



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:36 PM JST

PDB ID : 8YTX
Title : Tubulin-RB3-TTL in complex with compound SI9
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2024-03-26
Resolution : 2.53 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 types of validation reports are described at

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

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

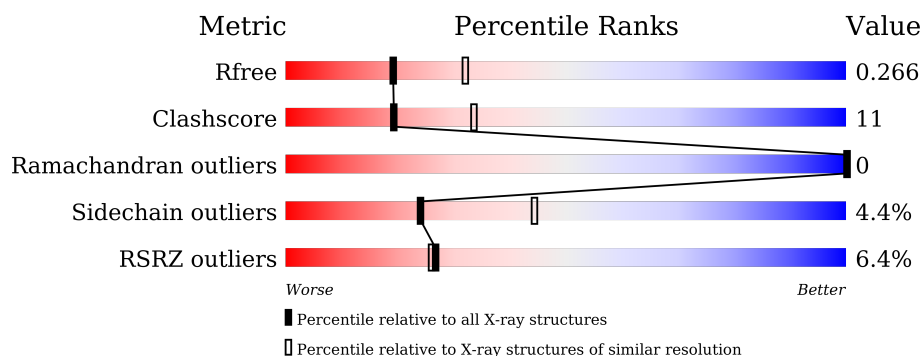
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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 $\leq 5\%$. 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>2%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
1	C	440	<div> <div>2%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	431	<div> <div>6%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
2	D	431	<div> <div>10%</div> <div>69%</div> <div>26%</div> <div>..</div> </div>
3	E	143	<div> <div>5%</div> <div>61%</div> <div>19%</div> <div>18%</div> </div>
4	F	380	<div> <div>11%</div> <div>48%</div> <div>20%</div> <div>29%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16858 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	117	Total	C	N	O	S	0	0	0
			962	594	176	187	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

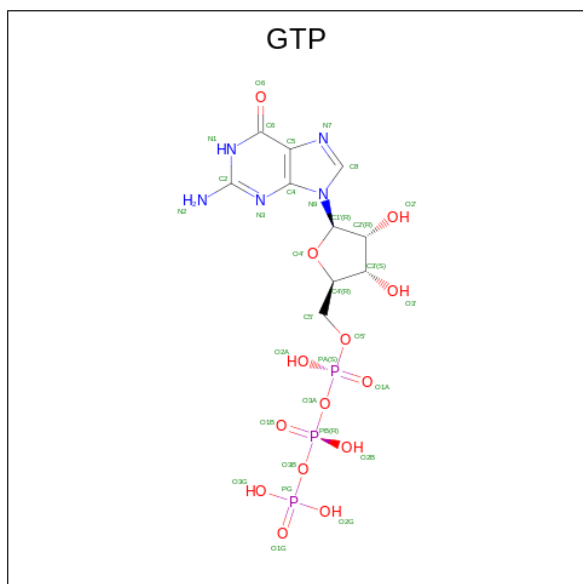
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	268	Total	C	N	O	S	0	0	0
			2166	1397	366	389	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).

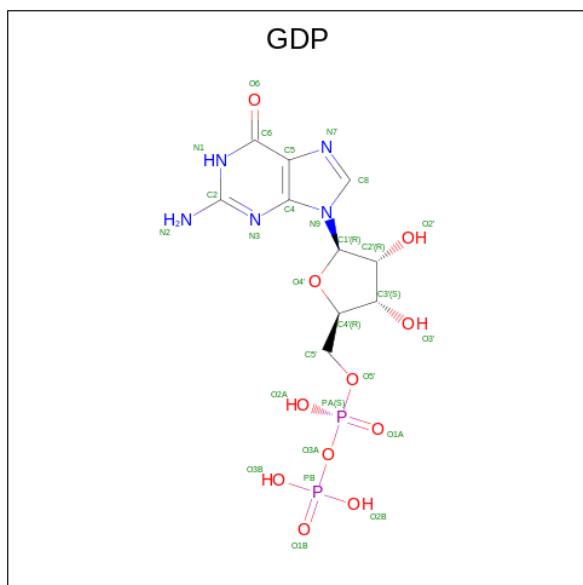
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

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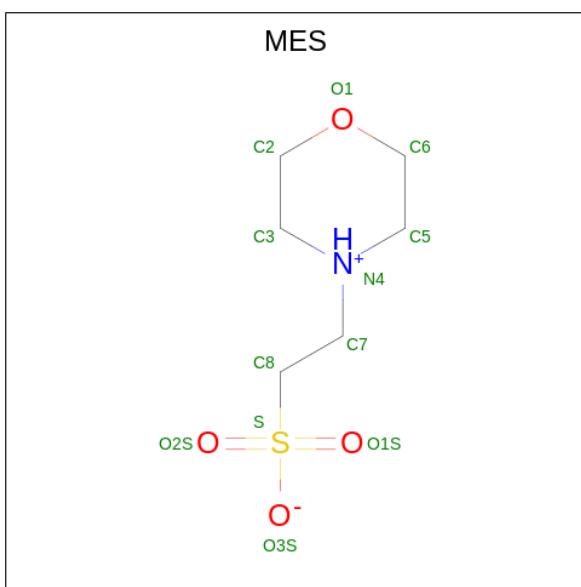
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

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



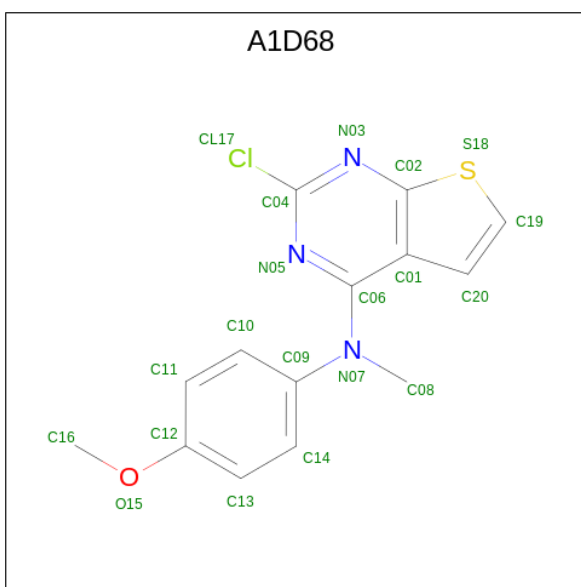
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	28	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	28	0
			28	10	5	11	2		

- 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[2,3-d]pyrimidin-4-a mine (three-letter code: A1D68) (formula: C₁₄H₁₂ClN₃OS) (labeled as "Ligand of Interest" by depositor).



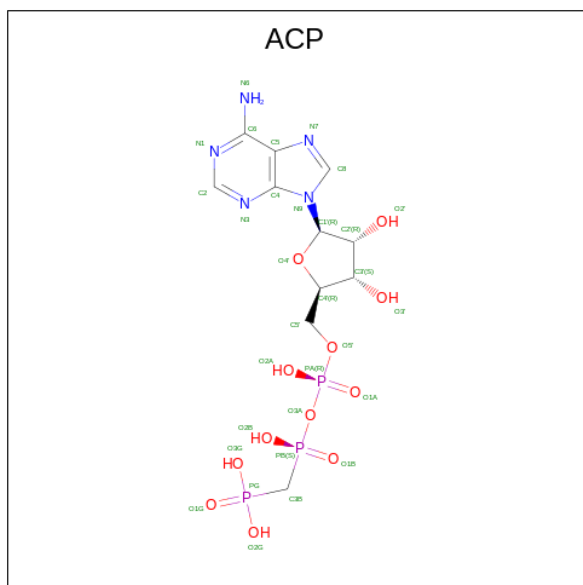
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	B	1	Total	C	Cl	H	N	O	S	0	0
			32	14	1	12	3	1	1		

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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		

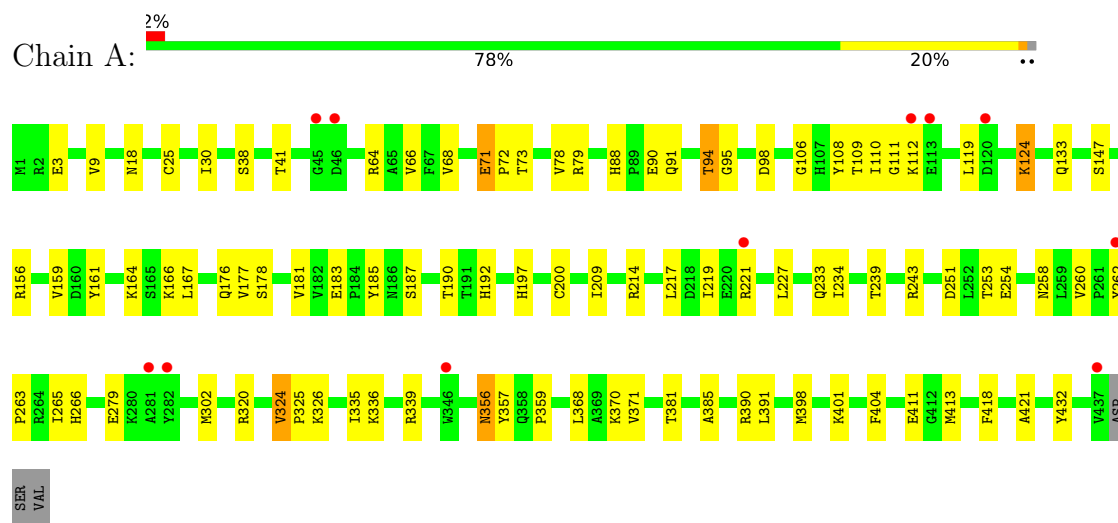
- Molecule 12 is water.

