Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 12:07 PM EDT

PDB ID	:	6XES
Title	:	Tubulin-RB3_SLD in complex with compound 40a
Authors	:	White, S.W.; Yun, M.
Deposited on	:	2020-06-13
Resolution	:	2.32 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:

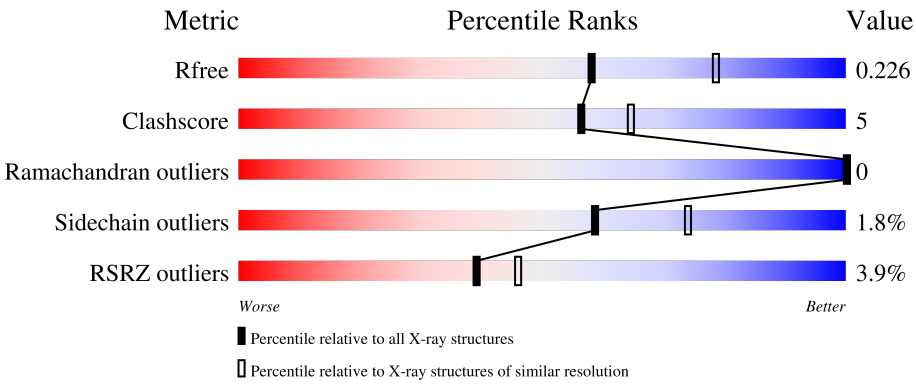
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	438	2%, 84%, 14%
1	C	438	%, 85%, 12%
2	B	433	8%, 84%, 14%
2	D	433	2%, 83%, 17%
3	E	143	11%, 85%, 13%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3344	2119	568	635	22	0	0	0
1	C	427	3343	2118	568	635	22	0	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	425	3335	2094	569	645	27	0	0	0
2	D	431	3389	2126	580	656	27	0	0	0

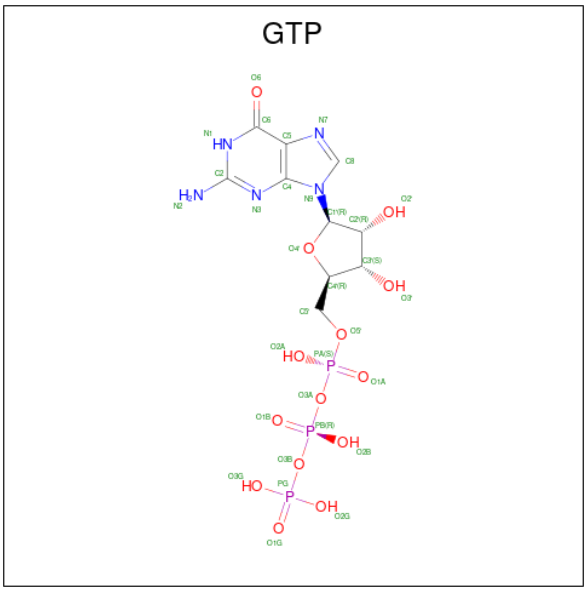
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	125	1027	638	186	199	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

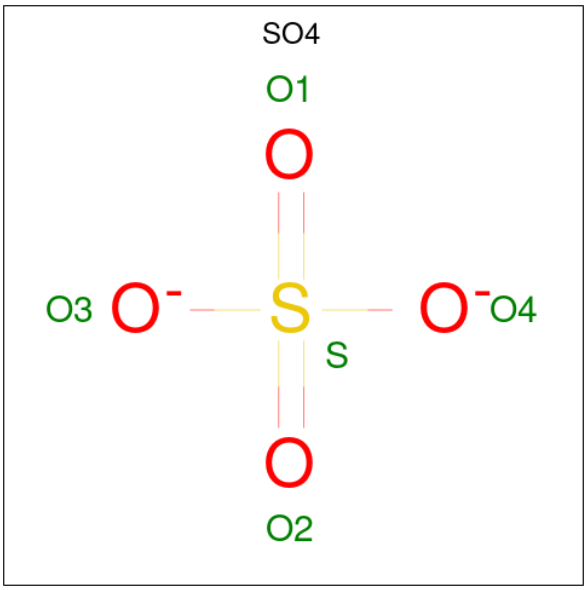
Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 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		
4	A	1	32	10	5	14	3	0	0
4	C	1	32	10	5	14	3	0	0
4	D	1	32	10	5	14	3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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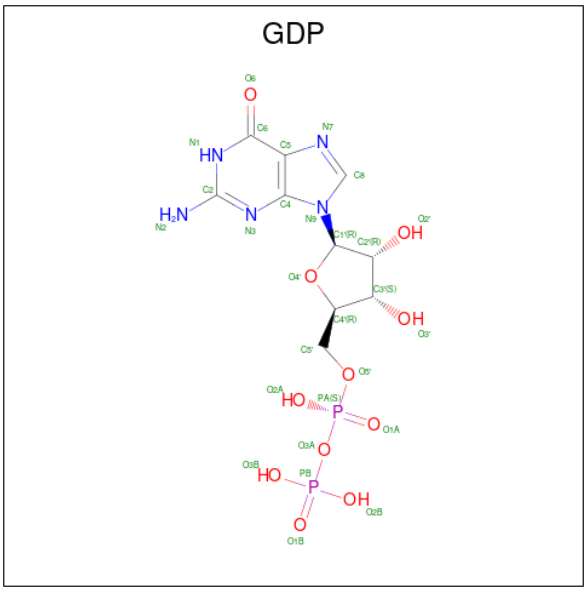
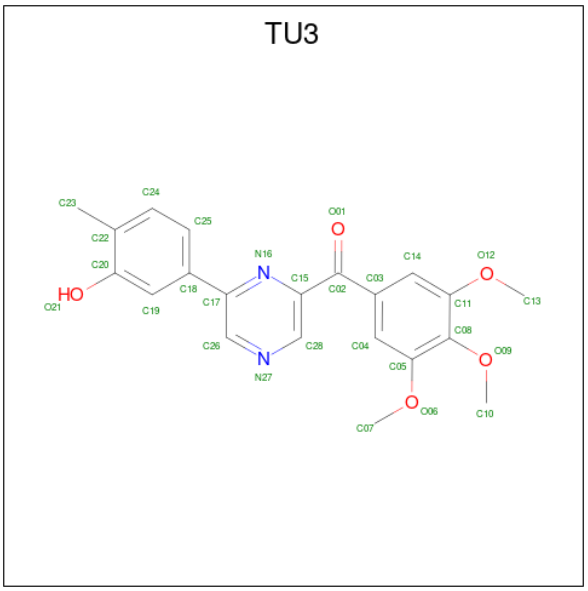
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	D	1	5	4	1	0	0

- Molecule 6 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		
6	B	1	28	10	5	11	2	0	0

- Molecule 7 is [6-(3-hydroxy-4-methylphenyl)pyrazin-2-yl](3,4,5-trimethoxyphenyl)methanone (three-letter code: TU3) (formula: $C_{21}H_{20}N_2O_5$) (labeled as "Ligand of Interest" by depositor).

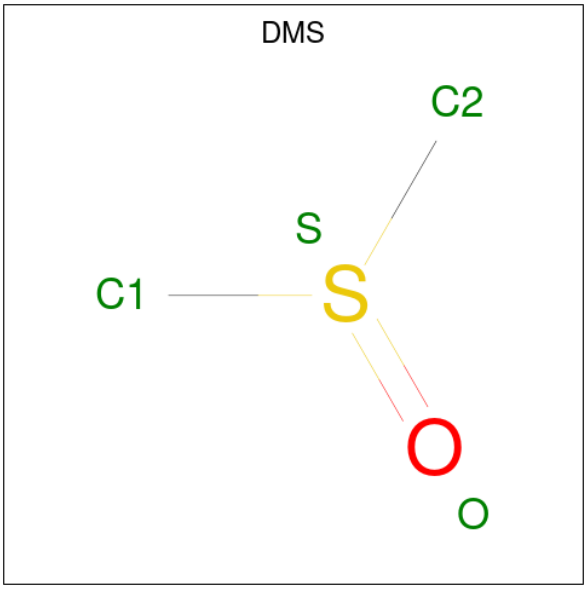


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	28	21	2	5	0	0
			Total	C	N	O		
7	D	1	28	21	2	5	0	0

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

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

- Molecule 9 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
9	D	1	4	2	1	1	0	0

- Molecule 10 is water.

