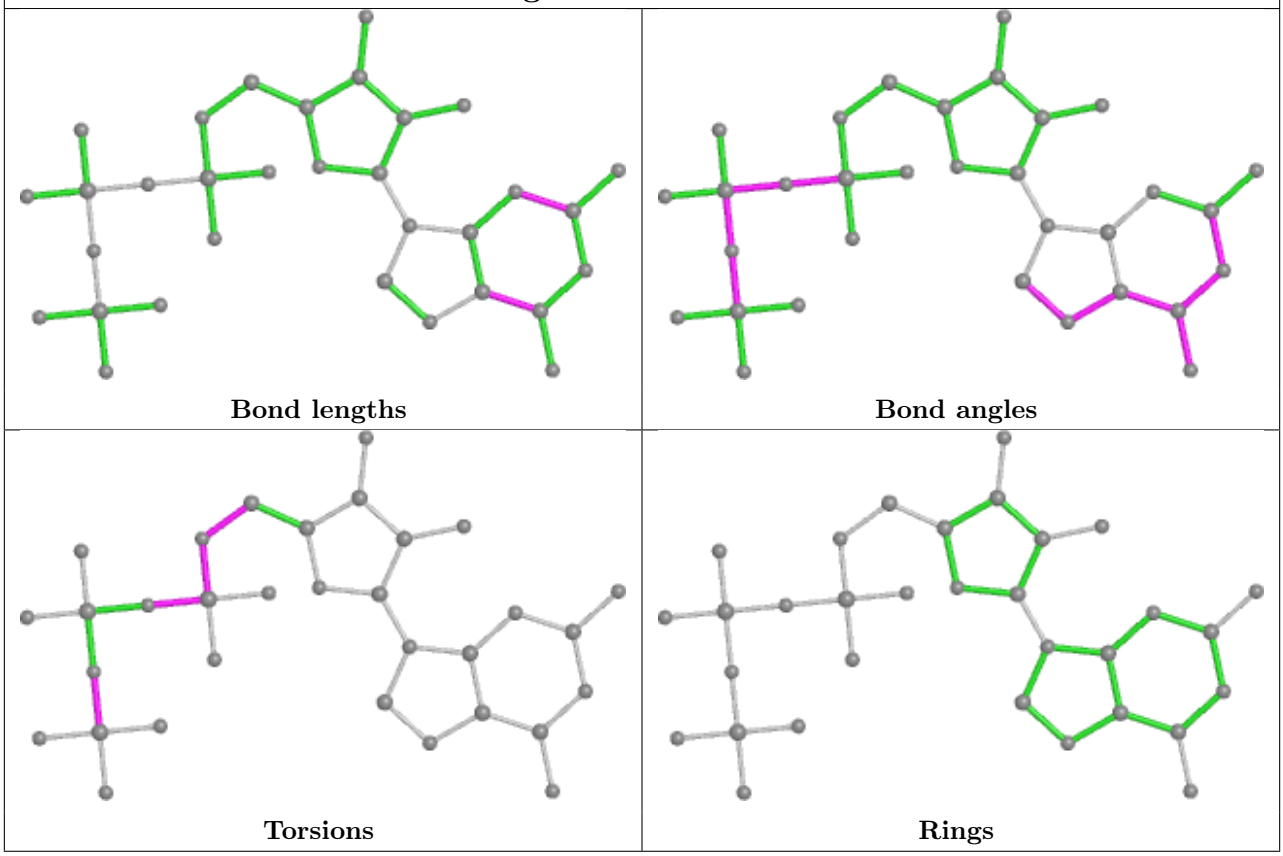
Ligand WV1 D 503



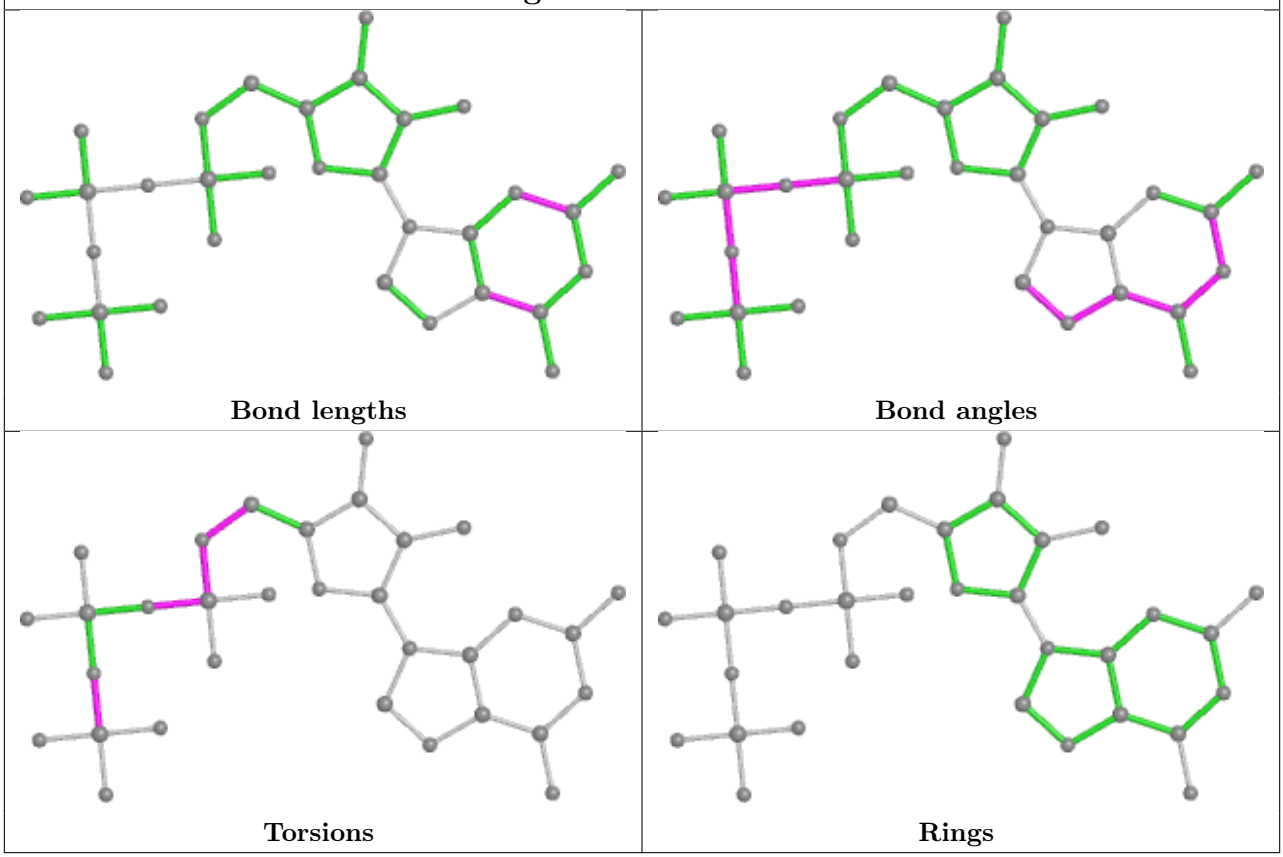
Ligand ACP F 401



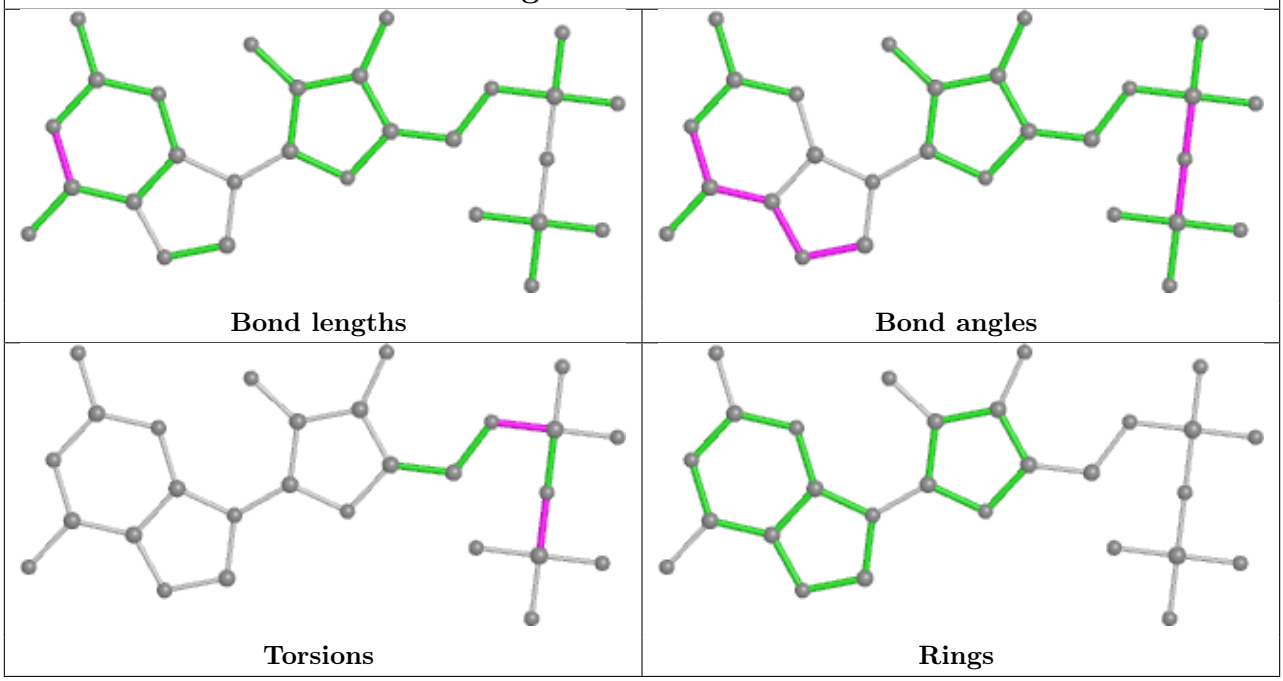
Ligand GTP A 501



Ligand GTP C 501



Ligand GDP D 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	438/451 (97%)	0.39	15 (3%)	45	52	48, 66, 100, 165	0
1	C	440/451 (97%)	0.55	4 (0%)	84	88	40, 53, 77, 109	0
2	B	425/445 (95%)	0.50	18 (4%)	36	43	43, 68, 108, 148	3 (0%)
2	D	431/445 (96%)	0.34	17 (3%)	39	46	47, 69, 105, 167	4 (0%)
3	E	123/143 (86%)	0.79	9 (7%)	15	20	52, 76, 115, 134	0
4	F	352/384 (91%)	0.79	52 (14%)	2	3	59, 88, 149, 187	0
All	All	2209/2319 (95%)	0.52	115 (5%)	27	34	40, 68, 119, 187	7 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	THR	7.5
3	E	6	MET	6.9
2	D	281	GLN	6.4
1	A	262	TYR	6.2
2	D	57	THR	6.1