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

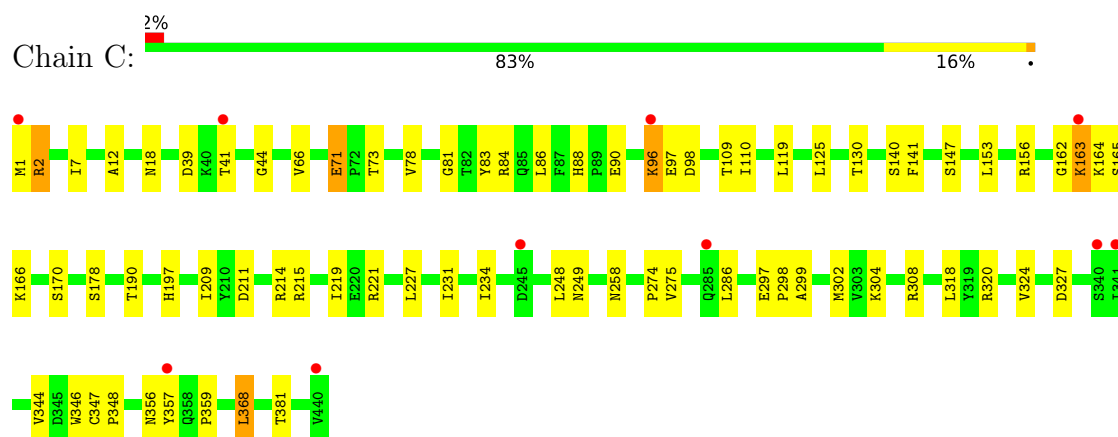
3 Residue-property plots

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.

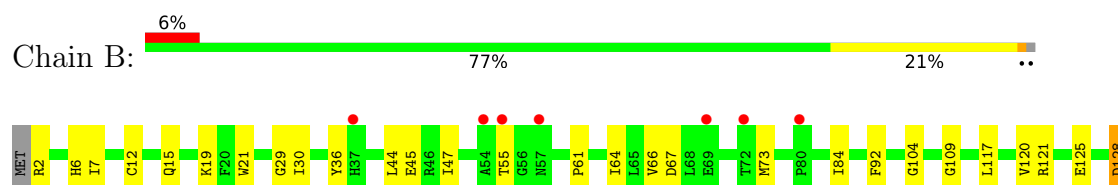
• Molecule 1: Detyrosinated tubulin alpha-1B chain

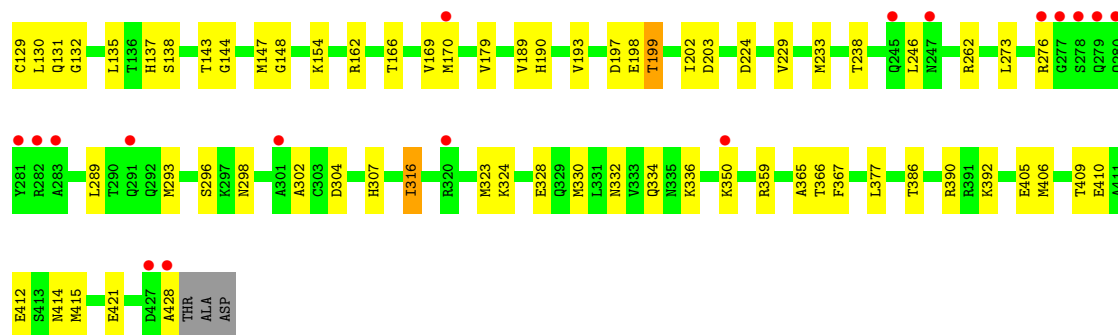


• Molecule 1: Detyrosinated tubulin alpha-1B chain

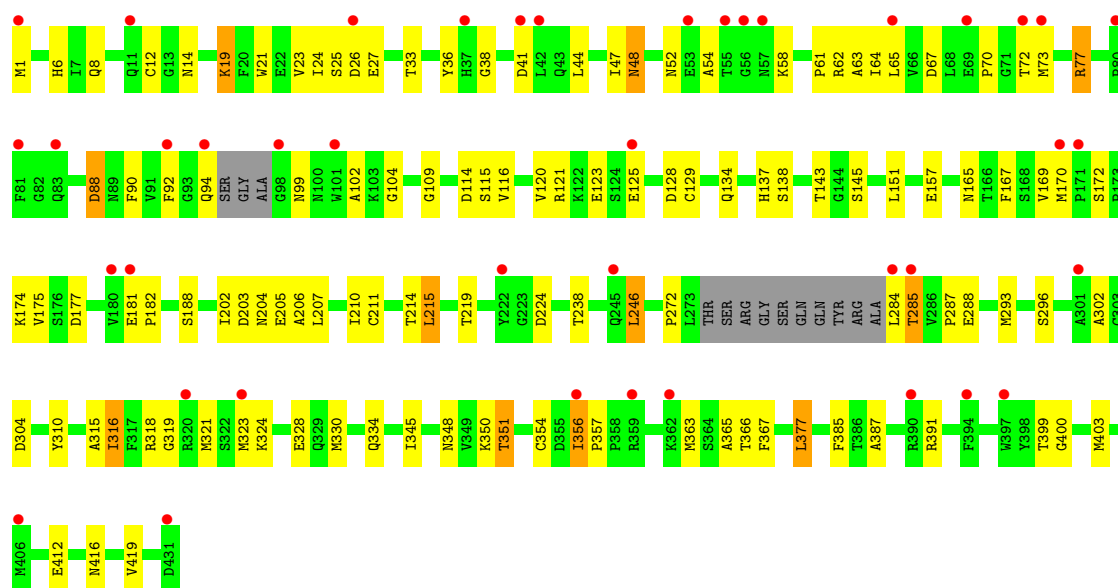


• Molecule 2: Tubulin beta chain

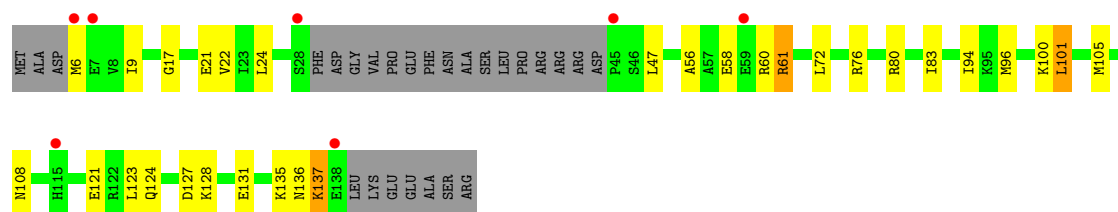




• Molecule 2: Tubulin beta chain

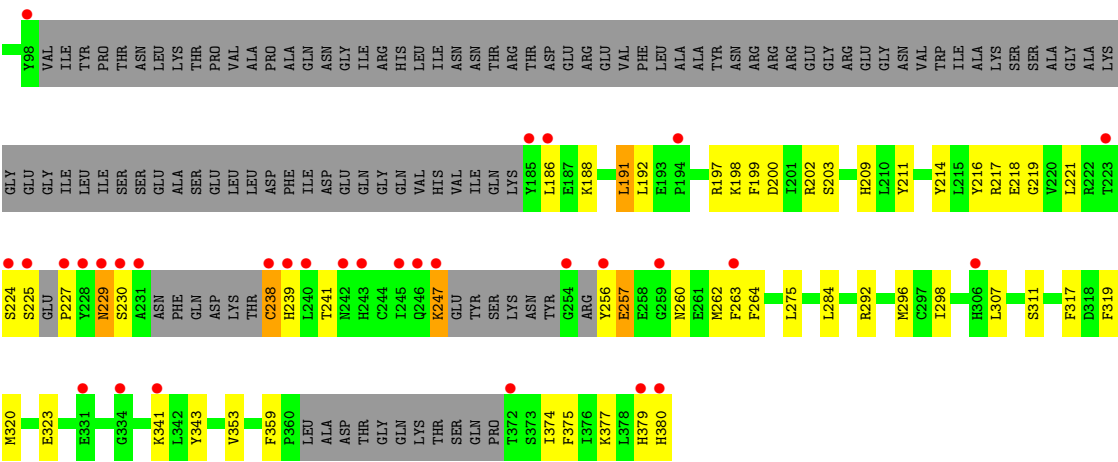


• Molecule 3: Stathmin-4



• 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, α , β , γ	105.37Å 158.31Å 180.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 2.53 45.56 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.56-2.53) 98.6 (45.56-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.222 , 0.266 0.222 , 0.266	Depositor DCC
R_{free} test set	99337 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	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	16858	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: CA, A1D68, MES, ACP, GDP, 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	0.46	0/3482	0.64	0/4728
1	C	0.52	0/3511	0.69	1/4768 (0.0%)
2	B	0.46	0/3426	0.64	1/4643 (0.0%)
2	D	0.40	0/3353	0.60	0/4543
3	E	0.45	0/970	0.59	0/1286
4	F	0.39	0/2215	0.60	0/2992
All	All	0.45	0/16957	0.63	2/22960 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	LEU	CB-CG-CD2	-5.91	100.95	111.00
2	B	350	LYS	CD-CE-NZ	5.03	123.26	111.70

