



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:10 pm BST

PDB ID : 3A60
Title : Crystal structure of unphosphorylated p70S6K1 (Form I)
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Deposited on : 2009-08-17
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

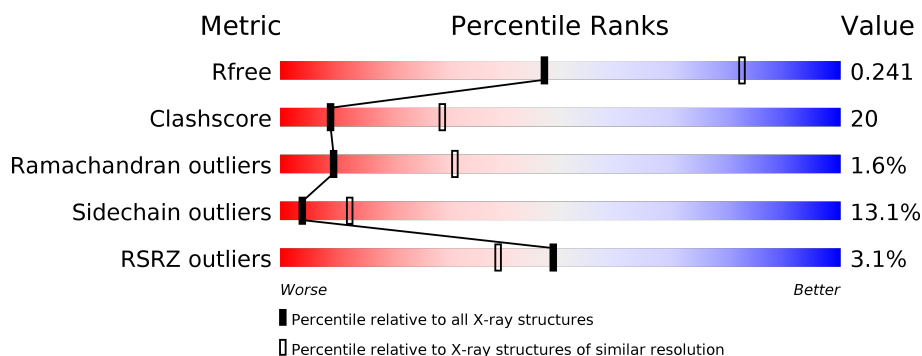
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>28%</div> <div>5%</div> <div>20%</div> </div> </div>
1	B	327	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>25%</div> <div>5%</div> <div>22%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

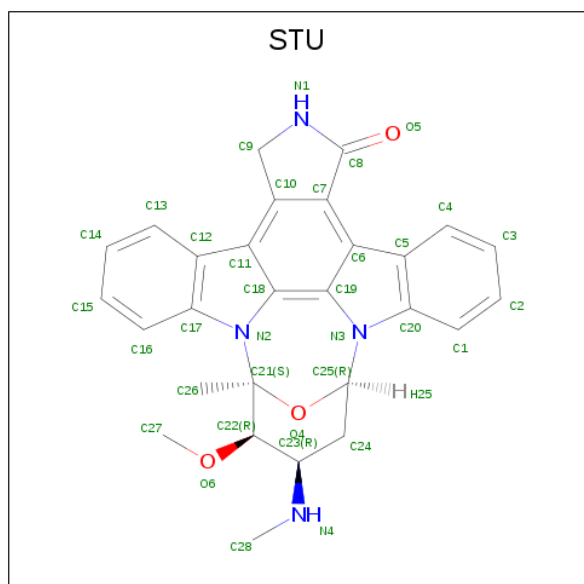
- Molecule 1 is a protein called Ribosomal protein S6 kinase beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2107	1365	365	363	14			
1	B	255	Total	C	N	O	S	0	0	0
			2035	1320	352	349	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLY	-	EXPRESSION TAG	UNP P23443
A	74	SER	-	EXPRESSION TAG	UNP P23443
B	73	GLY	-	EXPRESSION TAG	UNP P23443
B	74	SER	-	EXPRESSION TAG	UNP P23443

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		
2	B	1	Total	C	N	O	0	0
			35	28	4	3		

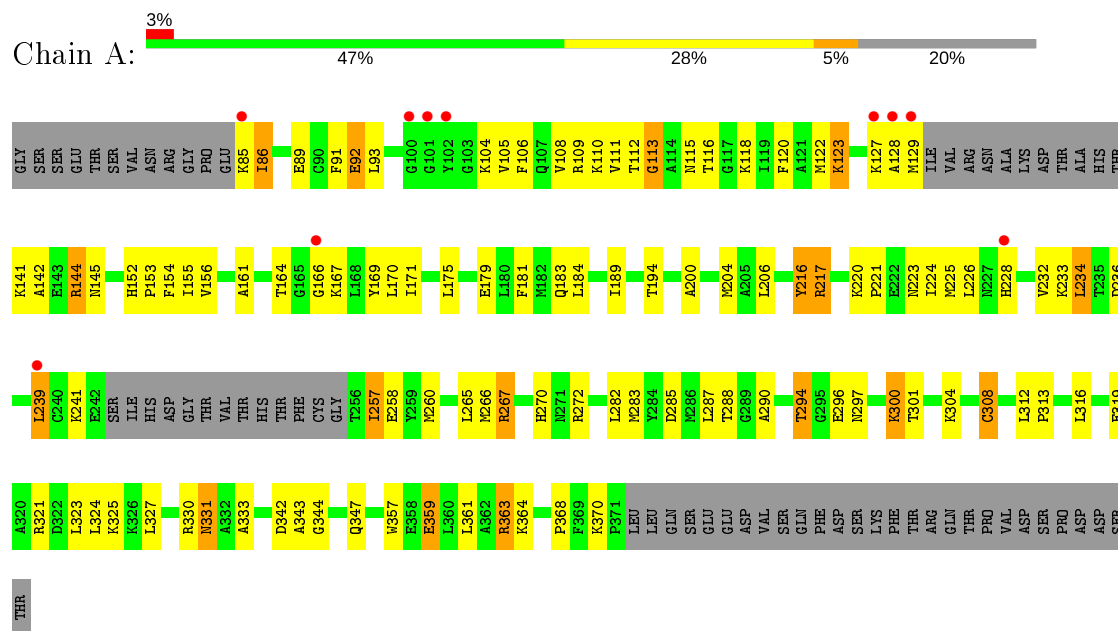
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	3	Total	O	0	0
			3	3		

