



## Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 02:01 PM JST

PDB ID : 8JY6 / pdb\_00008jy6  
EMDB ID : EMD-36721  
Title : Structure of TbAQP2 in complex with anti-trypanosomatid drug melarsoprol  
Authors : Chen, W.; Wang, C.  
Deposited on : 2023-07-03  
Resolution : 2.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

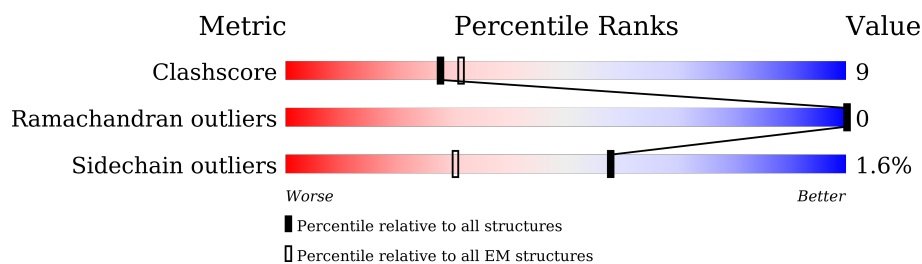
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	343	<div> <div>55%</div> <div>16%</div> <div>29%</div> </div>
1	B	343	<div> <div>55%</div> <div>16%</div> <div>29%</div> </div>
1	C	343	<div> <div>55%</div> <div>15%</div> <div>29%</div> </div>
1	D	343	<div> <div>55%</div> <div>15%</div> <div>29%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7440 atoms, of which 60 are hydrogens and 0 are deuteriums.

In the tables below, 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 Aquaglyceroporin 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	242	Total	C	N	O	S	0	0
			1823	1228	279	308	8		
1	B	242	Total	C	N	O	S	0	0
			1823	1228	279	308	8		
1	C	242	Total	C	N	O	S	0	0
			1823	1228	279	308	8		
1	D	242	Total	C	N	O	S	0	0
			1823	1228	279	308	8		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	SER	-	expression tag	UNP Q6ZXT3
A	314	ASN	-	expression tag	UNP Q6ZXT3
A	315	SER	-	expression tag	UNP Q6ZXT3
A	316	TRP	-	expression tag	UNP Q6ZXT3
A	317	SER	-	expression tag	UNP Q6ZXT3
A	318	HIS	-	expression tag	UNP Q6ZXT3
A	319	PRO	-	expression tag	UNP Q6ZXT3
A	320	GLN	-	expression tag	UNP Q6ZXT3
A	321	PHE	-	expression tag	UNP Q6ZXT3
A	322	GLU	-	expression tag	UNP Q6ZXT3
A	323	LYS	-	expression tag	UNP Q6ZXT3
A	324	GLY	-	expression tag	UNP Q6ZXT3
A	325	GLY	-	expression tag	UNP Q6ZXT3
A	326	GLY	-	expression tag	UNP Q6ZXT3
A	327	SER	-	expression tag	UNP Q6ZXT3
A	328	GLY	-	expression tag	UNP Q6ZXT3
A	329	GLY	-	expression tag	UNP Q6ZXT3
A	330	GLY	-	expression tag	UNP Q6ZXT3
A	331	SER	-	expression tag	UNP Q6ZXT3
A	332	GLY	-	expression tag	UNP Q6ZXT3
A	333	GLY	-	expression tag	UNP Q6ZXT3
A	334	SER	-	expression tag	UNP Q6ZXT3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ALA	-	expression tag	UNP Q6ZXT3
A	336	TRP	-	expression tag	UNP Q6ZXT3
A	337	SER	-	expression tag	UNP Q6ZXT3