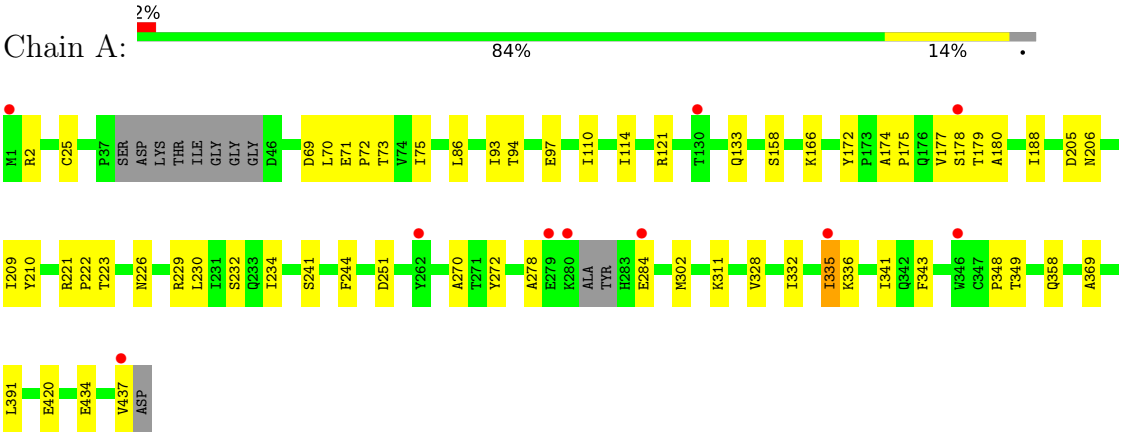
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	67	67	67	0	0
			Total	O		
10	B	39	39	39	0	0
			Total	O		
10	C	65	65	65	0	0
			Total	O		
10	D	55	55	55	0	0
			Total	O		
10	E	6	6	6	0	0

3 Residue-property plots (i)

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

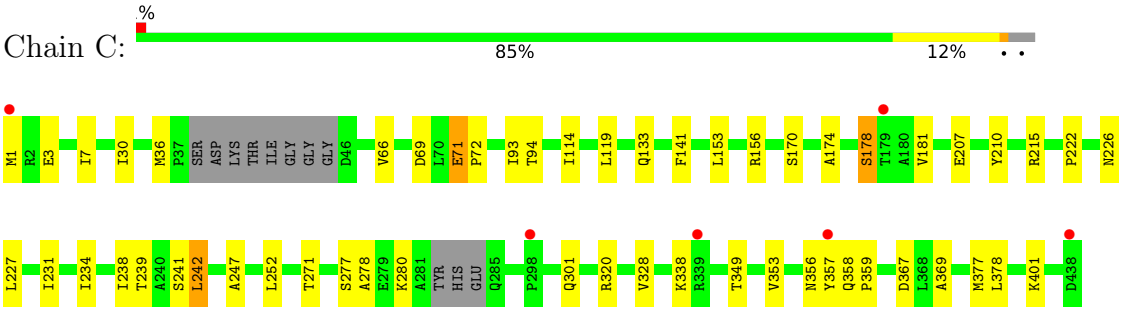
• Molecule 1: Tubulin alpha-1B chain

Chain A:



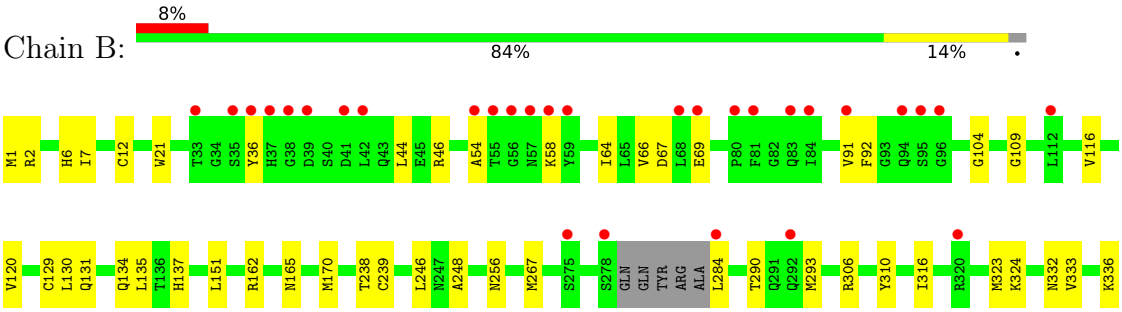
• Molecule 1: Tubulin alpha-1B chain

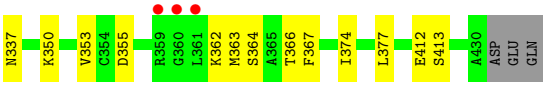
Chain C:



• Molecule 2: Tubulin beta chain

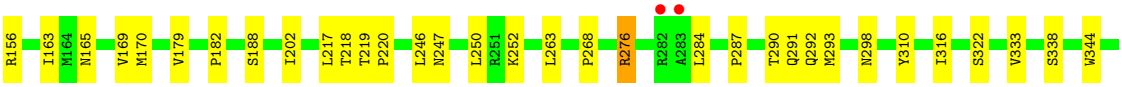
Chain B:





- Molecule 2: Tubulin beta chain

Chain D:



- Molecule 3: Stathmin-4

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.18Å 126.97Å 250.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.32 47.99 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.55-2.32) 91.5 (47.99-2.32)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.171 , 0.226 0.171 , 0.226	Depositor DCC
R_{free} test set	2000 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14870	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: GDP, SO4, TU3, DMS, GTP, MG

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	0.40	0/3418	0.55	0/4638
1	C	0.40	0/3417	0.54	0/4637
2	B	0.38	0/3408	0.54	0/4615
2	D	0.42	0/3464	0.57	0/4692
3	E	0.36	0/1038	0.45	0/1381
All	All	0.40	0/14745	0.54	0/19963