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	70	0
1	C	3433	0	3337	52	0
2	B	3351	0	3214	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3281	0	3151	110	0
3	E	962	0	981	27	0
4	F	2166	0	2110	70	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	0	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	16820	38	16192	375	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 11.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:MET:HE1	2:D:92:PHE:HB3	1.19	1.10
1:A:71:GLU:OE2	1:A:73:THR:HB	1.64	0.97
2:B:406:MET:HE3	2:B:409:THR:HB	1.48	0.95
2:D:73:MET:CE	2:D:92:PHE:HB3	1.96	0.95
2:B:238:THR:HB	2:B:316:ILE:HD13	1.46	0.93
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.49	0.92
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.03	0.91
1:A:109:THR:HG21	1:A:411:GLU:OE1	1.71	0.90
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.03	0.90
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.53	0.87
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.58	0.85
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.09	0.82
4:F:188:LYS:HD3	4:F:323:GLU:OE1	1.82	0.80
2:B:324:LYS:HE2	2:B:328:GLU:OE2	1.80	0.80
2:D:330:MET:HG3	2:D:351:THR:HG21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:THR:HG23	2:B:147:MET:HE2	1.63	0.79
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.17	0.77
2:B:238:THR:HB	2:B:316:ILE:CD1	2.15	0.77
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.02	0.77
1:A:370:LYS:HD3	1:A:371:VAL:N	2.00	0.76
2:B:238:THR:HG21	2:B:316:ILE:HD11	1.67	0.76
4:F:225:SER:O	4:F:227:PRO:HD3	1.88	0.74
2:D:285:THR:HG23	2:D:287:PRO:HD2	1.69	0.74
4:F:186:LEU:CD1	4:F:320:MET:HG2	2.16	0.74
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.88	0.74
3:E:101:LEU:O	3:E:105:MET:HG2	1.88	0.74
1:A:166:LYS:NZ	1:A:197:HIS:O	2.19	0.73
2:D:330:MET:O	2:D:334:GLN:HG3	1.89	0.73
4:F:70:LYS:O	4:F:76:SER:HB2	1.89	0.73
4:F:1:MET:HE1	4:F:28:LYS:HB3	1.70	0.73
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.24	0.72
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.71	0.72
2:B:262:ARG:NH2	2:B:414:ASN:OD1	2.21	0.72
1:A:147:SER:HB2	1:A:190:THR:HB	1.72	0.71
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.03	0.71
4:F:192:LEU:HD21	4:F:262:MET:HE2	1.74	0.69
1:C:221:ARG:CZ	2:D:323:MET:HB3	2.22	0.69
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.26	0.69
1:A:88:HIS:N	1:A:91:GLN:OE1	2.25	0.68
2:D:416:ASN:O	2:D:419:VAL:HG22	1.93	0.68
4:F:256:TYR:HB2	4:F:257:GLU:OE2	1.93	0.68
2:D:211:CYS:HA	2:D:215:LEU:HD23	1.76	0.67
4:F:192:LEU:HD21	4:F:262:MET:CE	2.24	0.67
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.28	0.67
2:B:238:THR:CG2	2:B:316:ILE:HD11	2.25	0.67
2:D:73:MET:HE1	2:D:92:PHE:CB	2.11	0.67
2:D:285:THR:HG22	2:D:288:GLU:HG3	1.75	0.67
1:A:112:LYS:HE3	3:E:61:ARG:HH22	1.60	0.66
4:F:224:SER:OG	4:F:238:CYS:HA	1.95	0.66
2:D:321:MET:HB3	2:D:363:MET:CE	2.26	0.66
4:F:247:LYS:NZ	4:F:247:LYS:HA	2.11	0.66
2:D:285:THR:HG22	2:D:288:GLU:CG	2.25	0.65
2:D:62:ARG:HG3	2:D:123:GLU:OE1	1.96	0.65
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.78	0.65
2:D:116:VAL:HG11	2:D:151:LEU:HD21	1.78	0.65
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.79	0.64
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.62	0.64
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.80	0.64
1:C:166:LYS:HE2	1:C:197:HIS:O	1.97	0.64
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.28	0.63
2:D:121:ARG:O	2:D:125:GLU:HG2	1.99	0.63
2:D:318:ARG:HH21	2:D:356:ILE:HG12	1.62	0.63
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.29	0.63
2:B:166:THR:OG1	2:B:199:THR:HB	1.99	0.62
2:D:63:ALA:C	2:D:64:ILE:HD13	2.19	0.62
2:D:157:GLU:HA	3:E:123:LEU:HD13	1.80	0.62
4:F:80:LEU:HD21	4:F:298:ILE:CG2	2.30	0.62
4:F:221:LEU:HD22	4:F:262:MET:CE	2.30	0.61
2:D:321:MET:HB3	2:D:363:MET:HE2	1.82	0.61
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.16	0.61
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.83	0.61
2:D:134:GLN:HA	2:D:165:ASN:O	2.01	0.61
2:D:324:LYS:HE2	2:D:328:GLU:OE2	2.00	0.61
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.83	0.60
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.36	0.60
2:D:73:MET:O	2:D:77:ARG:HG3	2.01	0.60
1:C:234:ILE:HD13	1:C:302:MET:SD	2.42	0.60
2:B:73:MET:CE	2:B:92:PHE:HB3	2.31	0.60
2:D:315:ALA:HB3	2:D:351:THR:CG2	2.31	0.60
4:F:296:MET:HE2	4:F:380:HIS:HB2	1.84	0.60
3:E:121:GLU:O	3:E:124:GLN:HG3	2.02	0.59
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.84	0.59
1:A:336:LYS:HD3	3:E:24:LEU:CD1	2.33	0.58
1:C:221:ARG:NH1	2:D:323:MET:HB3	2.16	0.58
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.04	0.58
1:A:177:VAL:HG12	1:A:177:VAL:O	2.03	0.58
2:B:30:ILE:HD12	2:B:30:ILE:N	2.19	0.58
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.84	0.57
4:F:14:TYR:HA	4:F:17:VAL:HB	1.86	0.57
2:B:189:VAL:HG21	2:B:415:MET:CE	2.34	0.57
4:F:191:LEU:HA	4:F:197:ARG:O	2.04	0.57
4:F:247:LYS:HA	4:F:247:LYS:CE	2.34	0.57
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.85	0.57
4:F:377:LYS:HE2	4:F:379:HIS:CD2	2.40	0.57
1:C:320:ARG:HA	1:C:356:ASN:O	2.05	0.56
1:A:178:SER:HB2	1:A:183:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:GLU:CA	3:E:123:LEU:HD13	2.36	0.56
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.39	0.56
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.05	0.56
2:D:23:VAL:O	2:D:27:GLU:HG3	2.06	0.56
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.87	0.56
2:D:210:ILE:O	2:D:215:LEU:HD22	2.06	0.56
2:B:169:VAL:HA	2:B:202:ILE:O	2.05	0.56
2:B:143:THR:CG2	2:B:147:MET:HE2	2.34	0.55
2:B:229:VAL:O	2:B:233:MET:HG3	2.04	0.55
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.88	0.55
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.55
2:D:323:MET:HE2	2:D:323:MET:H	1.70	0.55
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.88	0.55
2:D:102:ALA:HB2	2:D:403:MET:SD	2.47	0.55
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.37	0.55
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.89	0.55
2:D:316:ILE:HD12	2:D:366:THR:O	2.07	0.55
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.41	0.55
2:B:130:LEU:HB3	2:B:162:ARG:HE	1.72	0.55
2:D:88:ASP:OD1	2:D:88:ASP:N	2.39	0.55
1:A:119:LEU:HD11	1:A:156:ARG:CB	2.37	0.55
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.22	0.55
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.88	0.55
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.41	0.55
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.71	0.54
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.07	0.54
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.42	0.54
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.43	0.54
2:B:238:THR:CB	2:B:316:ILE:CD1	2.85	0.54
2:D:293:MET:CG	2:D:367:PHE:HB2	2.38	0.54
1:A:94:THR:HG23	1:A:95:GLY:O	2.07	0.54
1:C:110:ILE:HD13	1:C:110:ILE:N	2.22	0.54
4:F:1:MET:HE2	4:F:28:LYS:CD	2.37	0.54
4:F:18:SER:O	4:F:22:LEU:HD12	2.08	0.53
1:C:81:GLY:O	1:C:84:ARG:NH1	2.40	0.53
2:D:48:ASN:H	2:D:48:ASN:ND2	2.06	0.53
2:D:70:PRO:HD3	2:D:94:GLN:HA	1.90	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.89	0.53
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.23	0.53
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.43	0.53
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG22	3:E:61:ARG:HH11	1.73	0.53
2:B:262:ARG:NH1	2:B:421:GLU:OE1	2.37	0.53
1:C:178:SER:O	2:D:350:LYS:HE2	2.09	0.53
1:A:336:LYS:HD3	3:E:24:LEU:HD12	1.90	0.53
2:D:63:ALA:O	2:D:64:ILE:HD13	2.09	0.53
2:D:238:THR:OG1	2:D:318:ARG:HD2	2.09	0.53
2:D:1:MET:CE	2:D:128:ASP:HB2	2.39	0.53
2:D:285:THR:CG2	2:D:288:GLU:H	2.22	0.53
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.90	0.53
2:D:145:SER:OG	2:D:188:SER:OG	2.26	0.53
3:E:127:ASP:O	3:E:131:GLU:HG2	2.08	0.53
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.44	0.52
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.45	0.52
4:F:317:PHE:HB3	4:F:319:PHE:CE1	2.45	0.52
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.89	0.52
4:F:198:LYS:HE2	4:F:239:HIS:O	2.10	0.52
1:A:133:GLN:OE1	1:A:251:ASP:HA	2.09	0.52
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.89	0.52
2:D:318:ARG:NH2	2:D:356:ILE:HG12	2.24	0.52
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.92	0.52
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.25	0.52
4:F:209:HIS:HA	4:F:311:SER:O	2.10	0.52
2:D:138:SER:HA	2:D:169:VAL:HB	1.93	0.51
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.51
2:D:104:GLY:O	2:D:109:GLY:HA3	2.09	0.51
2:D:400:GLY:O	3:E:137:LYS:HD2	2.10	0.51
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.92	0.51
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.92	0.51
2:D:285:THR:HG23	2:D:287:PRO:CD	2.39	0.51
3:E:6:MET:HG3	3:E:24:LEU:CD2	2.41	0.51
4:F:353:VAL:HG21	4:F:375:PHE:CD2	2.46	0.51
2:D:67:ASP:HA	2:D:143:THR:HG21	1.92	0.51
1:A:401:LYS:HE3	2:B:428:ALA:HB1	1.92	0.50
2:D:206:ALA:HB2	2:D:302:ALA:HB2	1.93	0.50
2:D:206:ALA:O	2:D:210:ILE:HG13	2.11	0.50
1:A:25:CYS:HB3	1:A:30:ILE:O	2.11	0.50
2:B:332:ASN:ND2	2:B:336:LYS:HE2	2.26	0.50
1:C:1:MET:HB3	1:C:130:THR:OG1	2.12	0.50
1:C:41:THR:OG1	1:C:44:GLY:O	2.30	0.50
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.92	0.50
4:F:229:ASN:OD1	4:F:229:ASN:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:MET:HE2	2:D:377:LEU:HD11	1.94	0.50
1:C:71:GLU:OE1	1:C:73:THR:HB	2.11	0.50
1:A:109:THR:HG22	3:E:61:ARG:NH1	2.27	0.49
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.93	0.49
4:F:3:THR:HG22	4:F:28:LYS:CG	2.42	0.49
2:D:54:ALA:HB3	2:D:58:LYS:HB2	1.93	0.49
4:F:202:ARG:HG3	4:F:203:SER:N	2.27	0.49
2:D:1:MET:HE2	2:D:128:ASP:OD2	2.13	0.49
