



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:12 am BST

PDB ID : 5YLS
Title : Crystal structure of T2R-TTL-Y50 complex
Authors : Yang, J.H.; Chen, L.J.
Deposited on : 2017-10-18
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

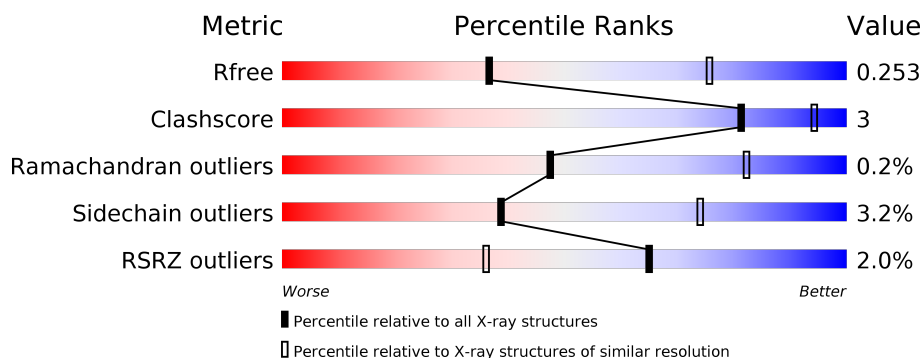
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>90%</div> <div>6%</div> </div>
1	C	451	<div> <div>92%</div> <div>6%</div> </div>
2	B	445	<div> <div>2%</div> <div>84%</div> <div>11%</div> </div>
2	D	445	<div> <div>2%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>
3	E	143	<div> <div>83%</div> <div>15%</div> </div>
4	F	384	<div> <div>8%</div> <div>76%</div> <div>9%</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 17527 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
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

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

Continued on next page...

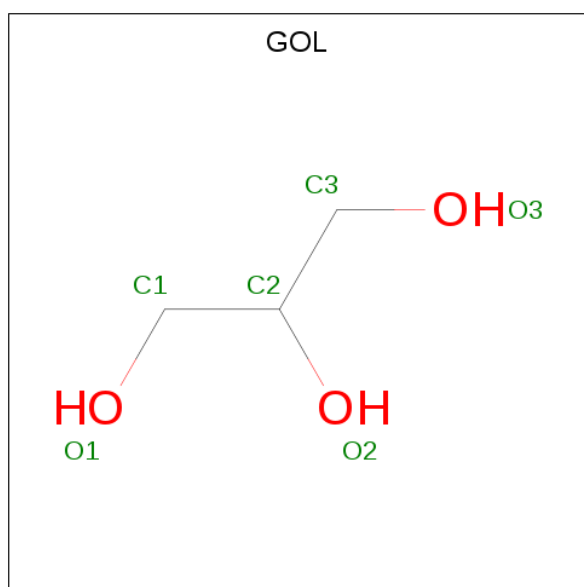
Continued from previous page...

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

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

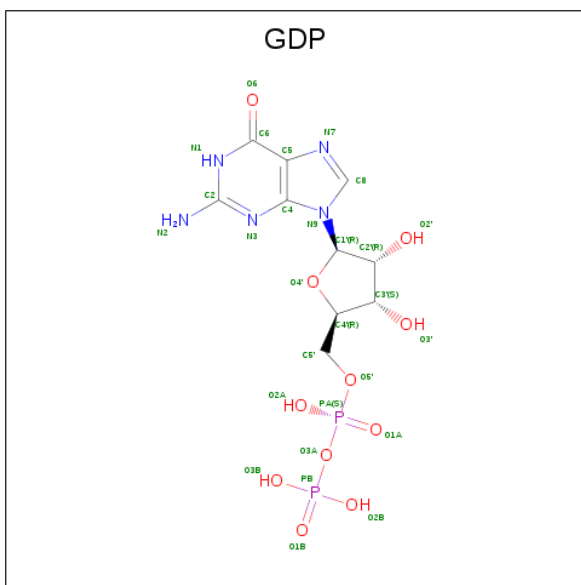
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



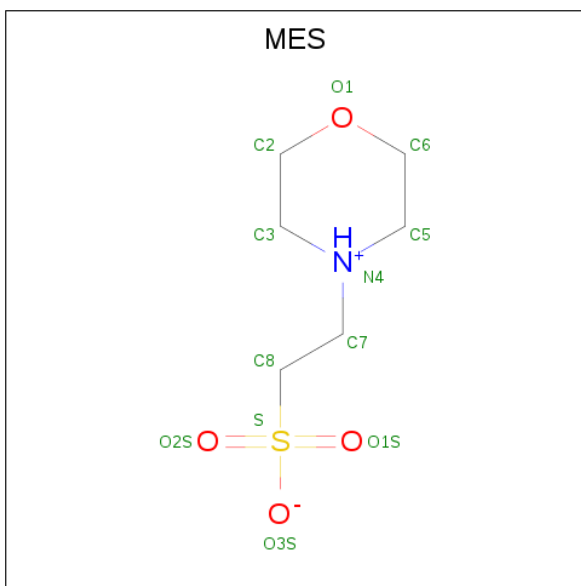
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

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



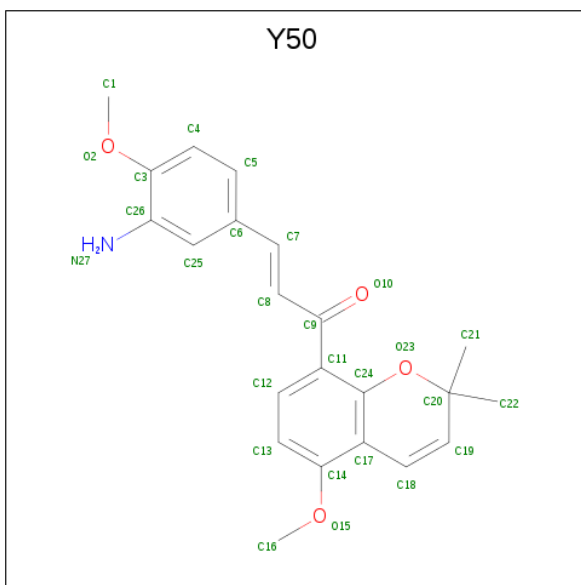
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



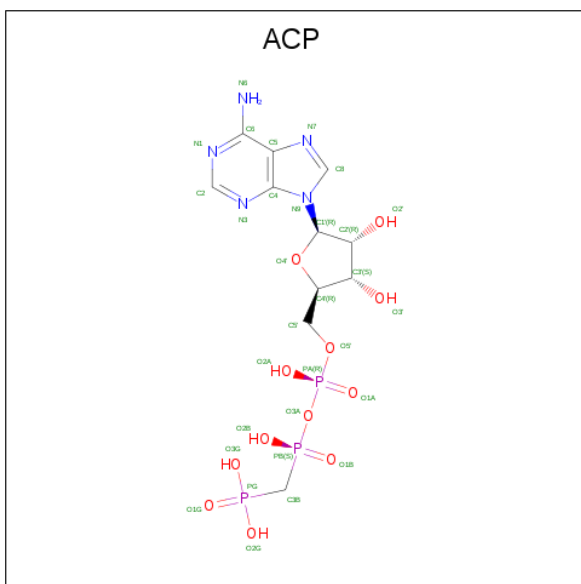
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is E-3-(3-azanyl-4-methoxy-phenyl)-1-(5-methoxy-2,2-dimethyl-chromen-8-yl)prop-2-en-1-one (three-letter code: Y50) (formula: $C_{22}H_{23}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	22	1	4		
11	D	1	Total	C	N	O	0	0
			27	22	1	4		

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



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

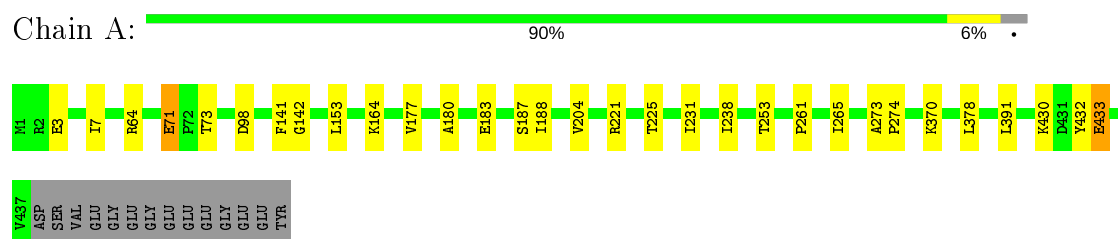
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	5	Total 5	O 5	0	0
13	B	7	Total 7	O 7	0	0
13	C	5	Total 5	O 5	0	0
13	D	2	Total 2	O 2	0	0

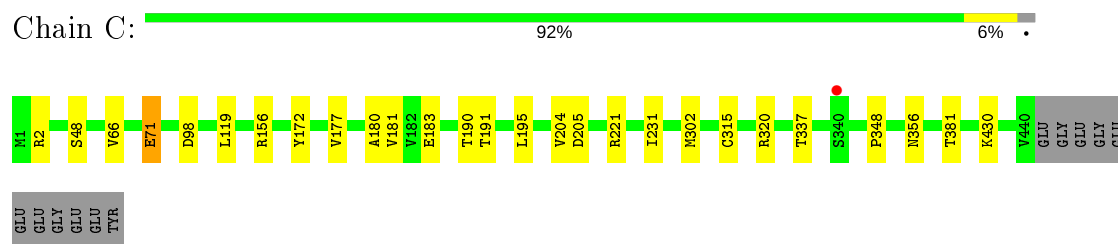
3 Residue-property plots [i](#)