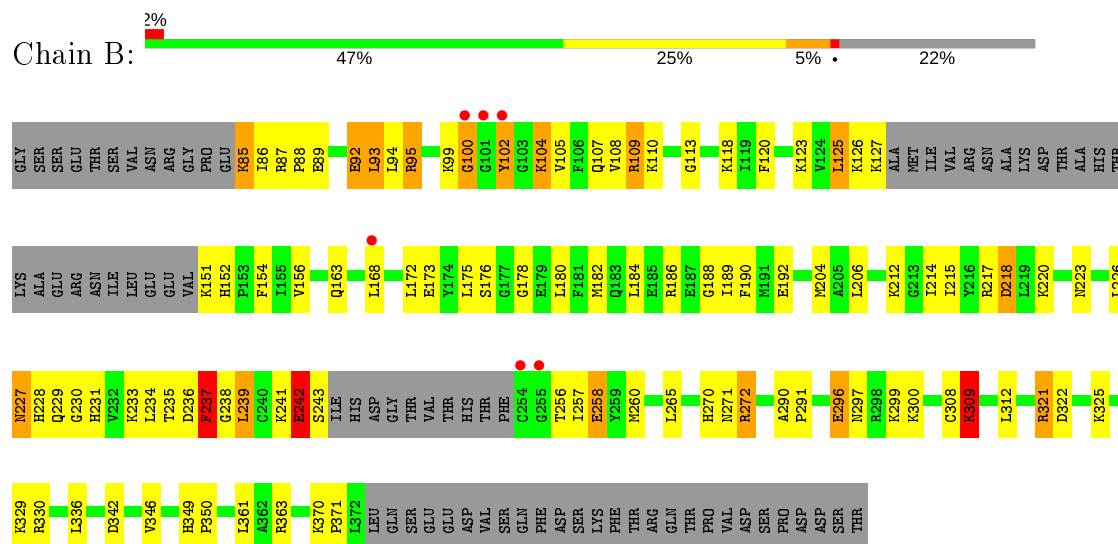
3 Residue-property plots [i](#)

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

• Molecule 1: Ribosomal protein S6 kinase beta-1



• Molecule 1: Ribosomal protein S6 kinase beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.60Å 62.89Å 86.99Å 90.00° 94.32° 90.00°	Depositor
Resolution (Å)	19.81 – 2.80 19.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.1 (19.81-2.80) 97.7 (19.83-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.79Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.210 , 0.268 0.235 , 0.241	Depositor DCC
R_{free} test set	1056 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	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	0.92	EDS
Total number of atoms	4218	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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: STU

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	0.42	0/2153	0.68	0/2891
1	B	0.44	0/2081	0.70	1/2795 (0.0%)
All	All	0.43	0/4234	0.69	1/5686 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	GLU	N-CA-C	6.35	128.14	111.00

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	2107	0	2169	88	0
1	B	2035	0	2093	86	0
2	A	35	0	26	0	0
2	B	35	0	26	2	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
All	All	4218	0	4314	172	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 20.