A	338	HIS	-	expression tag	UNP Q6ZXT3
A	339	PRO	-	expression tag	UNP Q6ZXT3
A	340	GLN	-	expression tag	UNP Q6ZXT3
A	341	PHE	-	expression tag	UNP Q6ZXT3
A	342	GLU	-	expression tag	UNP Q6ZXT3
A	343	LYS	-	expression tag	UNP Q6ZXT3
B	313	SER	-	expression tag	UNP Q6ZXT3
B	314	ASN	-	expression tag	UNP Q6ZXT3
B	315	SER	-	expression tag	UNP Q6ZXT3
B	316	TRP	-	expression tag	UNP Q6ZXT3
B	317	SER	-	expression tag	UNP Q6ZXT3
B	318	HIS	-	expression tag	UNP Q6ZXT3
B	319	PRO	-	expression tag	UNP Q6ZXT3
B	320	GLN	-	expression tag	UNP Q6ZXT3
B	321	PHE	-	expression tag	UNP Q6ZXT3
B	322	GLU	-	expression tag	UNP Q6ZXT3
B	323	LYS	-	expression tag	UNP Q6ZXT3
B	324	GLY	-	expression tag	UNP Q6ZXT3
B	325	GLY	-	expression tag	UNP Q6ZXT3
B	326	GLY	-	expression tag	UNP Q6ZXT3
B	327	SER	-	expression tag	UNP Q6ZXT3
B	328	GLY	-	expression tag	UNP Q6ZXT3
B	329	GLY	-	expression tag	UNP Q6ZXT3
B	330	GLY	-	expression tag	UNP Q6ZXT3
B	331	SER	-	expression tag	UNP Q6ZXT3
B	332	GLY	-	expression tag	UNP Q6ZXT3
B	333	GLY	-	expression tag	UNP Q6ZXT3
B	334	SER	-	expression tag	UNP Q6ZXT3
B	335	ALA	-	expression tag	UNP Q6ZXT3
B	336	TRP	-	expression tag	UNP Q6ZXT3
B	337	SER	-	expression tag	UNP Q6ZXT3
B	338	HIS	-	expression tag	UNP Q6ZXT3
B	339	PRO	-	expression tag	UNP Q6ZXT3
B	340	GLN	-	expression tag	UNP Q6ZXT3
B	341	PHE	-	expression tag	UNP Q6ZXT3
B	342	GLU	-	expression tag	UNP Q6ZXT3
B	343	LYS	-	expression tag	UNP Q6ZXT3
C	313	SER	-	expression tag	UNP Q6ZXT3
C	314	ASN	-	expression tag	UNP Q6ZXT3

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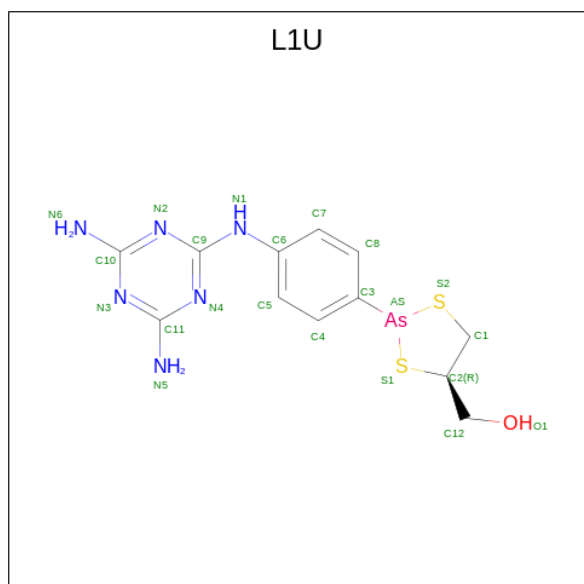
Chain	Residue	Modelled	Actual	Comment	Reference
C	315	SER	-	expression tag	UNP Q6ZXT3
C	316	TRP	-	expression tag	UNP Q6ZXT3
C	317	SER	-	expression tag	UNP Q6ZXT3
C	318	HIS	-	expression tag	UNP Q6ZXT3
C	319	PRO	-	expression tag	UNP Q6ZXT3
C	320	GLN	-	expression tag	UNP Q6ZXT3
C	321	PHE	-	expression tag	UNP Q6ZXT3
C	322	GLU	-	expression tag	UNP Q6ZXT3
C	323	LYS	-	expression tag	UNP Q6ZXT3
C	324	GLY	-	expression tag	UNP Q6ZXT3
C	325	GLY	-	expression tag	UNP Q6ZXT3
C	326	GLY	-	expression tag	UNP Q6ZXT3
C	327	SER	-	expression tag	UNP Q6ZXT3
C	328	GLY	-	expression tag	UNP Q6ZXT3
C	329	GLY	-	expression tag	UNP Q6ZXT3
