



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:38 PM JST

PDB ID : 8YUA  
Title : Tubulin-RB3-TTL in complex with compound SI10  
Authors : Wu, C.Y.; Wang, Y.X.  
Deposited on : 2024-03-27  
Resolution : 2.37 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

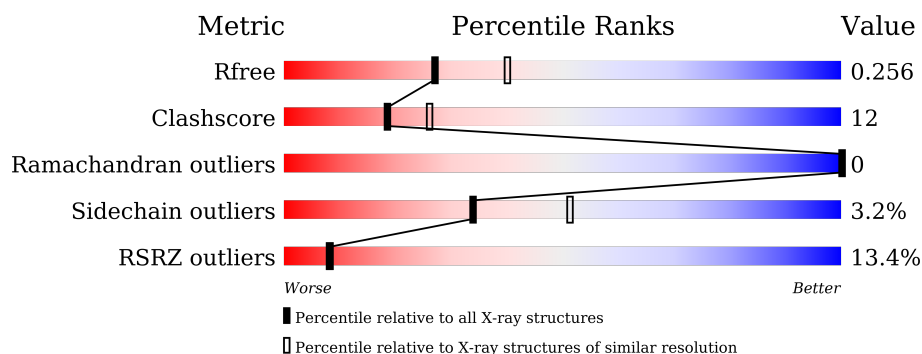
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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))
$R_{free}$	164625	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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  $\geq 3$ , 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	440	<div> <div>4%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	C	440	<div> <div>2%</div> <div>83%</div> <div>16%</div> </div>
2	B	431	<div> <div>9%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	D	431	<div> <div>23%</div> <div>67%</div> <div>28%</div> <div>..</div> </div>
3	E	143	<div> <div>13%</div> <div>64%</div> <div>17%</div> <div>..</div> <div>16%</div> </div>
4	F	380	<div> <div>27%</div> <div>55%</div> <div>23%</div> <div>.</div> <div>18%</div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17194 atoms, of which 38 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	418	Total	C	N	O	S	0	0	0
			3281	2065	555	634	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			988	611	180	192	5			

There are 2 discrepancies between the modelled and reference sequences:

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

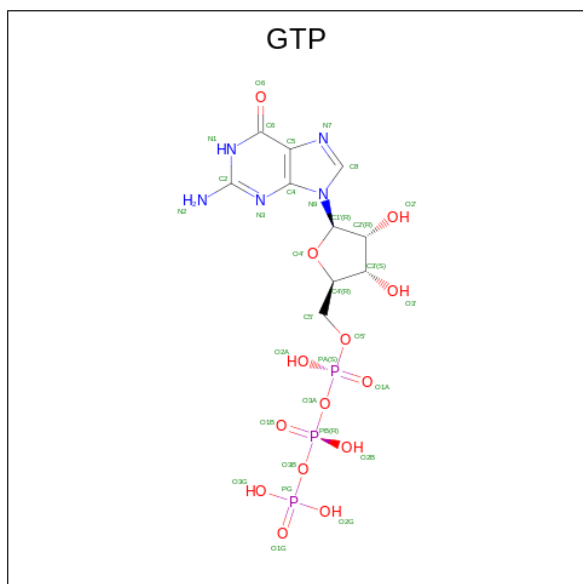
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	310	Total	C	N	O	S	0	0	0
			2476	1595	415	452	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1

- 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	32	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	32	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

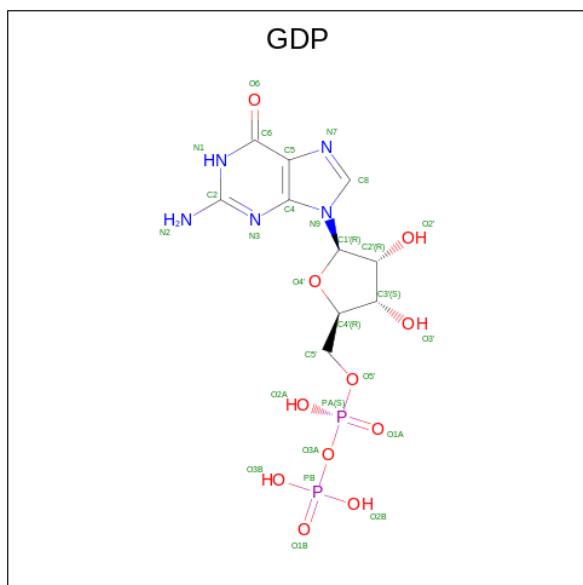
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

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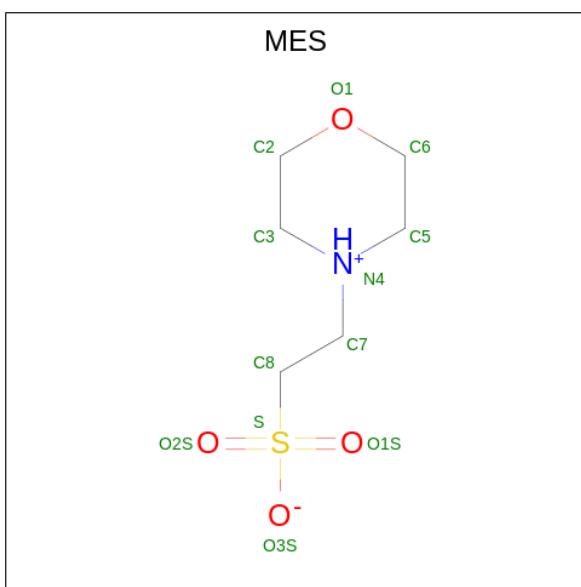
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

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



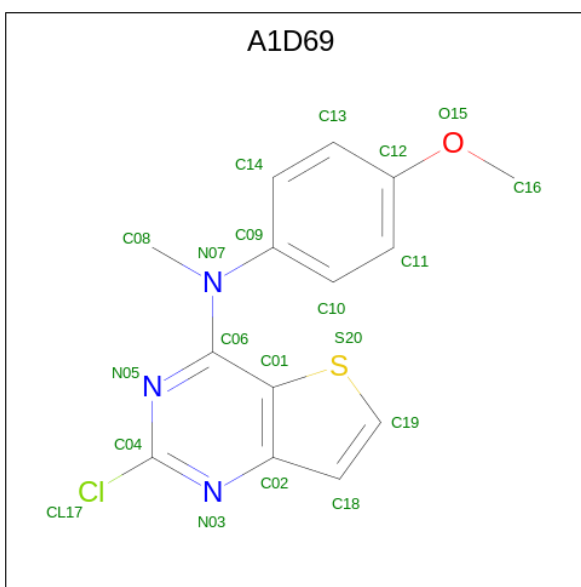
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	28	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	28	0
			28	10	5	11	2		

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



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

- Molecule 10 is 2-chloranyl- {N}-(4-methoxyphenyl)- {N}-methyl-thieno[3,2-d]pyrimidin-4-a mine (three-letter code: A1D69) (formula: C<sub>14</sub>H<sub>12</sub>ClN<sub>3</sub>OS) (labeled as "Ligand of Interest" by depositor).



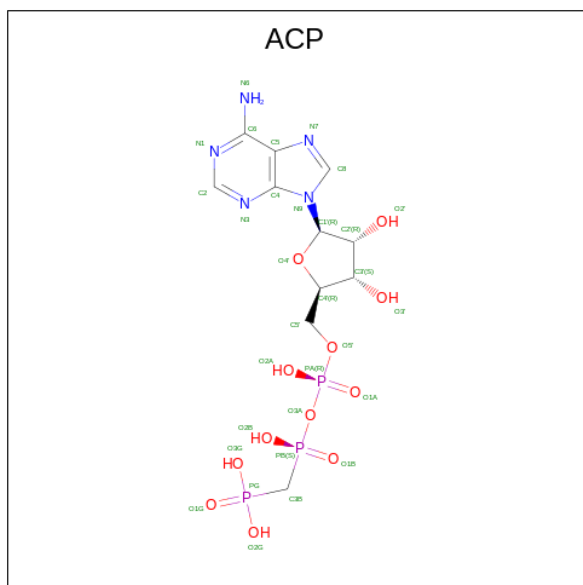
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	B	1	Total	C	Cl	H	N	O	S	0	0
			32	14	1	12	3	1	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	D	1	Total	C	Cl	H	N	O	S	0	0
			32	14	1	12	3	1	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		

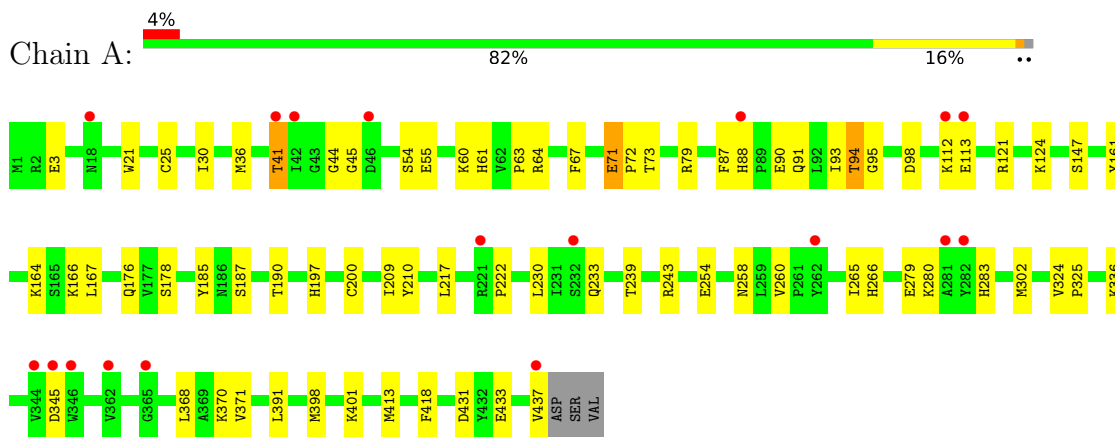
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total 1 O 1	0	0
12	D	1	Total 1 O 1	0	0

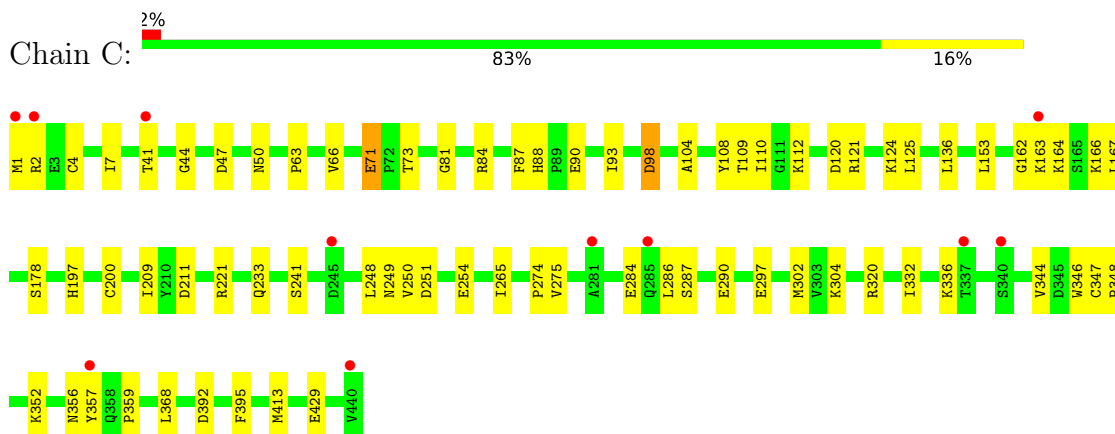
### 3 Residue-property plots [i](#)

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.