All (172) 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:B:217:ARG:HD2	1:B:241:LYS:HG2	1.54	0.89
1:B:237:PHE:HD1	1:B:238:GLY:H	1.24	0.86
1:B:102:TYR:H	1:B:102:TYR:HD1	1.24	0.85
1:A:105:VAL:HG22	1:A:123:LYS:HG2	1.61	0.82
1:A:118:LYS:HD2	1:A:120:PHE:CZ	2.16	0.80
1:B:215:ILE:HD11	1:B:241:LYS:HG3	1.62	0.79
1:B:297:ASN:HD21	1:B:299:LYS:HB3	1.48	0.78
1:B:152:HIS:HD2	1:B:154:PHE:H	1.32	0.76
1:B:125:LEU:HD23	1:B:168:LEU:HD22	1.68	0.75
1:B:296:GLU:HG2	1:B:300:LYS:HD3	1.67	0.75
1:A:142:ALA:HA	1:A:239:LEU:HD12	1.67	0.74
1:A:331:ASN:HD21	1:A:333:ALA:HB3	1.51	0.73
1:A:297:ASN:HD21	1:A:300:LYS:HE3	1.53	0.72
1:B:204:MET:HE1	1:B:361:LEU:HB2	1.70	0.72
1:A:347:GLN:HB3	1:A:357:TRP:CZ2	2.25	0.71
1:B:242:GLU:O	1:B:243:SER:HB2	1.91	0.70
1:B:95:ARG:HG2	1:B:107:GLN:HE21	1.55	0.70
1:B:227:ASN:HD21	1:B:231:HIS:H	1.40	0.69
1:B:87:ARG:HB2	1:B:88:PRO:HD2	1.75	0.69
1:A:331:ASN:HD21	1:A:333:ALA:CB	2.07	0.67
1:A:288:THR:HG22	1:A:313:PRO:HG2	1.76	0.67
1:B:156:VAL:HG11	1:B:235:THR:HG22	1.77	0.67
1:A:257:ILE:HD13	1:A:257:ILE:H	1.59	0.66
1:B:296:GLU:H	1:B:296:GLU:CD	1.98	0.66
1:A:85:LYS:HZ1	1:A:86:ILE:HD13	1.60	0.65
1:B:180:LEU:O	1:B:184:LEU:HD13	1.96	0.65
1:B:100:GLY:HA3	2:B:401:STU:C26	2.26	0.65
1:A:92:GLU:OE1	1:A:109:ARG:HD2	1.97	0.65
1:A:85:LYS:NZ	1:A:86:ILE:HD13	2.13	0.64
1:A:223:ASN:HD22	1:A:236:ASP:HB3	1.62	0.63
1:B:227:ASN:ND2	1:B:231:HIS:H	1.95	0.63
1:B:95:ARG:HD3	1:B:107:GLN:NE2	2.15	0.61
1:A:152:HIS:CD2	1:A:154:PHE:H	2.19	0.60
1:B:204:MET:CE	1:B:361:LEU:HD13	2.31	0.60
1:A:241:LYS:HZ1	1:A:270:HIS:HB3	1.67	0.59
1:B:105:VAL:HG22	1:B:123:LYS:HG3	1.83	0.59
1:A:104:LYS:HD2	1:A:106:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LYS:HG3	1:B:86:ILE:H	1.67	0.58
1:B:180:LEU:HD22	1:B:371:PRO:HB3	1.86	0.58
1:A:331:ASN:ND2	1:A:333:ALA:H	2.01	0.57
1:A:297:ASN:ND2	1:A:300:LYS:HE3	2.20	0.57
1:B:189:ILE:HG22	1:B:189:ILE:O	2.05	0.56
1:B:100:GLY:HA3	2:B:401:STU:H261	1.88	0.56
1:B:95:ARG:HD3	1:B:107:GLN:HE22	1.70	0.56
1:A:111:VAL:O	1:A:116:THR:HG23	2.06	0.56
1:A:164:THR:OG1	1:A:167:LYS:HB2	2.06	0.56
1:A:224:ILE:HD11	1:A:232:VAL:HG22	1.87	0.56
1:A:92:GLU:O	1:A:92:GLU:HG3	2.05	0.55
1:A:204:MET:HG2	1:A:347:GLN:HE22	1.72	0.55
1:B:349:HIS:CG	1:B:350:PRO:HD2	2.42	0.54
1:B:290:ALA:HB1	1:B:291:PRO:HD2	1.90	0.54
1:B:218:ASP:OD2	1:B:239:LEU:HD22	2.08	0.54
1:B:102:TYR:N	1:B:102:TYR:CD1	2.63	0.54
1:A:216:TYR:O	1:A:217:ARG:HB2	2.08	0.54
1:B:156:VAL:HG12	1:B:234:LEU:O	2.08	0.54
1:B:212:LYS:O	1:B:214:ILE:HD12	2.08	0.53
1:A:224:ILE:CD1	1:A:232:VAL:HG13	2.38	0.53
1:B:104:LYS:HE2	1:B:104:LYS:H	1.73	0.53
1:A:152:HIS:HD2	1:A:154:PHE:H	1.57	0.53
1:A:93:LEU:N	1:A:93:LEU:CD1	2.72	0.53
1:B:308:CYS:SG	1:B:330:ARG:HD3	2.49	0.53
1:A:363:ARG:HG3	1:A:363:ARG:NH1	2.24	0.52
1:B:227:ASN:ND2	1:B:230:GLY:H	2.07	0.52
1:A:225:MET:O	1:A:226:LEU:HD23	2.09	0.52
1:A:189:ILE:HB	1:A:287:LEU:O	2.09	0.52
1:A:330:ARG:NH2	1:B:330:ARG:NH2	2.57	0.52
1:A:343:ALA:O	1:A:347:GLN:HG3	2.10	0.51
1:B:176:SER:C	1:B:178:GLY:H	2.14	0.51
1:B:152:HIS:CD2	1:B:154:PHE:H	2.20	0.51
1:A:204:MET:HG2	1:A:347:GLN:NE2	2.25	0.51
1:A:156:VAL:HG13	1:A:156:VAL:O	2.11	0.51
1:A:181:PHE:CG	1:A:221:PRO:HB2	2.46	0.51
1:B:227:ASN:HD22	1:B:227:ASN:H	1.58	0.51
1:A:93:LEU:HD12	1:A:93:LEU:N	2.26	0.51
1:B:156:VAL:HG23	1:B:173:GLU:HG2	1.92	0.51
1:A:241:LYS:NZ	1:A:270:HIS:HB3	2.26	0.51
1:A:257:ILE:CD1	1:A:257:ILE:H	2.23	0.51
1:B:88:PRO:HG2	1:B:89:GLU:OE1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ALA:HA	1:A:169:TYR:O	2.11	0.50
1:A:144:ARG:HG3	1:A:170:LEU:HD11	1.93	0.50
1:A:283:MET:HG2	1:A:324:LEU:HD21	1.93	0.50
1:A:285:ASP:HA	1:A:290:ALA:O	2.10	0.50
1:A:288:THR:CG2	1:A:313:PRO:HG2	2.41	0.50
1:B:204:MET:HE2	1:B:361:LEU:HD13	1.94	0.50
1:B:104:LYS:NZ	1:B:126:LYS:NZ	2.60	0.49
1:B:226:LEU:HA	1:B:231:HIS:O	2.12	0.49
1:A:92:GLU:HG3	1:A:109:ARG:HB3	1.95	0.48
1:A:175:LEU:HD22	1:A:233:LYS:HG3	1.96	0.48
1:A:181:PHE:CD2	1:A:184:LEU:HD22	2.48	0.48