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	3344	0	3261	39	0
1	C	3343	0	3262	33	0
2	B	3335	0	3218	38	0
2	D	3389	0	3266	40	0
3	E	1027	0	1043	2	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	1	0
6	B	28	0	12	1	0
7	B	28	0	0	0	0
7	D	28	0	0	0	0
8	C	1	0	0	0	0
9	D	4	0	6	0	0
10	A	67	0	0	0	0
10	B	39	0	0	0	0
10	C	65	0	0	0	0
10	D	55	0	0	0	0
10	E	6	0	0	0	0
All	All	14870	0	14104	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HG2	2:B:377:LEU:HD11	1.58	0.83
2:B:1:MET:N	2:B:129:CYS:SG	2.51	0.83
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.64	0.79
2:D:1:MET:N	2:D:129:CYS:SG	2.53	0.78
1:A:70:LEU:HD21	1:A:114:ILE:HD13	1.68	0.73
1:A:158:SER:OG	1:A:166:LYS:NZ	2.26	0.69
1:A:177:VAL:HG11	1:A:206:ASN:HD22	1.59	0.67
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.76	0.66
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.38	0.63
1:C:239:THR:HA	1:C:242:LEU:HD12	1.79	0.63
1:C:277:SER:HB3	1:C:280:LYS:HG2	1.81	0.63
1:A:175:PRO:HA	1:A:179:THR:HG21	1.80	0.62
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.81	0.62
2:B:246:LEU:HD23	2:B:248:ALA:HB2	1.81	0.62
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.81	0.61
2:D:35:SER:OG	2:D:58:LYS:NZ	2.33	0.61
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.83	0.60
2:B:293:MET:SD	2:B:367:PHE:HB2	2.41	0.60
1:C:1:MET:N	1:C:3:GLU:OE2	2.33	0.60
2:B:310:TYR:CE1	2:B:367:PHE:HZ	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.84	0.58
2:D:276:ARG:NH2	5:D:502:SO4:O1	2.36	0.58
2:D:287:PRO:O	2:D:291:GLN:HG2	2.05	0.57
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.86	0.56
2:B:290:THR:HG22	2:B:333:VAL:HG21	1.87	0.56
1:A:97:GLU:HG3	2:B:1:MET:HG2	1.85	0.56
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.06	0.56
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.88	0.56
1:A:223:THR:HG23	1:A:226:ASN:H	1.71	0.55
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.24	0.55
2:B:64:ILE:HD13	2:B:120:VAL:HG22	1.87	0.55
1:A:188:ILE:HD11	1:A:391:LEU:HB3	1.89	0.55
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.88	0.54
2:B:54:ALA:HB3	2:B:58:LYS:HB2	1.88	0.54
1:A:72:PRO:HA	1:A:94:THR:HG21	1.89	0.54
2:B:134:GLN:HA	2:B:165:ASN:O	2.08	0.54
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.90	0.54
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.41	0.53
1:C:320:ARG:HA	1:C:356:ASN:O	2.09	0.53
2:D:292:GLN:HG2	2:D:298:ASN:ND2	2.24	0.53
1:A:2:ARG:HB3	1:A:133:GLN:CD	2.28	0.53
2:D:64:ILE:HD13	2:D:120:VAL:HG22	1.92	0.52
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.91	0.52
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.46	0.51
2:B:2:ARG:HH22	2:B:46:ARG:HG2	1.76	0.51
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.93	0.50
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.40	0.50
2:B:323:MET:HG3	2:B:353:VAL:HG21	1.93	0.50
2:D:218:THR:HG22	2:D:219:THR:HG23	1.94	0.49
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.41	0.49
1:C:271:THR:OG1	1:C:377:MET:HB3	2.12	0.49
2:D:64:ILE:HG12	2:D:119:VAL:HG12	1.92	0.49
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.49
2:D:386:THR:O	2:D:390:ARG:HG3	2.12	0.49
2:B:306:ARG:NH1	2:B:337:ASN:OD1	2.45	0.49
2:D:117:LEU:O	2:D:121:ARG:HG3	2.13	0.49
2:D:145:SER:HB2	2:D:188:SER:OG	2.13	0.49
1:C:238:ILE:HD12	1:C:378:LEU:HD11	1.95	0.48
2:D:292:GLN:HG2	2:D:298:ASN:HD21	1.78	0.48
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.48	0.48
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:LEU:HD23	2:D:47:ILE:HD13	1.95	0.48
2:D:293:MET:CG	2:D:367:PHE:HB2	2.44	0.47
2:B:36:TYR:CD1	2:B:44:LEU:HD21	2.50	0.47
2:B:238:THR:HB	2:B:316:ILE:HD13	1.96	0.47
2:B:332:ASN:O	2:B:336:LYS:HG2	2.14	0.47
1:C:133:GLN:HB3	1:C:252:LEU:HD12	1.95	0.47
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.97	0.47
1:A:2:ARG:HB3	1:A:133:GLN:NE2	2.31	0.46
1:C:30:ILE:HG12	1:C:36:MET:HE2	1.97	0.46
1:A:69:ASP:O	1:A:94:THR:HA	2.15	0.46
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.51	0.46
2:D:72:THR:O	2:D:76:VAL:HG23	2.14	0.46
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.46
2:B:130:LEU:O	2:B:162:ARG:NH1	2.45	0.46
1:C:238:ILE:HD11	1:C:378:LEU:HD21	1.98	0.46
1:A:221:ARG:HD2	2:B:324:LYS:N	2.30	0.46
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.97	0.46
1:A:335:ILE:HG13	1:A:336:LYS:N	2.29	0.46
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.98	0.45
1:A:75:ILE:HD12	1:A:94:THR:HG23	1.97	0.45
2:B:293:MET:CG	2:B:367:PHE:HB2	2.47	0.45
1:C:69:ASP:O	1:C:94:THR:HA	2.16	0.45
1:C:247:ALA:HB2	1:C:357:TYR:CE2	2.51	0.45
2:D:263:LEU:HD21	2:D:421:GLU:HG3	1.98	0.45
1:C:247:ALA:HB2	1:C:357:TYR:HE2	1.81	0.45
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.99	0.45
2:B:267:MET:HG2	2:B:374:ILE:HD13	1.99	0.45
2:D:69:GLU:OE2	2:D:70:PRO:HD2	2.17	0.45
1:A:234:ILE:HG21	1:A:302:MET:SD	2.57	0.44
1:A:180:ALA:HB1	2:B:256:ASN:OD1	2.17	0.44
1:A:174:ALA:O	1:A:177:VAL:HG12	2.18	0.44
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.45	0.44
2:D:316:ILE:HG23	2:D:366:THR:HB	2.00	0.44
1:A:335:ILE:HD12	1:A:341:ILE:HD11	2.00	0.44
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.44
2:B:67:ASP:O	2:B:92:PHE:HA	2.18	0.44
2:B:284:LEU:HD23	2:B:284:LEU:HA	1.75	0.43
1:C:36:MET:HB2	1:C:36:MET:HE3	1.89	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.43
1:C:238:ILE:CD1	1:C:378:LEU:HD21	2.49	0.43
2:B:2:ARG:NH2	2:B:46:ARG:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:CYS:SG	2:B:316:ILE:HD12	2.58	0.43
2:D:284:LEU:HD21	2:D:292:GLN:HE22	1.83	0.43
1:C:338:LYS:HD2	1:C:338:LYS:HA	1.77	0.43
2:B:66:VAL:HA	2:B:91:VAL:O	2.19	0.43
1:C:358:GLN:HG3	1:C:359:PRO:HD2	2.01	0.43
2:B:104:GLY:O	2:B:109:GLY:HA3	2.19	0.43
1:A:178:SER:HA	2:B:350:LYS:NZ	2.34	0.42
2:B:362:LYS:HA	2:B:362:LYS:HD3	1.70	0.42
1:A:244:PHE:CG	1:A:358:GLN:HG3	2.54	0.42
2:D:179:VAL:O	2:D:182:PRO:HD2	2.19	0.42
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.01	0.42
2:D:217:LEU:O	2:D:220:PRO:HD3	2.19	0.42
1:A:341:ILE:HD12	1:A:341:ILE:N	2.34	0.42
1:C:234:ILE:O	1:C:238:ILE:HG12	2.20	0.42
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.31	0.42
1:C:271:THR:HG22	1:C:301:GLN:HG2	2.01	0.41
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.02	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
1:A:229:ARG:O	1:A:232:SER:OG	2.29	0.41
2:B:316:ILE:HG23	2:B:366:THR:HB	2.01	0.41
2:B:116:VAL:HG11	2:B:151:LEU:HD11	2.03	0.41
2:B:267:MET:HE3	2:B:267:MET:HB3	1.82	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.41
1:C:178:SER:HB2	2:D:350:LYS:NZ	2.36	0.41
2:D:23:VAL:O	2:D:27:GLU:HG3	2.21	0.41
2:D:121:ARG:O	2:D:125:GLU:HG2	2.21	0.41
2:B:1:MET:CE	2:B:131:GLN:HG3	2.51	0.41
2:B:7:ILE:O	2:B:135:LEU:HA	2.21	0.41
2:D:154:LYS:HD2	2:D:154:LYS:HA	1.82	0.41
1:A:328:VAL:O	1:A:332:ILE:HG13	2.21	0.41
2:D:134:GLN:HA	2:D:165:ASN:O	2.21	0.41
2:D:163:ILE:HG21	2:D:250:LEU:HB3	2.03	0.41
1:A:221:ARG:HD2	2:B:323:MET:C	2.41	0.41
2:D:404:ASP:OD1	2:D:405:GLU:N	2.53	0.40
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.56	0.40
2:D:247:ASN:HB3	2:D:252:LYS:NZ	2.36	0.40
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.56	0.40
2:D:7:ILE:O	2:D:135:LEU:HA	2.21	0.40
1:A:234:ILE:HD12	1:A:272:TYR:HB2	2.04	0.40
1:A:311:LYS:NZ	1:A:437:VAL:O	2.26	0.40
2:D:73:MET:HE3	2:D:92:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/438 (96%)	413 (98%)	8 (2%)	0	100	100
1	C	421/438 (96%)	411 (98%)	10 (2%)	0	100	100
2	B	421/433 (97%)	410 (97%)	11 (3%)	0	100	100
2	D	429/433 (99%)	425 (99%)	4 (1%)	0	100	100
3	E	121/143 (85%)	121 (100%)	0	0	100	100
All	All	1813/1885 (96%)	1780 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/369 (98%)	356 (99%)	5 (1%)	67	80
1	C	361/369 (98%)	353 (98%)	8 (2%)	52	68
2	B	367/374 (98%)	360 (98%)	7 (2%)	57	73
2	D	372/374 (100%)	364 (98%)	8 (2%)	52	68
3	E	110/126 (87%)	109 (99%)	1 (1%)	78	89
All	All	1571/1612 (98%)	1542 (98%)	29 (2%)	59	74