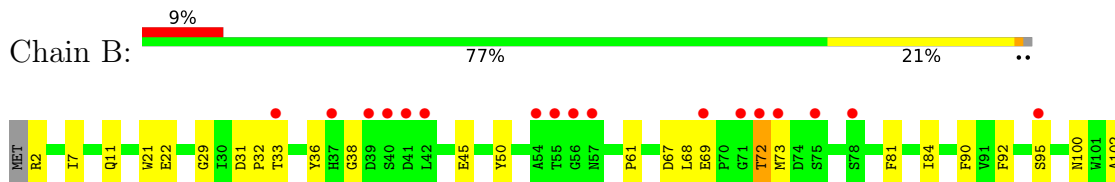
- Molecule 1: Detyrosinated tubulin alpha-1B chain



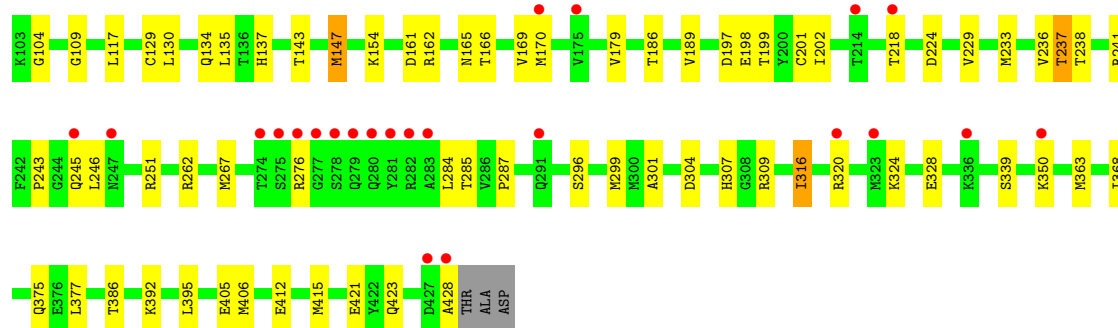
- Molecule 1: Detyrosinated tubulin alpha-1B chain



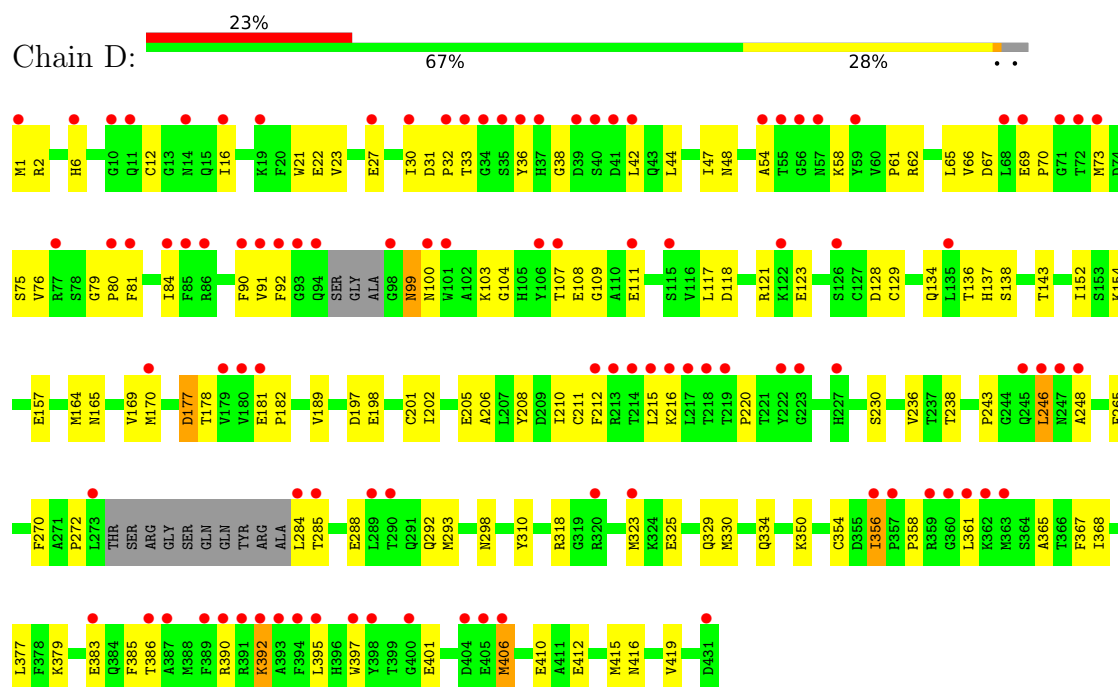
- Molecule 2: Tubulin beta chain



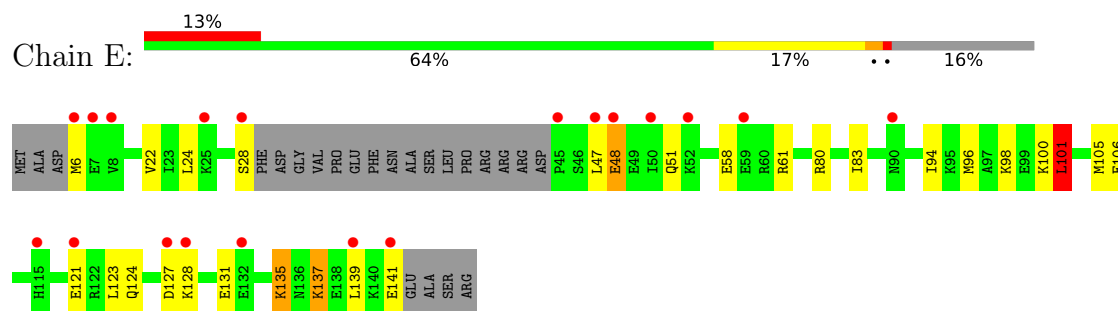




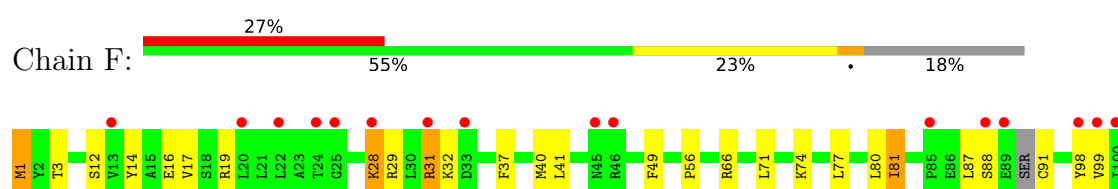
• Molecule 2: Tubulin beta chain

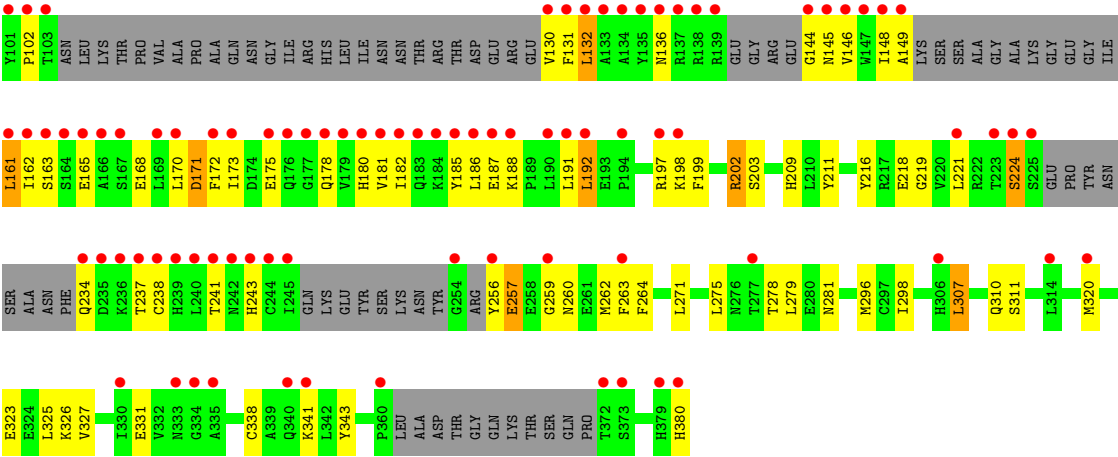


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.56Å 158.45Å 180.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.13 – 2.37 119.13 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.8 (119.13-2.37) 99.8 (119.13-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, $R_{free}$	0.229 , 0.254 0.229 , 0.256	Depositor DCC
$R_{free}$ test set	121385 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MES, GDP, GTP, MG, ACP, CA, A1D69

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	0.46	0/3482	0.64	0/4728
1	C	0.51	0/3511	0.68	2/4768 (0.0%)
2	B	0.47	1/3426 (0.0%)	0.63	0/4643
2	D	0.41	0/3353	0.60	1/4543 (0.0%)
3	E	0.43	0/996	0.59	1/1320 (0.1%)
4	F	0.39	0/2529	0.60	0/3424
All	All	0.45	1/17297 (0.0%)	0.63	4/23426 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	CYS	CB-SG	-5.25	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	246	LEU	CA-CB-CG	6.63	130.55	115.30
3	E	101	LEU	CA-CB-CG	6.56	130.39	115.30
1	C	98	ASP	CB-CG-OD1	6.14	123.83	118.30
1	C	98	ASP	CB-CG-OD2	-5.44	113.40	118.30

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	3405	0	3312	61	0
1	C	3433	0	3337	54	0
2	B	3351	0	3214	72	1
2	D	3281	0	3150	110	0
3	E	988	0	1011	26	1
4	F	2476	0	2388	87	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	11	0	0
9	B	24	0	26	0	0
10	B	20	12	0	1	0
10	D	20	12	0	0	0
11	F	31	14	14	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
All	All	17156	38	16499	395	1

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 12.