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

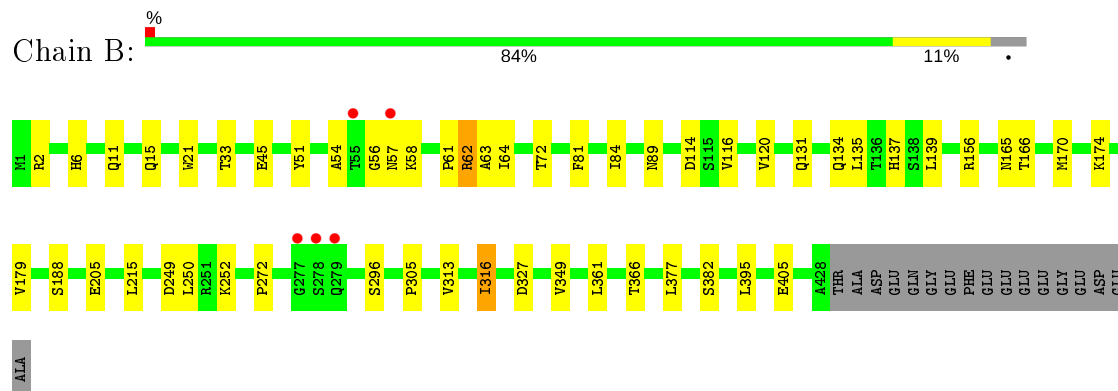
- Molecule 1: Tubulin alpha-1B chain



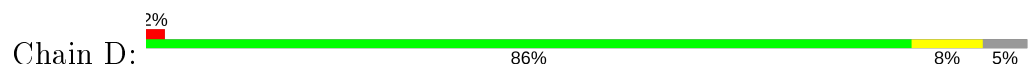
- Molecule 1: Tubulin alpha-1B chain

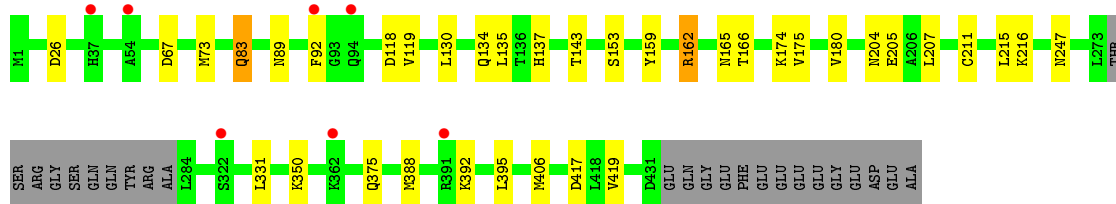


- Molecule 2: Tubulin beta chain



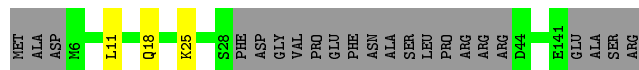
- Molecule 2: Tubulin beta chain





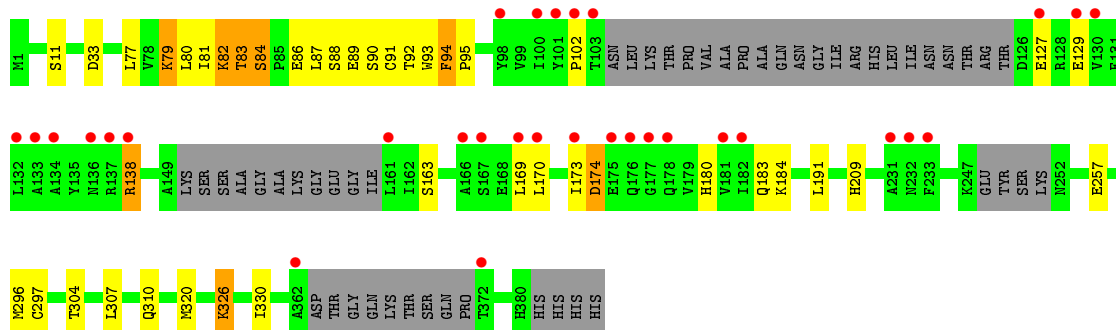
● Molecule 3: Stathmin-4

Chain E: 83% 15%



● Molecule 4: Tubulin tyrosine ligase

Chain F: 8% 76% 9% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.77Å 159.05Å 183.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 3.00 45.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.79-3.00) 99.8 (45.79-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.208 , 0.253 0.209 , 0.253	Depositor DCC
R_{free} test set	3126 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17527	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, Y50, CA, GTP, ACP, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/3494	0.59	0/4743
1	C	0.40	0/3515	0.61	0/4772
2	B	0.44	0/3444	0.61	1/4664 (0.0%)
2	D	0.41	0/3382	0.59	0/4581
3	E	0.36	0/1008	0.57	0/1337
4	F	0.45	0/2806	0.60	1/3791 (0.0%)
All	All	0.42	0/17649	0.60	2/23888 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	ARG	C-N-CA	-5.32	108.40	121.70
4	F	94	PHE	C-N-CD	5.06	139.02	128.40

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	3416	0	3331	11	0
1	C	3437	0	3348	8	0
2	B	3369	0	3250	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3309	0	3189	13	0
3	E	1000	0	1018	1	0
4	F	2744	0	2709	30	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	1	0
11	B	27	0	0	0	0
11	D	27	0	0	0	0
12	F	31	0	14	0	0
13	A	5	0	0	0	0
13	B	7	0	0	0	0
13	C	5	0	0	0	0
13	D	2	0	0	0	0
All	All	17527	0	16928	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (90) 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)
4:F:79:LYS:O	4:F:83:THR:OG1	1.86	0.94
4:F:81:ILE:HD13	4:F:87:LEU:HD12	1.58	0.83
4:F:81:ILE:HD13	4:F:87:LEU:CD1	2.08	0.83
2:B:63:ALA:O	2:B:89:ASN:ND2	2.12	0.82
4:F:92:THR:O	4:F:326:LYS:HE2	1.79	0.81
2:B:56:GLY:O	2:B:57:ASN:ND2	2.19	0.75
4:F:86:GLU:C	4:F:87:LEU:HD23	2.13	0.69
4:F:82:LYS:NZ	4:F:127:GLU:OE1	2.27	0.68
4:F:95:PRO:HG2	4:F:183:GLN:NE2	2.15	0.61
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.86	0.58
2:B:131:GLN:HE21	2:B:250:LEU:H	1.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:77:LEU:O	4:F:81:ILE:HG12	2.04	0.57
2:B:54:ALA:HB3	2:B:58:LYS:O	2.05	0.57
4:F:86:GLU:O	4:F:87:LEU:HD23	2.05	0.57
2:B:135:LEU:HB3	2:B:166:THR:HG22	1.87	0.56
4:F:81:ILE:C	4:F:83:THR:H	2.09	0.56
2:B:51:TYR:O	2:B:62:ARG:NH2	2.40	0.55
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.88	0.55
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.88	0.54
2:B:156:ARG:HG3	10:B:503:MES:H62	1.90	0.53
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.01	0.52
4:F:138:ARG:HH21	4:F:184:LYS:HD3	1.75	0.52
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.50
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.93	0.50
4:F:95:PRO:HG2	4:F:183:GLN:CG	2.42	0.49
2:B:64:ILE:HD13	2:B:120:VAL:HG22	1.94	0.49
4:F:89:GLU:O	4:F:91:CYS:N	2.40	0.49
2:D:135:LEU:HB3	2:D:166:THR:HG22	1.93	0.49
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.49
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.78	0.49
4:F:92:THR:O	4:F:326:LYS:CE	2.57	0.48
4:F:89:GLU:C	4:F:91:CYS:H	2.15	0.48
4:F:102:PRO:HG3	4:F:173:ILE:HG22	1.94	0.48
4:F:209:HIS:HB2	4:F:310:GLN:HG3	1.96	0.48
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.49	0.47
2:B:316:ILE:HG23	2:B:366:THR:HB	1.95	0.47
2:B:54:ALA:N	2:B:58:LYS:O	2.36	0.47
4:F:87:LEU:O	4:F:88:SER:OG	2.24	0.47
2:D:392:LYS:HB3	2:D:395:LEU:HD22	1.96	0.47
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.96	0.47
2:B:131:GLN:NE2	2:B:250:LEU:H	2.14	0.46
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.97	0.46
2:B:134:GLN:HA	2:B:165:ASN:O	2.14	0.46
2:B:54:ALA:HB3	2:B:58:LYS:C	2.35	0.46
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.96	0.46
4:F:80:LEU:HD12	4:F:80:LEU:O	2.16	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.45
2:B:139:LEU:HD22	2:B:188:SER:HB3	1.98	0.45
2:B:81:PHE:O	2:B:84:ILE:HG22	2.16	0.45
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.99	0.45
2:D:134:GLN:HA	2:D:165:ASN:O	2.17	0.45
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:163:SER:HB3	4:F:169:LEU:HG	1.98	0.45
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.99	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.52	0.44
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.99	0.44
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.98	0.44
4:F:84:SER:OG	4:F:297:CYS:SG	2.48	0.44
2:D:174:LYS:HD2	2:D:205:GLU:HG3	2.00	0.43
2:D:175:VAL:HG21	2:D:204:ASN:HB3	2.00	0.43
4:F:102:PRO:HB3	4:F:174:ASP:HA	2.00	0.43
4:F:94:PHE:CD1	4:F:95:PRO:CD	3.00	0.43
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.01	0.43
4:F:95:PRO:HG2	4:F:183:GLN:CD	2.39	0.43
1:A:273:ALA:HA	1:A:274:PRO:HA	1.81	0.43
1:A:430:LYS:HA	1:A:433:GLU:HB2	2.01	0.43
2:D:83:GLN:HG2	2:D:83:GLN:H	1.65	0.43
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.99	0.42
1:A:142:GLY:HA3	1:A:183:GLU:HG2	2.01	0.42
4:F:80:LEU:O	4:F:84:SER:HB2	2.19	0.42
2:B:56:GLY:C	2:B:57:ASN:ND2	2.73	0.42
2:D:67:ASP:HA	2:D:143:THR:HG21	2.02	0.42
2:B:11:GLN:HA	2:B:72:THR:HG21	2.01	0.41
2:D:89:ASN:HA	2:D:119:VAL:HG11	2.02	0.41
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.02	0.41
2:D:204:ASN:HA	2:D:207:LEU:HD12	2.02	0.41
2:B:296:SER:HB3	2:B:305:PRO:HD2	2.02	0.41
2:B:395:LEU:HD21	2:B:405:GLU:HG2	2.03	0.41
4:F:320:MET:HB2	4:F:330:ILE:HD11	2.02	0.41
2:B:116:VAL:O	2:B:120:VAL:HG23	2.21	0.41
4:F:81:ILE:C	4:F:83:THR:N	2.73	0.41
2:B:249:ASP:HB3	2:B:252:LYS:HB2	2.03	0.41
1:C:191:THR:O	1:C:195:LEU:HB2	2.21	0.41
1:C:320:ARG:HA	1:C:356:ASN:O	2.21	0.41
4:F:170:LEU:HA	4:F:173:ILE:HD12	2.02	0.41
2:B:272:PRO:HD2	2:B:361:LEU:HD13	2.02	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.50	0.41
1:C:71:GLU:HB3	1:C:98:ASP:HB3	2.03	0.40
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.02	0.40
2:D:159:TYR:HB3	2:D:162:ARG:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	435/451 (96%)	421 (97%)	13 (3%)	1 (0%)	47	82
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	426/445 (96%)	416 (98%)	10 (2%)	0	100	100
2	D	417/445 (94%)	406 (97%)	10 (2%)	1 (0%)	47	82
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	324/384 (84%)	304 (94%)	17 (5%)	3 (1%)	17	55
All	All	2157/2319 (93%)	2093 (97%)	59 (3%)	5 (0%)	47	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	216	LYS
4	F	11	SER
4	F	82	LYS
4	F	90	SER
1	A	261	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	357 (97%)	11 (3%)	41	75
1	C	371/379 (98%)	358 (96%)	13 (4%)	36	71
2	B	370/383 (97%)	360 (97%)	10 (3%)	44	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	364/383 (95%)	350 (96%)	14 (4%)	33	69
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	92
4	F	301/342 (88%)	289 (96%)	12 (4%)	31	68
All	All	1883/1993 (94%)	1822 (97%)	61 (3%)	39	74