1	A	346	TRP	6.0
4	F	173	ILE	5.9
1	A	340	SER	5.8
2	D	280	SER	5.8
3	E	26	PRO	5.7
2	B	59	ASN	5.2
2	D	285	ALA	5.0
2	D	277	SER	4.8
4	F	240	LEU	4.8
3	E	24	LEU	4.8
3	E	27	PRO	4.8
1	A	282	TYR	4.7
2	D	276	THR	4.7
3	E	25	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
4	F	103	THR	4.6
4	F	105	LEU	4.5
4	F	153	ALA	4.5
4	F	244	CYS	4.4
4	F	243	HIS	4.4
2	D	278	ARG	4.4
1	A	438	ASP	4.3
2	D	282	GLN	4.3
4	F	372	THR	4.3
4	F	154	GLY	4.3
4	F	177	GLY	4.0
4	F	251	LYS	4.0
2	D	1	MET	4.0
4	F	253	TYR	4.0
2	B	276	THR	3.9
4	F	169	LEU	3.9
2	B	281	GLN	3.8
2	B	1	MET	3.8
2	D	283	TYR	3.7
2	B	58	GLY	3.7
4	F	233	PHE	3.5
4	F	249	TYR	3.5
4	F	89	GLU	3.5
3	E	28	SER	3.5
4	F	20	LEU	3.4
2	D	284	ARG	3.4
1	A	348	PRO	3.4
4	F	245	ILE	3.4
4	F	142	ARG	3.3
4	F	99	VAL	3.2
4	F	250	SER	3.2
4	F	362	ALA	3.2
4	F	259	GLY	3.1