All (395) 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:A:239:THR:OG1	1:A:243:ARG:NH1	1.96	0.98
2:D:54:ALA:HB3	2:D:58:LYS:HB2	1.50	0.93
2:B:68:LEU:HG	2:B:147:MET:HE1	1.55	0.89
4:F:98:TYR:O	4:F:181:VAL:HG23	1.75	0.86
4:F:256:TYR:HB2	4:F:257:GLU:OE1	1.74	0.86
2:D:318:ARG:HH21	2:D:356:ILE:HG12	1.41	0.85
1:A:71:GLU:OE2	1:A:73:THR:HB	1.77	0.84
3:E:121:GLU:HG3	3:E:124:GLN:HE21	1.45	0.81
1:C:88:HIS:HD2	1:C:90:GLU:H	1.26	0.81
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.82	0.79
2:D:107:THR:O	2:D:111:GLU:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HE3	2:B:377:LEU:HD21	1.66	0.77
2:B:11:GLN:HG3	2:B:72:THR:HG21	1.67	0.77
4:F:188:LYS:HD3	4:F:323:GLU:OE1	1.84	0.77
1:A:112:LYS:NZ	1:A:113:GLU:OE2	2.19	0.75
2:B:143:THR:HG23	2:B:147:MET:HE3	1.68	0.75
2:B:143:THR:HG23	2:B:147:MET:CE	2.18	0.74
1:C:88:HIS:CD2	1:C:90:GLU:H	2.05	0.73
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.17	0.73
2:D:285:THR:HG23	2:D:288:GLU:H	1.53	0.72
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.71	0.72
4:F:149:ALA:CB	4:F:161:LEU:HB3	2.20	0.72
4:F:278:THR:HG23	4:F:281:ASN:H	1.54	0.71
2:B:68:LEU:HG	2:B:147:MET:CE	2.20	0.71
2:B:238:THR:HG21	2:B:316:ILE:HD11	1.72	0.70
2:B:262:ARG:NH1	2:B:421:GLU:OE2	2.24	0.70
4:F:149:ALA:HB3	4:F:161:LEU:HB3	1.71	0.70
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.25	0.70
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.72	0.70
4:F:186:LEU:CD1	4:F:320:MET:HG2	2.20	0.70
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.91	0.70
3:E:121:GLU:O	3:E:124:GLN:HG3	1.91	0.70
4:F:131:PHE:CZ	4:F:182:ILE:HD11	2.26	0.70
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.73	0.69
2:B:386:THR:HG22	2:B:412:GLU:OE2	1.93	0.69
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.28	0.69
2:D:104:GLY:O	2:D:109:GLY:HA3	1.91	0.69
1:A:336:LYS:HD3	3:E:24:LEU:CD1	2.22	0.69
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.75	0.69
4:F:1:MET:HE1	4:F:28:LYS:HB3	1.76	0.68
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.74	0.67
3:E:101:LEU:O	3:E:105:MET:HG2	1.94	0.67
4:F:148:ILE:HD12	4:F:161:LEU:HB2	1.77	0.67
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.78	0.65
2:B:189:VAL:CB	2:B:415:MET:HE2	2.26	0.65
2:D:1:MET:CE	2:D:128:ASP:HB2	2.25	0.65
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.26	0.65
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.78	0.65
1:C:108:TYR:O	1:C:112:LYS:HG2	1.97	0.65
1:C:178:SER:O	2:D:350:LYS:HE2	1.97	0.65
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.79	0.64
2:D:73:MET:HG3	2:D:90:PHE:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:CE	2:B:377:LEU:HD21	2.28	0.64
3:E:121:GLU:HA	3:E:124:GLN:HG2	1.80	0.63
4:F:148:ILE:CD1	4:F:161:LEU:HB2	2.27	0.63
2:D:416:ASN:O	2:D:419:VAL:HG22	1.98	0.63
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.80	0.63
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.33	0.62
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.29	0.62
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.35	0.62
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.34	0.62
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.18	0.62
2:D:285:THR:HG22	2:D:288:GLU:HB2	1.81	0.62
2:B:189:VAL:HG21	2:B:415:MET:HE2	1.82	0.62
4:F:144:GLY:C	4:F:145:ASN:HD22	2.02	0.62
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.81	0.62
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.82	0.62
4:F:144:GLY:O	4:F:145:ASN:ND2	2.24	0.62
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.65	0.62
4:F:257:GLU:OE1	4:F:257:GLU:N	2.33	0.62
2:B:189:VAL:HB	2:B:415:MET:CE	2.30	0.61
2:D:392:LYS:HG3	2:D:395:LEU:HD12	1.81	0.61
3:E:121:GLU:HG3	3:E:124:GLN:NE2	2.15	0.61
4:F:74:LYS:HE3	4:F:331:GLU:HG3	1.80	0.61
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.00	0.61
1:C:332:ILE:HG22	1:C:336:LYS:HE2	1.82	0.61
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.36	0.61
2:B:31:ASP:OD1	2:B:33:THR:HG22	2.00	0.61
2:D:23:VAL:O	2:D:27:GLU:HG3	2.00	0.60
2:B:81:PHE:O	2:B:84:ILE:HG22	2.01	0.60
2:D:330:MET:O	2:D:334:GLN:HG3	2.01	0.60
4:F:80:LEU:HD21	4:F:298:ILE:HG22	1.84	0.60
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.37	0.60
1:A:370:LYS:HD3	1:A:371:VAL:O	2.02	0.60
2:D:134:GLN:HA	2:D:165:ASN:O	2.00	0.60
4:F:338:CYS:O	4:F:343:TYR:HE1	1.85	0.60
2:D:285:THR:HG22	2:D:288:GLU:CG	2.32	0.59
2:D:42:LEU:HD22	2:D:243:PRO:HG2	1.85	0.59
2:B:233:MET:O	2:B:237:THR:OG1	2.21	0.59
4:F:161:LEU:HD23	4:F:172:PHE:CZ	2.37	0.59
1:C:41:THR:O	1:C:41:THR:OG1	2.21	0.59
1:C:41:THR:OG1	1:C:44:GLY:O	2.19	0.59
2:D:293:MET:CG	2:D:367:PHE:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.33	0.59
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.84	0.59
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.67	0.58
4:F:1:MET:HE2	4:F:28:LYS:CD	2.33	0.58
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.38	0.58
2:D:170:MET:CE	2:D:377:LEU:HD21	2.33	0.58
4:F:29:ARG:HH21	4:F:31:ARG:HH22	1.51	0.58
4:F:171:ASP:O	4:F:175:GLU:HG3	2.03	0.58
1:A:71:GLU:HG2	1:A:72:PRO:N	2.18	0.58
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.84	0.58
4:F:80:LEU:HD21	4:F:298:ILE:CG2	2.33	0.58
4:F:202:ARG:HG3	4:F:203:SER:N	2.19	0.58
2:B:245:GLN:O	2:B:245:GLN:HG2	2.03	0.58
3:E:48:GLU:OE2	3:E:48:GLU:HA	2.04	0.58
2:B:324:LYS:HE2	2:B:328:GLU:OE2	2.04	0.57
2:D:170:MET:HE3	2:D:377:LEU:HD21	1.86	0.57
2:D:189:VAL:HG21	2:D:415:MET:HE2	1.85	0.57
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.85	0.57
4:F:88:SER:HG	4:F:91:CYS:N	2.02	0.57
1:A:25:CYS:HB3	1:A:30:ILE:O	2.05	0.57
2:D:246:LEU:HD12	2:D:248:ALA:HB2	1.87	0.57
2:D:30:ILE:HG21	2:D:84:ILE:HD11	1.87	0.56
2:D:386:THR:O	2:D:390:ARG:HG2	2.05	0.56
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.22	0.56
2:B:67:ASP:O	2:B:92:PHE:HA	2.06	0.56
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.87	0.56
2:D:1:MET:HG3	2:D:128:ASP:HB3	1.88	0.56
1:A:72:PRO:HA	1:A:94:THR:OG1	2.06	0.56
1:C:221:ARG:NH1	2:D:323:MET:HB3	2.20	0.56
2:B:406:MET:HE3	2:B:406:MET:O	2.06	0.56
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.88	0.56
4:F:146:VAL:HG12	4:F:185:TYR:HB2	1.88	0.56
1:A:79:ARG:HH22	1:A:94:THR:HB	1.71	0.56
2:B:285:THR:HB	2:B:287:PRO:HD2	1.86	0.56
2:D:189:VAL:HG11	2:D:415:MET:HE2	1.88	0.56
2:D:285:THR:CG2	2:D:288:GLU:H	2.19	0.55
1:A:41:THR:HB	1:A:44:GLY:O	2.07	0.55
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.21	0.55
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.89	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.42	0.55
1:A:63:PRO:HG2	1:A:87:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:THR:HG22	2:D:288:GLU:CB	2.36	0.55
4:F:148:ILE:O	4:F:182:ILE:HA	2.06	0.55
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.42	0.55
2:D:31:ASP:OD1	2:D:33:THR:HG22	2.06	0.55
3:E:47:LEU:O	3:E:51:GLN:HG2	2.07	0.55
2:B:238:THR:HG21	2:B:316:ILE:CD1	2.35	0.55
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.89	0.55
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.88	0.55
1:A:336:LYS:HD3	3:E:24:LEU:HD12	1.89	0.55
1:C:88:HIS:HD2	1:C:90:GLU:N	2.03	0.55
3:E:106:GLU:HA	3:E:106:GLU:OE1	2.05	0.55
1:C:265:ILE:N	1:C:265:ILE:HD12	2.21	0.54
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.22	0.54
2:D:318:ARG:NH2	2:D:356:ILE:HG12	2.18	0.54
3:E:47:LEU:O	3:E:47:LEU:HD23	2.07	0.54
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.43	0.54
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.72	0.54
2:B:143:THR:CG2	2:B:147:MET:HE3	2.38	0.54
2:D:73:MET:HG3	2:D:90:PHE:HD2	1.73	0.54
1:C:1:MET:O	1:C:2:ARG:HB2	2.08	0.54
1:C:221:ARG:CZ	2:D:323:MET:HB3	2.37	0.54
2:D:177:ASP:N	2:D:177:ASP:OD1	2.41	0.54
2:D:189:VAL:HB	2:D:415:MET:HE3	1.89	0.54
2:B:189:VAL:CG1	2:B:415:MET:HE2	2.38	0.54
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.08	0.54
2:D:69:GLU:HG3	2:D:70:PRO:HD2	1.89	0.54
2:B:104:GLY:O	2:B:109:GLY:HA3	2.08	0.53
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.42	0.53
1:C:81:GLY:O	1:C:84:ARG:NH1	2.41	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.53
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.22	0.53
2:B:169:VAL:HA	2:B:202:ILE:O	2.08	0.53
2:B:189:VAL:CG2	2:B:415:MET:HE2	2.38	0.53
2:D:386:THR:HG22	2:D:412:GLU:OE2	2.08	0.53
1:A:345:ASP:HB2	3:E:28:SER:HB2	1.91	0.53
3:E:127:ASP:O	3:E:131:GLU:HG2	2.09	0.53
4:F:131:PHE:CE2	4:F:182:ILE:HD11	2.43	0.53
2:B:309:ARG:NH1	2:B:339:SER:O	2.42	0.53
4:F:192:LEU:HD21	4:F:262:MET:CE	2.38	0.53
1:C:320:ARG:HA	1:C:356:ASN:O	2.09	0.53
2:D:44:LEU:HA	2:D:47:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ASN:ND2	2:D:397:TRP:HB3	2.24	0.52
4:F:275:LEU:N	4:F:275:LEU:HD22	2.23	0.52
2:D:12:CYS:CB	2:D:138:SER:HB3	2.38	0.52
2:B:73:MET:HE3	2:B:90:PHE:CD2	2.44	0.52
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.90	0.52
2:D:212:PHE:O	2:D:216:LYS:HA	2.09	0.52
4:F:14:TYR:HA	4:F:17:VAL:HB	1.90	0.52
4:F:224:SER:OG	4:F:238:CYS:HA	2.09	0.52
2:D:65:LEU:N	2:D:65:LEU:HD12	2.25	0.52
2:D:236:VAL:HG12	2:D:368:ILE:HG12	1.92	0.52
2:B:29:GLY:O	2:B:36:TYR:HA	2.10	0.51
1:A:112:LYS:HE2	3:E:61:ARG:HH22	1.72	0.51
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.25	0.51
2:B:31:ASP:OD1	2:B:33:THR:CG2	2.58	0.51
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.46	0.51
2:D:416:ASN:O	2:D:419:VAL:CG2	2.59	0.51
1:C:357:TYR:O	1:C:359:PRO:HD3	2.10	0.51
2:D:118:ASP:HA	2:D:121:ARG:NH1	2.26	0.51
2:D:377:LEU:C	2:D:377:LEU:HD23	2.31	0.51
1:C:104:ALA:HB2	1:C:413:MET:SD	2.50	0.51
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.91	0.51
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.41	0.51