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	73	THR
1	A	141	PHE
1	A	164	LYS
1	A	177	VAL
1	A	188	ILE
1	A	221	ARG
1	A	225	THR
1	A	253	THR
1	A	370	LYS
1	A	433	GLU
2	B	2	ARG
2	B	15	GLN
2	B	33	THR
2	B	45	GLU
2	B	114	ASP
2	B	137	HIS
2	B	215	LEU
2	B	316	ILE
2	B	327	ASP
2	B	382	SER
1	C	2	ARG
1	C	48	SER
1	C	66	VAL
1	C	71	GLU
1	C	177	VAL
1	C	181	VAL
1	C	190	THR
1	C	221	ARG
1	C	302	MET
1	C	315	CYS
1	C	337	THR
1	C	381	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	430	LYS
2	D	26	ASP
2	D	83	GLN
2	D	118	ASP
2	D	130	LEU
2	D	137	HIS
2	D	153	SER
2	D	162	ARG
2	D	180	VAL
2	D	247	ASN
2	D	331	LEU
2	D	350	LYS
2	D	388	MET
2	D	406	MET
2	D	417	ASP
3	E	25	LYS
4	F	33	ASP
4	F	79	LYS
4	F	83	THR
4	F	84	SER
4	F	129	GLU
4	F	138	ARG
4	F	174	ASP
4	F	180	HIS
4	F	191	LEU
4	F	257	GLU
4	F	296	MET
4	F	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	329	ASN
2	B	57	ASN
2	B	131	GLN
2	B	190	HIS
2	B	375	GLN
1	C	11	GLN
1	C	293	ASN
2	D	99	ASN
2	D	165	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	247	ASN
3	E	18	GLN
3	E	92	ASN
4	F	183	GLN
4	F	196	HIS
4	F	260	ASN
4	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	Y50	B	504	-	29,29,29	3.13	13 (44%)	41,42,42	1.92	10 (24%)
11	Y50	D	503	-	29,29,29	3.15	14 (48%)	41,42,42	2.05	10 (24%)
10	MES	B	503	-	12,12,12	2.08	1 (8%)	14,16,16	7.18	6 (42%)
8	GOL	A	504	-	5,5,5	0.23	0	5,5,5	0.39	0
5	GTP	D	501	-	26,34,34	1.27	2 (7%)	33,54,54	1.96	9 (27%)
9	GDP	B	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.98	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	501	6	26,34,34	1.19	2 (7%)	33,54,54	1.97	6 (18%)
5	GTP	A	501	6	26,34,34	1.28	2 (7%)	33,54,54	1.94	7 (21%)
12	ACP	F	401	-	27,33,33	1.48	6 (22%)	32,52,52	1.36	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	Y50	B	504	-	-	6/13/24/24	0/3/3/3
11	Y50	D	503	-	-	6/13/24/24	0/3/3/3
10	MES	B	503	-	-	3/6/14/14	0/1/1/1
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	D	501	-	-	4/18/38/38	0/3/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3
12	ACP	F	401	-	-	1/15/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	Y50	C18-C19	9.54	1.45	1.33
11	B	504	Y50	C18-C19	9.45	1.45	1.33
11	D	503	Y50	O23-C24	8.72	1.51	1.37
11	B	504	Y50	O23-C24	8.46	1.50	1.37
10	B	503	MES	C8-S	-6.55	1.68	1.77
5	A	501	GTP	C6-C5	4.85	1.49	1.41
5	D	501	GTP	C6-C5	4.59	1.49	1.41
11	B	504	Y50	O15-C14	4.49	1.44	1.37
11	D	503	Y50	O15-C14	4.49	1.44	1.37
11	B	504	Y50	C6-C7	4.48	1.60	1.47
5	C	501	GTP	C6-C5	4.35	1.48	1.41
11	D	503	Y50	C6-C7	4.32	1.60	1.47
9	B	501	GDP	C6-C5	3.89	1.48	1.41
12	F	401	ACP	PB-O3A	3.24	1.62	1.58
11	D	503	Y50	C11-C9	3.22	1.54	1.48
11	B	504	Y50	C11-C9	3.19	1.54	1.48
11	D	503	Y50	O10-C9	-3.17	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	Y50	O10-C9	-3.04	1.17	1.24
11	B	504	Y50	C20-C19	3.00	1.55	1.50
11	D	503	Y50	C20-C19	2.94	1.55	1.50
12	F	401	ACP	PG-O3G	2.86	1.61	1.54
12	F	401	ACP	PG-O2G	2.83	1.61	1.54
11	D	503	Y50	C13-C12	2.80	1.43	1.38
11	B	504	Y50	O2-C3	2.76	1.41	1.37
5	D	501	GTP	C5-C4	2.75	1.48	1.40
12	F	401	ACP	C5-C4	2.74	1.48	1.40
5	A	501	GTP	C5-C4	2.68	1.48	1.40
11	B	504	Y50	C13-C12	2.60	1.43	1.38
5	C	501	GTP	C5-C4	2.46	1.47	1.40
11	D	503	Y50	C17-C14	2.45	1.45	1.41
9	B	501	GDP	C5-C4	2.45	1.47	1.40
11	D	503	Y50	O2-C3	2.43	1.41	1.37
11	B	504	Y50	C17-C14	2.38	1.45	1.41
11	B	504	Y50	C8-C9	2.33	1.51	1.47
11	D	503	Y50	C11-C24	2.29	1.45	1.40
11	B	504	Y50	C26-N27	2.28	1.45	1.37
12	F	401	ACP	PB-O2B	2.21	1.61	1.56
12	F	401	ACP	C2-N3	2.20	1.35	1.32
11	D	503	Y50	C26-N27	2.14	1.45	1.37
11	B	504	Y50	C25-C6	2.10	1.43	1.39
11	D	503	Y50	C25-C6	2.07	1.43	1.39
11	D	503	Y50	C8-C9	2.01	1.50	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O1S-S-C8	-18.40	84.76	106.92
10	B	503	MES	O3S-S-O1S	-11.07	84.24	111.27
10	B	503	MES	O2S-S-C8	9.89	118.82	106.92
11	D	503	Y50	O2-C3-C26	8.74	119.82	114.05
10	B	503	MES	O2S-S-O1S	-8.72	83.77	113.95
10	B	503	MES	O3S-S-C8	8.21	119.05	105.77
11	B	504	Y50	O2-C3-C26	8.10	119.40	114.05
9	B	501	GDP	C2-N3-C4	4.92	120.97	115.36
5	A	501	GTP	C2-N3-C4	4.79	120.83	115.36
5	D	501	GTP	C2-N3-C4	4.76	120.79	115.36
5	C	501	GTP	C5-C6-N1	-4.65	117.06	123.43
5	C	501	GTP	C6-N1-C2	4.65	123.32	115.93
9	B	501	GDP	C6-N1-C2	4.49	123.07	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	4.48	120.48	115.36
5	A	501	GTP	C5-C6-N1	-4.41	117.40	123.43
5	A	501	GTP	C6-N1-C2	4.29	122.75	115.93
5	D	501	GTP	C6-N1-C2	4.27	122.71	115.93
5	C	501	GTP	C6-C5-C4	-4.15	116.83	120.80
5	D	501	GTP	C5-C6-N1	-4.12	117.80	123.43
9	B	501	GDP	C5-C6-N1	-4.12	117.80	123.43
9	B	501	GDP	N3-C2-N1	-3.97	121.93	127.22
11	B	504	Y50	C22-C20-C21	-3.90	100.20	111.29
9	B	501	GDP	C6-C5-C4	-3.88	117.09	120.80
11	D	503	Y50	C22-C20-C21	-3.88	100.24	111.29
5	A	501	GTP	C6-C5-C4	-3.84	117.13	120.80
5	D	501	GTP	C6-C5-C4	-3.79	117.17	120.80
5	C	501	GTP	N3-C2-N1	-3.61	122.41	127.22
5	D	501	GTP	N3-C2-N1	-3.45	122.62	127.22
12	F	401	ACP	C3'-C2'-C1'	3.43	106.14	100.98
12	F	401	ACP	N3-C2-N1	-3.41	123.34	128.68
5	A	501	GTP	N3-C2-N1	-3.27	122.87	127.22
11	D	503	Y50	C16-O15-C14	-3.26	112.60	117.53
10	B	503	MES	O3S-S-O2S	3.23	119.16	111.27
5	A	501	GTP	C4-C5-N7	-3.10	106.17	109.40
11	B	504	Y50	C16-O15-C14	-3.09	112.86	117.53
11	B	504	Y50	O15-C14-C17	2.88	120.82	115.26
11	B	504	Y50	O15-C14-C13	-2.87	119.44	124.37
12	F	401	ACP	PA-O3A-PB	-2.85	123.53	132.56
11	D	503	Y50	O15-C14-C13	-2.81	119.56	124.37
11	D	503	Y50	O2-C3-C4	-2.75	119.66	124.37
5	C	501	GTP	C4-C5-N7	-2.70	106.58	109.40
11	D	503	Y50	O15-C14-C17	2.66	120.41	115.26
5	D	501	GTP	C4-C5-N7	-2.61	106.68	109.40
12	F	401	ACP	C4-C5-N7	-2.58	106.71	109.40
5	D	501	GTP	PB-O3B-PG	-2.58	123.99	132.83
5	D	501	GTP	PA-O3A-PB	-2.54	124.13	132.83
11	D	503	Y50	C25-C26-C3	2.46	120.16	118.18
5	A	501	GTP	PA-O3A-PB	-2.44	124.46	132.83
11	B	504	Y50	C25-C26-C3	2.44	120.15	118.18
11	B	504	Y50	O2-C3-C4	-2.34	120.36	124.37
9	B	501	GDP	C4-C5-N7	-2.32	106.98	109.40
11	D	503	Y50	O23-C20-C21	2.30	110.74	105.98
11	D	503	Y50	C7-C8-C9	-2.28	117.92	121.64
11	B	504	Y50	O23-C20-C21	2.26	110.65	105.98
11	B	504	Y50	C22-C20-C19	2.25	115.61	111.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	Y50	C7-C8-C9	-2.16	118.11	121.64
9	B	501	GDP	PA-O3A-PB	-2.12	125.54	132.83
11	D	503	Y50	C22-C20-C19	2.11	115.33	111.45
5	D	501	GTP	C3'-C2'-C1'	2.08	104.10	100.98