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	SER
1	A	284	GLU
1	A	335	ILE
1	A	420	GLU
1	A	434	GLU
2	B	69	GLU
2	B	137	HIS
2	B	355	ASP
2	B	363	MET
2	B	364	SER
2	B	412	GLU
2	B	413	SER
1	C	66	VAL
1	C	71	GLU
1	C	178	SER
1	C	181	VAL
1	C	215	ARG
1	C	241	SER
1	C	242	LEU
1	C	349	THR
2	D	115	SER
2	D	137	HIS
2	D	246	LEU
2	D	268	PRO
2	D	276	ARG
2	D	322	SER
2	D	338	SER
2	D	413	SER
3	E	28	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
2	B	247	ASN
2	D	48	ASN
2	D	292	GLN
2	D	298	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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	TU3	B	503	-	30,30,30	1.23	4 (13%)	41,42,42	1.88	7 (17%)
9	DMS	D	504	-	3,3,3	0.75	0	3,3,3	0.85	0
5	SO4	B	502	-	4,4,4	0.16	0	6,6,6	0.18	0
4	GTP	A	501	-	26,34,34	1.14	2 (7%)	32,54,54	1.38	5 (15%)
4	GTP	D	501	-	26,34,34	1.09	2 (7%)	32,54,54	1.50	6 (18%)
5	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.09	0
7	TU3	D	503	-	30,30,30	1.23	3 (10%)	41,42,42	1.40	5 (12%)
4	GTP	C	501	8	26,34,34	1.12	2 (7%)	32,54,54	1.51	5 (15%)
5	SO4	D	502	-	4,4,4	0.20	0	6,6,6	0.30	0
6	GDP	B	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.19	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
7	TU3	B	503	-	-	4/18/18/18	0/3/3/3
4	GTP	A	501	-	-	7/18/38/38	0/3/3/3
4	GTP	D	501	-	-	5/18/38/38	0/3/3/3
7	TU3	D	503	-	-	0/18/18/18	0/3/3/3
4	GTP	C	501	8	-	6/18/38/38	0/3/3/3
6	GDP	B	501	-	-	5/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	C5-C6	-3.88	1.39	1.47
4	C	501	GTP	C5-C6	-3.74	1.39	1.47
4	D	501	GTP	C5-C6	-3.33	1.40	1.47
7	D	503	TU3	C18-C17	3.06	1.53	1.48
7	B	503	TU3	C18-C17	2.88	1.53	1.48
7	D	503	TU3	O01-C02	-2.79	1.17	1.22
4	D	501	GTP	C2-N3	2.73	1.39	1.33
7	B	503	TU3	O06-C05	2.47	1.41	1.37
6	B	501	GDP	C6-N1	-2.42	1.34	1.37
7	B	503	TU3	O01-C02	-2.40	1.18	1.22
4	C	501	GTP	C2-N3	2.35	1.38	1.33
7	B	503	TU3	O21-C20	2.31	1.41	1.36
7	D	503	TU3	O12-C11	2.28	1.40	1.37
4	A	501	GTP	C2-N3	2.16	1.38	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	503	TU3	O06-C05-C08	5.22	124.33	115.16
7	B	503	TU3	O09-C08-C05	4.31	126.33	120.12
7	B	503	TU3	O06-C05-C04	-4.26	116.78	124.12
7	B	503	TU3	O09-C08-C11	-4.11	114.20	120.12
4	D	501	GTP	PB-O3B-PG	-3.64	120.34	132.83
7	D	503	TU3	C02-C15-N16	3.48	121.72	116.90
4	C	501	GTP	C5-C6-N1	3.37	119.91	113.95
4	A	501	GTP	C8-N7-C5	3.14	108.97	102.99
7	D	503	TU3	O06-C05-C08	3.05	120.52	115.16
4	D	501	GTP	C8-N7-C5	3.05	108.80	102.99
4	C	501	GTP	PA-O3A-PB	-3.04	122.40	132.83
4	D	501	GTP	C5-C6-N1	3.03	119.30	113.95
4	C	501	GTP	PB-O3B-PG	-2.94	122.73	132.83
4	D	501	GTP	PA-O3A-PB	-2.92	122.81	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	GTP	C8-N7-C5	2.90	108.51	102.99
4	A	501	GTP	C5-C6-N1	2.87	119.02	113.95
7	B	503	TU3	C13-O12-C11	-2.86	113.21	117.53
4	C	501	GTP	C2-N1-C6	-2.77	119.99	125.10
7	D	503	TU3	O06-C05-C04	-2.73	119.42	124.12
4	A	501	GTP	PA-O3A-PB	-2.64	123.78	132.83
6	B	501	GDP	C8-N7-C5	2.58	107.91	102.99
7	D	503	TU3	C18-C17-N16	2.56	119.66	116.02
6	B	501	GDP	O3B-PB-O3A	2.53	113.13	104.64
4	D	501	GTP	C2-N1-C6	-2.45	120.59	125.10
4	A	501	GTP	O2G-PG-O3B	2.40	112.69	104.64
4	A	501	GTP	C2-N1-C6	-2.37	120.74	125.10
6	B	501	GDP	PA-O3A-PB	-2.23	125.17	132.83
7	D	503	TU3	C28-N27-C26	2.13	120.39	117.48
7	B	503	TU3	C02-C15-N16	2.02	119.71	116.90
4	D	501	GTP	O6-C6-N1	-2.01	118.27	120.65
7	B	503	TU3	O12-C11-C14	-2.01	120.66	124.12

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
7	B	503	TU3	C11-C08-O09-C10
7	B	503	TU3	C05-C08-O09-C10
4	A	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O3A
7	B	503	TU3	C08-C11-O12-C13
4	A	501	GTP	PB-O3A-PA-O1A
4	D	501	GTP	PB-O3B-PG-O1G
4	C	501	GTP	C4'-C5'-O5'-PA
4	A	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
7	B	503	TU3	C14-C11-O12-C13
4	A	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	PB-O3B-PG-O2G
4	C	501	GTP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	PB-O3A-PA-O1A
6	B	501	GDP	PB-O3A-PA-O2A

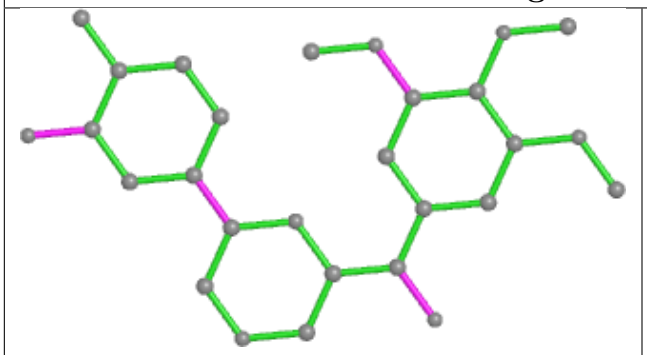
There are no ring outliers.

2 monomers are involved in 2 short contacts:

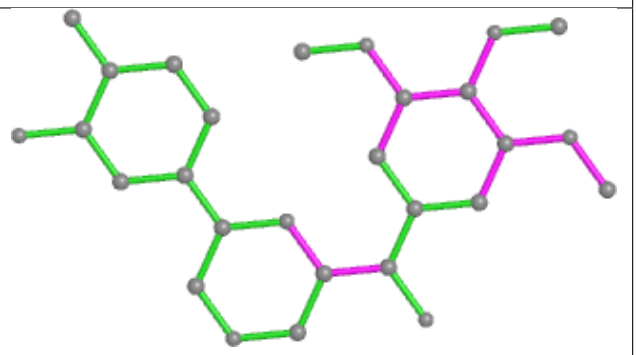
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	SO4	1	0
6	B	501	GDP	1	0

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.