1:A:265:ILE:HD12	1:A:265:ILE:N	2.25	0.51
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.26	0.51
2:B:50:TYR:OH	2:B:237:THR:CG2	2.59	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
1:A:71:GLU:HG2	1:A:73:THR:H	1.75	0.50
1:A:147:SER:HB2	1:A:190:THR:HB	1.93	0.50
2:B:237:THR:HB	2:B:241:ARG:HE	1.77	0.50
4:F:192:LEU:HD21	4:F:262:MET:HE2	1.93	0.50
2:B:161:ASP:O	2:B:251:ARG:NH2	2.44	0.50
2:D:80:PRO:O	2:D:81:PHE:HB2	2.11	0.50
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.91	0.50
2:D:401:GLU:HA	3:E:137:LYS:HD3	1.94	0.50
4:F:198:LYS:HG2	4:F:199:PHE:N	2.27	0.50
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.93	0.50
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.92	0.50
2:B:284:LEU:N	2:B:284:LEU:HD12	2.26	0.50
4:F:271:LEU:O	4:F:275:LEU:O	2.30	0.50
1:A:94:THR:HG23	1:A:95:GLY:O	2.12	0.49
1:A:88:HIS:N	1:A:91:GLN:OE1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:VAL:CB	2:B:415:MET:CE	2.90	0.49
4:F:161:LEU:HD23	4:F:172:PHE:CE2	2.47	0.49
2:B:284:LEU:O	2:B:363:MET:CE	2.61	0.49
4:F:149:ALA:HB2	4:F:161:LEU:HB3	1.94	0.49
1:A:209:ILE:HD11	1:A:302:MET:SD	2.52	0.49
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.47	0.49
4:F:192:LEU:CD2	4:F:262:MET:HE2	2.42	0.49
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.95	0.49
1:A:401:LYS:HE3	2:B:428:ALA:HB1	1.95	0.49
1:C:71:GLU:OE1	1:C:73:THR:HB	2.13	0.49
4:F:148:ILE:HG13	4:F:149:ALA:N	2.28	0.49
2:B:134:GLN:HA	2:B:165:ASN:O	2.13	0.48
4:F:191:LEU:HA	4:F:197:ARG:O	2.12	0.48
2:B:130:LEU:HB3	2:B:162:ARG:HE	1.79	0.48
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.48	0.48
2:B:166:THR:OG1	2:B:199:THR:HB	2.13	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.48
1:C:287:SER:OG	1:C:290:GLU:HG3	2.14	0.48
2:B:236:VAL:HG12	2:B:368:ILE:HG12	1.96	0.48
4:F:102:PRO:HG3	4:F:178:GLN:O	2.14	0.48
4:F:326:LYS:HD2	4:F:327:VAL:N	2.28	0.48
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.96	0.48
3:E:135:LYS:HB3	3:E:135:LYS:HE3	1.39	0.48
1:A:280:LYS:NZ	1:A:283:HIS:HD2	2.12	0.48
2:D:169:VAL:HA	2:D:202:ILE:O	2.13	0.48
2:B:2:ARG:HA	2:B:129:CYS:O	2.14	0.47
2:B:7:ILE:O	2:B:135:LEU:HA	2.14	0.47
2:D:99:ASN:OD1	2:D:178:THR:HG21	2.15	0.47
2:B:117:LEU:HD11	2:B:154:LYS:HD3	1.96	0.47
4:F:165:GLU:HB2	4:F:168:GLU:HG3	1.96	0.47
1:C:286:LEU:N	1:C:286:LEU:HD12	2.29	0.47
2:D:325:GLU:O	2:D:329:GLN:HG2	2.14	0.47
2:D:379:LYS:O	2:D:383:GLU:HG3	2.14	0.47
1:A:185:TYR:CZ	1:A:398:MET:HE2	2.50	0.47
4:F:275:LEU:HD22	4:F:275:LEU:H	1.79	0.47
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.97	0.47
2:D:189:VAL:HG21	2:D:415:MET:CE	2.44	0.47
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.32	0.47
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.97	0.47
2:D:238:THR:OG1	2:D:318:ARG:HD2	2.15	0.47
2:D:358:PRO:HG2	2:D:361:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:170:LEU:O	4:F:173:ILE:HG12	2.14	0.47
1:A:178:SER:O	2:B:350:LYS:NZ	2.37	0.47
2:D:1:MET:CB	2:D:48:ASN:HD22	2.28	0.47
2:D:81:PHE:O	2:D:84:ILE:HG22	2.15	0.47
4:F:296:MET:HE2	4:F:380:HIS:HB2	1.97	0.47
1:C:136:LEU:HD12	1:C:136:LEU:N	2.30	0.46
2:D:385:PHE:CE1	2:D:412:GLU:HB2	2.50	0.46
4:F:192:LEU:CD2	4:F:262:MET:CE	2.94	0.46
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.97	0.46
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.14	0.46
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.46
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.38	0.46
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.97	0.46
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.27	0.46
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.49	0.46
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.50	0.46
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.96	0.46
2:D:272:PRO:HG3	2:D:284:LEU:HD13	1.98	0.46
2:D:406:MET:O	2:D:410:GLU:HG3	2.16	0.46
1:A:55:GLU:HA	1:A:60:LYS:O	2.16	0.46
2:D:208:TYR:CD1	2:D:220:PRO:HG2	2.50	0.46
1:A:324:VAL:HG13	1:A:325:PRO:CD	2.45	0.46
4:F:148:ILE:HD12	4:F:149:ALA:H	1.81	0.46
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.46	0.45
2:D:206:ALA:O	2:D:210:ILE:HG13	2.15	0.45
2:B:45:GLU:OE2	2:B:243:PRO:HG3	2.16	0.45
4:F:192:LEU:CD1	4:F:192:LEU:N	2.79	0.45
4:F:209:HIS:HA	4:F:311:SER:O	2.16	0.45
2:B:229:VAL:O	2:B:233:MET:HG3	2.16	0.45
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.50	0.45
2:D:270:PHE:O	2:D:298:ASN:HB3	2.16	0.45
4:F:162:ILE:HG22	4:F:163:SER:N	2.32	0.45
1:C:166:LYS:HE2	1:C:197:HIS:O	2.17	0.45
4:F:1:MET:HE1	4:F:28:LYS:CB	2.45	0.45
4:F:259:GLY:O	4:F:260:ASN:HB2	2.17	0.45
2:B:375:GLN:OE1	2:B:423:GLN:HG2	2.17	0.45
2:D:16:ILE:HD11	2:D:136:THR:HB	1.99	0.45
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.00	0.44
1:A:41:THR:HG21	1:A:45:GLY:CA	2.47	0.44
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.98	0.44
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.52	0.44
4:F:338:CYS:O	4:F:343:TYR:CE1	2.70	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.00	0.44
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.57	0.44
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.98	0.44
4:F:130:VAL:C	4:F:132:LEU:HD23	2.38	0.44
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.44
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.52	0.44
2:D:288:GLU:O	2:D:292:GLN:HG3	2.18	0.44
1:C:274:PRO:HB3	1:C:286:LEU:HD22	1.99	0.44
1:A:370:LYS:HD3	1:A:371:VAL:N	2.31	0.44
2:D:354:CYS:SG	2:D:356:ILE:HG23	2.58	0.44
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.51	0.44
2:B:267:MET:HE1	2:B:299:MET:HG3	2.00	0.44
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.36	0.44
1:C:265:ILE:N	1:C:265:ILE:CD1	2.81	0.43
2:D:285:THR:HG22	2:D:288:GLU:CD	2.39	0.43
4:F:130:VAL:O	4:F:132:LEU:HD23	2.18	0.43
1:A:413:MET:CE	1:A:418:PHE:CE1	3.00	0.43
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.99	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.00	0.43
2:D:23:VAL:HG21	2:D:230:SER:HB2	2.01	0.43
1:A:41:THR:HG21	1:A:45:GLY:HA2	2.00	0.43
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.49	0.43
2:D:75:SER:O	2:D:79:GLY:N	2.49	0.43
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.99	0.43
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.53	0.43
2:B:100:ASN:OD1	2:B:102:ALA:HB3	2.19	0.43
2:B:189:VAL:HB	2:B:415:MET:HE3	1.99	0.43
10:B:505:A1D69:S20	10:B:505:A1D69:C09	3.06	0.43
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.99	0.43
2:D:31:ASP:OD1	2:D:33:THR:CG2	2.67	0.43
1:C:47:ASP:O	1:C:50:ASN:HB2	2.18	0.43
2:D:66:VAL:HA	2:D:91:VAL:O	2.19	0.43
2:D:67:ASP:O	2:D:92:PHE:HA	2.18	0.43
2:D:181:GLU:HB2	2:D:182:PRO:HD3	2.00	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.42
2:D:152:ILE:HG23	2:D:164:MET:HG2	2.01	0.42
3:E:6:MET:HG3	3:E:24:LEU:CD2	2.48	0.42
4:F:49:PHE:CD2	4:F:66:ARG:HG3	2.54	0.42
2:B:197:ASP:C	2:B:198:GLU:HG3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:29:ARG:NH2	4:F:31:ARG:HH22	2.16	0.42
1:C:88:HIS:NE2	1:C:90:GLU:HG3	2.34	0.42
4:F:74:LYS:HB3	4:F:181:VAL:HG11	2.01	0.42
4:F:178:GLN:N	4:F:178:GLN:OE1	2.53	0.42
4:F:199:PHE:HA	4:F:241:THR:HG21	2.01	0.42
2:D:170:MET:HE2	2:D:377:LEU:HD21	2.01	0.42
2:D:350:LYS:HD2	2:D:350:LYS:HA	1.88	0.42
1:A:437:VAL:O	1:A:437:VAL:CG1	2.67	0.42
2:D:157:GLU:HA	3:E:123:LEU:HD13	2.01	0.42
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.50	0.42
2:D:293:MET:SD	2:D:365:ALA:HB1	2.60	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.42
1:A:437:VAL:O	1:A:437:VAL:HG12	2.20	0.41
1:C:164:LYS:HE2	1:C:164:LYS:HB2	1.70	0.41
2:D:197:ASP:C	2:D:198:GLU:HG3	2.40	0.41
4:F:71:LEU:HD12	4:F:77:LEU:HD13	2.02	0.41
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.83	0.41
4:F:16:GLU:OE2	4:F:19:ARG:HD3	2.21	0.41
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.55	0.41
2:D:285:THR:HG22	2:D:288:GLU:OE1	2.21	0.41
4:F:197:ARG:HB3	4:F:224:SER:O	2.21	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.50	0.41
4:F:81:ILE:O	4:F:87:LEU:O	2.39	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.60	0.41
1:A:54:SER:O	1:A:61:HIS:HA	2.21	0.41
2:B:395:LEU:HD23	2:B:395:LEU:HA	1.88	0.41
2:D:54:ALA:N	2:D:58:LYS:O	2.41	0.41
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.49	0.41
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.95	0.41
4:F:148:ILE:CG1	4:F:149:ALA:N	2.84	0.41
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.56	0.41
2:B:285:THR:CB	2:B:287:PRO:HD2	2.50	0.41
1:C:71:GLU:CG	1:C:98:ASP:HB3	2.47	0.41
1:C:221:ARG:NH1	2:D:323:MET:CB	2.83	0.41
1:C:241:SER:HA	1:C:249:ASN:OD1	2.20	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.56	0.41
2:D:103:LYS:O	2:D:108:GLU:HB2	2.19	0.41
3:E:98:LYS:O	3:E:101:LEU:HD12	2.21	0.41
4:F:131:PHE:CZ	4:F:182:ILE:CD1	3.00	0.41
4:F:192:LEU:HD11	4:F:199:PHE:CD1	2.56	0.41
1:A:67:PHE:CD1	1:A:67:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:THR:HA	2:B:415:MET:HE1	2.03	0.41
1:C:109:THR:HG22	1:C:110:ILE:HD13	2.03	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.02	0.40
1:C:395:PHE:CD1	1:C:395:PHE:C	2.94	0.40
3:E:47:LEU:HD23	3:E:51:GLN:HG2	2.03	0.40
4:F:186:LEU:HD13	4:F:320:MET:CG	2.51	0.40
2:B:50:TYR:OH	2:B:237:THR:HG21	2.22	0.40
2:D:401:GLU:HA	3:E:137:LYS:CD	2.51	0.40
1:C:120:ASP:O	1:C:124:LYS:HG2	2.21	0.40
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.51	0.40
2:D:67:ASP:HA	2:D:143:THR:HG21	2.04	0.40
2:D:189:VAL:HB	2:D:415:MET:CE	2.52	0.40
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.56	0.40
2:B:186:THR:HA	2:B:415:MET:CE	2.51	0.40
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ARG:NH2	3:E:131:GLU:OE2[4_545]	2.11	0.09