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	503	MES	N4-C7-C8-S
10	B	503	MES	C7-C8-S-O2S
9	B	501	GDP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O1A
11	D	503	Y50	C26-C3-O2-C1
11	D	503	Y50	C7-C8-C9-O10
11	D	503	Y50	C7-C8-C9-C11
11	B	504	Y50	C13-C14-O15-C16
11	D	503	Y50	C13-C14-O15-C16
11	D	503	Y50	C17-C14-O15-C16
11	B	504	Y50	C17-C14-O15-C16
11	B	504	Y50	C7-C8-C9-O10
11	B	504	Y50	C7-C8-C9-C11
11	B	504	Y50	C26-C3-O2-C1
11	D	503	Y50	C4-C3-O2-C1
8	A	504	GOL	O2-C2-C3-O3
11	B	504	Y50	C4-C3-O2-C1
8	A	504	GOL	C1-C2-C3-O3
10	B	503	MES	C7-C8-S-O3S
5	C	501	GTP	PB-O3B-PG-O3G
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
12	F	401	ACP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	D	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C3'-C4'-C5'-O5'

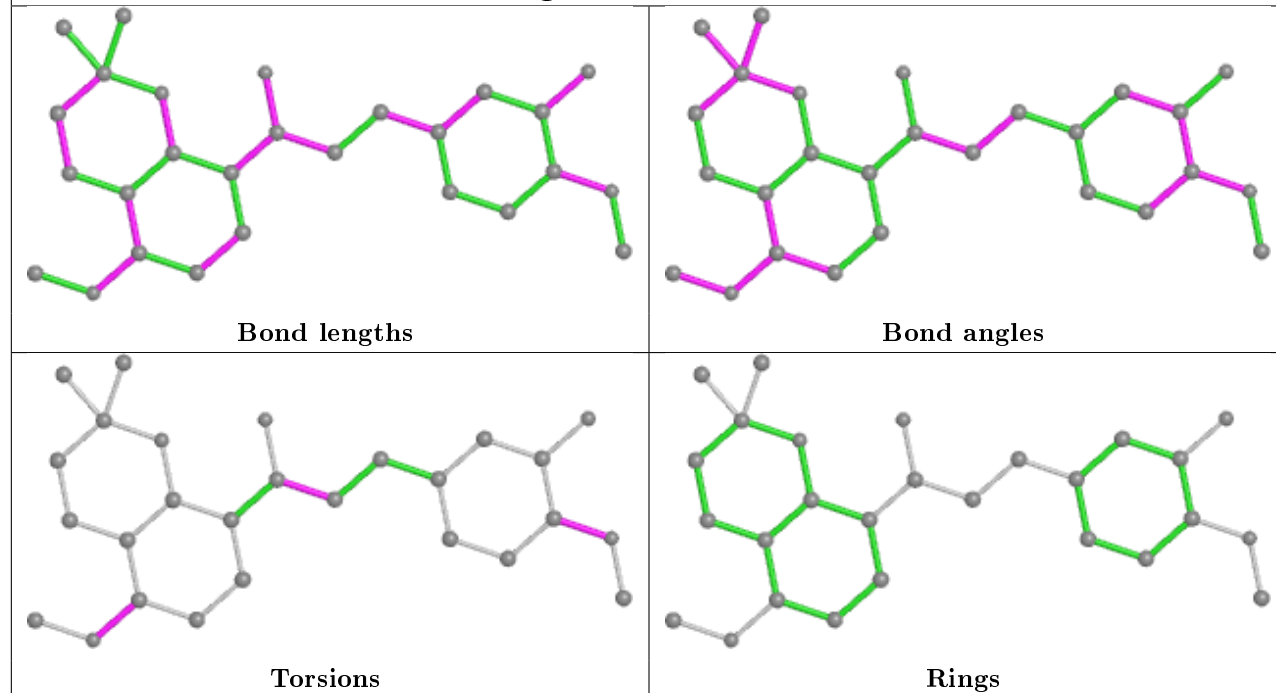
There are no ring outliers.