1:A:312:LEU:HD11	1:A:325:LYS:HG3	1.95	0.48
1:B:260:MET:HG3	1:B:265:LEU:HD21	1.95	0.48
1:A:312:LEU:HD11	1:A:325:LYS:CG	2.44	0.48
1:A:118:LYS:HD2	1:A:120:PHE:CE1	2.49	0.47
1:B:227:ASN:HD22	1:B:227:ASN:N	2.09	0.47
1:A:194:THR:HG23	1:A:368:PRO:HG3	1.95	0.47
1:A:363:ARG:HH11	1:A:363:ARG:HG3	1.79	0.47
1:B:217:ARG:NE	1:B:241:LYS:HD3	2.29	0.47
1:B:215:ILE:HD11	1:B:241:LYS:CG	2.40	0.47
1:B:127:LYS:HB3	1:B:127:LYS:NZ	2.29	0.47
1:B:272:ARG:HD2	1:B:342:ASP:OD1	2.15	0.47
1:A:127:LYS:HB2	1:A:166:GLY:C	2.35	0.46
1:B:241:LYS:NZ	1:B:270:HIS:ND1	2.63	0.46
1:A:89:GLU:C	1:A:91:PHE:H	2.19	0.46
1:B:110:LYS:NZ	1:B:113:GLY:HA3	2.31	0.46
1:B:118:LYS:HD3	1:B:120:PHE:CZ	2.49	0.46
1:A:200:ALA:HB1	1:A:357:TRP:CZ3	2.51	0.46
1:B:228:HIS:CE1	1:B:229:GLN:HE21	2.33	0.46
1:B:127:LYS:HZ3	1:B:127:LYS:HB3	1.80	0.46
1:A:108:VAL:HG23	1:A:120:PHE:HB2	1.98	0.46
1:A:220:LYS:HB3	1:A:221:PRO:HD2	1.97	0.46
1:B:227:ASN:HD22	1:B:227:ASN:C	2.19	0.46
1:A:92:GLU:CG	1:A:109:ARG:HB3	2.46	0.46
1:B:93:LEU:H	1:B:93:LEU:HD22	1.81	0.46
1:A:155:ILE:HG12	1:A:234:LEU:HB2	1.98	0.46
1:A:308:CYS:SG	1:A:330:ARG:HB2	2.56	0.45
1:B:227:ASN:C	1:B:227:ASN:ND2	2.69	0.45
1:B:336:LEU:HG	1:B:346:VAL:HG22	1.98	0.45
1:A:128:ALA:O	1:A:129:MET:HG2	2.16	0.45
1:B:188:GLY:C	1:B:190:PHE:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:HIS:CD2	1:B:229:GLN:HG3	2.52	0.45
1:B:180:LEU:HB3	1:B:226:LEU:HD12	1.99	0.45
1:A:316:LEU:HB2	1:A:321:ARG:HG3	1.99	0.45
1:B:89:GLU:OE1	1:B:89:GLU:N	2.51	0.44
1:A:241:LYS:HB3	1:A:241:LYS:HE3	1.61	0.44
1:A:181:PHE:CE1	1:A:224:ILE:HG21	2.53	0.44
1:A:331:ASN:ND2	1:A:331:ASN:C	2.70	0.44
1:A:257:ILE:HD13	1:A:257:ILE:N	2.31	0.44
1:A:257:ILE:HA	1:A:260:MET:HG3	1.99	0.44
1:A:294:THR:HA	1:A:301:THR:HG23	2.00	0.43
1:B:296:GLU:N	1:B:296:GLU:OE2	2.51	0.43
1:B:94:LEU:HD11	1:B:109:ARG:HG3	2.00	0.43
1:B:204:MET:HE1	1:B:361:LEU:HD13	2.00	0.43
1:A:194:THR:HG23	1:A:368:PRO:CG	2.48	0.43
1:B:227:ASN:O	1:B:230:GLY:N	2.50	0.43
1:A:181:PHE:HD2	1:A:184:LEU:HD22	1.83	0.43
1:A:323:LEU:HG	1:A:327:LEU:CD1	2.48	0.43
1:A:266:MET:O	1:A:267:ARG:HB2	2.19	0.43
1:A:179:GLU:HG2	1:A:225:MET:CE	2.49	0.43
1:B:99:LYS:O	1:B:100:GLY:C	2.56	0.43
1:B:92:GLU:CG	1:B:109:ARG:HB2	2.49	0.43
1:B:217:ARG:CD	1:B:241:LYS:HG2	2.39	0.42
1:B:308:CYS:HB3	1:B:309:LYS:H	1.49	0.42
1:A:127:LYS:HE3	1:A:167:LYS:N	2.34	0.42
1:A:110:LYS:HE3	1:A:113:GLY:HA3	2.00	0.42
1:A:342:ASP:C	1:A:344:GLY:N	2.72	0.42
1:B:227:ASN:H	1:B:227:ASN:ND2	2.17	0.42
1:B:271:ASN:HB2	3:B:5:HOH:O	2.18	0.42
1:A:142:ALA:H	1:A:145:ASN:HB2	1.84	0.42
1:A:258:GLU:HG2	1:B:291:PRO:HG3	2.01	0.42
1:A:359:GLU:HG3	1:A:364:LYS:HB2	2.00	0.42
1:B:256:THR:HB	1:B:258:GLU:OE2	2.19	0.42
1:A:224:ILE:HG23	1:A:224:ILE:O	2.19	0.42
1:A:323:LEU:HG	1:A:327:LEU:HD12	2.02	0.42
1:B:118:LYS:HB3	1:B:120:PHE:CE1	2.54	0.42
1:B:312:LEU:HD11	1:B:325:LYS:HG3	2.02	0.41
1:A:221:PRO:C	1:A:224:ILE:HG22	2.40	0.41
1:A:152:HIS:CG	1:A:153:PRO:HD2	2.56	0.41
1:A:331:ASN:ND2	1:A:333:ALA:HB3	2.26	0.41
1:A:316:LEU:CB	1:A:321:ARG:HG3	2.49	0.41
1:B:118:LYS:HB3	1:B:120:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HB3	1:B:226:LEU:O	2.20	0.41
1:B:297:ASN:ND2	1:B:299:LYS:HB3	2.27	0.41
1:B:87:ARG:CB	1:B:88:PRO:HD2	2.49	0.41
1:B:241:LYS:HZ2	1:B:270:HIS:CG	2.38	0.41
1:B:92:GLU:O	1:B:92:GLU:HG3	2.20	0.41
1:A:111:VAL:O	1:A:116:THR:CG2	2.68	0.41
1:B:321:ARG:HG3	1:B:322:ASP:N	2.36	0.41
1:B:182:MET:O	1:B:186:ARG:HG3	2.21	0.41
1:A:272:ARG:HD2	1:A:342:ASP:OD1	2.20	0.41
1:A:363:ARG:CG	1:A:363:ARG:HH11	2.34	0.40
1:B:241:LYS:HZ2	1:B:270:HIS:CB	2.34	0.40
1:A:122:MET:HG3	1:A:171:ILE:HD13	2.03	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	257/327 (79%)	227 (88%)	26 (10%)	4 (2%)	9	31
1	B	249/327 (76%)	221 (89%)	24 (10%)	4 (2%)	9	31
All	All	506/654 (77%)	448 (88%)	50 (10%)	8 (2%)	9	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	B	237	PHE
1	A	112	THR
1	A	113	GLY
1	B	100	GLY
1	B	218	ASP