C	330	GLY	-	expression tag	UNP Q6ZXT3
C	331	SER	-	expression tag	UNP Q6ZXT3
C	332	GLY	-	expression tag	UNP Q6ZXT3
C	333	GLY	-	expression tag	UNP Q6ZXT3
C	334	SER	-	expression tag	UNP Q6ZXT3
C	335	ALA	-	expression tag	UNP Q6ZXT3
C	336	TRP	-	expression tag	UNP Q6ZXT3
C	337	SER	-	expression tag	UNP Q6ZXT3
C	338	HIS	-	expression tag	UNP Q6ZXT3
C	339	PRO	-	expression tag	UNP Q6ZXT3
C	340	GLN	-	expression tag	UNP Q6ZXT3
C	341	PHE	-	expression tag	UNP Q6ZXT3
C	342	GLU	-	expression tag	UNP Q6ZXT3
C	343	LYS	-	expression tag	UNP Q6ZXT3
D	313	SER	-	expression tag	UNP Q6ZXT3
D	314	ASN	-	expression tag	UNP Q6ZXT3
D	315	SER	-	expression tag	UNP Q6ZXT3
D	316	TRP	-	expression tag	UNP Q6ZXT3
D	317	SER	-	expression tag	UNP Q6ZXT3
D	318	HIS	-	expression tag	UNP Q6ZXT3
D	319	PRO	-	expression tag	UNP Q6ZXT3
D	320	GLN	-	expression tag	UNP Q6ZXT3
D	321	PHE	-	expression tag	UNP Q6ZXT3
D	322	GLU	-	expression tag	UNP Q6ZXT3
D	323	LYS	-	expression tag	UNP Q6ZXT3
D	324	GLY	-	expression tag	UNP Q6ZXT3
D	325	GLY	-	expression tag	UNP Q6ZXT3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	326	GLY	-	expression tag	UNP Q6ZXT3
D	327	SER	-	expression tag	UNP Q6ZXT3
D	328	GLY	-	expression tag	UNP Q6ZXT3
D	329	GLY	-	expression tag	UNP Q6ZXT3
D	330	GLY	-	expression tag	UNP Q6ZXT3
D	331	SER	-	expression tag	UNP Q6ZXT3
D	332	GLY	-	expression tag	UNP Q6ZXT3
D	333	GLY	-	expression tag	UNP Q6ZXT3
D	334	SER	-	expression tag	UNP Q6ZXT3
D	335	ALA	-	expression tag	UNP Q6ZXT3
D	336	TRP	-	expression tag	UNP Q6ZXT3
D	337	SER	-	expression tag	UNP Q6ZXT3
D	338	HIS	-	expression tag	UNP Q6ZXT3
D	339	PRO	-	expression tag	UNP Q6ZXT3
D	340	GLN	-	expression tag	UNP Q6ZXT3
D	341	PHE	-	expression tag	UNP Q6ZXT3
D	342	GLU	-	expression tag	UNP Q6ZXT3
D	343	LYS	-	expression tag	UNP Q6ZXT3

- Molecule 2 is [(4 {R})-2-[4-[[4,6-bis(azanyl)-1,3,5-triazin-2-yl]amino]phenyl]-1,3,2-dithiarsolan-4-yl]methanol (CCD ID: L1U) (formula: C<sub>12</sub>H<sub>15</sub>AsN<sub>6</sub>OS<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total	As	C	H	N	O	S	0
			37	1	12	15	6	1	2	

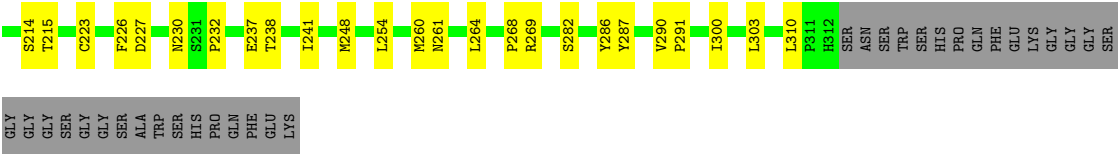
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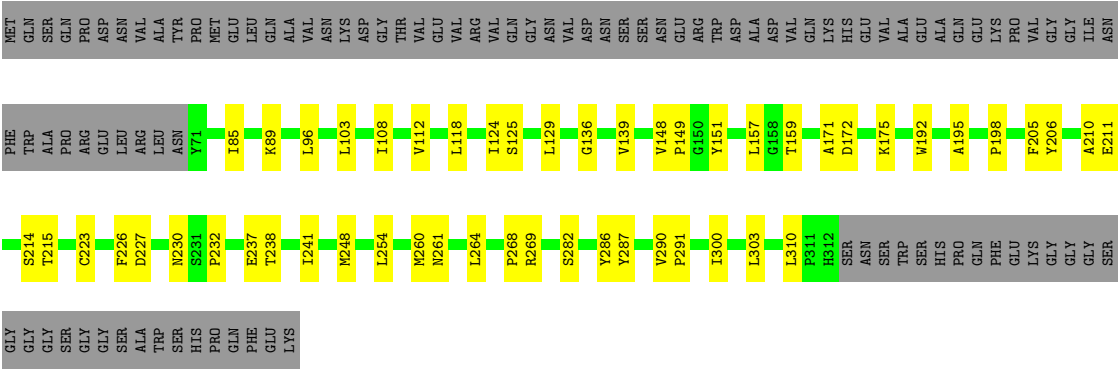
Mol	Chain	Residues	Atoms								AltConf