1 monomer is involved in 1 short contact:

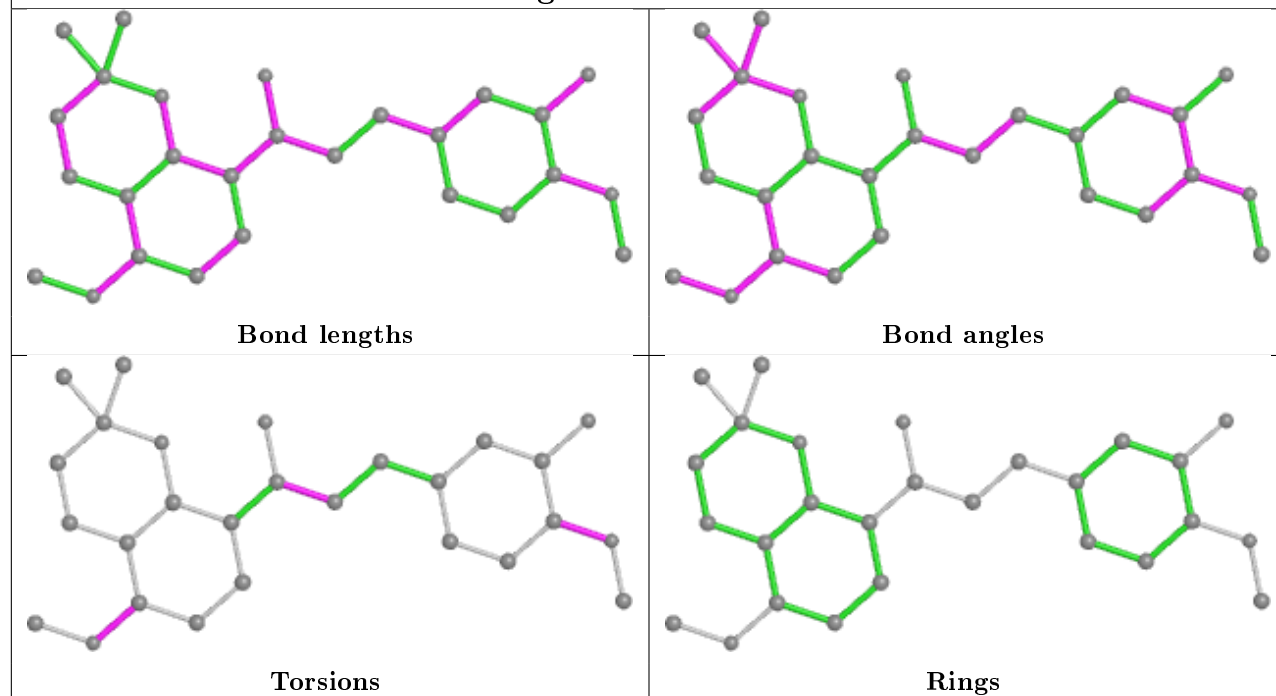
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	1	0

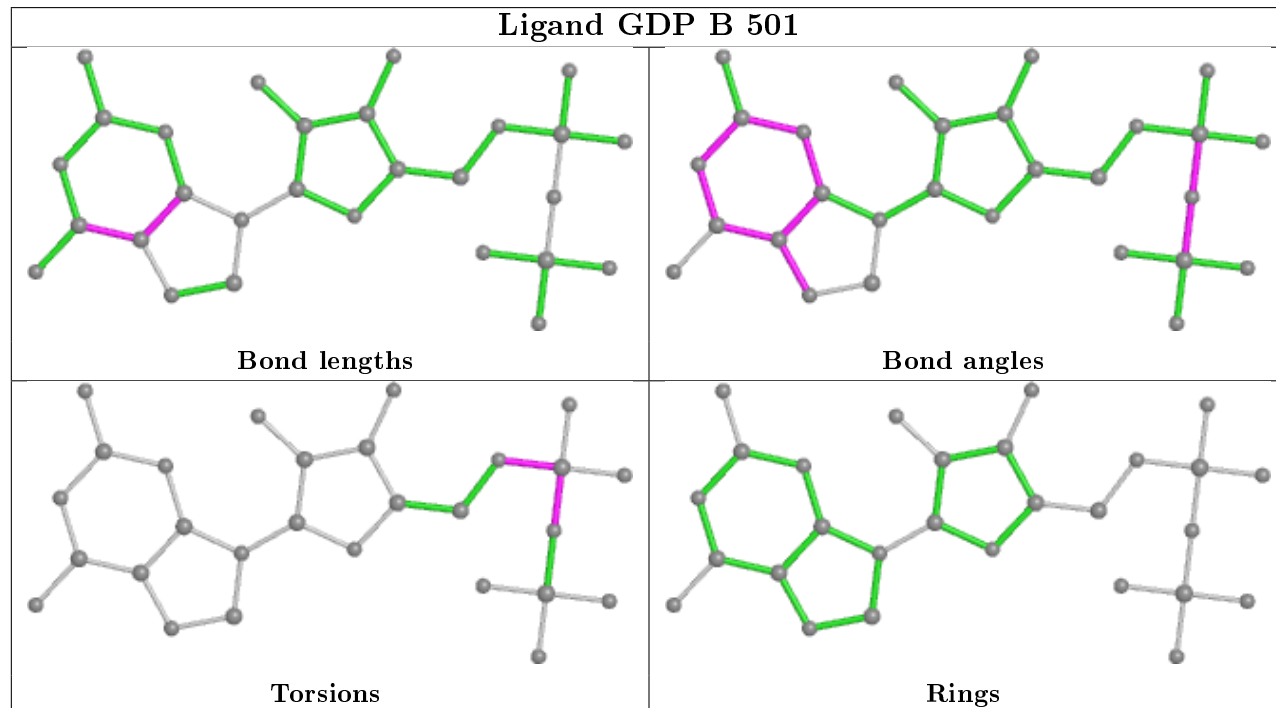
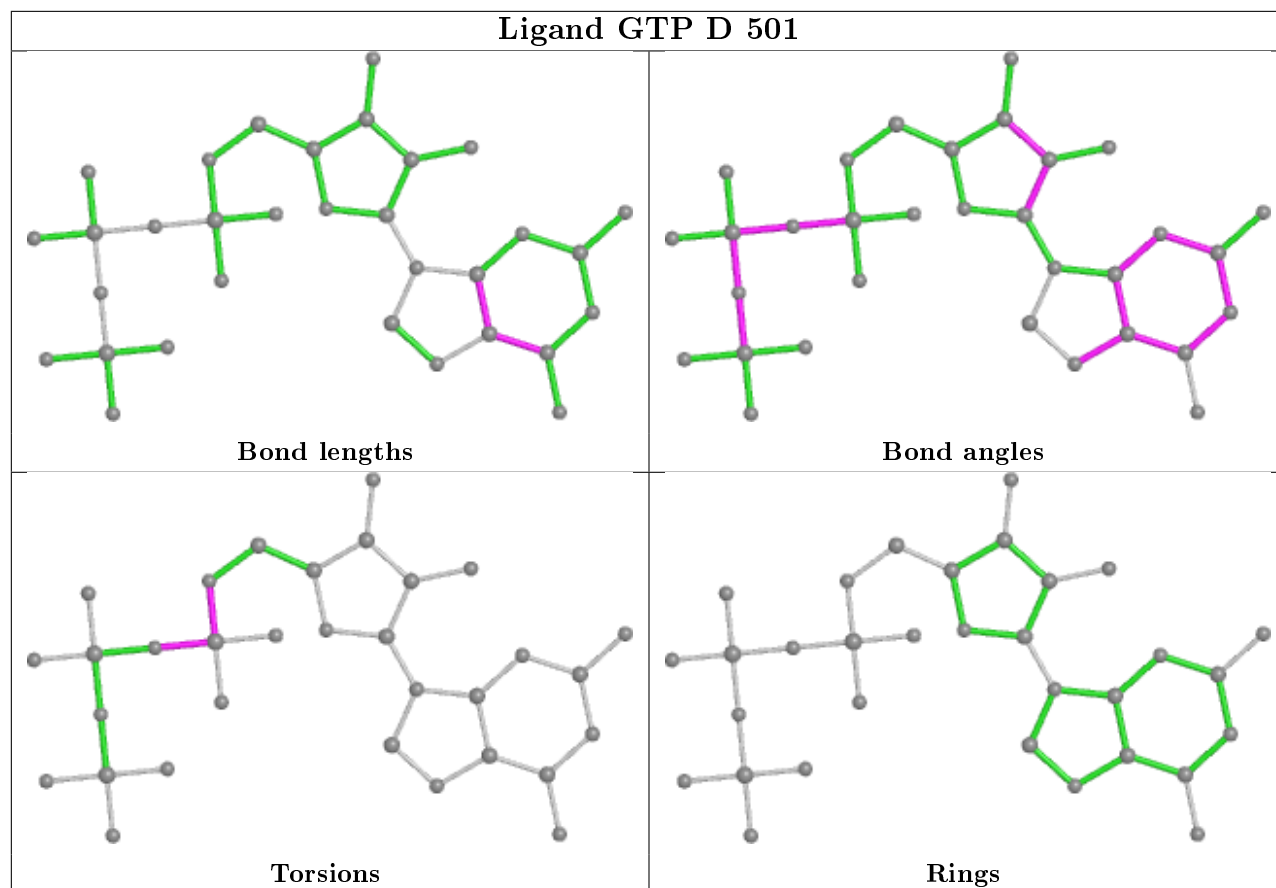
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand Y50 B 504