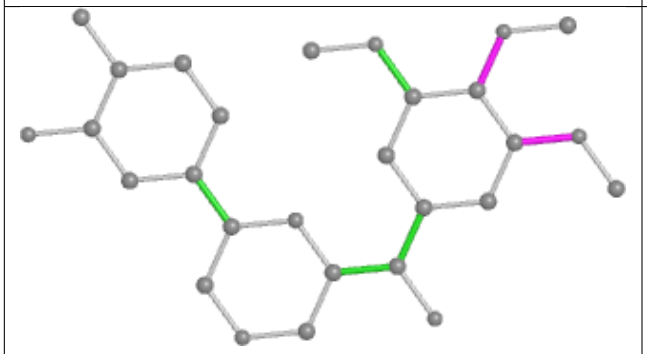
Ligand TU3 B 503



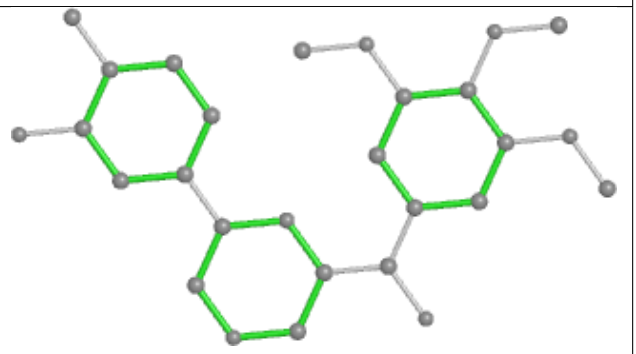
Bond lengths



Bond angles

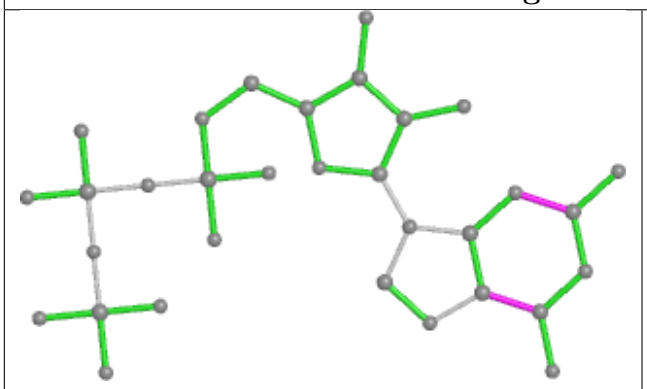


Torsions

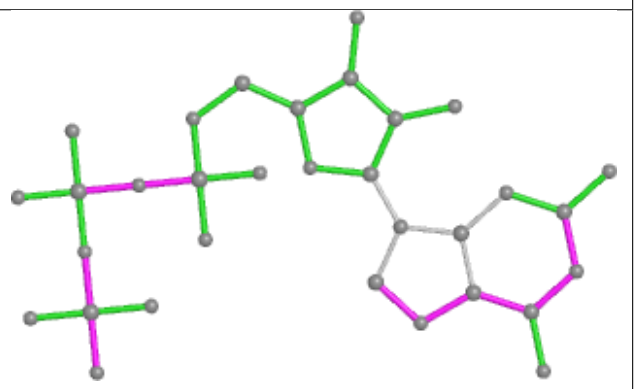


Rings

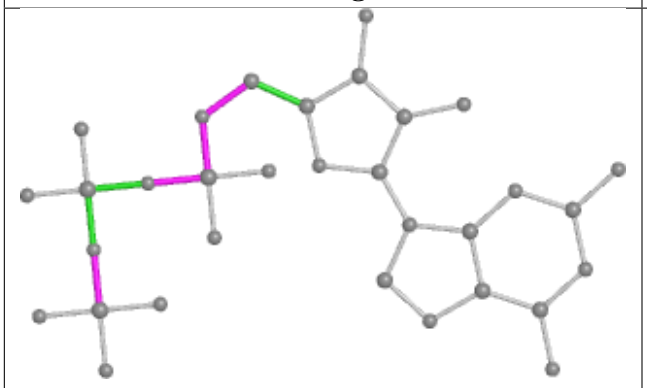
Ligand GTP A 501