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Mol	Chain	Res	Type
1	B	309	LYS
1	A	86	ILE

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	221/279 (79%)	195 (88%)	26 (12%)	5	16
1	B	214/279 (77%)	183 (86%)	31 (14%)	3	9
All	All	435/558 (78%)	378 (87%)	57 (13%)	4	12

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	GLU
1	A	115	ASN
1	A	123	LYS
1	A	141	LYS
1	A	144	ARG
1	A	183	GLN
1	A	206	LEU
1	A	216	TYR
1	A	217	ARG
1	A	228	HIS
1	A	234	LEU
1	A	257	ILE
1	A	265	LEU
1	A	267	ARG
1	A	282	LEU
1	A	294	THR
1	A	296	GLU
1	A	300	LYS
1	A	304	LYS
1	A	308	CYS
1	A	319	GLU

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Mol	Chain	Res	Type
1	A	331	ASN
1	A	359	GLU
1	A	361	LEU
1	A	363	ARG
1	A	370	LYS
1	B	85	LYS
1	B	92	GLU
1	B	93	LEU
1	B	95	ARG
1	B	102	TYR
1	B	104	LYS
1	B	108	VAL
1	B	109	ARG
1	B	125	LEU
1	B	151	LYS
1	B	163	GLN
1	B	172	LEU
1	B	192	GLU
1	B	206	LEU
1	B	220	LYS
1	B	223	ASN
1	B	227	ASN
1	B	233	LYS
1	B	236	ASP
1	B	237	PHE
1	B	239	LEU
1	B	242	GLU
1	B	257	ILE
1	B	258	GLU
1	B	272	ARG
1	B	296	GLU
1	B	309	LYS
1	B	321	ARG
1	B	329	LYS
1	B	363	ARG
1	B	370	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	152	HIS
1	A	270	HIS
1	A	331	ASN
1	B	107	GLN
1	B	152	HIS
1	B	227	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	STU	B	401	-	30,42,42	2.73	19 (63%)	31,68,68	1.90	9 (29%)
2	STU	A	400	-	30,42,42	2.70	19 (63%)	31,68,68	1.94	9 (29%)