2	B	57	THR	3.0
3	E	50	ILE	3.0
2	D	279	GLY	3.0
4	F	248	GLU	2.9
2	B	325	MET	2.9
4	F	104	ASN	2.9
2	B	437	ASP	2.9
1	A	345	ASP	2.8
1	C	245	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	90	SER	2.7
4	F	254	GLY	2.7
4	F	152	SER	2.6
4	F	256	TYR	2.6
3	E	45	PRO	2.6
4	F	130	VAL	2.6
4	F	234	GLN	2.6
2	B	277	SER	2.5
4	F	135	TYR	2.5
1	A	281	ALA	2.5
4	F	231	ALA	2.5
1	A	335	ILE	2.5
2	D	404	PHE	2.5
2	B	337	ASN	2.5
2	D	400	ARG	2.5
4	F	241	THR	2.5
4	F	44	ARG	2.4
4	F	155	ALA	2.4
3	E	59	GLU	2.4
1	A	349	THR	2.4
2	D	37	HIS	2.3
4	F	340	GLN	2.3
1	C	284	GLU	2.3
4	F	379	HIS	2.3
4	F	337	ALA	2.3
2	D	407	TRP	2.3
2	B	333	LEU	2.2
4	F	176	GLN	2.2
4	F	246	GLN	2.2
2	B	318	ILE	2.2
4	F	339	ALA	2.2
2	B	336	GLN	2.2
1	C	357	TYR	2.2
1	A	78	VAL	2.2
4	F	137	ARG	2.1
4	F	197	ARG	2.1
2	B	124	LYS	2.1
4	F	179	VAL	2.1