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.95	0.49
2:B:406:MET:CE	2:B:409:THR:HB	2.31	0.49
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.94	0.49
4:F:88:SER:HG	4:F:91:CYS:N	2.11	0.49
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.28	0.49
2:D:296:SER:OG	2:D:304:ASP:HA	2.12	0.49
4:F:217:ARG:HG2	4:F:374:ILE:O	2.13	0.49
2:B:189:VAL:O	2:B:193:VAL:HG23	2.12	0.49
2:B:293:MET:CE	2:B:365:ALA:HB1	2.42	0.49
4:F:1:MET:CE	4:F:28:LYS:HB3	2.40	0.49
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.94	0.48
2:B:330:MET:O	2:B:334:GLN:HG3	2.12	0.48
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.31	0.48
1:A:187:SER:CB	1:A:391:LEU:HD21	2.44	0.48
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.94	0.48
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.94	0.48
4:F:1:MET:HE2	4:F:28:LYS:CG	2.44	0.48
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.96	0.48
2:D:73:MET:HB3	2:D:90:PHE:CD2	2.49	0.48
2:B:29:GLY:O	2:B:36:TYR:HA	2.14	0.48
2:B:386:THR:O	2:B:390:ARG:HG2	2.13	0.48
1:C:83:TYR:CD1	1:C:86:LEU:HD22	2.48	0.48
1:C:357:TYR:O	1:C:359:PRO:HD3	2.14	0.48
2:D:134:GLN:HG3	2:D:167:PHE:HE1	1.78	0.48
4:F:225:SER:O	4:F:227:PRO:CD	2.59	0.48
2:B:104:GLY:O	2:B:109:GLY:HA3	2.14	0.47
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.95	0.47
1:C:2:ARG:N	1:C:2:ARG:HD2	2.29	0.47
2:D:285:THR:HG22	2:D:288:GLU:CB	2.44	0.47
1:C:83:TYR:HD1	1:C:86:LEU:HD22	1.78	0.47
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.41	0.47
2:D:170:MET:CE	2:D:377:LEU:HD11	2.44	0.47
2:D:181:GLU:HB2	2:D:182:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HD2	2:B:323:MET:HB3	1.96	0.47
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.60	0.47
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.80	0.47
1:C:274:PRO:CB	1:C:286:LEU:HD22	2.45	0.47
4:F:377:LYS:HE2	4:F:379:HIS:HD2	1.78	0.47
2:B:66:VAL:HG12	2:B:147:MET:CE	2.45	0.47
2:B:189:VAL:HG21	2:B:415:MET:HE3	1.96	0.47
2:B:67:ASP:O	2:B:92:PHE:HA	2.15	0.47
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.97	0.47
2:D:285:THR:CG2	2:D:288:GLU:HG3	2.43	0.47
1:C:97:GLU:O	1:C:110:ILE:HG21	2.15	0.46
1:A:71:GLU:HG2	1:A:72:PRO:N	2.29	0.46
2:B:197:ASP:C	2:B:198:GLU:HG3	2.35	0.46
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.97	0.46
4:F:80:LEU:HD21	4:F:298:ILE:HG22	1.96	0.46
1:A:398:MET:HE3	1:A:404:PHE:HD2	1.79	0.46
2:D:33:THR:O	2:D:58:LYS:HD2	2.15	0.46
1:A:234:ILE:HD13	1:A:302:MET:SD	2.55	0.46
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.97	0.46
2:D:416:ASN:O	2:D:419:VAL:CG2	2.61	0.46
1:C:147:SER:HB2	1:C:190:THR:HB	1.97	0.46
2:D:172:SER:HB2	2:D:205:GLU:HB2	1.97	0.46
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.51	0.46
4:F:214:TYR:CD2	4:F:353:VAL:HG11	2.50	0.46
4:F:214:TYR:CE2	4:F:353:VAL:CG1	2.99	0.46
2:B:64:ILE:HD12	2:B:120:VAL:HG22	1.97	0.46
2:B:117:LEU:HD11	2:B:154:LYS:HD3	1.96	0.46
4:F:47:LEU:HD23	4:F:48:PRO:HD2	1.97	0.46
1:A:185:TYR:CZ	1:A:398:MET:HE2	2.51	0.46
2:B:144:GLY:O	2:B:148:GLY:HA3	2.16	0.46
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.97	0.46
1:C:96:LYS:HB2	1:C:96:LYS:NZ	2.31	0.46
2:D:318:ARG:O	2:D:363:MET:HA	2.17	0.45
1:C:39:ASP:OD1	1:C:41:THR:OG1	2.35	0.45
2:D:385:PHE:CE1	2:D:412:GLU:HB2	2.51	0.45
2:D:387:ALA:O	2:D:391:ARG:HD3	2.17	0.45
1:C:163:LYS:HA	1:C:163:LYS:HD3	1.45	0.45
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.46	0.45
2:D:293:MET:SD	2:D:365:ALA:HB1	2.56	0.45
1:A:72:PRO:HB3	1:A:94:THR:HG21	1.99	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:ASP:O	2:D:207:LEU:HG	2.17	0.45
4:F:12:SER:HB2	4:F:343:TYR:CE1	2.51	0.45
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.51	0.45
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.98	0.45
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.32	0.45
2:D:246:LEU:HD12	2:D:246:LEU:C	2.38	0.45
4:F:5:VAL:HG13	4:F:37:PHE:HB3	1.98	0.45
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.47	0.45
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.97	0.45
2:D:321:MET:HB3	2:D:363:MET:HE1	1.96	0.44
2:B:132:GLY:HA2	2:B:162:ARG:HB3	2.00	0.44
2:D:44:LEU:HA	2:D:47:ILE:HB	2.00	0.44
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.47	0.44
2:D:65:LEU:N	2:D:65:LEU:HD12	2.33	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.44
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.47	0.44
2:D:151:LEU:HD12	2:D:151:LEU:HA	1.87	0.44
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.20	0.44
1:C:41:THR:OG1	1:C:41:THR:O	2.34	0.44
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.44
4:F:377:LYS:HG2	4:F:379:HIS:CD2	2.52	0.44
2:B:316:ILE:HG23	2:B:366:THR:HB	1.99	0.44
2:B:2:ARG:HA	2:B:129:CYS:O	2.18	0.44
1:C:221:ARG:NH1	2:D:323:MET:CB	2.81	0.44
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.52	0.43
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.18	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
2:B:332:ASN:OD1	2:B:336:LYS:HD3	2.18	0.43
2:D:24:ILE:HG13	2:D:25:SER:N	2.32	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.43
1:C:274:PRO:HB3	1:C:286:LEU:HD22	2.00	0.43
1:A:18:ASN:HD21	1:A:78:VAL:HG21	1.81	0.43
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.01	0.43
2:D:73:MET:O	2:D:77:ARG:CG	2.65	0.43
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.57	0.43
2:D:316:ILE:HD13	2:D:366:THR:HB	2.00	0.43
2:D:116:VAL:O	2:D:120:VAL:HG23	2.19	0.43
2:D:318:ARG:HA	2:D:354:CYS:O	2.19	0.43
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.93	0.43
1:A:413:MET:CE	1:A:418:PHE:CE1	3.02	0.43
2:D:157:GLU:HA	3:E:123:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.49	0.42
2:B:12:CYS:HB3	2:B:138:SER:HB3	2.01	0.42
2:B:406:MET:HE2	2:B:410:GLU:HG3	2.01	0.42
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.42
4:F:198:LYS:HG2	4:F:199:PHE:N	2.34	0.42
2:B:7:ILE:O	2:B:135:LEU:HA	2.19	0.42
2:D:285:THR:HG22	2:D:288:GLU:H	1.84	0.42
2:D:315:ALA:HB3	2:D:351:THR:HG23	1.99	0.42
2:B:128:ASP:OD1	2:B:128:ASP:N	2.52	0.42
4:F:191:LEU:HD23	4:F:197:ARG:O	2.20	0.42
2:D:73:MET:HB3	2:D:90:PHE:HD2	1.84	0.42
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.82	0.42
2:B:19:LYS:HD3	2:B:19:LYS:HA	1.80	0.42
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.54	0.42
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.86	0.42
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.28	0.42
1:A:357:TYR:O	1:A:359:PRO:HD3	2.20	0.42
1:C:234:ILE:CD1	1:C:302:MET:SD	3.08	0.42
2:B:143:THR:HG23	2:B:147:MET:CE	2.43	0.42
4:F:353:VAL:HG21	4:F:375:PHE:CE2	2.53	0.42
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.61	0.41
2:B:332:ASN:HD21	2:B:336:LYS:HE2	1.85	0.41
1:A:370:LYS:HD3	1:A:370:LYS:C	2.40	0.41
2:B:121:ARG:HG2	2:B:125:GLU:OE2	2.20	0.41
2:B:324:LYS:O	2:B:328:GLU:HG3	2.20	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.61	0.41
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.55	0.41
4:F:17:VAL:O	4:F:21:LEU:HG	2.21	0.41
4:F:74:LYS:HA	4:F:74:LYS:HD3	1.88	0.41
1:A:79:ARG:HH22	1:A:94:THR:HB	1.86	0.41
1:A:320:ARG:HA	1:A:356:ASN:O	2.21	0.41
1:C:88:HIS:ND1	1:C:90:GLU:HB2	2.36	0.41
1:C:96:LYS:HG3	2:D:129:CYS:HB2	2.03	0.41
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.56	0.41
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.84	0.41
2:B:66:VAL:HG12	2:B:147:MET:HE3	2.03	0.41
2:D:52:ASN:ND2	2:D:123:GLU:OE1	2.53	0.41
2:D:210:ILE:HG22	2:D:215:LEU:CD2	2.51	0.41
4:F:292:ARG:O	4:F:296:MET:HG2	2.21	0.41
1:A:112:LYS:HE3	3:E:61:ARG:NH2	2.31	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ASP:HA	2:B:143:THR:HG21	2.02	0.41
2:B:392:LYS:HE3	2:B:405:GLU:OE2	2.20	0.41
2:D:214:THR:HG22	2:D:215:LEU:HD13	2.03	0.41
2:D:321:MET:O	2:D:323:MET:HE2	2.20	0.41
2:D:354:CYS:SG	2:D:356:ILE:HG23	2.60	0.41
4:F:12:SER:HB2	4:F:343:TYR:OH	2.19	0.41
4:F:89:GLU:O	4:F:91:CYS:N	2.53	0.41
4:F:217:ARG:NH1	4:F:374:ILE:HA	2.36	0.41
2:D:64:ILE:HD13	2:D:64:ILE:N	2.36	0.41
1:A:106:GLY:O	1:A:111:GLY:HA3	2.21	0.40
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.36	0.40
2:D:19:LYS:HD3	2:D:19:LYS:HA	1.85	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.40
2:D:175:VAL:HG21	2:D:204:ASN:ND2	2.36	0.40
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.21	0.40
1:A:68:VAL:O	1:A:68:VAL:HG13	2.22	0.40
1:A:71:GLU:CB	1:A:98:ASP:HB3	2.51	0.40
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.57	0.40
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.40
2:B:203:ASP:OD2	2:B:302:ALA:HB3	2.21	0.40
2:D:134:GLN:HG3	2:D:167:PHE:CE1	2.55	0.40
4:F:8:ASP:HB2	4:F:43:GLU:HA	2.03	0.40
2:B:44:LEU:HA	2:B:47:ILE:HB	2.04	0.40
4:F:1:MET:HE1	4:F:28:LYS:CB	2.45	0.40
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.89	0.40
2:B:406:MET:HE3	2:B:406:MET:O	2.21	0.40
3:E:135:LYS:HE2	3:E:135:LYS:HB3	1.61	0.40
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.55	0.40
1:A:214:ARG:HG2	1:A:219:ILE:O	2.21	0.40
2:D:1:MET:HG3	2:D:128:ASP:HB3	2.04	0.40
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.37	0.40
4:F:214:TYR:CE2	4:F:353:VAL:HG11	2.57	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	435/440 (99%)	427 (98%)	8 (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
3	E	113/143 (79%)	111 (98%)	2 (2%)	0	100	100
4	F	253/380 (67%)	247 (98%)	6 (2%)	0	100	100
All	All	2076/2265 (92%)	2033 (98%)	43 (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%)	354 (97%)	12 (3%)	33	57
1	C	370/371 (100%)	361 (98%)	9 (2%)	44	68
2	B	367/372 (99%)	357 (97%)	10 (3%)	40	65
2	D	360/372 (97%)	337 (94%)	23 (6%)	14	28
3	E	104/127 (82%)	95 (91%)	9 (9%)	8	16
4	F	235/338 (70%)	219 (93%)	16 (7%)	13	25
All	All	1802/1951 (92%)	1723 (96%)	79 (4%)	24	44