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/440 (99%)	428 (98%)	7 (2%)	0	100	100
1	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
2	B	425/431 (99%)	418 (98%)	7 (2%)	0	100	100
2	D	412/431 (96%)	405 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	116/143 (81%)	116 (100%)	0	0	100	100
4	F	293/380 (77%)	283 (97%)	10 (3%)	0	100	100
All	All	2119/2265 (94%)	2075 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	366/371 (99%)	362 (99%)	4 (1%)	70	83
1	C	370/371 (100%)	364 (98%)	6 (2%)	58	75
2	B	367/372 (99%)	357 (97%)	10 (3%)	40	58
2	D	360/372 (97%)	353 (98%)	7 (2%)	52	70
3	E	107/127 (84%)	97 (91%)	10 (9%)	7	10
4	F	266/338 (79%)	244 (92%)	22 (8%)	9	13
All	All	1836/1951 (94%)	1777 (97%)	59 (3%)	34	51

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	71	GLU
1	A	94	THR
1	A	433	GLU
2	B	69	GLU
2	B	72	THR
2	B	95	SER
2	B	137	HIS
2	B	147	MET
2	B	218	THR
2	B	237	THR
2	B	246	LEU

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Mol	Chain	Res	Type
2	B	296	SER
2	B	316	ILE
1	C	71	GLU
1	C	163	LYS
1	C	251	ASP
1	C	284	GLU
1	C	297	GLU
1	C	347	CYS
2	D	99	ASN
2	D	137	HIS
2	D	177	ASP
2	D	205	GLU
2	D	356	ILE
2	D	392	LYS
2	D	406	MET
3	E	22	VAL
3	E	48	GLU
3	E	96	MET
3	E	100	LYS
3	E	101	LEU
3	E	128	LYS
3	E	135	LYS
3	E	137	LYS
3	E	139	LEU
3	E	141	GLU
4	F	1	MET
4	F	12	SER
4	F	28	LYS
4	F	31	ARG
4	F	81	ILE
4	F	99	VAL
4	F	132	LEU
4	F	136	ASN
4	F	161	LEU
4	F	171	ASP
4	F	180	HIS
4	F	192	LEU
4	F	202	ARG
4	F	211	TYR
4	F	224	SER
4	F	234	GLN
4	F	237	THR

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Mol	Chain	Res	Type
4	F	243	HIS
4	F	257	GLU
4	F	279	LEU
4	F	307	LEU
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	C	88	HIS
1	C	133	GLN
3	E	124	GLN
3	E	129	HIS
4	F	145	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MES	B	502	-	12,12,12	1.24	1 (8%)	14,16,16	0.78	1 (7%)
8	GDP	D	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.43	5 (16%)
9	MES	B	503	-	12,12,12	1.17	1 (8%)	14,16,16	0.86	0
5	GTP	A	501	7	26,34,34	1.11	2 (7%)	32,54,54	1.60	7 (21%)
8	GDP	B	501	7	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
5	GTP	C	501	7	26,34,34	1.12	2 (7%)	32,54,54	1.61	7 (21%)
10	A1D69	B	505	-	20,22,22	0.98	1 (5%)	21,31,31	2.79	5 (23%)
10	A1D69	D	502	-	20,22,22	1.08	1 (5%)	21,31,31	2.85	4 (19%)
11	ACP	F	401	-	27,33,33	2.19	3 (11%)	32,52,52	1.12	3 (9%)

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
9	MES	B	502	-	-	5/6/14/14	0/1/1/1
8	GDP	D	501	-	-	4/12/32/32	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
5	GTP	A	501	7	-	9/18/38/38	0/3/3/3
8	GDP	B	501	7	-	3/12/32/32	0/3/3/3
5	GTP	C	501	7	-	6/18/38/38	0/3/3/3
10	A1D69	B	505	-	-	0/9/16/16	0/3/3/3
10	A1D69	D	502	-	-	0/9/16/16	0/3/3/3
11	ACP	F	401	-	-	2/15/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	10.15	1.69	1.58
5	C	501	GTP	C5-C6	-3.99	1.39	1.47
5	A	501	GTP	C5-C6	-3.97	1.39	1.47
9	B	502	MES	C8-S	3.35	1.82	1.77
10	D	502	A1D69	C06-N07	3.26	1.46	1.39
9	B	503	MES	C8-S	3.15	1.82	1.77
10	B	505	A1D69	C04-N03	2.37	1.32	1.30
8	B	501	GDP	C6-N1	-2.36	1.34	1.37
11	F	401	ACP	C8-N7	-2.20	1.30	1.34
5	C	501	GTP	C2-N3	2.20	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O2B	-2.18	1.51	1.56
5	A	501	GTP	C2-N3	2.10	1.38	1.33
8	D	501	GDP	C6-N1	-2.05	1.34	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	A1D69	C18-C02-C01	8.94	117.14	110.62
10	B	505	A1D69	N03-C04-N05	-7.50	123.07	130.62
10	D	502	A1D69	N03-C04-N05	-6.97	123.60	130.62
10	B	505	A1D69	CL17-C04-N03	6.39	121.15	115.70
10	B	505	A1D69	C18-C02-C01	5.89	114.92	110.62
10	D	502	A1D69	CL17-C04-N03	3.77	118.92	115.70
8	D	501	GDP	PA-O3A-PB	-3.69	120.16	132.83
10	B	505	A1D69	N05-C06-N07	3.65	119.92	116.09
5	A	501	GTP	PB-O3B-PG	-3.58	120.53	132.83
5	C	501	GTP	PB-O3B-PG	-3.57	120.57	132.83
5	C	501	GTP	PA-O3A-PB	-3.54	120.66	132.83
5	A	501	GTP	PA-O3A-PB	-3.53	120.70	132.83
10	D	502	A1D69	C04-N05-C06	3.47	121.35	111.04
8	B	501	GDP	PA-O3A-PB	-3.40	121.17	132.83
8	B	501	GDP	C3'-C2'-C1'	3.24	105.86	100.98
5	C	501	GTP	C5-C6-N1	3.20	119.61	113.95
5	A	501	GTP	C5-C6-N1	3.15	119.52	113.95
11	F	401	ACP	O2B-PB-O1B	3.05	120.26	110.07
5	A	501	GTP	C3'-C2'-C1'	3.04	105.56	100.98
5	C	501	GTP	C3'-C2'-C1'	3.02	105.52	100.98
5	A	501	GTP	C8-N7-C5	3.01	108.73	102.99
8	D	501	GDP	C3'-C2'-C1'	2.99	105.49	100.98
5	C	501	GTP	C8-N7-C5	2.99	108.68	102.99
11	F	401	ACP	PB-O3A-PA	-2.89	123.39	132.56
5	A	501	GTP	C2-N1-C6	-2.88	119.79	125.10
5	C	501	GTP	C2-N1-C6	-2.85	119.84	125.10
10	B	505	A1D69	C04-N05-C06	2.81	119.39	111.04
11	F	401	ACP	O1G-PG-C3B	-2.63	105.58	111.24
8	D	501	GDP	C5-C6-N1	2.55	118.46	113.95
8	D	501	GDP	C8-N7-C5	2.38	107.53	102.99
8	B	501	GDP	C8-N7-C5	2.31	107.40	102.99
9	B	502	MES	O2S-S-C8	-2.31	104.14	106.92
8	B	501	GDP	C5-C6-N1	2.27	117.96	113.95
5	C	501	GTP	O6-C6-C5	-2.10	120.26	124.37
5	A	501	GTP	O6-C6-C5	-2.08	120.31	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	N2-C2-N1	2.07	121.13	116.71

There are no chirality outliers.