2	B	335	VAL	2.1
2	B	284	ARG	2.1
2	B	358	ILE	2.1
4	F	320	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	344	VAL	2.1
2	D	124	LYS	2.1
4	F	101	TYR	2.1
4	F	236	LYS	2.1
2	B	286	LEU	2.1
4	F	381	HIS	2.1
4	F	31	ARG	2.0
4	F	283	ILE	2.0
4	F	232	ASN	2.0
1	A	77	GLU	2.0
1	C	340	SER	2.0
1	A	339	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	B	503	1/1	0.68	0.29	117,117,117,117	0
6	MG	D	502	1/1	0.72	0.11	66,66,66,66	0
7	CA	A	504	1/1	0.79	0.15	93,93,93,93	0
9	MES	B	504	12/12	0.80	0.20	97,104,116,122	0
6	MG	F	402	1/1	0.86	0.11	84,84,84,84	0
10	WV1	D	503	15/15	0.87	0.39	72,81,94,97	0
11	ACP	F	401	31/31	0.87	0.14	87,97,105,108	0
6	MG	A	502	1/1	0.92	0.09	49,49,49,49	0
6	MG	B	502	1/1	0.95	0.17	41,41,41,41	0
6	MG	C	502	1/1	0.95	0.09	43,43,43,43	0
8	GDP	D	501	28/28	0.95	0.14	62,67,72,78	0