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	41	THR
1	A	66	VAL

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Mol	Chain	Res	Type
1	A	71	GLU
1	A	94	THR
1	A	110	ILE
1	A	124	LYS
1	A	181	VAL
1	A	253	THR
1	A	324	VAL
1	A	356	ASN
1	A	381	THR
2	B	15	GLN
2	B	45	GLU
2	B	55	THR
2	B	128	ASP
2	B	137	HIS
2	B	199	THR
2	B	246	LEU
2	B	296	SER
2	B	316	ILE
2	B	359	ARG
1	C	2	ARG
1	C	71	GLU
1	C	96	LYS
1	C	163	LYS
1	C	165	SER
1	C	297	GLU
1	C	318	LEU
1	C	347	CYS
1	C	381	THR
2	D	19	LYS
2	D	26	ASP
2	D	41	ASP
2	D	48	ASN
2	D	72	THR
2	D	77	ARG
2	D	88	ASP
2	D	99	ASN
2	D	114	ASP
2	D	115	SER
2	D	137	HIS
2	D	174	LYS
2	D	177	ASP
2	D	215	LEU

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Mol	Chain	Res	Type
2	D	219	THR
2	D	224	ASP
2	D	246	LEU
2	D	285	THR
2	D	316	ILE
2	D	351	THR
2	D	356	ILE
2	D	377	LEU
2	D	399	THR
3	E	22	VAL
3	E	61	ARG
3	E	96	MET
3	E	100	LYS
3	E	101	LEU
3	E	108	ASN
3	E	128	LYS
3	E	136	ASN
3	E	137	LYS
4	F	12	SER
4	F	19	ARG
4	F	28	LYS
4	F	31	ARG
4	F	74	LYS
4	F	76	SER
4	F	191	LEU
4	F	211	TYR
4	F	229	ASN
4	F	230	SER
4	F	238	CYS
4	F	247	LYS
4	F	257	GLU
4	F	260	ASN
4	F	275	LEU
4	F	307	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	301	GLN
4	F	269	GLN
4	F	379	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
10	A1D68	D	502	-	20,22,22	1.33	3 (15%)	25,31,31	2.65	10 (40%)
5	GTP	A	501	7	26,34,34	1.12	2 (7%)	32,54,54	1.59	7 (21%)
11	ACP	F	401	-	27,33,33	2.21	3 (11%)	32,52,52	1.09	3 (9%)
8	GDP	B	501	7	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
8	GDP	D	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.42	5 (16%)
9	MES	B	502	-	12,12,12	1.25	1 (8%)	14,16,16	0.82	1 (7%)
5	GTP	C	501	7	26,34,34	1.12	2 (7%)	32,54,54	1.61	7 (21%)
10	A1D68	B	505	-	20,22,22	1.42	4 (20%)	25,31,31	2.68	8 (32%)
9	MES	B	503	-	12,12,12	1.25	1 (8%)	14,16,16	0.83	0

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
10	A1D68	D	502	-	-	2/10/10/10	0/3/3/3
5	GTP	A	501	7	-	9/18/38/38	0/3/3/3
11	ACP	F	401	-	-	2/15/38/38	0/3/3/3
8	GDP	B	501	7	-	3/12/32/32	0/3/3/3
8	GDP	D	501	-	-	3/12/32/32	0/3/3/3
9	MES	B	502	-	-	5/6/14/14	0/1/1/1
5	GTP	C	501	7	-	6/18/38/38	0/3/3/3
10	A1D68	B	505	-	-	2/10/10/10	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	10.30	1.69	1.58
5	A	501	GTP	C5-C6	-4.00	1.39	1.47
5	C	501	GTP	C5-C6	-3.97	1.39	1.47
10	B	505	A1D68	C04-N03	3.64	1.33	1.30
9	B	503	MES	C8-S	3.41	1.82	1.77
9	B	502	MES	C8-S	3.35	1.82	1.77
10	D	502	A1D68	C06-N07	3.35	1.46	1.39
10	D	502	A1D68	C04-N03	2.98	1.32	1.30
10	B	505	A1D68	C02-C01	-2.78	1.38	1.42
8	B	501	GDP	C6-N1	-2.38	1.34	1.37
5	C	501	GTP	C2-N3	2.21	1.38	1.33
11	F	401	ACP	PB-O2B	-2.20	1.51	1.56
11	F	401	ACP	C8-N7	-2.18	1.30	1.34
10	D	502	A1D68	C02-C01	-2.17	1.39	1.42
10	B	505	A1D68	C04-CL17	2.14	1.79	1.73
5	A	501	GTP	C2-N3	2.14	1.38	1.33
10	B	505	A1D68	C06-N07	2.07	1.43	1.39
8	D	501	GDP	C6-N1	-2.07	1.34	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	A1D68	N03-C04-N05	-7.99	122.58	130.62
10	D	502	A1D68	N03-C04-N05	-7.53	123.03	130.62
10	D	502	A1D68	C04-N03-C02	6.63	119.34	114.09
10	B	505	A1D68	C04-N03-C02	6.17	118.98	114.09
10	B	505	A1D68	C19-S18-C02	4.55	96.87	91.00
10	D	502	A1D68	C19-S18-C02	3.98	96.13	91.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	PA-O3A-PB	-3.79	119.81	132.83
5	C	501	GTP	PB-O3B-PG	-3.59	120.52	132.83
5	C	501	GTP	PA-O3A-PB	-3.57	120.58	132.83
5	A	501	GTP	PA-O3A-PB	-3.53	120.71	132.83
5	A	501	GTP	PB-O3B-PG	-3.53	120.71	132.83
8	B	501	GDP	PA-O3A-PB	-3.43	121.07	132.83
10	D	502	A1D68	C04-N05-C06	3.41	121.15	111.04
10	B	505	A1D68	CL17-C04-N05	3.23	119.77	115.15
8	B	501	GDP	C3'-C2'-C1'	3.23	105.83	100.98
10	B	505	A1D68	C20-C01-C02	3.22	116.20	105.90
5	C	501	GTP	C5-C6-N1	3.20	119.60	113.95
5	A	501	GTP	C5-C6-N1	3.18	119.57	113.95
10	B	505	A1D68	C04-N05-C06	3.08	120.19	111.04
5	C	501	GTP	C3'-C2'-C1'	3.08	105.61	100.98
5	A	501	GTP	C3'-C2'-C1'	3.05	105.57	100.98
11	F	401	ACP	O2B-PB-O1B	3.01	120.12	110.07
5	A	501	GTP	C8-N7-C5	3.01	108.72	102.99
5	C	501	GTP	C8-N7-C5	3.00	108.70	102.99
5	A	501	GTP	C2-N1-C6	-2.89	119.77	125.10
10	D	502	A1D68	CL17-C04-N03	2.88	118.16	115.70
5	C	501	GTP	C2-N1-C6	-2.84	119.87	125.10
8	D	501	GDP	C3'-C2'-C1'	2.80	105.19	100.98
10	D	502	A1D68	C20-C01-C02	2.77	114.75	105.90
10	D	502	A1D68	C01-C02-N03	-2.71	120.43	124.94
11	F	401	ACP	O1G-PG-C3B	-2.61	105.61	111.24
11	F	401	ACP	PB-O3A-PA	-2.58	124.37	132.56
10	D	502	A1D68	CL17-C04-N05	2.56	118.81	115.15
8	D	501	GDP	C5-C6-N1	2.55	118.46	113.95
9	B	502	MES	O2S-S-C8	-2.43	103.99	106.92
10	D	502	A1D68	C16-O15-C12	-2.40	112.29	117.51
8	D	501	GDP	C8-N7-C5	2.36	107.49	102.99
8	B	501	GDP	C8-N7-C5	2.32	107.41	102.99
8	B	501	GDP	C5-C6-N1	2.29	117.99	113.95
10	B	505	A1D68	CL17-C04-N03	2.29	117.65	115.70
10	B	505	A1D68	C01-C02-N03	-2.21	121.25	124.94
10	D	502	A1D68	C01-C06-N05	-2.18	118.01	122.66
5	C	501	GTP	O6-C6-C5	-2.14	120.20	124.37
5	A	501	GTP	O6-C6-C5	-2.11	120.24	124.37
8	D	501	GDP	N2-C2-N1	2.06	121.10	116.71