All (32) torsion outliers are listed below:

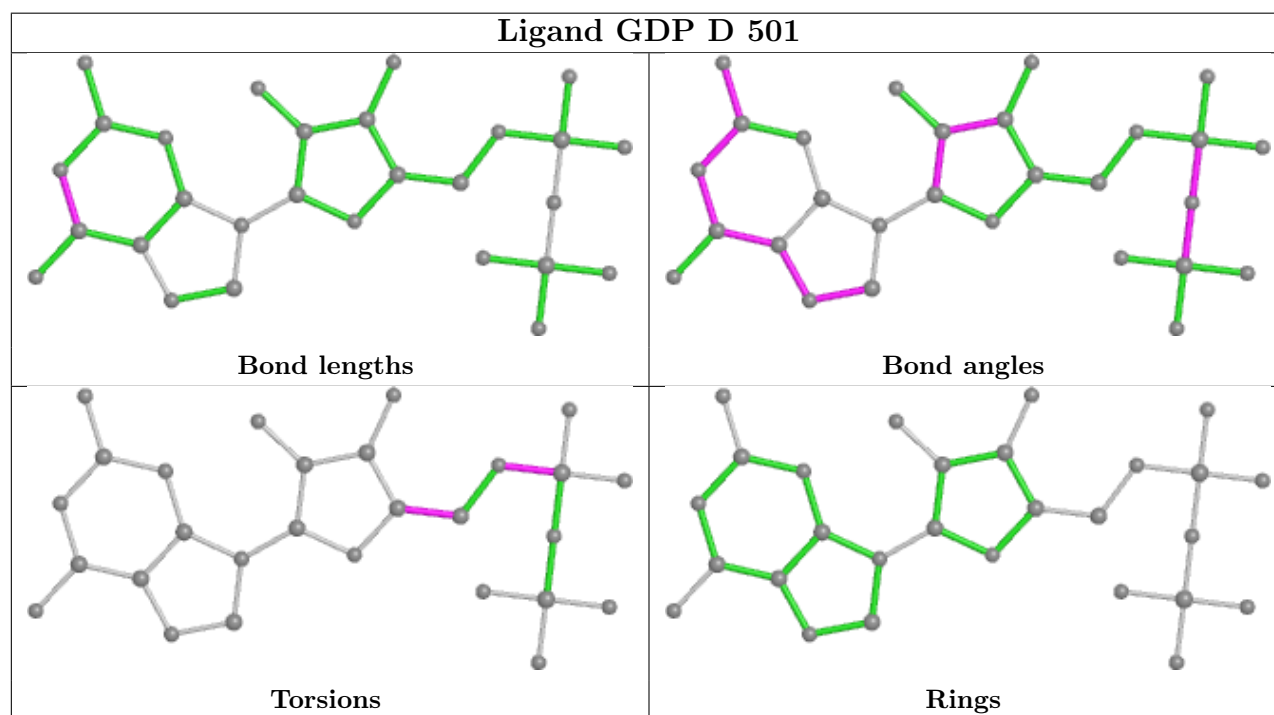
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	502	MES	C7-C8-S-O1S
9	B	502	MES	C7-C8-S-O2S
9	B	502	MES	C7-C8-S-O3S
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
9	B	502	MES	C8-C7-N4-C3
9	B	502	MES	C8-C7-N4-C5
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
8	D	501	GDP	C3'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	O4'-C4'-C5'-O5'
8	D	501	GDP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G

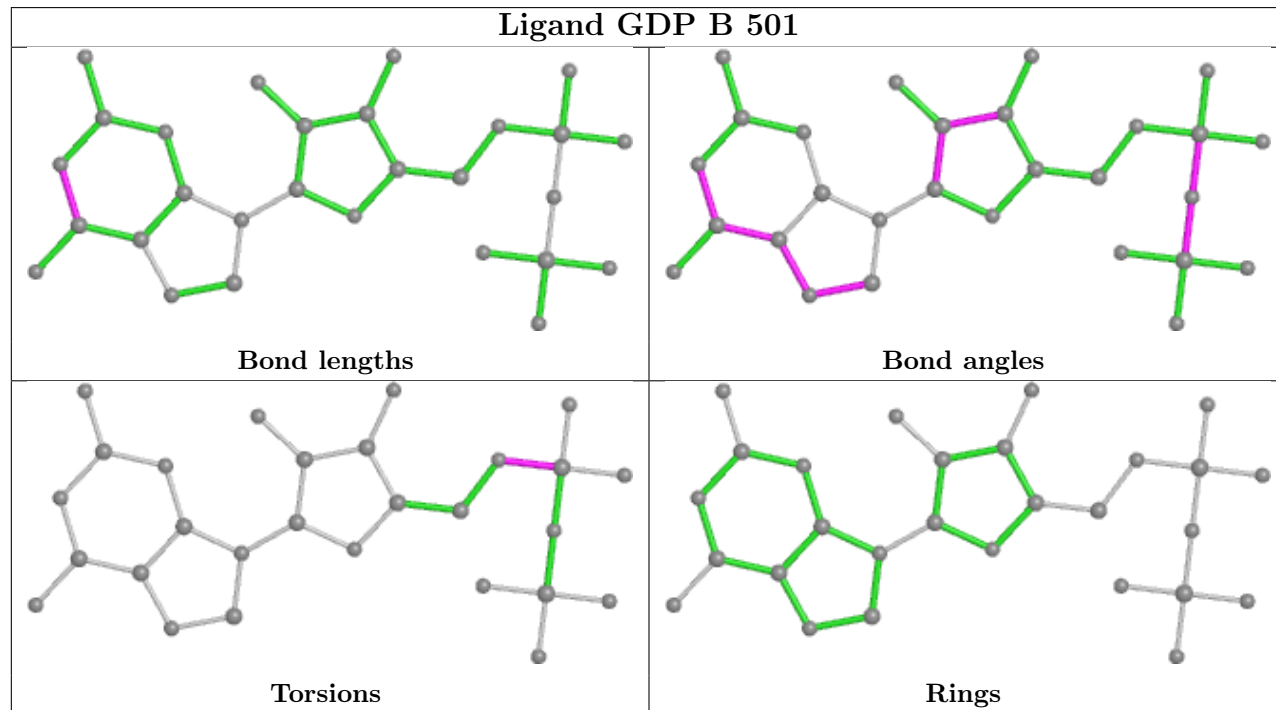
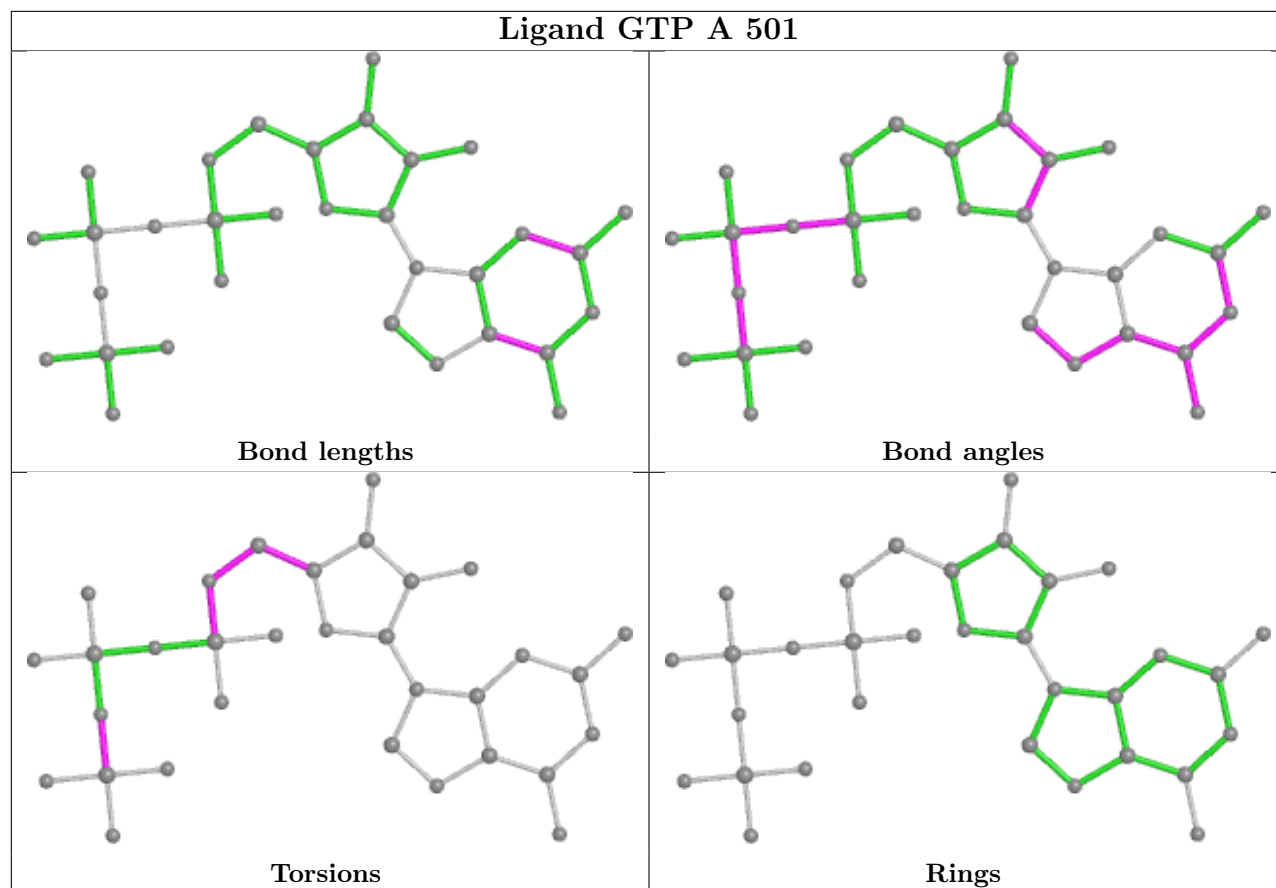
There are no ring outliers.