2	B	1	Total	As	C	H	N	O	S	0	
			37	1	12	15	6	1	2		
2	C	1	Total	As	C	H	N	O	S	0	
			37	1	12	15	6	1	2		
2	D	1	Total	As	C	H	N	O	S	0	
			37	1	12	15	6	1	2		







● Molecule 1: Aquaglyceroporin 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	379082	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	71	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 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: L1U

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	0.13	0/1880	0.30	0/2566
1	B	0.14	0/1880	0.30	0/2566
1	C	0.13	0/1880	0.31	0/2566
1	D	0.13	0/1880	0.30	0/2566
All	All	0.13	0/7520	0.30	0/10264

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1823	0	1826	36	0
1	B	1823	0	1826	40	0
1	C	1823	0	1826	39	0
1	D	1823	0	1826	36	0
2	A	22	15	0	1	0
2	B	22	15	0	1	0
2	C	22	15	0	1	0
2	D	22	15	0	1	0
All	All	7380	60	7304	139	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 9.

All (139) 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:248:MET:HB3	1:A:260:MET:HE1	1.56	0.88
1:D:248:MET:HB3	1:D:260:MET:HE1	1.56	0.88
1:B:248:MET:HB3	1:B:260:MET:HE1	1.56	0.87
1:C:248:MET:HB3	1:C:260:MET:HE1	1.56	0.87
1:A:124:ILE:HD12	1:D:310:LEU:HD22	1.73	0.71
1:A:310:LEU:HD22	1:B:124:ILE:HD12	1.73	0.71
1:C:310:LEU:HD22	1:D:124:ILE:HD12	1.73	0.70
1:B:310:LEU:HD22	1:C:124:ILE:HD12	1.73	0.70
1:B:159:THR:HB	1:B:268:PRO:HD3	1.77	0.67
1:A:159:THR:HB	1:A:268:PRO:HD3	1.77	0.67
1:D:85:ILE:HG13	1:D:159:THR:HG22	1.77	0.67
1:A:85:ILE:HG13	1:A:159:THR:HG22	1.77	0.67
1:C:85:ILE:HG13	1:C:159:THR:HG22	1.77	0.66
1:C:159:THR:HB	1:C:268:PRO:HD3	1.77	0.66
1:B:85:ILE:HG13	1:B:159:THR:HG22	1.77	0.66
1:D:159:THR:HB	1:D:268:PRO:HD3	1.77	0.66
1:B:118:LEU:HB3	1:B:238:THR:HG22	1.84	0.60
1:D:118:LEU:HB3	1:D:238:THR:HG22	1.84	0.60
1:A:118:LEU:HB3	1:A:238:THR:HG22	1.83	0.60
1:C:118:LEU:HB3	1:C:238:THR:HG22	1.84	0.59
1:C:85:ILE:HG13	1:C:159:THR:HA	1.88	0.56
1:D:85:ILE:HG13	1:D:159:THR:HA	1.88	0.56
1:B:85:ILE:HG13	1:B:159:THR:HA	1.88	0.56
1:A:85:ILE:HG13	1:A:159:THR:HA	1.88	0.56
1:D:226:PHE:CE2	1:D:241:ILE:HD11	2.44	0.53
1:A:226:PHE:CE2	1:A:241:ILE:HD11	2.44	0.52
1:B:226:PHE:CE2	1:B:241:ILE:HD11	2.45	0.51
1:C:226:PHE:CE2	1:C:241:ILE:HD11	2.45	0.51
1:B:290:VAL:HB	1:B:291:PRO:HD3	1.92	0.51