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
2	STU	B	401	-	-	2/4/42/42	-
2	STU	A	400	-	-	1/4/42/42	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	STU	C22-C23	4.54	1.57	1.52
2	A	400	STU	C7-C6	4.47	1.50	1.43
2	A	400	STU	C6-C19	4.41	1.48	1.42
2	B	401	STU	C7-C6	4.31	1.50	1.43
2	B	401	STU	C6-C19	4.31	1.48	1.42
2	A	400	STU	C24-C25	4.29	1.60	1.51
2	A	400	STU	C5-C20	3.90	1.47	1.41
2	B	401	STU	C14-C15	3.76	1.48	1.38
2	B	401	STU	C14-C13	3.75	1.45	1.36
2	B	401	STU	C11-C18	3.61	1.47	1.42
2	B	401	STU	C24-C25	3.60	1.58	1.51
2	A	400	STU	C14-C15	3.54	1.47	1.38
2	A	400	STU	C14-C13	3.46	1.44	1.36
2	A	400	STU	C24-C23	3.40	1.58	1.53
2	B	401	STU	C12-C17	3.38	1.46	1.41
2	B	401	STU	C5-C20	3.34	1.46	1.41
2	A	400	STU	C8-N1	-3.33	1.32	1.35
2	A	400	STU	C3-C2	3.32	1.46	1.38
2	A	400	STU	C12-C17	3.23	1.46	1.41
2	A	400	STU	C2-C1	3.21	1.44	1.36
2	B	401	STU	C3-C2	3.20	1.46	1.38
2	B	401	STU	C10-C11	3.13	1.47	1.42
2	A	400	STU	C22-C23	3.11	1.56	1.52
2	B	401	STU	C2-C1	3.00	1.43	1.36
2	B	401	STU	C24-C23	2.97	1.57	1.53
2	A	400	STU	C11-C18	2.94	1.46	1.42
2	A	400	STU	C3-C4	2.74	1.42	1.36
2	B	401	STU	O6-C22	2.62	1.47	1.42
2	B	401	STU	C1-C20	2.50	1.46	1.41
2	A	400	STU	C15-C16	2.44	1.42	1.36
2	A	400	STU	C1-C20	2.38	1.45	1.41
2	A	400	STU	C26-C21	2.35	1.54	1.51
2	B	401	STU	C15-C16	2.28	1.41	1.36
2	B	401	STU	C3-C4	2.24	1.41	1.36
2	B	401	STU	O4-C25	-2.23	1.40	1.43
2	B	401	STU	C8-N1	-2.15	1.33	1.35
2	A	400	STU	O6-C22	2.10	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	STU	C10-C11	2.02	1.46	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	STU	C9-N1-C8	4.86	118.53	113.85
2	A	400	STU	O4-C25-C24	-4.55	105.75	112.31
2	B	401	STU	C9-N1-C8	4.49	118.17	113.85
2	B	401	STU	O4-C25-C24	-4.17	106.28	112.31
2	B	401	STU	C7-C8-N1	-3.45	102.88	106.37
2	A	400	STU	C7-C8-N1	-3.29	103.04	106.37
2	B	401	STU	C24-C23-N4	-3.09	105.32	112.17
2	A	400	STU	C10-C9-N1	-3.08	98.63	101.76
2	A	400	STU	C15-C14-C13	-2.82	116.48	120.44
2	B	401	STU	C11-C12-C17	2.76	109.39	106.37
2	B	401	STU	C10-C9-N1	-2.76	98.96	101.76
2	A	400	STU	C24-C23-N4	-2.73	106.10	112.17
2	A	400	STU	C11-C12-C17	2.67	109.28	106.37
2	B	401	STU	C15-C14-C13	-2.64	116.74	120.44
2	A	400	STU	C1-C20-N3	-2.53	129.22	132.25
2	B	401	STU	O5-C8-N1	2.43	128.11	125.27
2	B	401	STU	C1-C20-N3	-2.23	129.58	132.25
2	A	400	STU	O5-C8-N1	2.08	127.70	125.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	STU	C22-C23-N4-C28
2	B	401	STU	C24-C23-N4-C28
2	A	400	STU	C22-C23-N4-C28

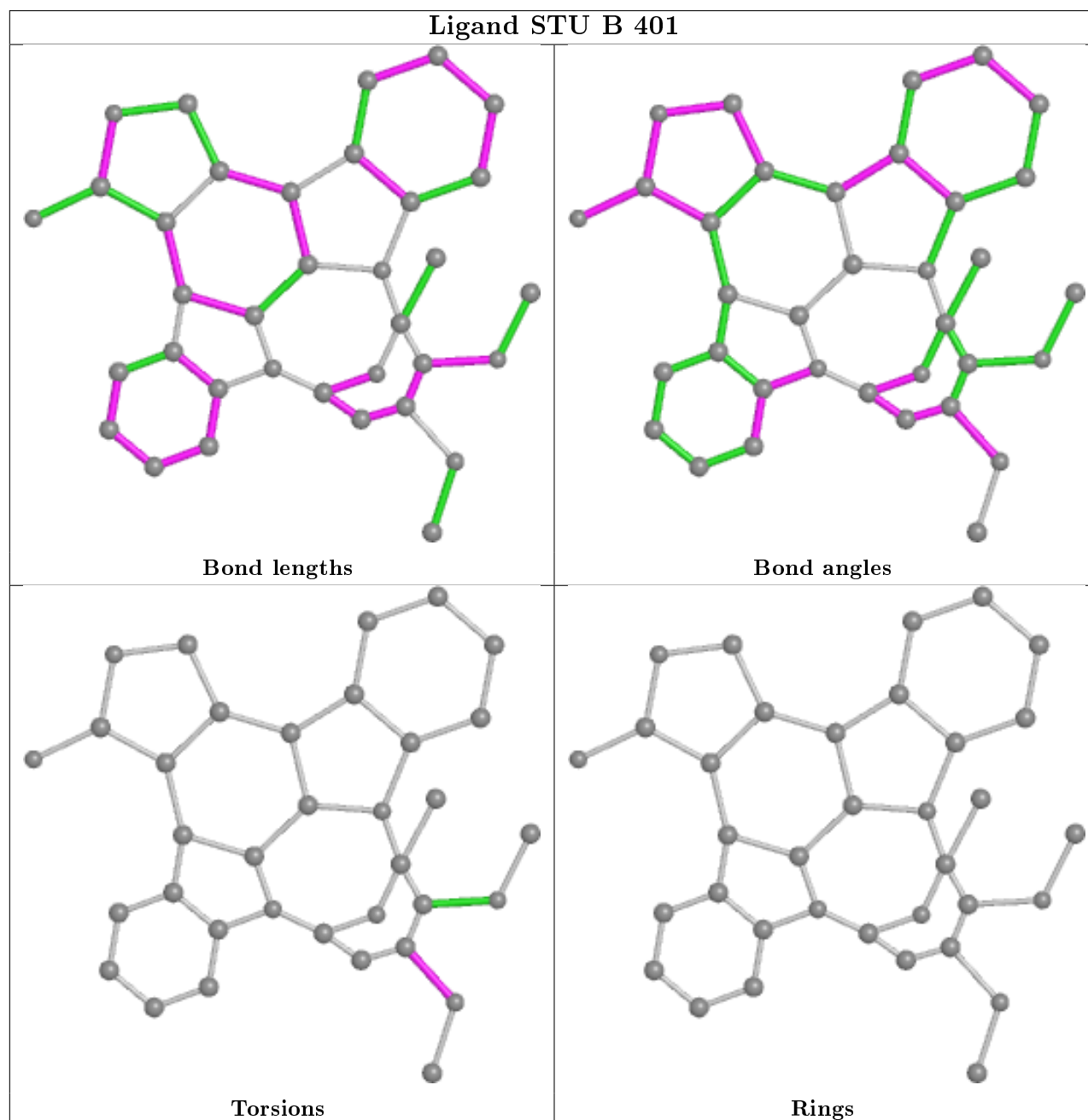
There are no ring outliers.