There are no chirality outliers.

All (35) torsion outliers are listed below:

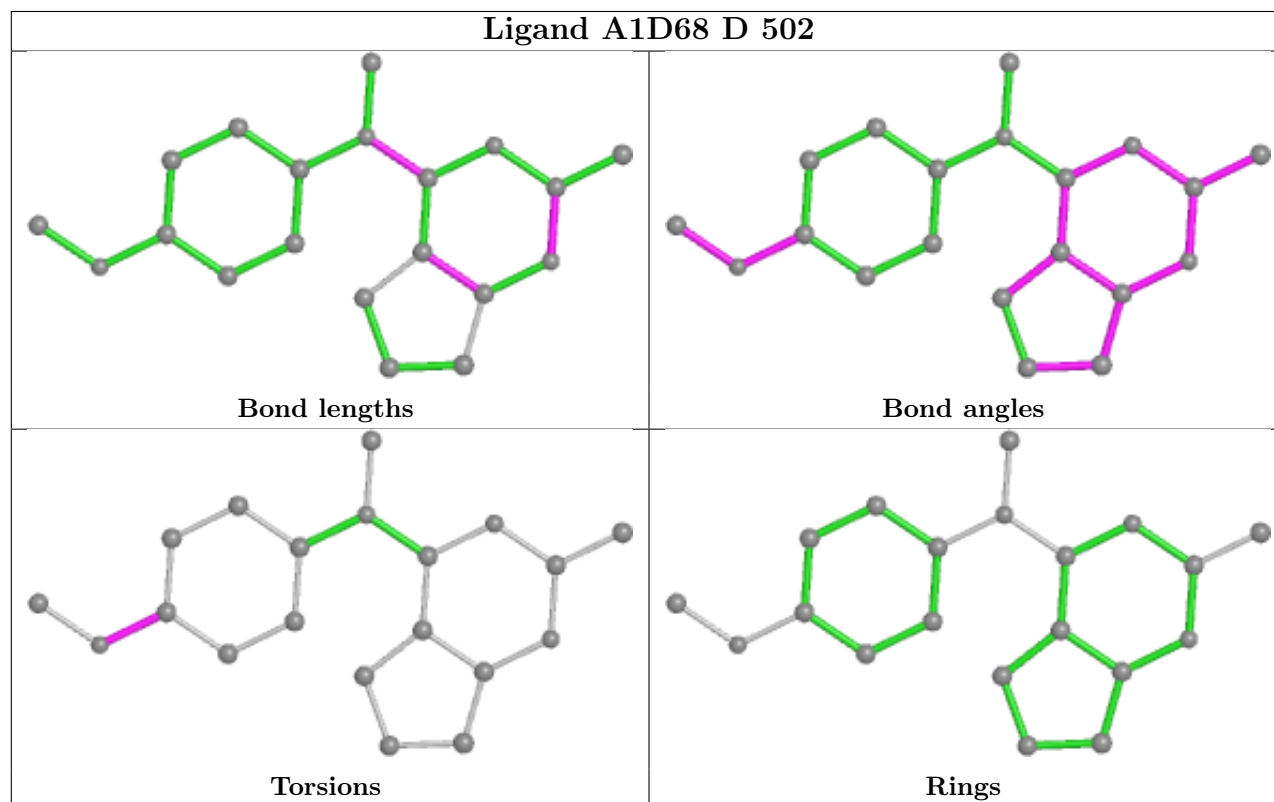
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
10	D	502	A1D68	C11-C12-O15-C16
10	D	502	A1D68	C13-C12-O15-C16
9	B	502	MES	C7-C8-S-O3S
10	B	505	A1D68	C13-C12-O15-C16
10	B	505	A1D68	C11-C12-O15-C16
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O1A
9	B	502	MES	C7-C8-S-O1S
9	B	502	MES	C7-C8-S-O2S
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	O4'-C4'-C5'-O5'
11	F	401	ACP	C4'-C5'-O5'-PA
9	B	502	MES	C8-C7-N4-C3
9	B	502	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C3'-C4'-C5'-O5'
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G

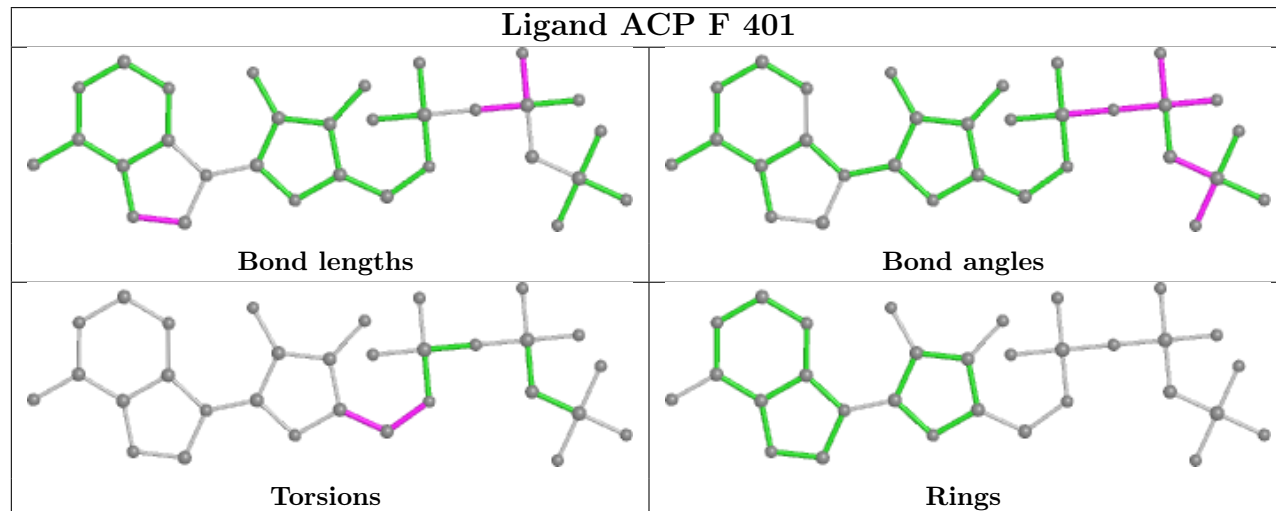
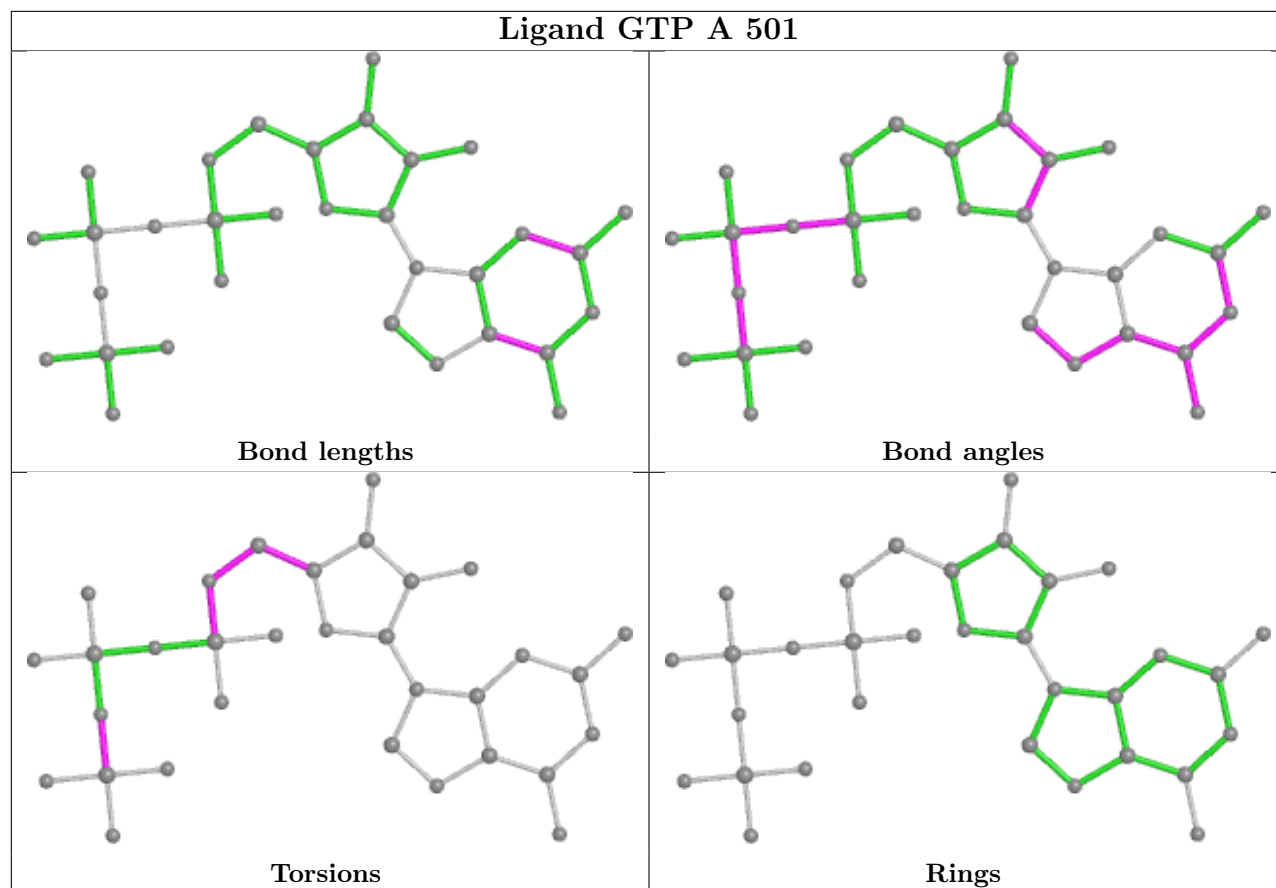
There are no ring outliers.