1:A:248:MET:HA	1:A:248:MET:HE2	1.92	0.51
1:C:290:VAL:HB	1:C:291:PRO:HD3	1.92	0.51
1:D:248:MET:HA	1:D:248:MET:HE2	1.93	0.51
1:B:85:ILE:CG1	1:B:159:THR:HG22	2.41	0.50
1:C:248:MET:HA	1:C:248:MET:HE2	1.92	0.50
1:C:85:ILE:CG1	1:C:159:THR:HG22	2.41	0.50
1:B:248:MET:HE2	1:B:248:MET:HA	1.93	0.50
1:B:261:ASN:HB3	1:B:264:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:GLU:O	1:C:215:THR:OG1	2.24	0.50
1:D:85:ILE:CG1	1:D:159:THR:HG22	2.41	0.50
1:A:85:ILE:CG1	1:A:159:THR:HG22	2.41	0.50
1:A:261:ASN:HB3	1:A:264:LEU:HB3	1.94	0.50
1:D:290:VAL:HB	1:D:291:PRO:HD3	1.92	0.50
1:A:290:VAL:HB	1:A:291:PRO:HD3	1.93	0.49
1:B:129:LEU:HB2	2:B:401:L1U:S2	2.52	0.49
1:C:261:ASN:HB3	1:C:264:LEU:HB3	1.94	0.49
1:B:125:SER:HB2	1:B:151:TYR:OH	2.13	0.49
1:A:129:LEU:HB2	2:A:401:L1U:S2	2.52	0.49
1:C:129:LEU:HB2	2:C:401:L1U:S2	2.52	0.49
1:B:230:ASN:O	1:B:232:PRO:HD3	2.13	0.49
1:D:129:LEU:HB2	2:D:401:L1U:S2	2.52	0.49
1:D:261:ASN:HB3	1:D:264:LEU:HB3	1.94	0.49
1:A:125:SER:HB2	1:A:151:TYR:OH	2.13	0.49
1:C:125:SER:HB2	1:C:151:TYR:OH	2.13	0.49
1:D:85:ILE:O	1:D:89:LYS:HB2	2.13	0.48
1:D:125:SER:HB2	1:D:151:TYR:OH	2.13	0.48
1:B:206:TYR:HE2	1:C:171:ALA:HB3	1.78	0.48
1:C:85:ILE:O	1:C:89:LYS:HB2	2.13	0.48
1:A:85:ILE:O	1:A:89:LYS:HB2	2.13	0.48
1:C:198:PRO:HG3	1:C:287:TYR:CD1	2.49	0.48
1:A:171:ALA:HB3	1:D:206:TYR:HE2	1.78	0.48
1:A:206:TYR:HE2	1:B:171:ALA:HB3	1.78	0.48
1:C:230:ASN:O	1:C:232:PRO:HD3	2.13	0.48
1:D:230:ASN:O	1:D:232:PRO:HD3	2.13	0.48
1:B:85:ILE:O	1:B:89:LYS:HB2	2.13	0.47
1:B:198:PRO:HG3	1:B:287:TYR:CD1	2.49	0.47
1:A:230:ASN:O	1:A:232:PRO:HD3	2.13	0.47
1:D:198:PRO:HG3	1:D:287:TYR:CD1	2.49	0.47
1:A:198:PRO:HG3	1:A:287:TYR:CD1	2.49	0.47
1:C:206:TYR:HE2	1:D:171:ALA:HB3	1.78	0.47
1:D:211:GLU:O	1:D:215:THR:OG1	2.24	0.46
1:B:248:MET:CB	1:B:260:MET:HE1	2.39	0.46
1:A:211:GLU:O	1:A:215:THR:OG1	2.24	0.45
1:D:248:MET:CB	1:D:260:MET:HE1	2.38	0.45
1:A:108:ILE:O	1:A:112:VAL:HG23	2.17	0.45
1:B:136:GLY:HA2	1:B:300:ILE:CD1	2.47	0.45
1:A:136:GLY:HA2	1:A:300:ILE:CD1	2.47	0.45
1:B:148:VAL:HB	1:B:149:PRO:HD3	1.99	0.45
1:C:108:ILE:O	1:C:112:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ILE:O	1:D:112:VAL:HG23	2.17	0.45
1:D:136:GLY:HA2	1:D:300:ILE:CD1	2.47	0.45
1:D:148:VAL:HB	1:D:149:PRO:HD3	1.99	0.44
1:B:108:ILE:O	1:B:112:VAL:HG23	2.16	0.44