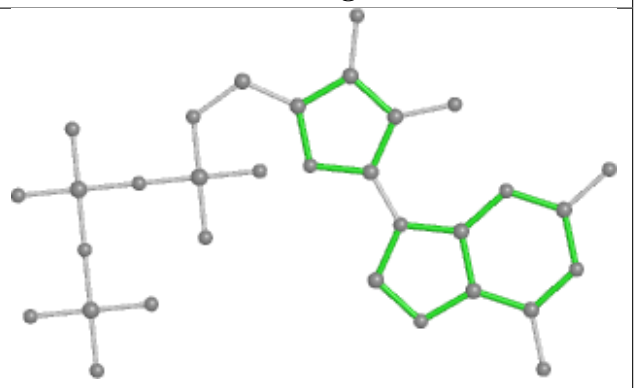
Bond lengths



Bond angles

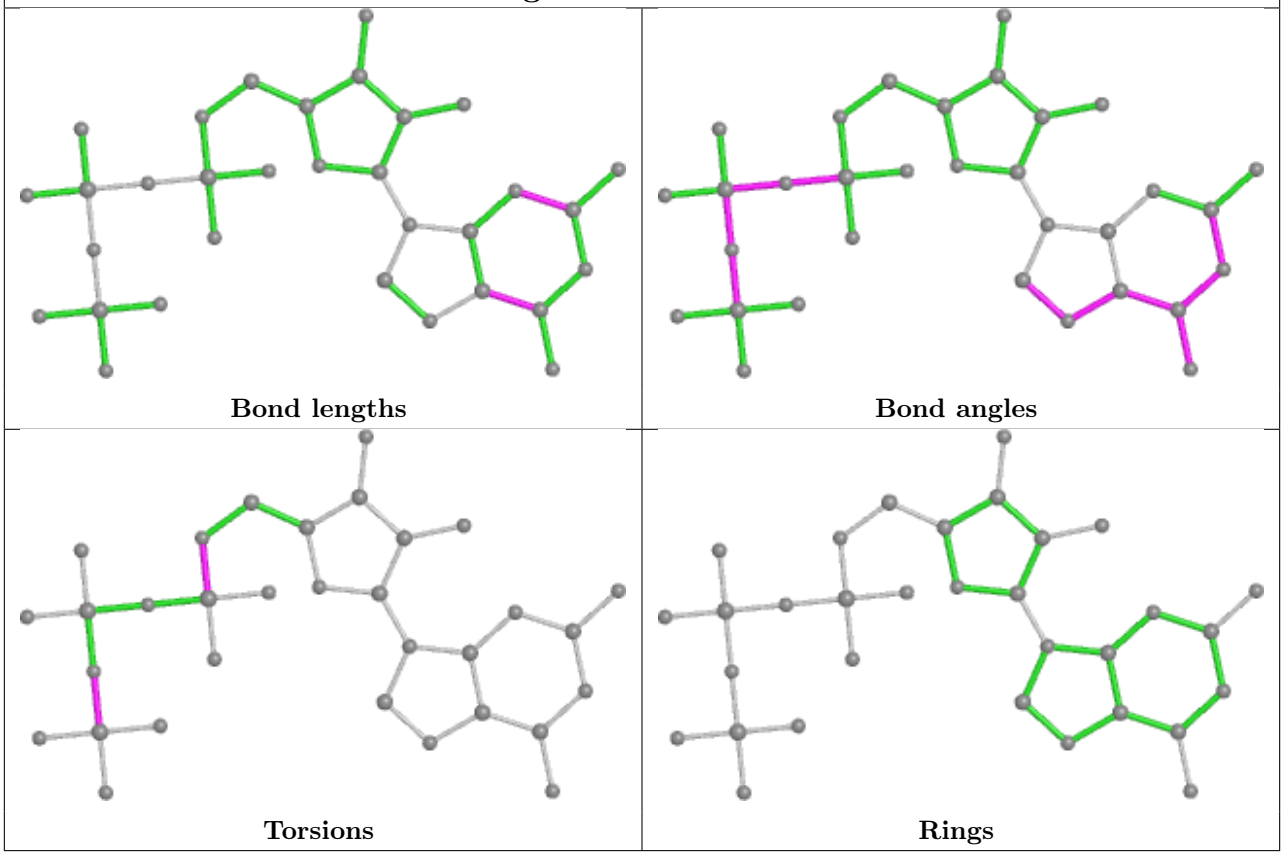


Torsions



Rings

Ligand GTP D 501



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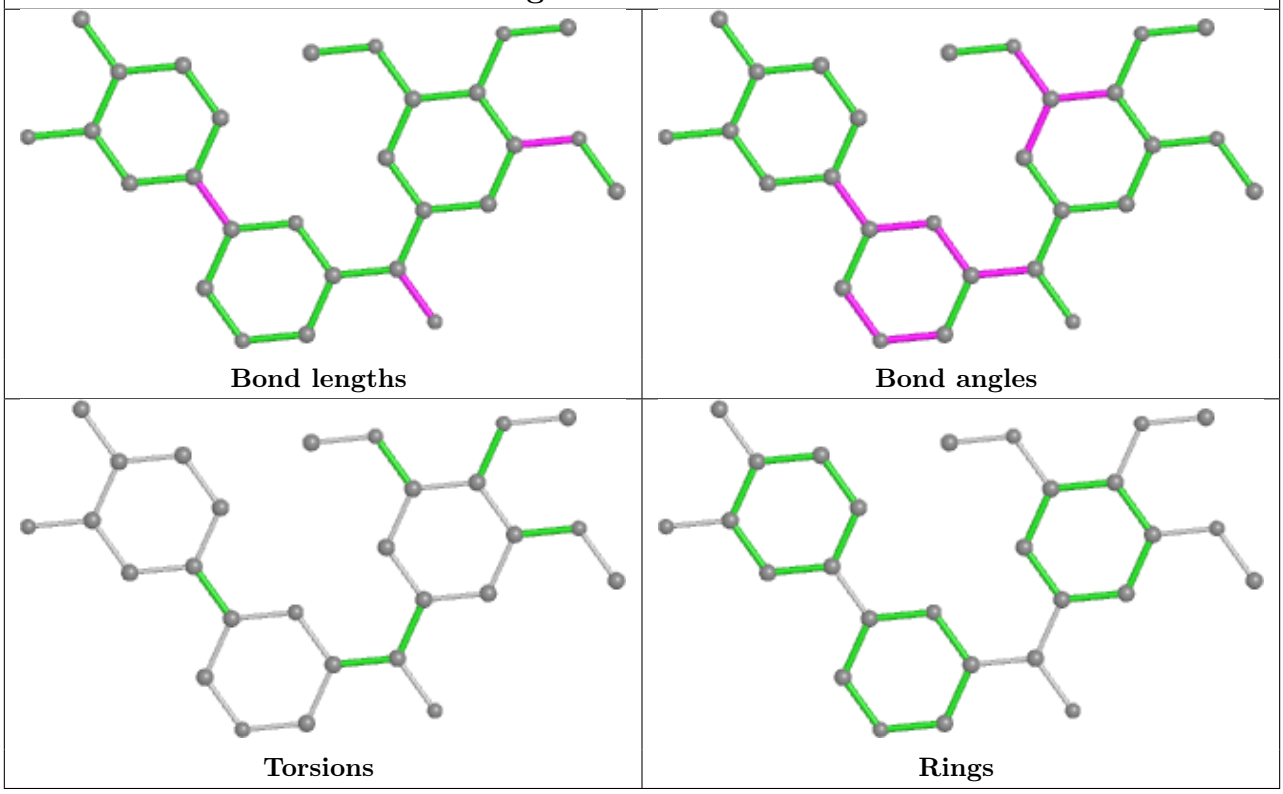
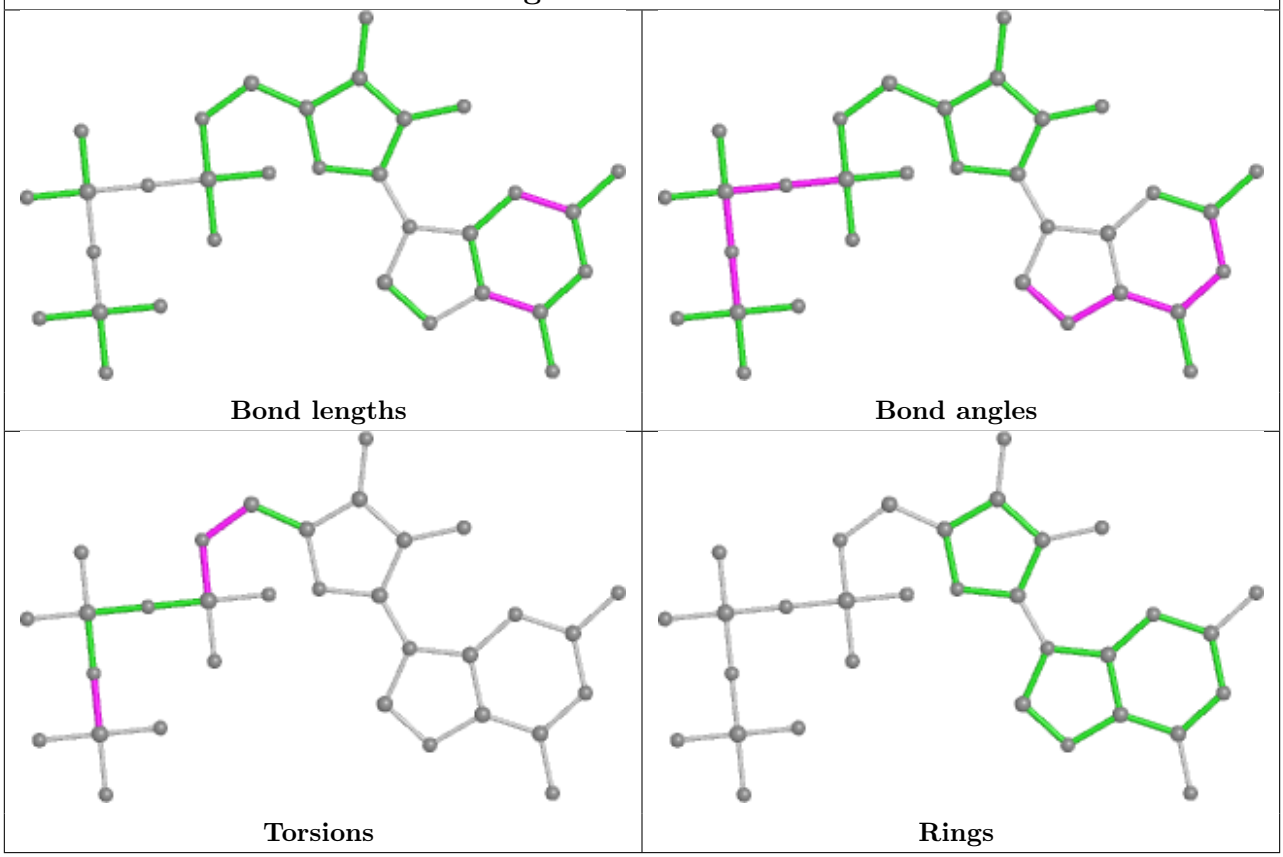
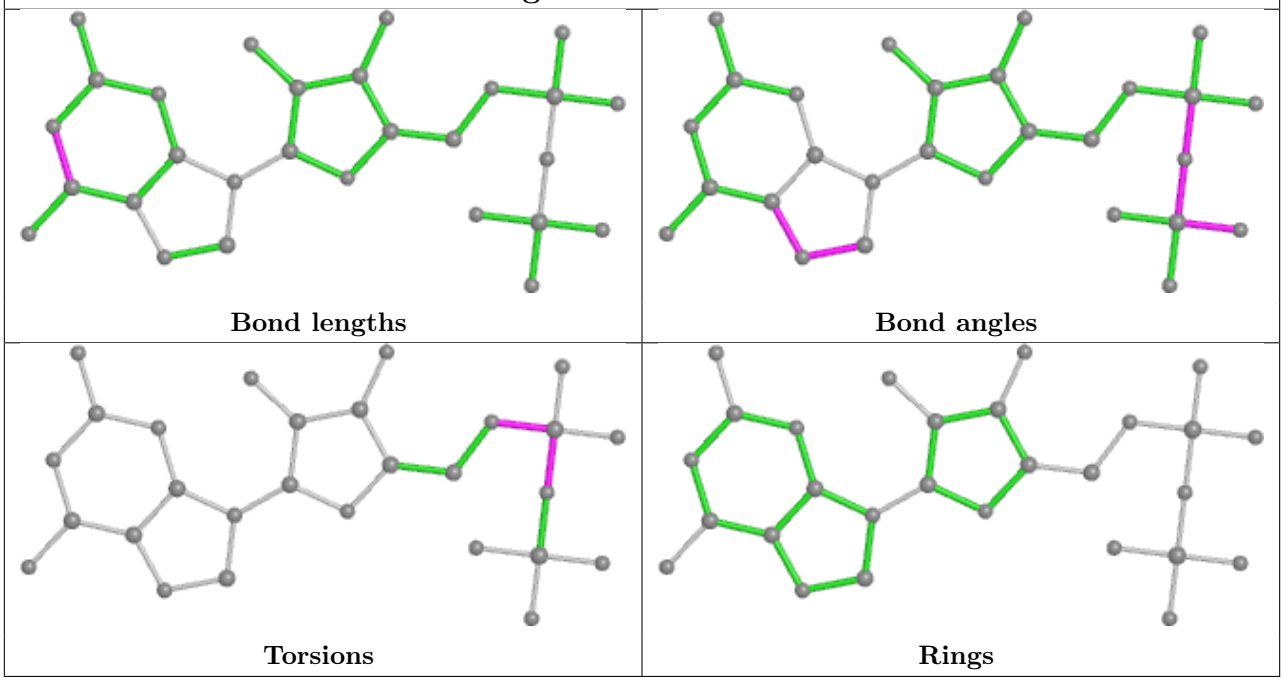