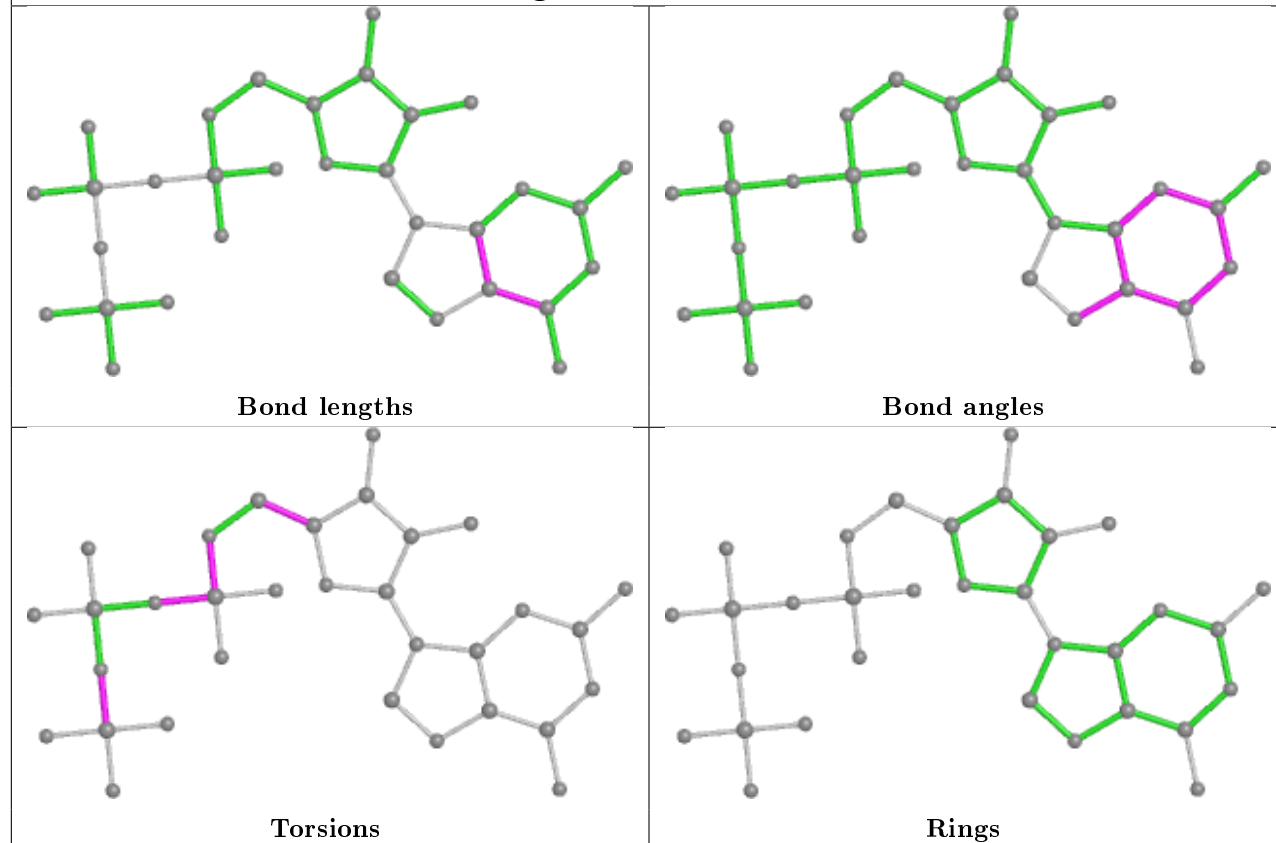


Ligand Y50 D 503

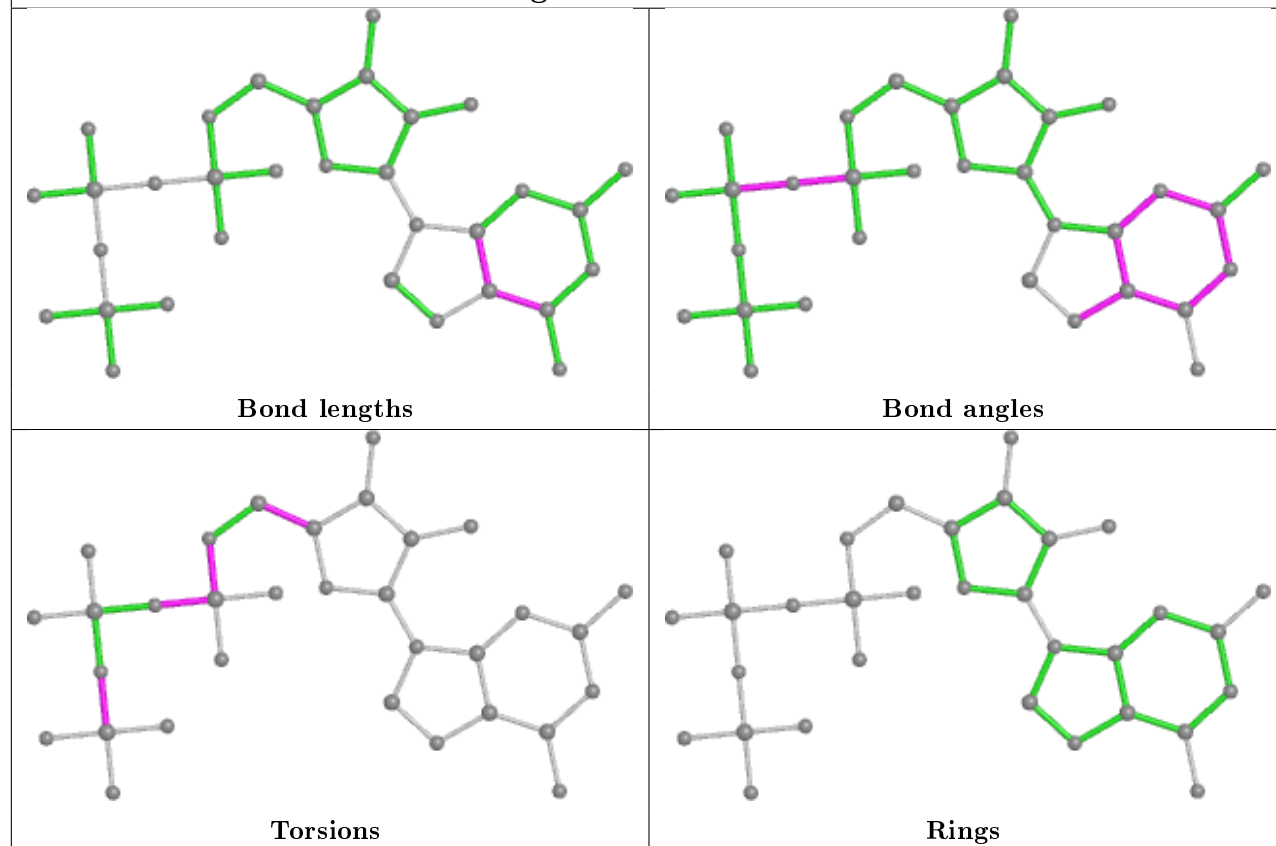


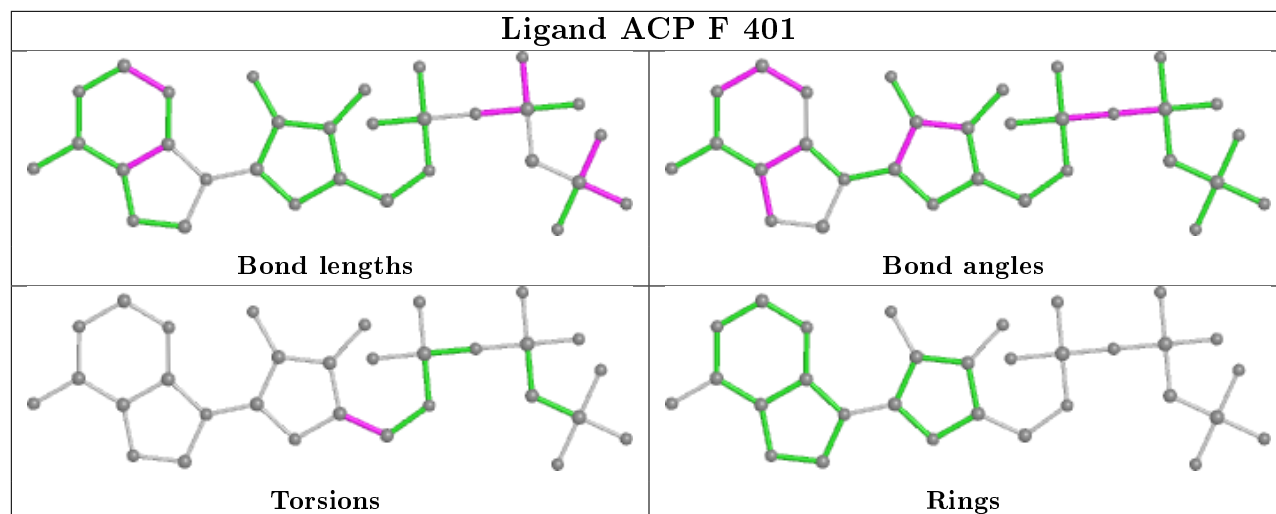


Ligand GTP C 501



Ligand GTP A 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	-0.28	0 100 100	42, 63, 88, 112	0
1	C	440/451 (97%)	-0.36	1 (0%) 95 87	34, 52, 76, 97	0
2	B	428/445 (96%)	-0.21	5 (1%) 79 54	38, 59, 91, 136	0
2	D	421/445 (94%)	0.08	7 (1%) 70 41	48, 90, 130, 155	0
3	E	121/143 (84%)	0.01	0 100 100	50, 81, 117, 138	0
4	F	334/384 (86%)	0.38	31 (9%) 8 3	55, 96, 157, 169	0
All	All	2181/2319 (94%)	-0.10	44 (2%) 65 36	34, 69, 128, 169	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	5.4
4	F	133	ALA	4.8
4	F	173	ILE	4.4
4	F	132	LEU	4.1
4	F	167	SER	3.9
4	F	100	ILE	3.9
4	F	178	GLN	3.8
2	D	37	HIS	3.6
4	F	231	ALA	3.5
4	F	232	ASN	3.3
4	F	134	ALA	3.3
4	F	169	LEU	3.3
4	F	166	ALA	3.3
4	F	372	THR	3.2
2	D	94	GLN	3.2
4	F	136	ASN	3.2
4	F	103	THR	3.1
2	B	279	GLN	3.1
4	F	161	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	101	TYR	3.0
4	F	129	GLU	2.9
4	F	170	LEU	2.9
4	F	102	PRO	2.8
2	B	278	SER	2.8
2	B	57	ASN	2.7
2	B	55	THR	2.7
4	F	127	GLU	2.7
4	F	362	ALA	2.5
2	D	391	ARG	2.5
4	F	176	GLN	2.5
4	F	137	ARG	2.3
4	F	182	ILE	2.2
1	C	340	SER	2.2
4	F	233	PHE	2.2
2	D	362	LYS	2.2
4	F	177	GLY	2.2
2	D	92	PHE	2.1
4	F	138	ARG	2.1
4	F	98	TYR	2.1
2	D	322	SER	2.1
2	B	277	GLY	2.0
4	F	175	GLU	2.0
2	D	54	ALA	2.0
4	F	181	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