1:C:136:GLY:HA2	1:C:300:ILE:CD1	2.47	0.44
1:C:148:VAL:HB	1:C:149:PRO:HD3	1.99	0.44
1:A:148:VAL:HB	1:A:149:PRO:HD3	1.99	0.44
1:A:206:TYR:CE2	1:B:171:ALA:HB3	2.53	0.44
1:C:248:MET:CB	1:C:260:MET:HE1	2.39	0.44
1:B:206:TYR:CE2	1:C:171:ALA:HB3	2.53	0.43
1:A:171:ALA:HB3	1:D:206:TYR:CE2	2.53	0.43
1:C:206:TYR:CE2	1:D:171:ALA:HB3	2.53	0.43
1:A:96:LEU:HD12	1:A:192:TRP:HZ2	1.84	0.43
1:B:96:LEU:HD12	1:B:192:TRP:HZ2	1.84	0.42
1:B:226:PHE:HE2	1:B:241:ILE:HD11	1.84	0.42
1:C:227:ASP:O	1:C:232:PRO:HG3	2.19	0.42
1:B:89:LYS:HA	1:B:89:LYS:HD2	1.84	0.42
1:D:223:CYS:SG	1:D:303:LEU:HD23	2.60	0.42
1:D:227:ASP:O	1:D:232:PRO:HG3	2.19	0.42
1:A:227:ASP:O	1:A:232:PRO:HG3	2.19	0.42
1:B:195:ALA:HB1	1:B:269:ARG:CZ	2.50	0.42
1:D:96:LEU:HD12	1:D:192:TRP:HZ2	1.84	0.42
1:A:195:ALA:HB1	1:A:269:ARG:CZ	2.50	0.42
1:A:223:CYS:SG	1:A:303:LEU:HD23	2.60	0.42
1:D:195:ALA:HB1	1:D:269:ARG:CZ	2.50	0.42
1:B:223:CYS:SG	1:B:303:LEU:HD23	2.60	0.42
1:B:227:ASP:O	1:B:232:PRO:HG3	2.19	0.42
1:D:172:ASP:O	1:D:175:LYS:HG2	2.20	0.42
1:B:211:GLU:O	1:B:215:THR:OG1	2.24	0.41
1:B:214:SER:HB3	1:B:260:MET:SD	2.60	0.41
1:C:172:ASP:O	1:C:175:LYS:HG2	2.20	0.41
1:C:223:CYS:SG	1:C:303:LEU:HD23	2.60	0.41
1:D:210:ALA:O	1:D:214:SER:HB2	2.20	0.41
1:C:210:ALA:O	1:C:214:SER:HB2	2.20	0.41
1:C:226:PHE:HE2	1:C:241:ILE:HD11	1.84	0.41
1:A:210:ALA:O	1:A:214:SER:HB2	2.20	0.41
1:C:195:ALA:HB1	1:C:269:ARG:CZ	2.50	0.41
1:D:214:SER:HB3	1:D:260:MET:SD	2.60	0.41
1:C:214:SER:HB3	1:C:260:MET:SD	2.60	0.41
1:A:237:GLU:O	1:A:241:ILE:HG13	2.21	0.41
1:B:103:LEU:HD22	1:B:254:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASP:O	1:B:175:LYS:HG2	2.20	0.41
1:C:96:LEU:HD12	1:C:192:TRP:HZ2	1.84	0.41
1:D:282:SER:HA	1:D:286:TYR:CD1	2.56	0.41
1:A:177:HIS:O	1:A:188:LYS:NZ	2.31	0.41
1:B:210:ALA:O	1:B:214:SER:HB2	2.20	0.41
1:B:282:SER:HA	1:B:286:TYR:CD1	2.56	0.41
1:A:172:ASP:O	1:A:175:LYS:HG2	2.20	0.41
1:C:103:LEU:HD22	1:C:254:LEU:HD22	2.03	0.41
1:D:237:GLU:O	1:D:241:ILE:HG13	2.21	0.41
1:A:214:SER:HB3	1:A:260:MET:SD	2.60	0.41
1:B:177:HIS:O	1:B:188:LYS:NZ	2.31	0.41
1:B:237:GLU:O	1:B:241:ILE:HG13	2.21	0.41
1:B:309:PHE:HD1	1:B:309:PHE:HA	1.75	0.41
1:C:89:LYS:HD2	1:C:89:LYS:HA	1.84	0.41
1:C:282:SER:HA	1:C:286:TYR:CD1	2.56	0.41
1:C:118:LEU:HD11	1:C:241:ILE:HG21	2.03	0.40