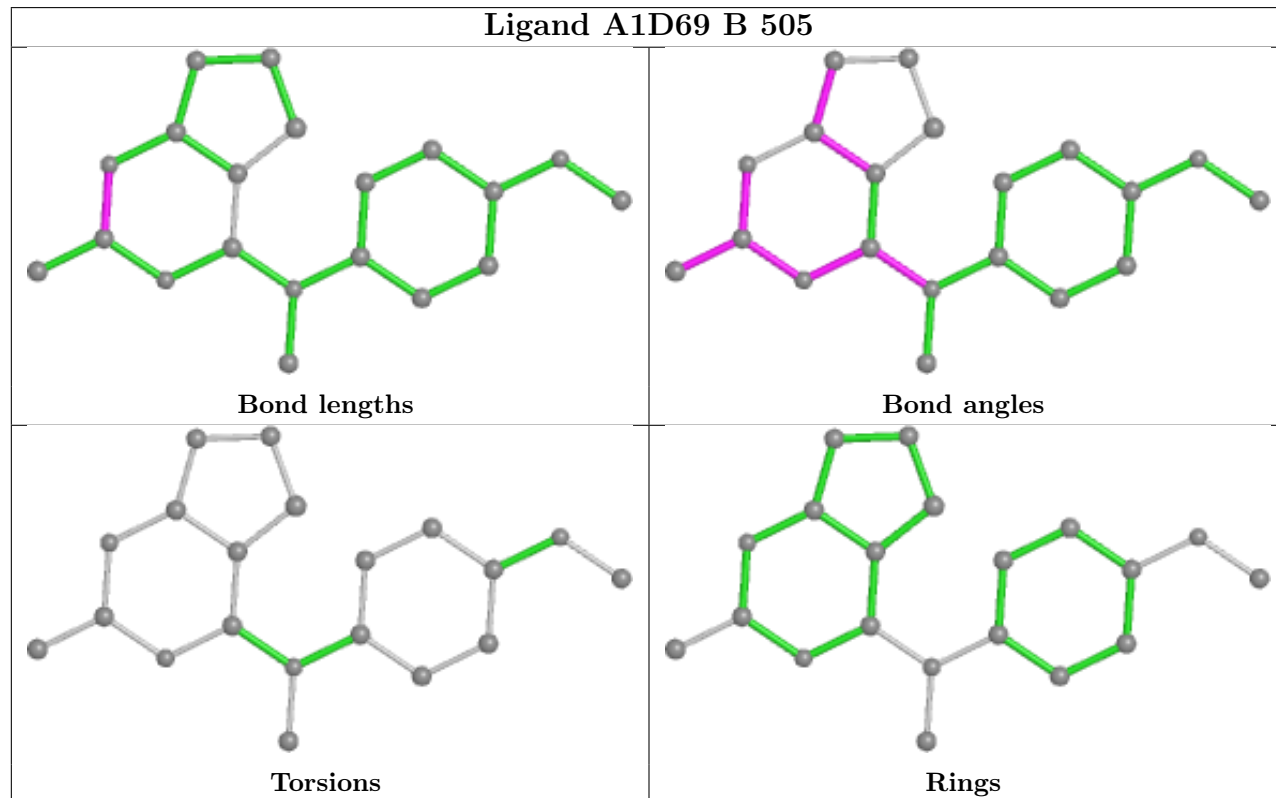
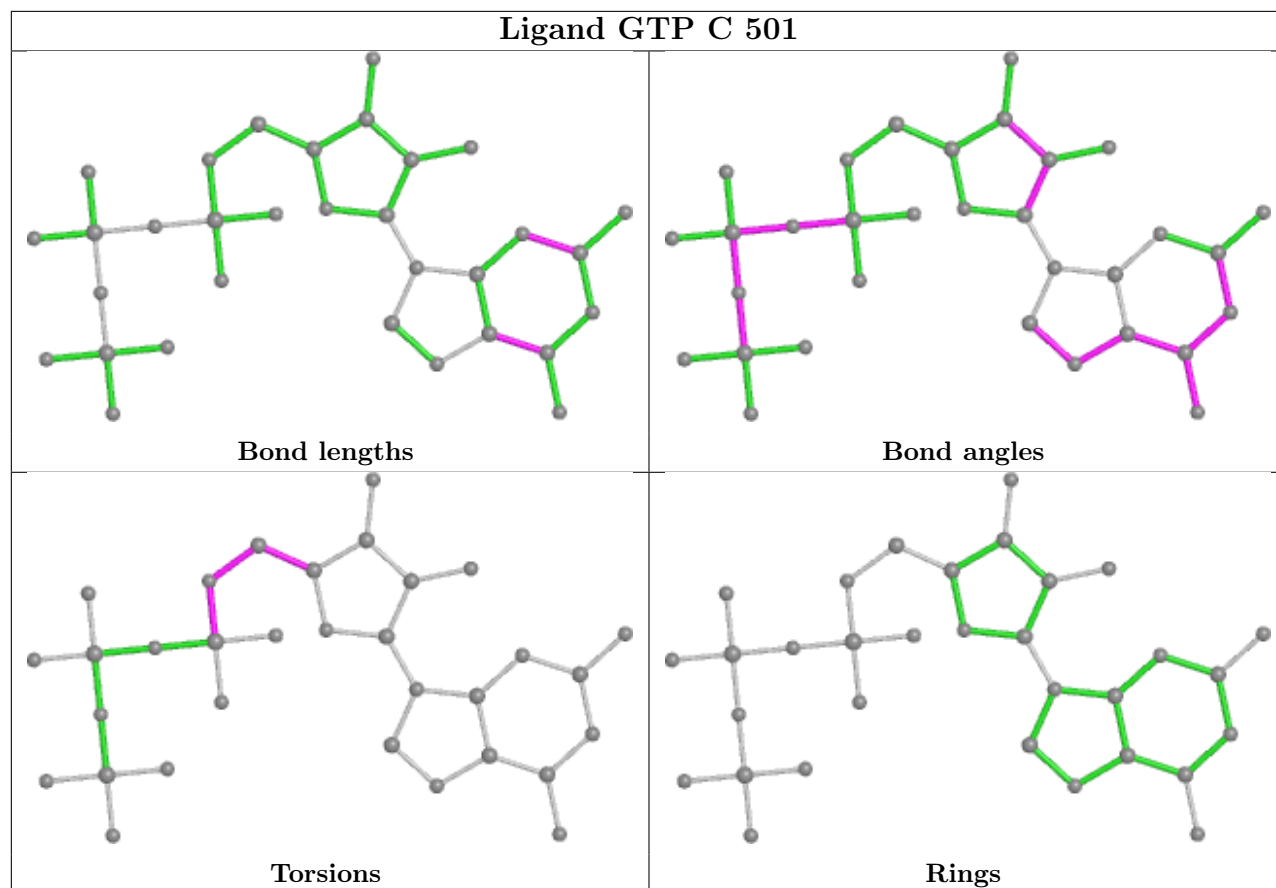
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	A1D69	1	0