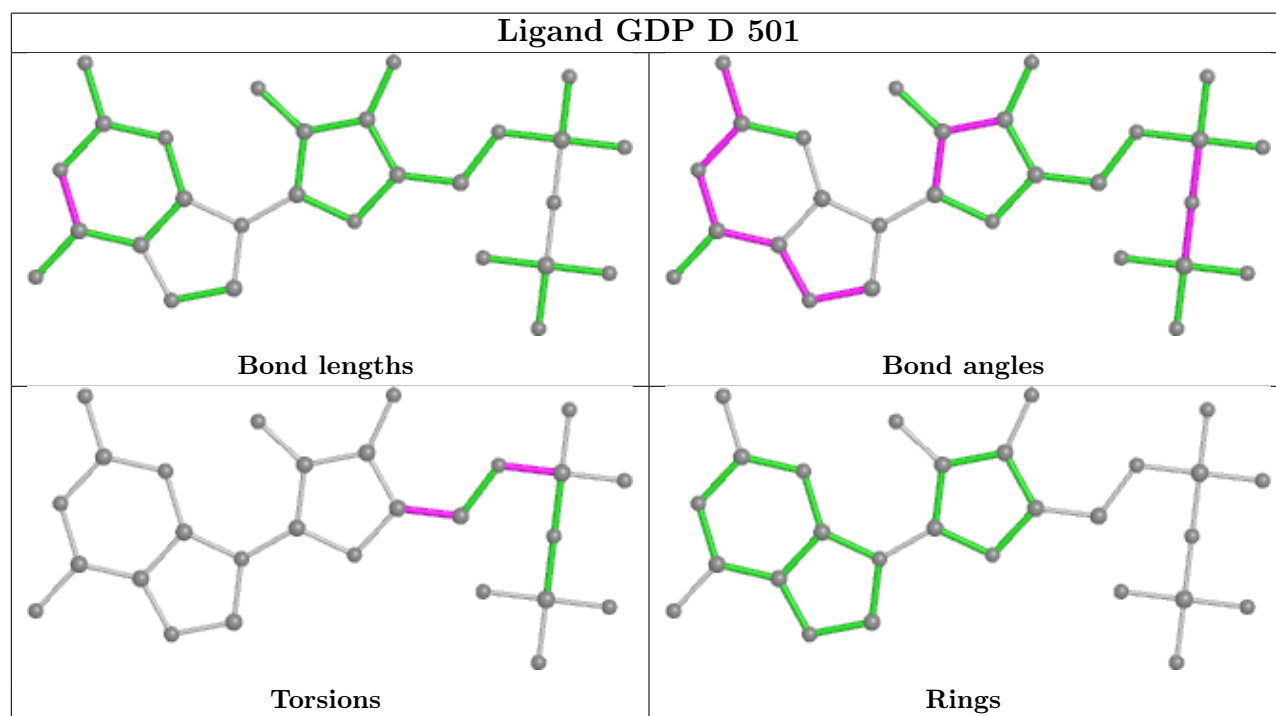
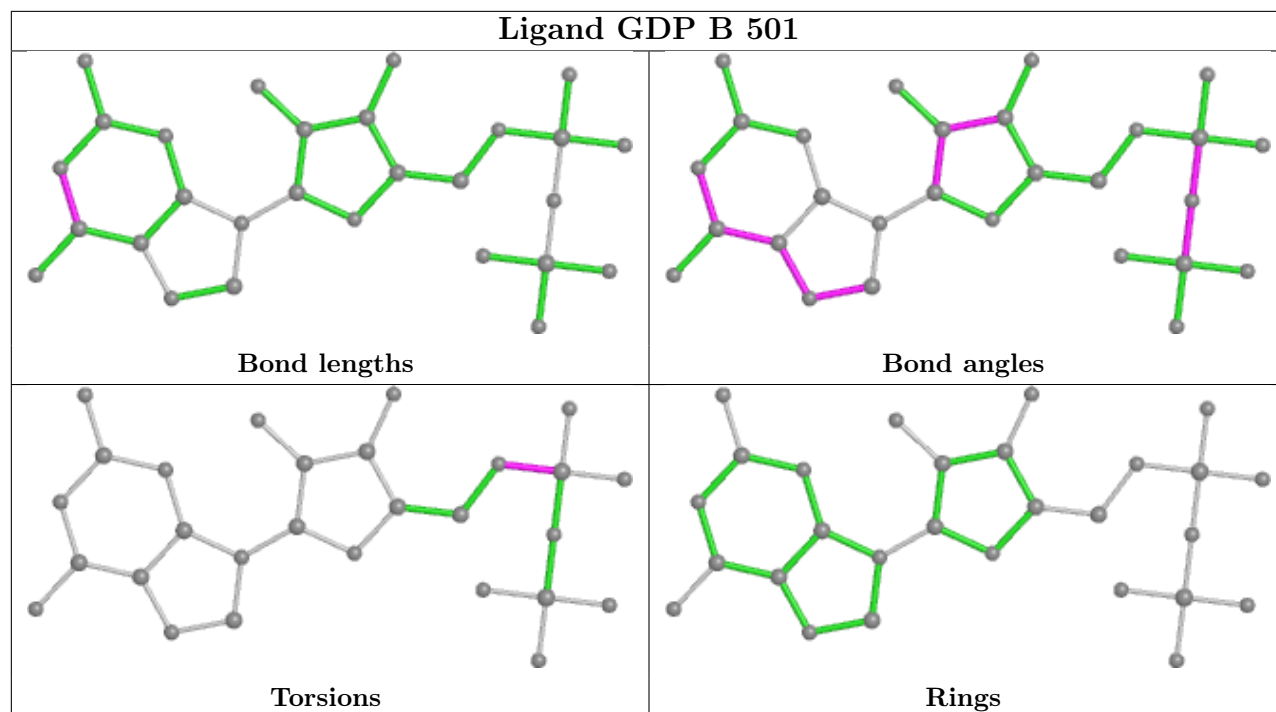
No monomer is involved in short contacts.