1:A:282:SER:HA	1:A:286:TYR:CD1	2.56	0.40
1:C:237:GLU:O	1:C:241:ILE:HG13	2.21	0.40
1:A:103:LEU:HD22	1:A:254:LEU:HD22	2.03	0.40
1:D:103:LEU:HD22	1:D:254:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	240/343 (70%)	232 (97%)	8 (3%)	0	100	100
1	B	240/343 (70%)	232 (97%)	8 (3%)	0	100	100
1	C	240/343 (70%)	232 (97%)	8 (3%)	0	100	100
1	D	240/343 (70%)	232 (97%)	8 (3%)	0	100	100
All	All	960/1372 (70%)	928 (97%)	32 (3%)	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 PDB entries followed by that with respect to all EM entries.

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	182/264 (69%)	179 (98%)	3 (2%)	58	80
1	B	182/264 (69%)	179 (98%)	3 (2%)	58	80
1	C	182/264 (69%)	179 (98%)	3 (2%)	58	80
1	D	182/264 (69%)	179 (98%)	3 (2%)	58	80
All	All	728/1056 (69%)	716 (98%)	12 (2%)	58	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	157	LEU
1	A	205	PHE
1	B	139	VAL
1	B	157	LEU
1	B	205	PHE
1	C	139	VAL
1	C	157	LEU
1	C	205	PHE
1	D	139	VAL
1	D	157	LEU
1	D	205	PHE

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	250	ASN
1	B	250	ASN
1	C	250	ASN
1	D	250	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	L1U	D	401	-	20,24,24	4.76	16 (80%)	23,33,33	2.27	7 (30%)
2	L1U	C	401	-	20,24,24	4.76	16 (80%)	23,33,33	2.28	7 (30%)
2	L1U	A	401	-	20,24,24	4.76	16 (80%)	23,33,33	2.28	7 (30%)
2	L1U	B	401	-	20,24,24	4.76	16 (80%)	23,33,33	2.29	7 (30%)

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	L1U	D	401	-	-	5/10/19/19	0/3/3/3
2	L1U	C	401	-	-	5/10/19/19	0/3/3/3
2	L1U	A	401	-	-	5/10/19/19	0/3/3/3
2	L1U	B	401	-	-	5/10/19/19	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	L1U	C7-C6	8.28	1.53	1.39
2	C	401	L1U	C7-C6	8.28	1.53	1.39
2	A	401	L1U	C7-C6	8.23	1.53	1.39
2	D	401	L1U	C7-C6	8.23	1.53	1.39
2	A	401	L1U	C4-C5	8.02	1.53	1.38
2	B	401	L1U	C4-C5	7.97	1.53	1.38
2	C	401	L1U	C4-C5	7.97	1.53	1.38
2	D	401	L1U	C4-C5	7.97	1.53	1.38
2	C	401	L1U	C10-N6	5.93	1.45	1.33
2	A	401	L1U	C10-N6	5.90	1.45	1.33
2	B	401	L1U	C10-N6	5.89	1.45	1.33
2	D	401	L1U	C10-N6	5.89	1.45	1.33
2	B	401	L1U	C11-N5	5.85	1.45	1.33
2	C	401	L1U	C11-N5	5.85	1.45	1.33
2	D	401	L1U	C11-N5	5.85	1.45	1.33
2	A	401	L1U	C11-N5	5.80	1.45	1.33
2	C	401	L1U	C11-N4	5.75	1.45	1.35