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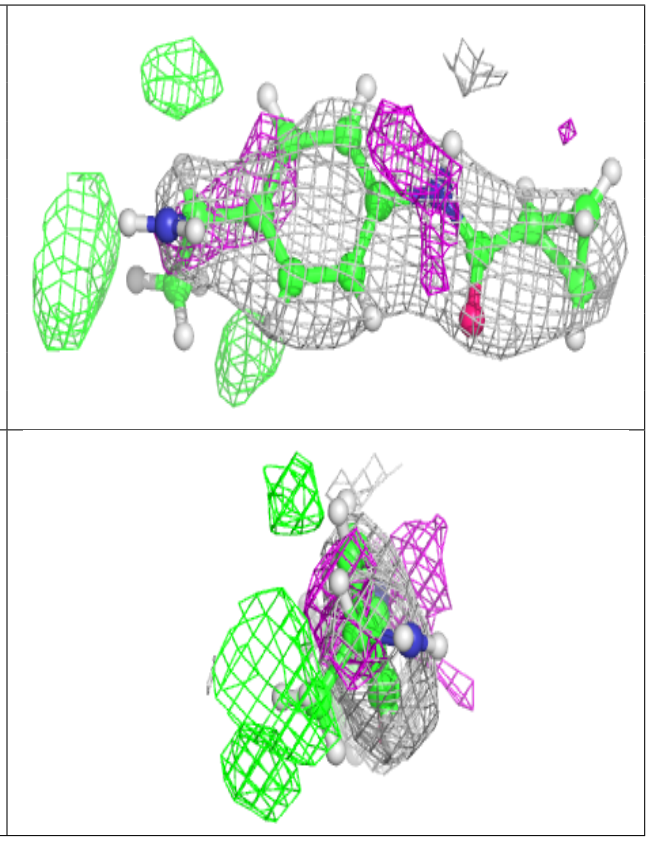
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GTP	A	501	32/32	0.96	0.15	43,51,57,57	0
7	CA	A	503	1/1	0.97	0.08	85,85,85,85	0
7	CA	C	503	1/1	0.98	0.14	68,68,68,68	0
8	GDP	B	501	28/28	0.98	0.16	43,51,55,61	0
5	GTP	C	501	32/32	0.98	0.18	40,45,48,50	0

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.

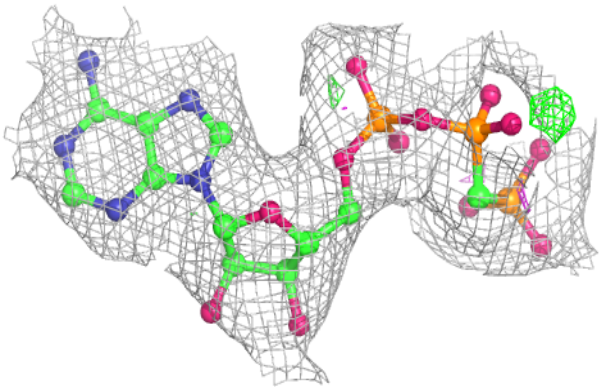
Electron density around WV1 D 503:

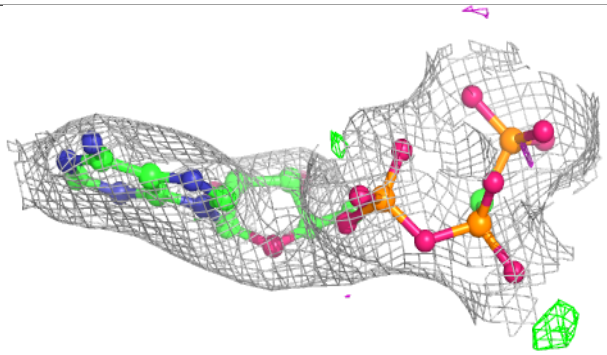
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

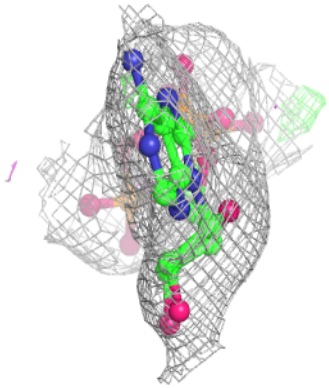


Electron density around ACP F 401:

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

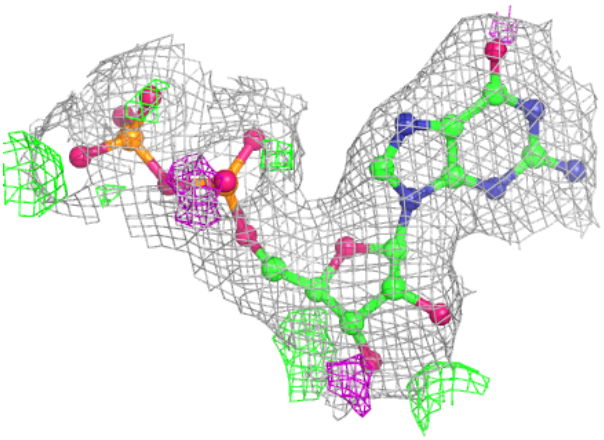


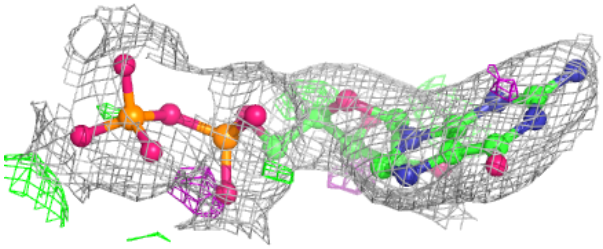


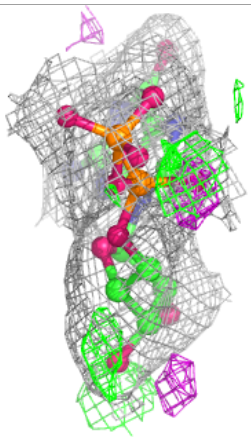


Electron density around GDP D 501:

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

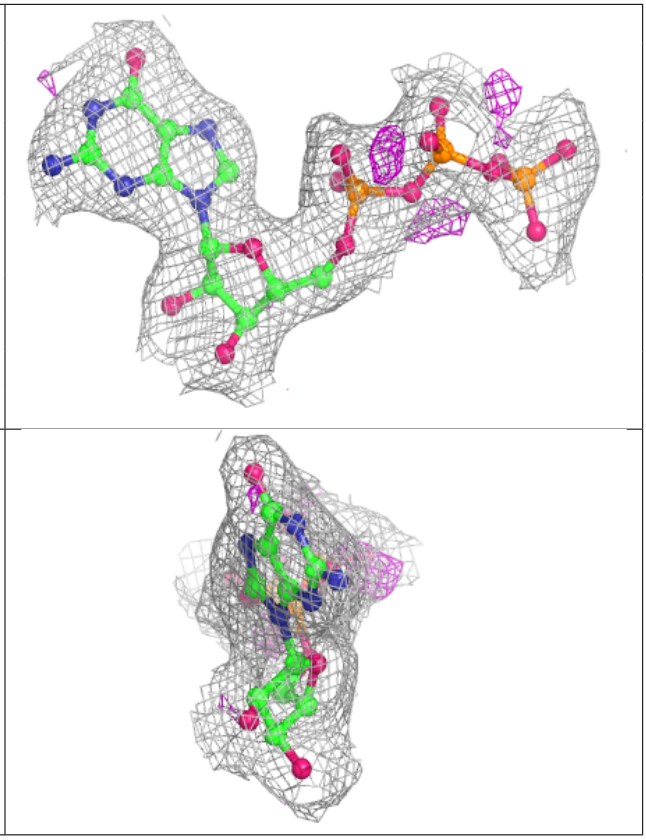


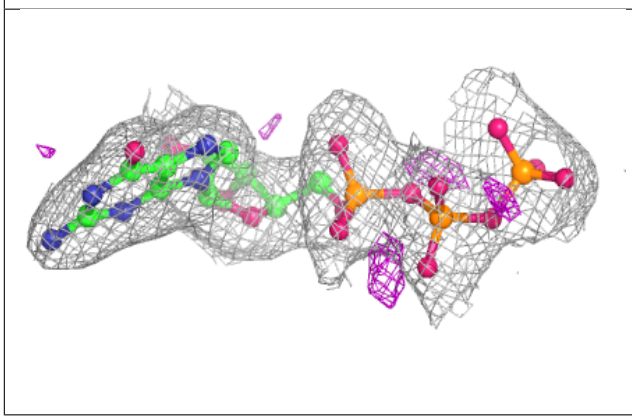




Electron density around GTP A 501:

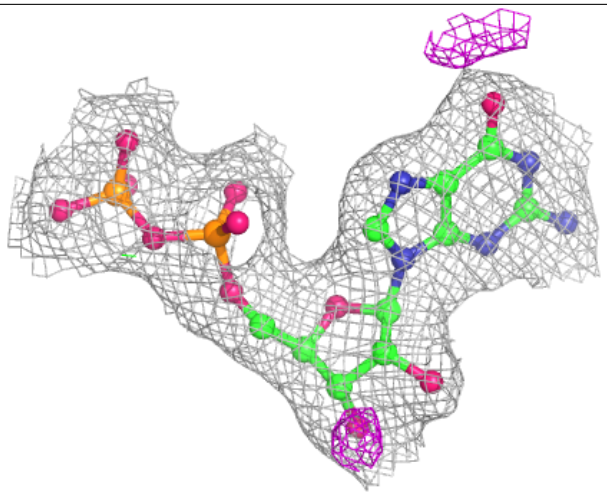
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

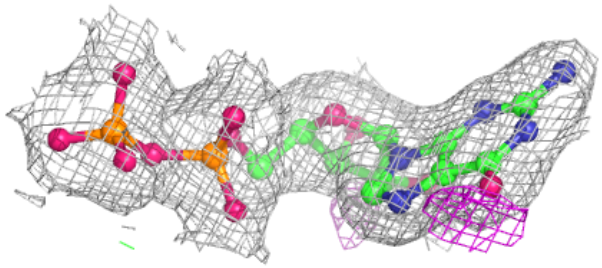


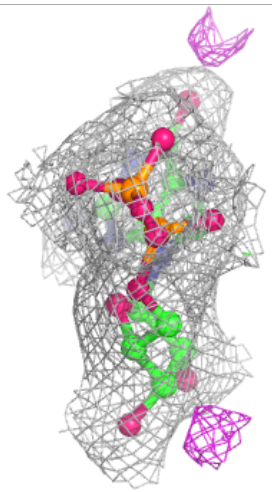


Electron density around GDP B 501:

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

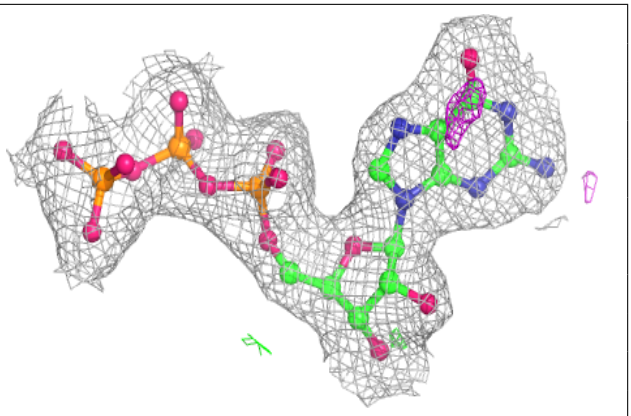


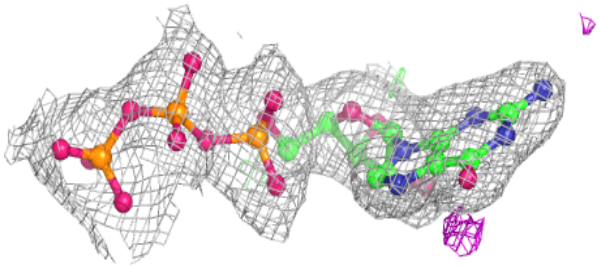




Electron density around GTP C 501:

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





6.5 Other polymers (i)

There are no such residues in this entry.