Ligand GTP C 501



Ligand GDP B 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	427/438 (97%)	-0.08	10 (2%)	60	67	37, 56, 88, 137	0
1	C	427/438 (97%)	-0.03	6 (1%)	75	80	37, 57, 95, 124	0
2	B	425/433 (98%)	0.30	33 (7%)	13	17	37, 56, 98, 132	0
2	D	431/433 (99%)	-0.08	7 (1%)	72	78	32, 50, 91, 122	0
3	E	125/143 (87%)	0.62	16 (12%)	3	5	57, 73, 98, 112	0
All	All	1835/1885 (97%)	0.07	72 (3%)	39	46	32, 56, 95, 137	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	360	GLY	4.8
2	B	37	HIS	4.7
1	A	1	MET	4.6
3	E	9	ILE	4.5
2	D	55	THR	4.5
2	B	36	TYR	4.4
3	E	6	MET	4.4
3	E	8	VAL	4.0
3	E	32	VAL	3.9
1	A	284	GLU	3.9
2	B	33	THR	3.9
2	B	55	THR	3.8
2	B	81	PHE	3.8
2	B	35	SER	3.8
2	B	39	ASP	3.7
2	B	284	LEU	3.6
2	B	80	PRO	3.5
1	A	346	TRP	3.4
2	B	361	LEU	3.4
2	B	42	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	3.4
3	E	45	PRO	3.3
3	E	48	GLU	3.3
2	B	57	ASN	3.2
2	B	95	SER	3.2
2	B	278	SER	3.1
3	E	7	GLU	3.1
2	B	38	GLY	3.1
2	D	54	ALA	3.0
2	B	94	GLN	2.9
1	C	357	TYR	2.7
1	C	179	THR	2.7
2	B	96	GLY	2.7
1	A	437	VAL	2.7
1	A	335	ILE	2.6
2	B	58	LYS	2.6
2	D	80	PRO	2.6
3	E	30	ASP	2.5
2	D	92	PHE	2.4
3	E	29	PHE	2.4
3	E	33	PRO	2.4
2	B	59	TYR	2.4
2	B	83	GLN	2.3
3	E	47	LEU	2.3
1	A	280	LYS	2.3
2	B	41	ASP	2.3
3	E	31	GLY	2.3
2	D	57	ASN	2.3
1	A	130	THR	2.2
2	B	91	VAL	2.2
1	C	1	MET	2.2
1	A	279	GLU	2.2
2	B	292	GLN	2.2
2	D	282	ARG	2.2
2	B	68	LEU	2.2
2	D	283	ALA	2.2
3	E	55	GLU	2.2
3	E	113	GLU	2.2
1	C	339	ARG	2.1
2	B	69	GLU	2.1
2	B	112	LEU	2.1
2	B	54	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	56	GLY	2.1
2	B	359	ARG	2.1
3	E	96	MET	2.1
1	C	298	PRO	2.1
1	C	438	ASP	2.0
1	A	178	SER	2.0
2	B	320	ARG	2.0
3	E	24	LEU	2.0
2	B	275	SER	2.0
2	B	84	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

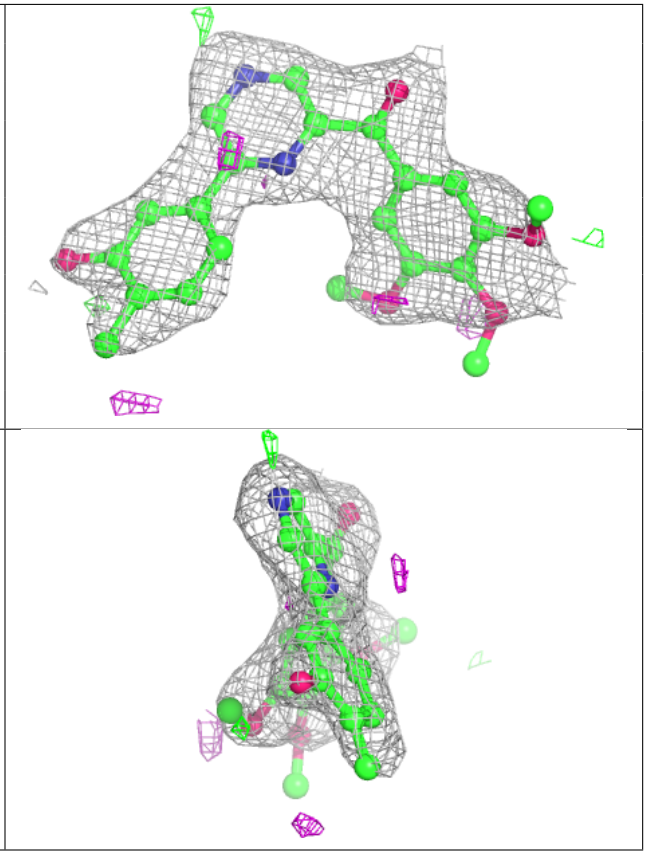
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	DMS	D	504	4/4	0.85	0.16	71,74,85,86	0
5	SO4	B	502	5/5	0.88	0.14	93,97,102,107	0
7	TU3	B	503	28/28	0.90	0.18	63,80,91,94	0
5	SO4	D	502	5/5	0.93	0.11	72,87,92,97	0
5	SO4	A	502	5/5	0.94	0.12	116,116,117,122	0
8	MG	C	502	1/1	0.96	0.06	47,47,47,47	0
7	TU3	D	503	28/28	0.97	0.20	36,56,75,82	0
4	GTP	A	501	32/32	0.98	0.16	34,41,56,58	0
4	GTP	C	501	32/32	0.98	0.15	37,43,48,51	0
4	GTP	D	501	32/32	0.98	0.10	28,38,73,82	0
6	GDP	B	501	28/28	0.98	0.15	38,43,52,55	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.

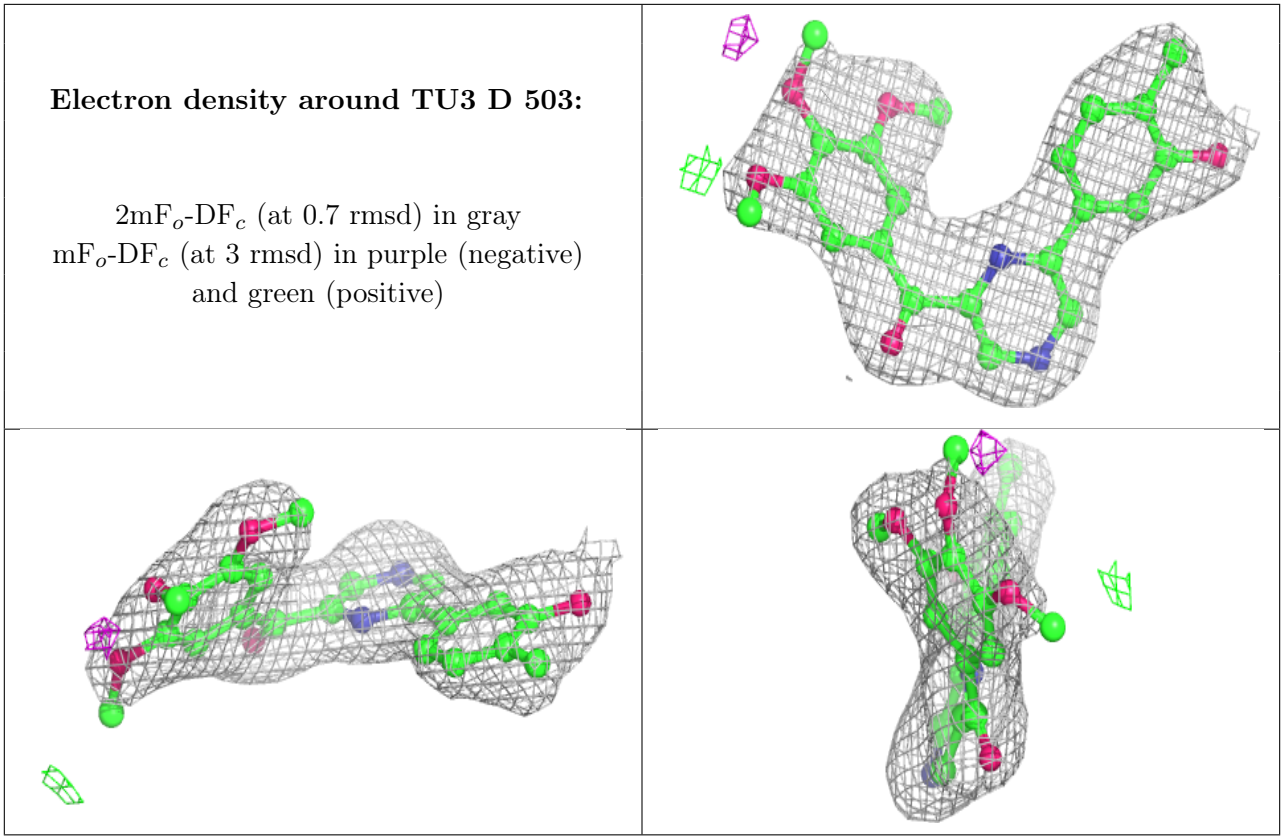
Electron density around TU3 B 503:

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



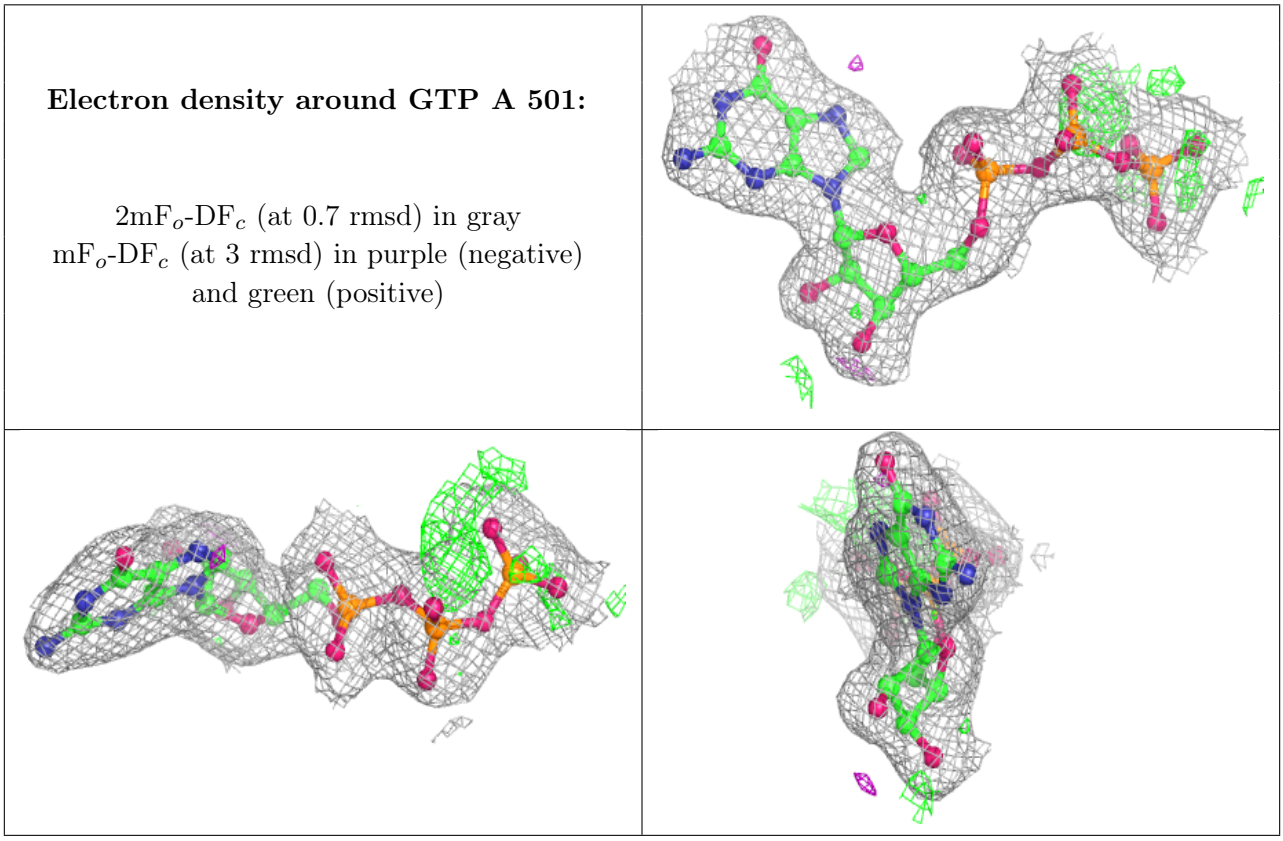
Electron density around TU3 D 503:

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



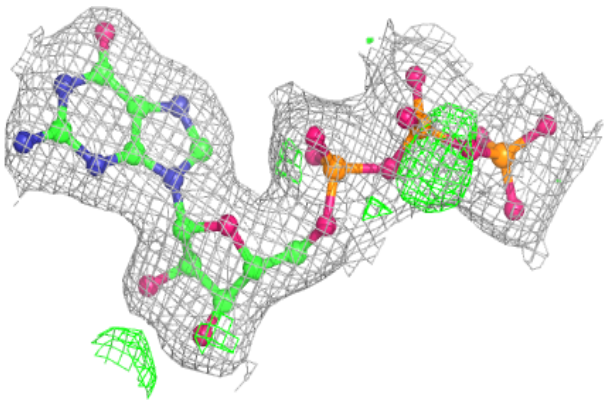
Electron density around GTP A 501:

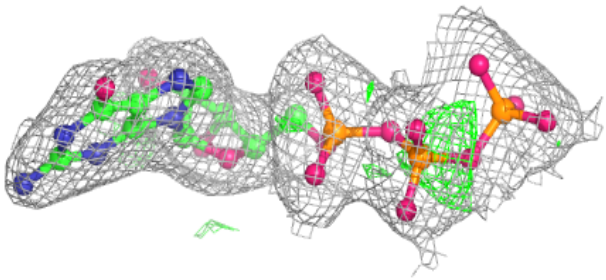
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

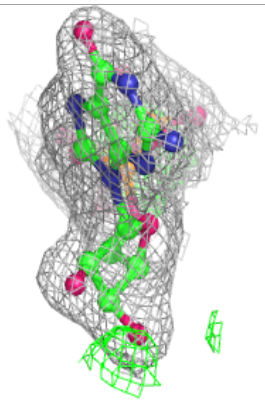


Electron density around GTP C 501:

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







Electron density around GTP D 501:

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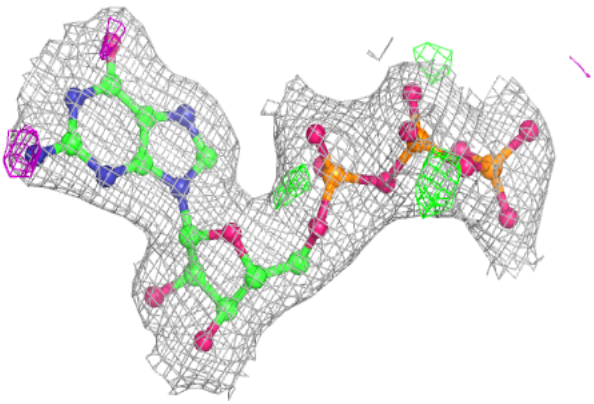
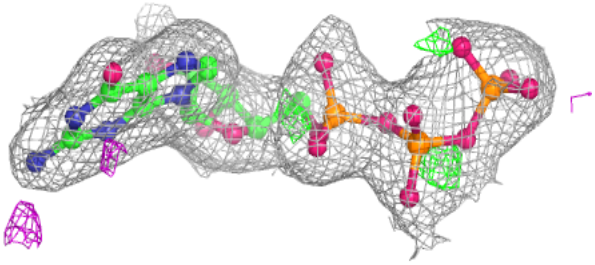
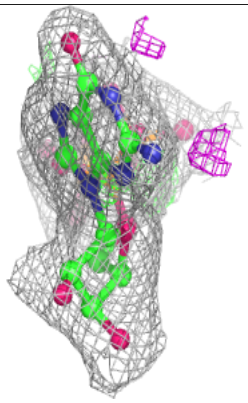
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

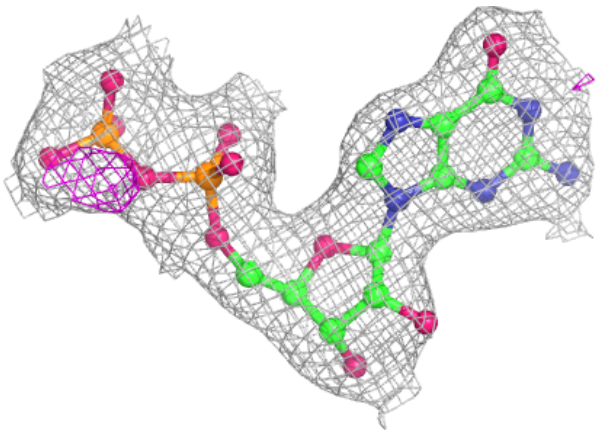


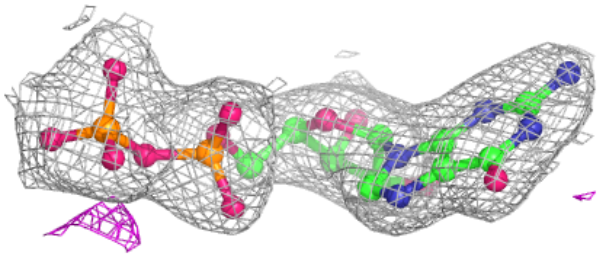


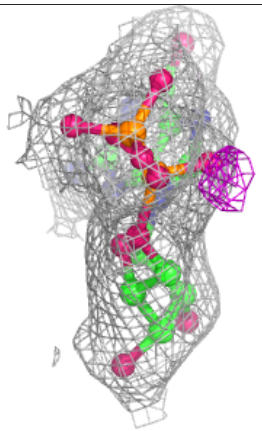


Electron density around GDP B 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.