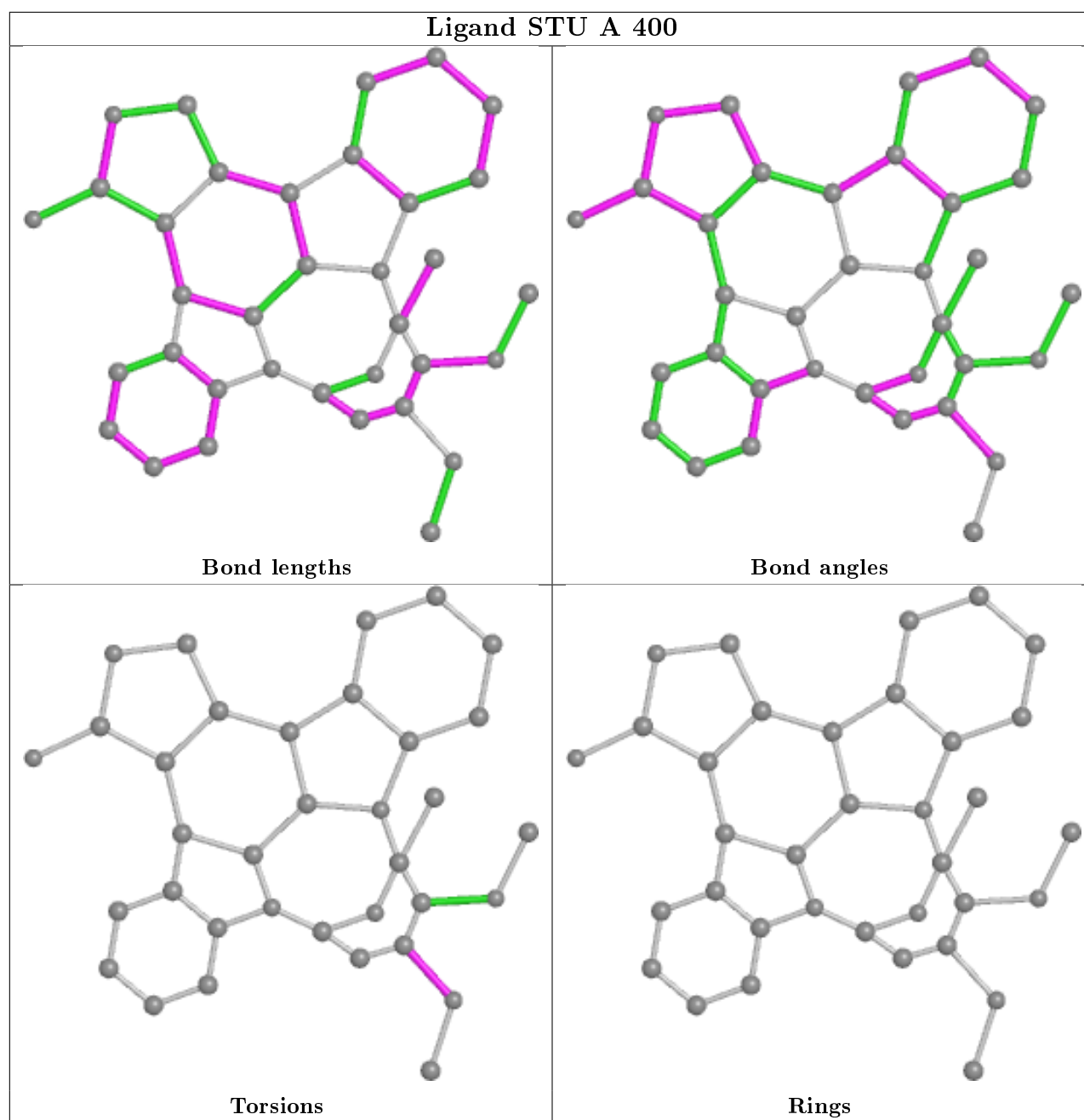
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	STU	2	0

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

also be included. For torsion angles, if less 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/327 (80%)	0.01	10 (3%) 40 30	22, 51, 80, 97	0
1	B	255/327 (77%)	-0.05	6 (2%) 59 49	24, 48, 77, 89	0
All	All	518/654 (79%)	-0.02	16 (3%) 49 39	22, 50, 78, 97	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	254	CYS	5.6
1	A	129	MET	4.3
1	A	166	GLY	4.3
1	B	255	GLY	4.2
1	A	102	TYR	3.6
1	A	228	HIS	3.6
1	A	101	GLY	3.3
1	B	100	GLY	2.7
1	B	102	TYR	2.6
1	B	101	GLY	2.5
1	A	128	ALA	2.5
1	B	168	LEU	2.5
1	A	127	LYS	2.4
1	A	239	LEU	2.3
1	A	100	GLY	2.2
1	A	85	LYS	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

There are no carbohydrates in this entry.