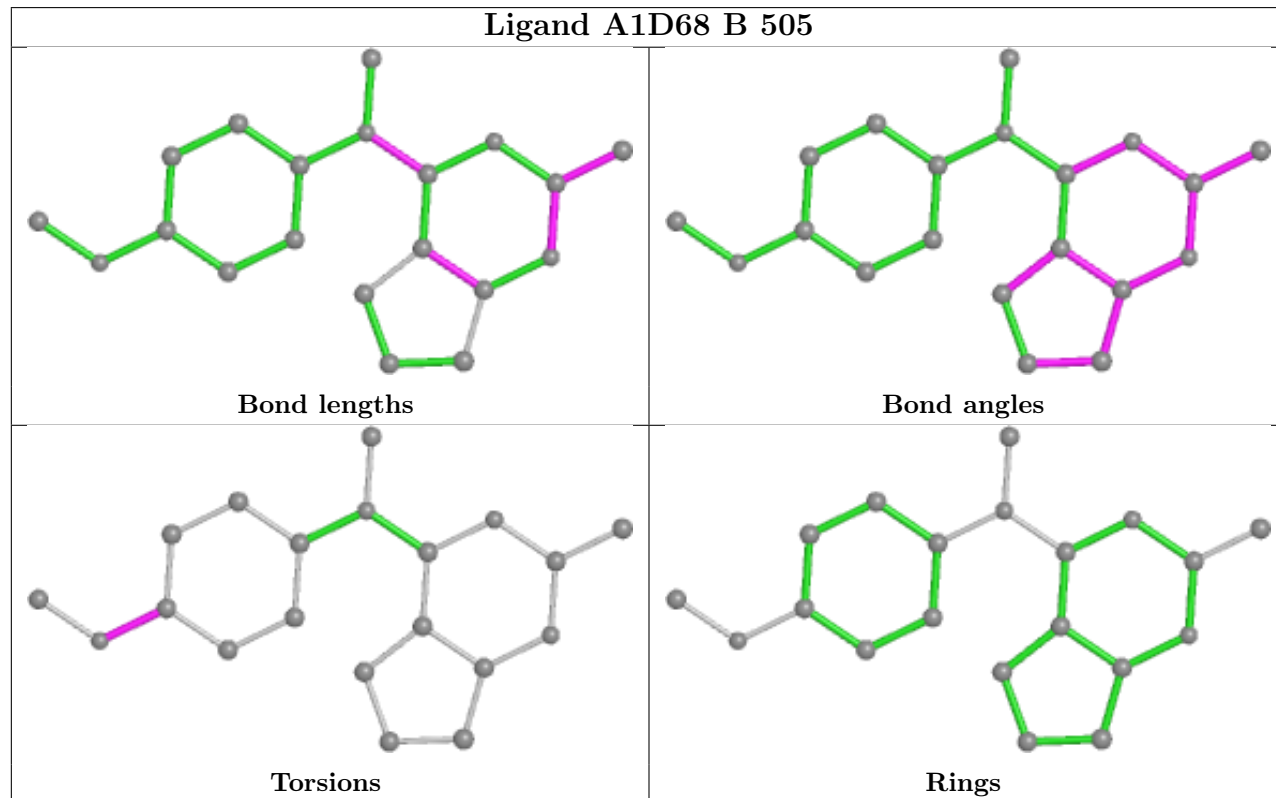
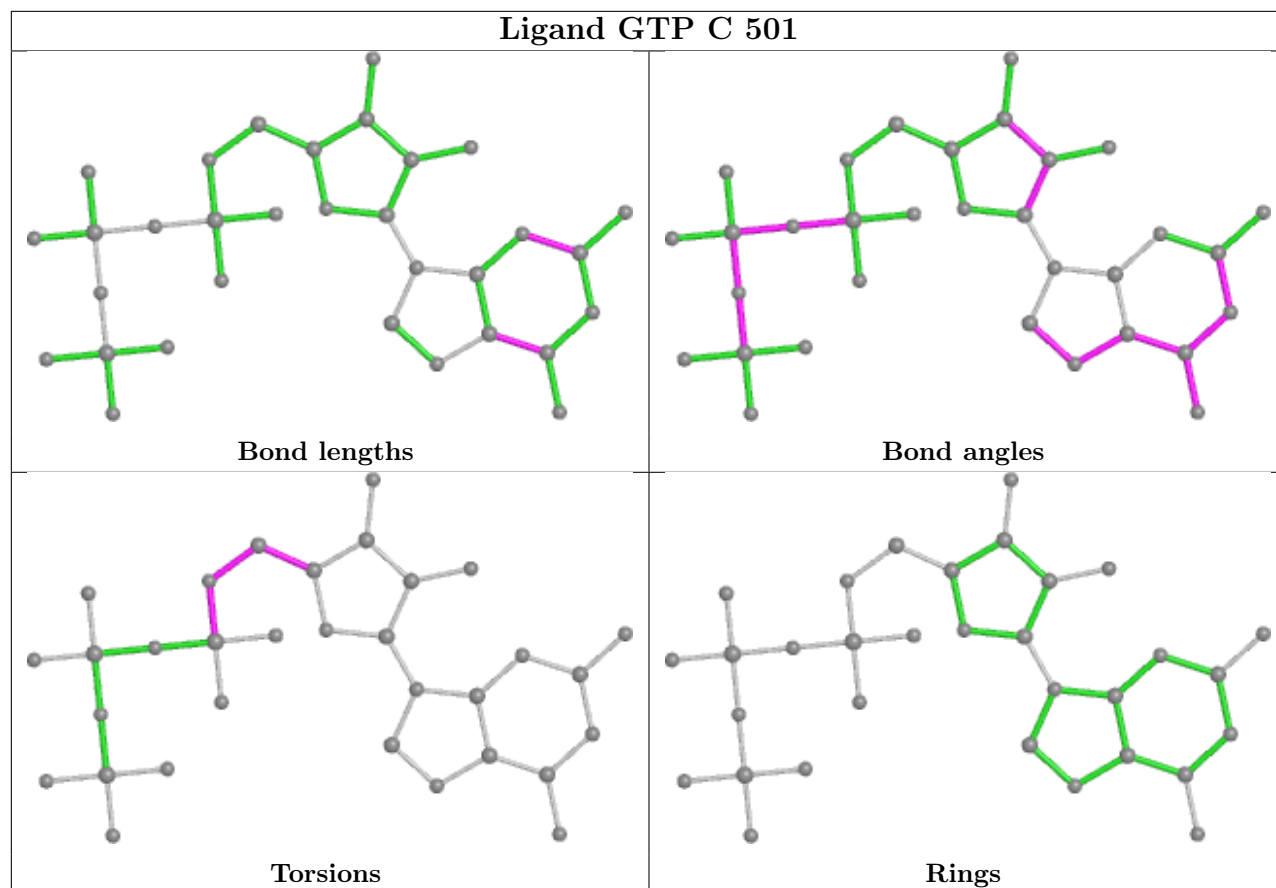
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	437/440 (99%)	0.10	11 (2%) 58 56	37, 53, 79, 96	0
1	C	440/440 (100%)	-0.10	10 (2%) 61 59	30, 43, 66, 110	0
2	B	427/431 (99%)	0.24	24 (5%) 31 30	32, 51, 87, 140	0
2	D	418/431 (96%)	0.69	41 (9%) 14 14	39, 69, 101, 132	0
3	E	117/143 (81%)	0.64	7 (5%) 29 28	44, 64, 100, 113	0
4	F	268/380 (70%)	0.87	41 (15%) 6 6	45, 69, 104, 130	0
All	All	2107/2265 (93%)	0.33	134 (6%) 27 26	30, 57, 93, 140	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	5.1
4	F	225	SER	5.0
4	F	238	CYS	4.9
2	B	428	ALA	4.6
4	F	254	GLY	4.4
3	E	45	PRO	4.3
4	F	246	GLN	4.1
4	F	239	HIS	4.1
2	D	397	TRP	4.1
2	D	92	PHE	4.0
1	C	340	SER	3.9
2	D	1	MET	3.9
1	A	437	VAL	3.8
4	F	89	GLU	3.8
3	E	28	SER	3.7
1	C	1	MET	3.7
2	B	278	SER	3.7
4	F	186	LEU	3.7
4	F	194	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	E	138	GLU	3.6
4	F	256	TYR	3.6
3	E	6	MET	3.6
1	C	357	TYR	3.5
4	F	230	SER	3.5
4	F	380	HIS	3.5
2	D	170	MET	3.5
4	F	46	ARG	3.4
2	B	55	THR	3.4
2	D	284	LEU	3.4
4	F	229	ASN	3.4
4	F	33	ASP	3.3
2	D	181	GLU	3.3
4	F	240	LEU	3.2
1	A	282	TYR	3.2
2	D	72	THR	3.2
2	D	431	ASP	3.2
2	D	42	LEU	3.2
4	F	247	LYS	3.2
2	B	280	GLN	3.1
2	B	57	ASN	3.1
4	F	372	THR	3.1
4	F	306	HIS	3.0
4	F	227	PRO	3.0
2	B	320	ARG	3.0
2	D	94	GLN	3.0
4	F	20	LEU	2.9
4	F	185	TYR	2.9
2	D	56	GLY	2.9
4	F	245	ILE	2.9
2	B	69	GLU	2.9
2	D	53	GLU	2.8
2	B	245	GLN	2.8
2	D	394	PHE	2.7
1	C	440	VAL	2.7
2	B	54	ALA	2.7
1	C	41	THR	2.7
2	B	427	ASP	2.7
4	F	224	SER	2.7
1	C	96	LYS	2.6
2	D	57	ASN	2.6
2	D	301	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	334	GLY	2.6
4	F	74	LYS	2.6
2	B	301	ALA	2.6
3	E	7	GLU	2.6
4	F	259	GLY	2.6
1	A	113	GLU	2.5
1	A	346	TRP	2.5
2	D	356	ILE	2.5
2	D	98	GLY	2.5
2	D	362	LYS	2.5
2	B	281	TYR	2.5
2	B	350	LYS	2.5
4	F	228	TYR	2.5
3	E	59	GLU	2.5
1	A	112	LYS	2.4
2	D	80	PRO	2.4
4	F	73	ARG	2.4
1	C	245	ASP	2.4
2	D	37	HIS	2.4
4	F	13	VAL	2.4
2	D	55	THR	2.4
2	D	41	ASP	2.4
2	D	323	MET	2.4
2	B	282	ARG	2.4
2	B	72	THR	2.4
4	F	242	ASN	2.3
2	B	170	MET	2.3
2	D	101	TRP	2.3
2	D	73	MET	2.3
2	D	285	THR	2.3
2	D	406	MET	2.3
2	B	80	PRO	2.3
1	A	262	TYR	2.3
2	D	26	ASP	2.3
2	D	320	ARG	2.3
2	B	37	HIS	2.2
2	D	81	PHE	2.2
1	A	120	ASP	2.2
2	D	171	PRO	2.2
2	D	125	GLU	2.2
4	F	331	GLU	2.2
4	F	243	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	276	ARG	2.2
2	D	359	ARG	2.2
1	A	46	ASP	2.2
3	E	115	HIS	2.2
4	F	341	LYS	2.2
2	B	277	GLY	2.2
2	D	180	VAL	2.2
4	F	223	THR	2.2
4	F	263	PHE	2.2
2	D	11	GLN	2.2
2	D	245	GLN	2.2
1	A	281	ALA	2.2
4	F	27	TRP	2.1
4	F	379	HIS	2.1
2	B	247	ASN	2.1
2	B	283	ALA	2.1
2	D	65	LEU	2.1
1	C	285	GLN	2.1
2	B	279	GLN	2.1
1	C	163	LYS	2.1
2	D	83	GLN	2.1
4	F	82	LYS	2.0
2	B	291	GLN	2.0
2	D	69	GLU	2.0
2	D	390	ARG	2.0
1	A	45	GLY	2.0
4	F	85	PRO	2.0
2	D	222	TYR	2.0
4	F	98	TYR	2.0
1	C	341	ILE	2.0
1	A	221	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.