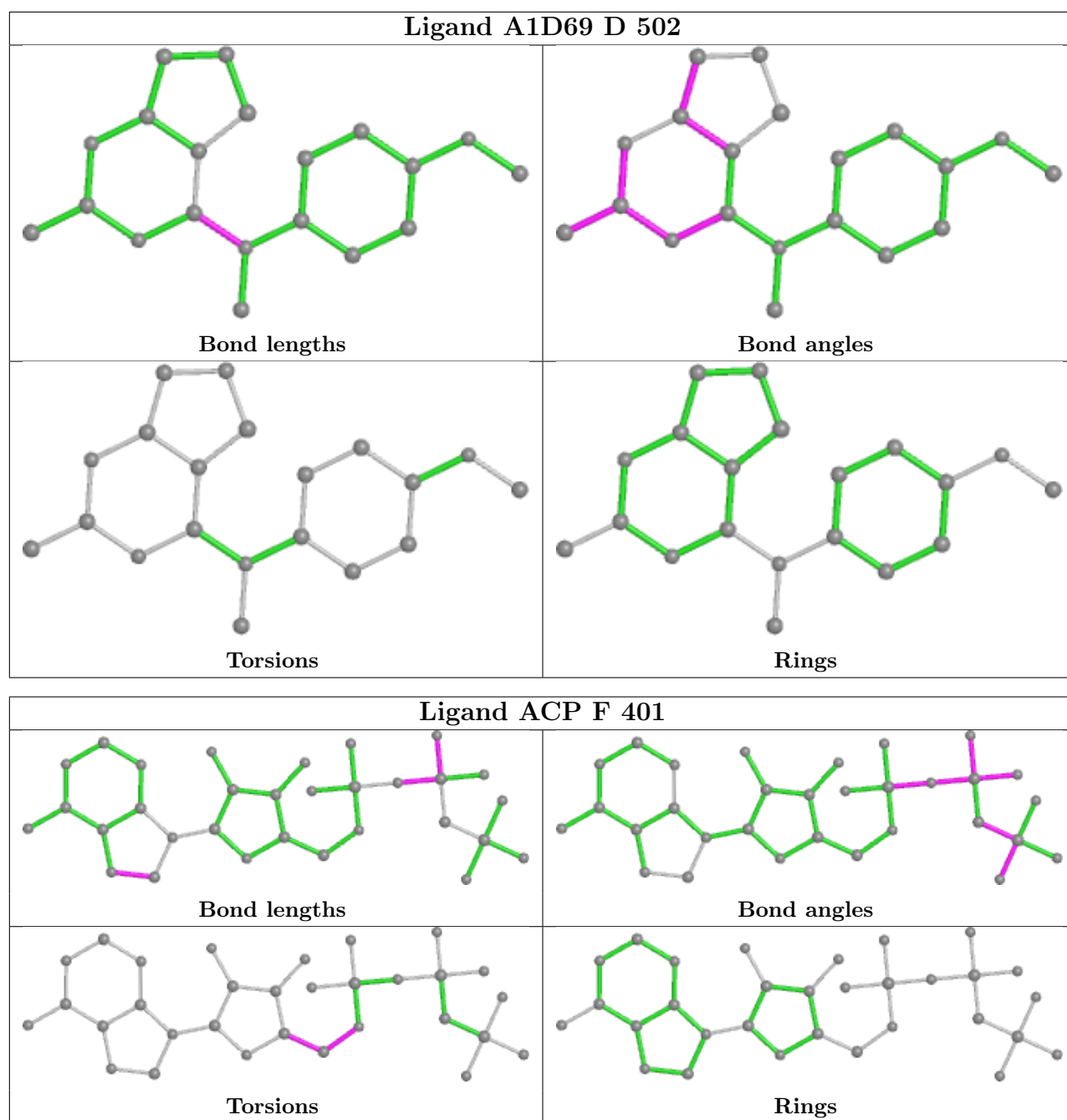
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/440 (99%)	0.43	18 (4%) 42 42	36, 51, 77, 97	0
1	C	440/440 (100%)	0.15	11 (2%) 58 58	29, 42, 63, 100	0
2	B	427/431 (99%)	0.60	40 (9%) 15 15	31, 50, 86, 146	0
2	D	418/431 (96%)	1.27	100 (23%) 2 2	40, 68, 103, 142	0
3	E	120/143 (83%)	1.12	19 (15%) 6 6	44, 63, 97, 105	0
4	F	310/380 (81%)	1.83	101 (32%) 1 1	44, 69, 133, 170	0
All	All	2152/2265 (95%)	0.81	289 (13%) 8 8	29, 55, 99, 170	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	148	ILE	9.2
4	F	162	ILE	9.1
4	F	245	ILE	9.1
4	F	130	VAL	8.8
4	F	146	VAL	7.7
4	F	169	LEU	6.8
4	F	161	LEU	6.6
4	F	254	GLY	6.5
4	F	149	ALA	6.4
4	F	99	VAL	6.3
4	F	103	THR	6.2
2	D	247	ASN	6.2
1	A	437	VAL	6.1
4	F	166	ALA	6.0
4	F	186	LEU	6.0
4	F	180	HIS	5.9
4	F	240	LEU	5.8
4	F	239	HIS	5.8
4	F	184	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
2	D	73	MET	5.7
4	F	134	ALA	5.7
4	F	256	TYR	5.6
4	F	170	LEU	5.5
2	B	428	ALA	5.5
4	F	172	PHE	5.5
4	F	182	ILE	5.4
4	F	147	TRP	5.4
4	F	173	ILE	5.4
2	D	72	THR	5.2
4	F	98	TYR	5.1
4	F	101	TYR	5.1
3	E	45	PRO	5.1
4	F	179	VAL	5.0
2	D	92	PHE	4.9
4	F	132	LEU	4.9
2	D	55	THR	4.8
2	D	397	TRP	4.7
4	F	238	CYS	4.7
4	F	181	VAL	4.7
3	E	139	LEU	4.7
4	F	89	GLU	4.6
2	D	284	LEU	4.5
4	F	135	TYR	4.5
2	B	72	THR	4.5
4	F	131	PHE	4.5
2	D	42	LEU	4.5
4	F	236	LYS	4.4
4	F	164	SER	4.4
2	D	219	THR	4.3
2	D	11	GLN	4.3
4	F	163	SER	4.3
4	F	185	TYR	4.2
4	F	100	ILE	4.2
4	F	243	HIS	4.2
4	F	225	SER	4.2
4	F	380	HIS	4.2
2	B	280	GLN	4.1
2	D	32	PRO	4.1
3	E	141	GLU	4.1
2	D	1	MET	4.0
4	F	244	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	98	GLY	4.0
1	C	440	VAL	3.9
2	D	394	PHE	3.9
2	D	37	HIS	3.9
2	D	246	LEU	3.9
2	D	245	GLN	3.9
4	F	194	PRO	3.9
4	F	139	ARG	3.9
4	F	237	THR	3.8
3	E	28	SER	3.8
2	D	56	GLY	3.8
1	C	41	THR	3.8
1	A	282	TYR	3.8
1	C	357	TYR	3.8
2	B	279	GLN	3.8
1	A	112	LYS	3.8
2	B	218	THR	3.8
2	D	81	PHE	3.7
2	B	55	THR	3.7
1	C	340	SER	3.7
4	F	133	ALA	3.6
4	F	138	ARG	3.6
1	C	1	MET	3.6
2	B	277	GLY	3.6
2	D	80	PRO	3.6
4	F	277	THR	3.5
2	D	170	MET	3.5
2	B	276	ARG	3.5
4	F	242	ASN	3.5
3	E	6	MET	3.4
4	F	102	PRO	3.4
2	B	427	ASP	3.4
2	D	395	LEU	3.4
4	F	379	HIS	3.4
2	D	94	GLN	3.3
4	F	241	THR	3.3
4	F	372	THR	3.3
2	D	391	ARG	3.3
2	D	222	TYR	3.3
2	D	57	ASN	3.3
4	F	224	SER	3.3
2	B	278	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	390	ARG	3.2
2	B	247	ASN	3.2
4	F	145	ASN	3.2
2	D	33	THR	3.2
2	B	41	ASP	3.2
2	D	248	ALA	3.1
1	C	245	ASP	3.1
2	B	281	TYR	3.1
2	D	115	SER	3.1
2	D	389	PHE	3.1
2	D	405	GLU	3.1
4	F	183	GLN	3.0
2	B	40	SER	3.0
4	F	167	SER	3.0
4	F	263	PHE	3.0
1	A	46	ASP	3.0
2	B	37	HIS	3.0
2	D	217	LEU	3.0
2	D	91	VAL	3.0
2	D	404	ASP	3.0
4	F	33	ASP	3.0
2	D	362	LYS	3.0
1	A	42	ILE	2.9
4	F	341	LYS	2.9
2	D	387	ALA	2.9
1	A	365	GLY	2.9
4	F	320	MET	2.9
4	F	28	LYS	2.9
2	B	245	GLN	2.9
2	D	431	ASP	2.9
4	F	187	GLU	2.9
2	D	386	THR	2.9
2	D	356	ILE	2.9
4	F	46	ARG	2.9
1	C	163	LYS	2.9
2	D	39	ASP	2.8
2	D	323	MET	2.8
1	A	41	THR	2.8
1	A	262	TYR	2.8
2	D	69	GLU	2.8
2	D	285	THR	2.8
4	F	88	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	56	GLY	2.8
2	B	275	SER	2.8
2	B	336	LYS	2.8
1	A	113	GLU	2.8
3	E	7	GLU	2.8
4	F	165	GLU	2.8
2	D	361	LEU	2.8
4	F	197	ARG	2.7
2	D	218	THR	2.7
2	D	215	LEU	2.7
2	D	100	ASN	2.7
4	F	175	GLU	2.7
2	D	68	LEU	2.7
4	F	221	LEU	2.7
2	B	282	ARG	2.7
2	D	406	MET	2.7
4	F	235	ASP	2.7
4	F	334	GLY	2.7
2	D	393	ALA	2.7
2	D	84	ILE	2.6
2	D	90	PHE	2.6
2	D	180	VAL	2.6
2	D	398	TYR	2.6
4	F	136	ASN	2.6
2	D	30	ILE	2.6
2	D	392	LYS	2.6
3	E	52	LYS	2.6
4	F	333	ASN	2.6
4	F	234	GLN	2.6
2	D	383	GLU	2.6
3	E	59	GLU	2.6
2	B	69	GLU	2.5
4	F	20	LEU	2.5
3	E	115	HIS	2.5
4	F	330	ILE	2.5
1	A	362	VAL	2.5
2	D	212	PHE	2.5
3	E	8	VAL	2.5
2	D	290	THR	2.5
2	D	216	LYS	2.5
2	D	77	ARG	2.5
2	D	359	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	2.5
3	E	48	GLU	2.5
2	D	122	LYS	2.5
3	E	25	LYS	2.5
4	F	191	LEU	2.5
4	F	223	THR	2.5
4	F	85	PRO	2.5
4	F	177	GLY	2.5
1	C	2	ARG	2.5
4	F	178	GLN	2.5
2	D	36	TYR	2.4
2	D	35	SER	2.4
2	B	323	MET	2.4
4	F	198	LYS	2.4
4	F	259	GLY	2.4
1	A	281	ALA	2.4
2	B	42	LEU	2.4
2	D	179	VAL	2.4
2	D	273	LEU	2.4
2	D	289	LEU	2.4
4	F	306	HIS	2.4
4	F	24	THR	2.4
2	D	16	ILE	2.4
3	E	121	GLU	2.4
2	D	227	HIS	2.4
1	C	337	THR	2.4
2	D	40	SER	2.4
2	D	360	GLY	2.4
4	F	335	ALA	2.4
2	D	101	TRP	2.4
2	B	214	THR	2.4
2	B	71	GLY	2.4
4	F	176	GLN	2.4
2	B	54	ALA	2.4
2	B	57	ASN	2.4
2	D	54	ALA	2.4
2	D	135	LEU	2.4
4	F	314	LEU	2.4
2	D	71	GLY	2.3
2	D	400	GLY	2.3
4	F	25	GLY	2.3
4	F	340	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	190	LEU	2.3
2	B	283	ALA	2.3
2	D	111	GLU	2.3
1	A	345	ASP	2.3
2	D	213	ARG	2.3
2	B	291	GLN	2.3
4	F	144	GLY	2.3
2	B	175	VAL	2.3
1	A	232	SER	2.3
2	B	78	SER	2.3
1	C	285	GLN	2.3
3	E	128	LYS	2.3
2	D	14	ASN	2.3
3	E	50	ILE	2.3
2	D	34	GLY	2.3
2	B	33	THR	2.2
2	D	107	THR	2.2
2	D	223	GLY	2.2
3	E	132	GLU	2.2
4	F	22	LEU	2.2
1	A	221	ARG	2.2
2	D	6	HIS	2.2
4	F	188	LYS	2.2
2	D	93	GLY	2.2
2	D	181	GLU	2.2
2	B	320	ARG	2.2
2	D	357	PRO	2.2
2	B	39	ASP	2.2
2	D	41	ASP	2.2
2	D	86	ARG	2.2
4	F	31	ARG	2.1
3	E	47	LEU	2.1
1	C	281	ALA	2.1
2	D	214	THR	2.1
2	B	95	SER	2.1
2	D	10	GLY	2.1
4	F	45	ASN	2.1
4	F	192	LEU	2.1
4	F	13	VAL	2.1
2	D	85	PHE	2.1
2	D	126	SER	2.1
2	D	320	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	127	ASP	2.1
1	A	18	ASN	2.1
3	E	90	ASN	2.1
4	F	360	PRO	2.1
2	D	363	MET	2.1
1	A	344	VAL	2.1
2	D	59	TYR	2.1
2	B	274	THR	2.1
2	D	27	GLU	2.0
2	D	106	TYR	2.0
4	F	373	SER	2.0
1	A	88	HIS	2.0
2	B	73	MET	2.0
4	F	137	ARG	2.0
2	B	75	SER	2.0
2	B	350	LYS	2.0
2	D	19	LYS	2.0
2	B	170	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

## 6.5 Other polymers [i](#)

There are no such residues in this entry.