6.4 Ligands

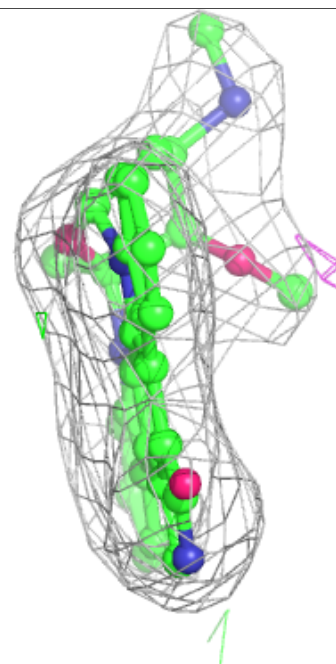
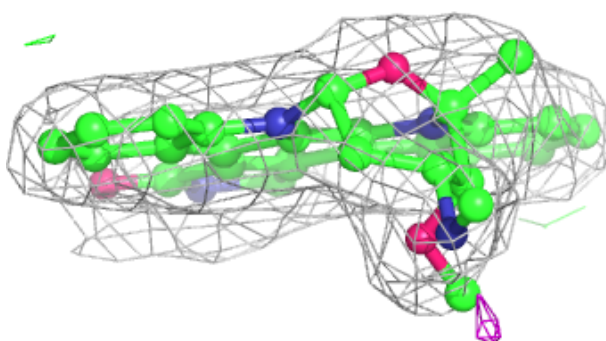
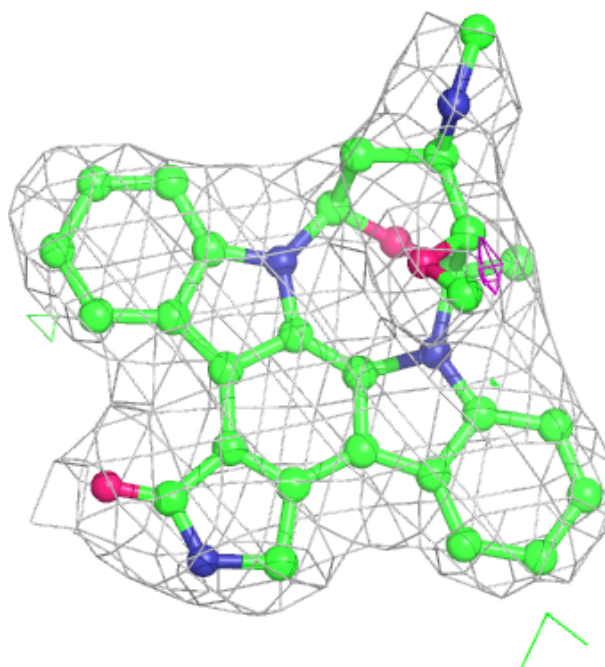
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	STU	A	400	35/35	0.94	0.16	33,38,41,46	0
2	STU	B	401	35/35	0.95	0.21	46,48,55,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

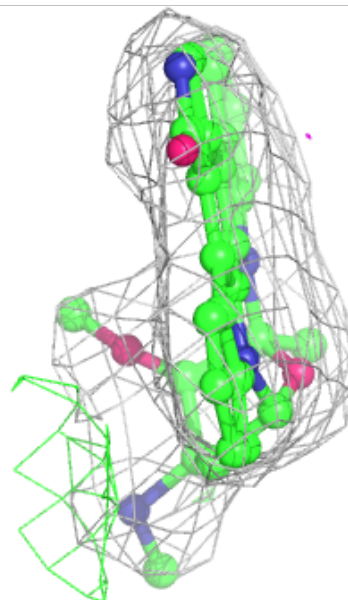
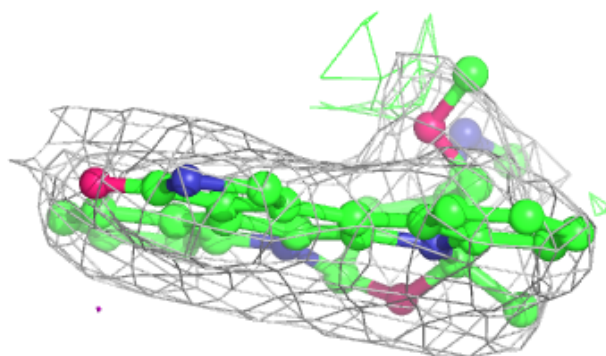
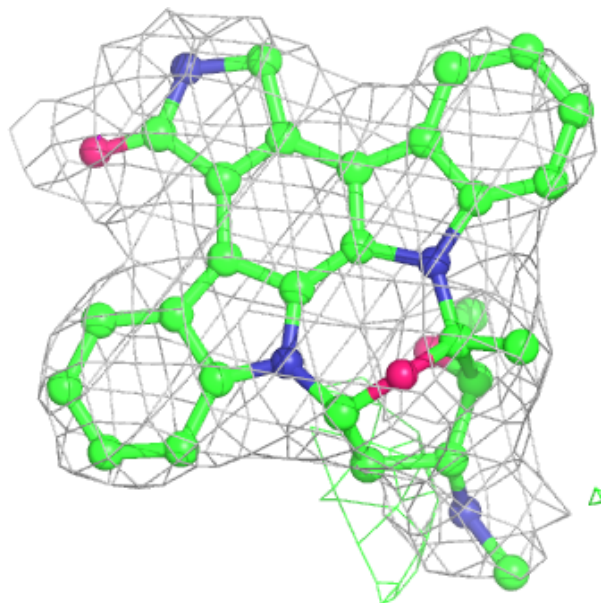
Electron density around STU A 400:

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



Electron density around STU B 401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.