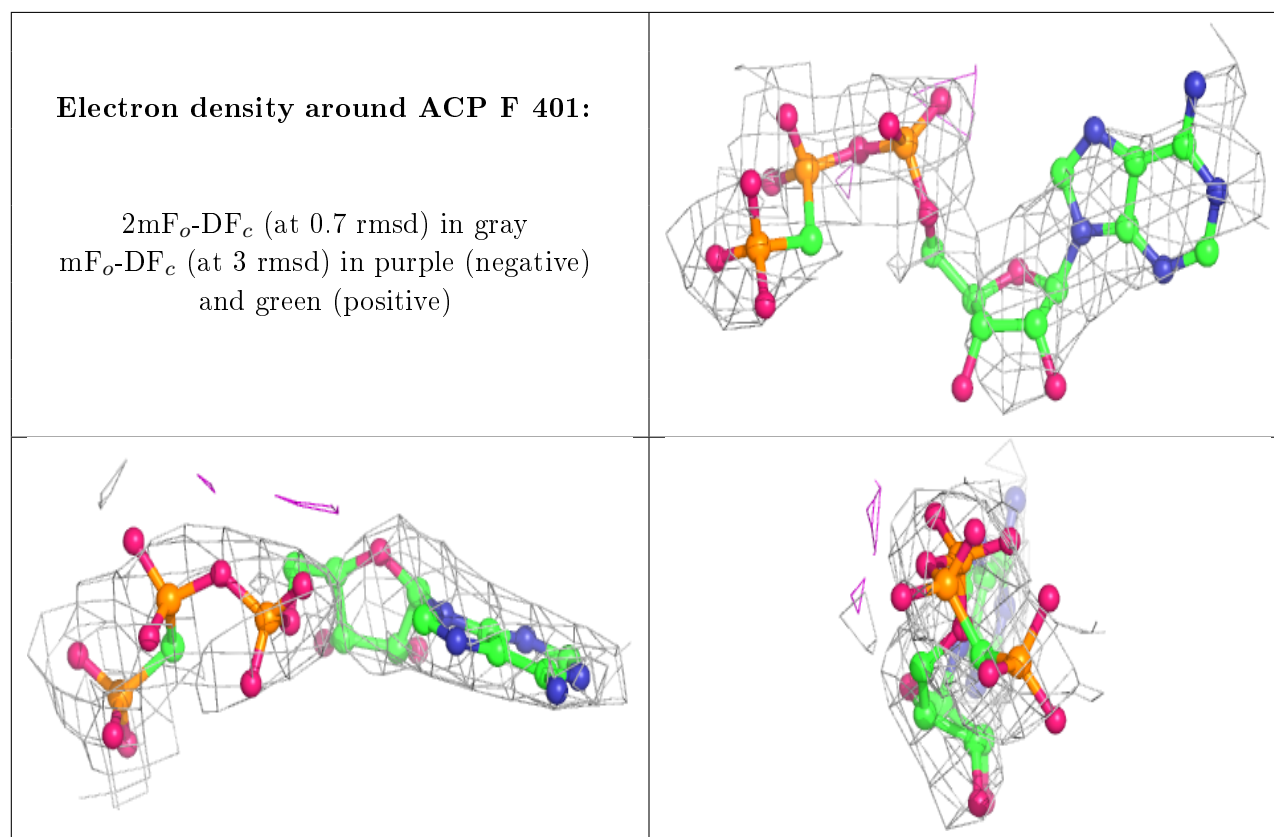
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

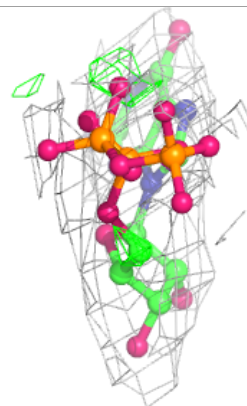
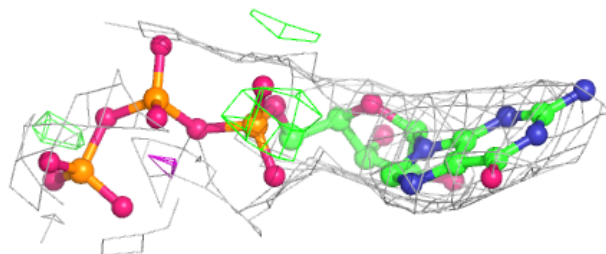
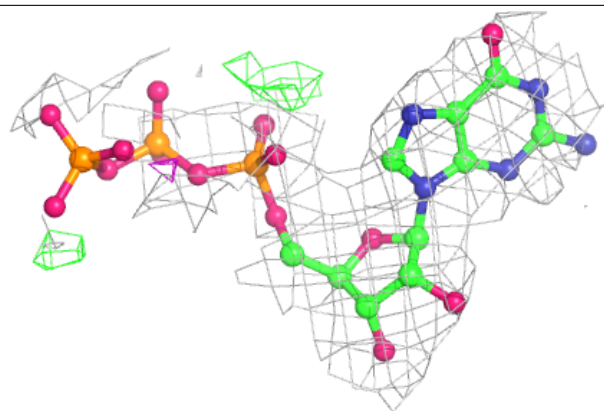
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	502	1/1	0.74	0.14	90,90,90,90	0
10	MES	B	503	12/12	0.81	0.31	112,126,141,143	0
12	ACP	F	401	31/31	0.82	0.26	118,131,160,161	0
7	CA	A	503	1/1	0.86	0.09	84,84,84,84	0
8	GOL	A	504	6/6	0.91	0.23	62,64,65,68	0
5	GTP	D	501	32/32	0.93	0.16	75,82,96,99	0
11	Y50	D	503	27/27	0.95	0.24	77,90,102,106	0
7	CA	C	503	1/1	0.96	0.12	75,75,75,75	0
11	Y50	B	504	27/27	0.96	0.25	52,68,72,74	0
5	GTP	C	501	32/32	0.97	0.18	37,41,45,46	0
9	GDP	B	501	28/28	0.97	0.18	39,42,44,48	0
5	GTP	A	501	32/32	0.98	0.20	39,43,45,45	0
6	MG	A	502	1/1	0.99	0.16	49,49,49,49	0
6	MG	B	502	1/1	0.99	0.15	48,48,48,48	0
6	MG	C	502	1/1	0.99	0.19	40,40,40,40	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.

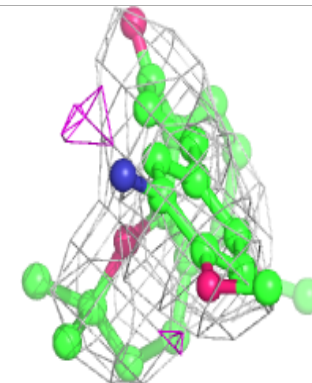
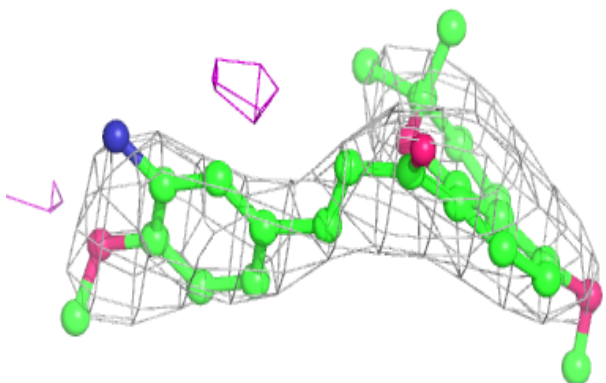
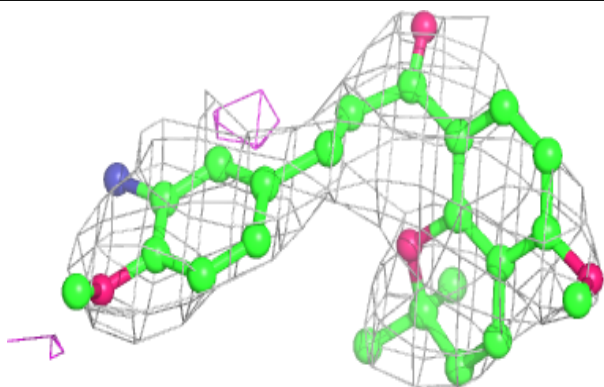


Electron density around GTP D 501:

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

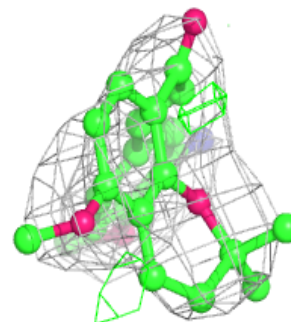
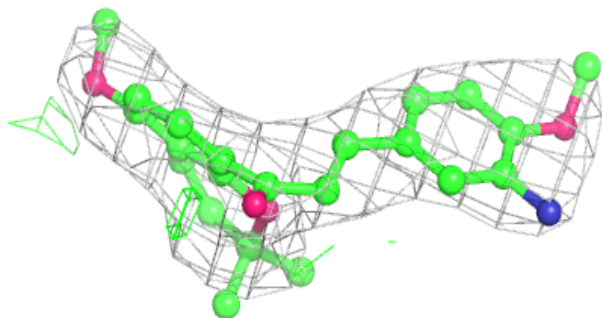
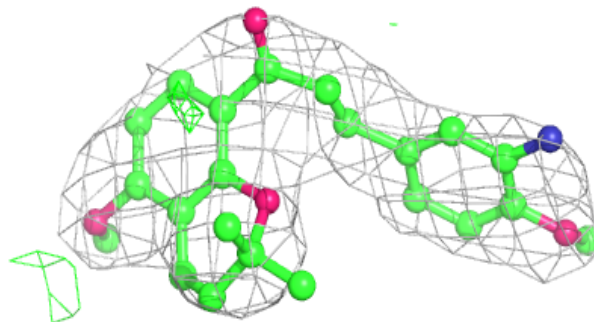
**Electron density around Y50 D 503:**

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

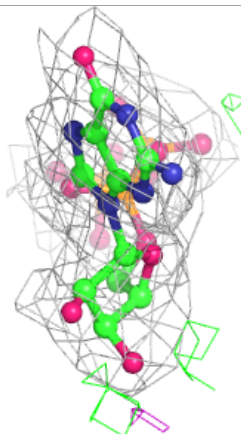
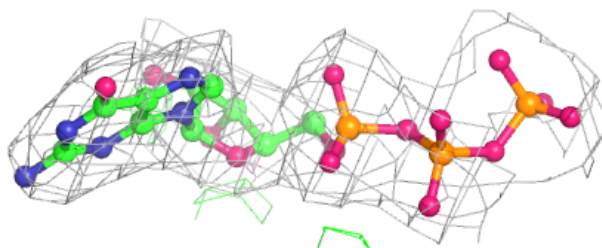
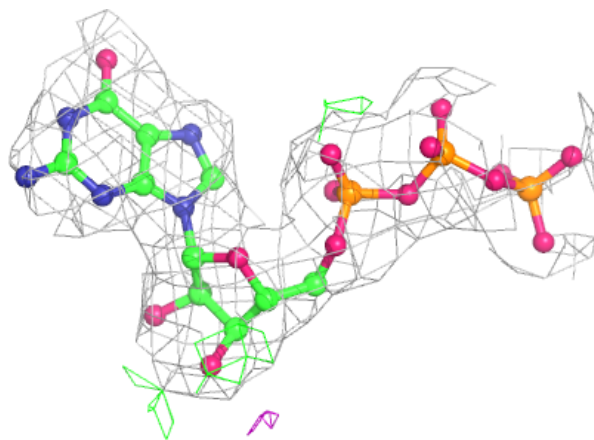


Electron density around Y50 B 504:

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

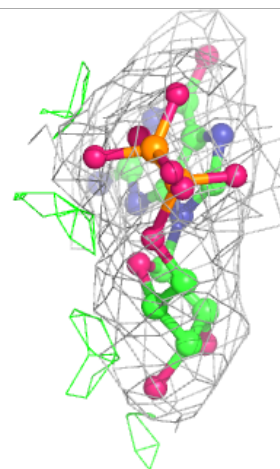
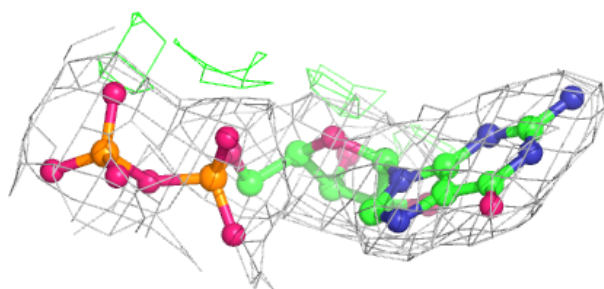
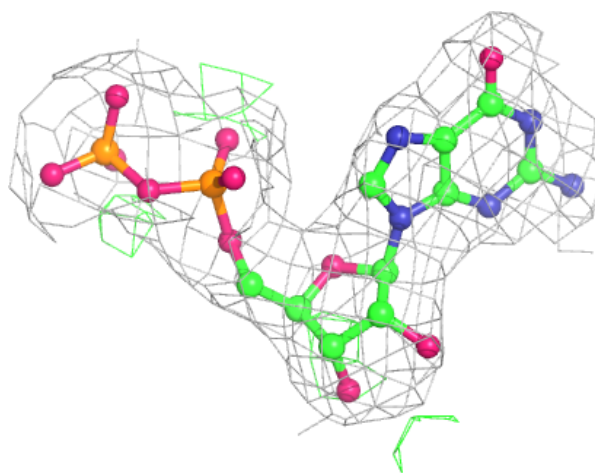
**Electron density around GTP C 501:**

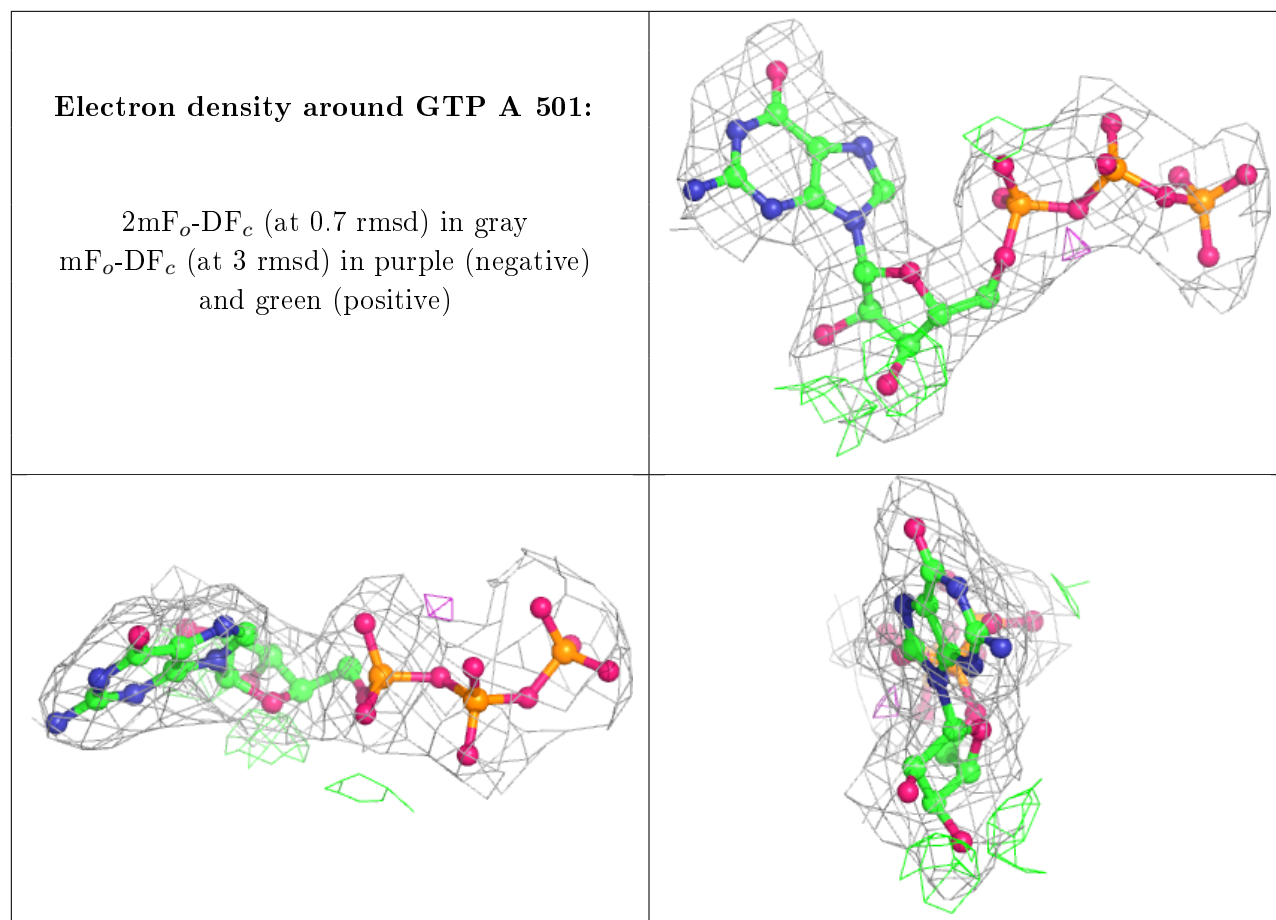
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.