2	A	401	L1U	C11-N4	5.73	1.45	1.35
2	D	401	L1U	C11-N3	-5.73	1.25	1.35
2	B	401	L1U	C11-N4	5.72	1.45	1.35
2	B	401	L1U	C11-N3	-5.72	1.25	1.35
2	A	401	L1U	C11-N3	-5.71	1.25	1.35
2	C	401	L1U	C11-N3	-5.71	1.25	1.35
2	D	401	L1U	C11-N4	5.68	1.45	1.35
2	A	401	L1U	C10-N2	-5.68	1.25	1.35
2	D	401	L1U	C10-N2	-5.68	1.25	1.35
2	B	401	L1U	C10-N2	-5.67	1.25	1.35
2	C	401	L1U	C10-N2	-5.65	1.25	1.35
2	A	401	L1U	C10-N3	5.62	1.45	1.35
2	D	401	L1U	C10-N3	5.62	1.45	1.35
2	B	401	L1U	C10-N3	5.61	1.45	1.35
2	C	401	L1U	C10-N3	5.56	1.45	1.35
2	A	401	L1U	C8-C3	5.27	1.52	1.39
2	B	401	L1U	C8-C3	5.26	1.52	1.39
2	C	401	L1U	C8-C3	5.24	1.52	1.39
2	D	401	L1U	C8-C3	5.24	1.52	1.39
2	C	401	L1U	C9-N1	5.03	1.46	1.36
2	A	401	L1U	C9-N1	5.01	1.46	1.36
2	B	401	L1U	C9-N1	5.01	1.46	1.36
2	D	401	L1U	C9-N1	5.01	1.46	1.36
2	B	401	L1U	C7-C8	-3.98	1.31	1.38
2	A	401	L1U	C7-C8	-3.98	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	L1U	C7-C8	-3.98	1.31	1.38
2	C	401	L1U	C7-C8	-3.98	1.31	1.38
2	B	401	L1U	C5-C6	-3.88	1.32	1.39
2	C	401	L1U	C5-C6	-3.88	1.32	1.39
2	D	401	L1U	C5-C6	-3.88	1.32	1.39
2	A	401	L1U	C5-C6	-3.82	1.32	1.39
2	C	401	L1U	C9-N2	3.62	1.45	1.34
2	A	401	L1U	C9-N2	3.60	1.45	1.34
2	B	401	L1U	C9-N2	3.60	1.45	1.34
2	D	401	L1U	C9-N2	3.60	1.45	1.34
2	C	401	L1U	C9-N4	-3.15	1.25	1.34
2	A	401	L1U	C9-N4	-3.11	1.25	1.34
2	D	401	L1U	C9-N4	-3.09	1.25	1.34
2	B	401	L1U	C9-N4	-3.09	1.25	1.34
2	A	401	L1U	C4-C3	-2.98	1.31	1.39
2	B	401	L1U	C4-C3	-2.94	1.31	1.39
2	D	401	L1U	C4-C3	-2.94	1.32	1.39
2	C	401	L1U	C4-C3	-2.90	1.32	1.39
2	B	401	L1U	C6-N1	2.78	1.46	1.40
2	C	401	L1U	C6-N1	2.77	1.46	1.40
2	A	401	L1U	C6-N1	2.77	1.46	1.40
2	D	401	L1U	C6-N1	2.77	1.46	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	L1U	N4-C9-N2	-4.85	118.56	126.23
2	D	401	L1U	N4-C9-N2	-4.84	118.58	126.23
2	C	401	L1U	N4-C9-N2	-4.83	118.59	126.23
2	A	401	L1U	N4-C9-N2	-4.82	118.61	126.23
2	B	401	L1U	C10-N2-C9	4.27	120.98	113.75
2	A	401	L1U	C10-N2-C9	4.27	120.98	113.75
2	D	401	L1U	C10-N2-C9	4.27	120.97	113.75
2	C	401	L1U	C10-N2-C9	4.23	120.92	113.75
2	C	401	L1U	C11-N4-C9	4.18	120.83	113.75
2	B	401	L1U	C11-N4-C9	4.17	120.81	113.75
2	A	401	L1U	C11-N4-C9	4.16	120.79	113.75
2	D	401	L1U	C11-N4-C9	4.14	120.76	113.75
2	A	401	L1U	N3-C10-N2	-3.57	119.82	125.42
2	B	401	L1U	N3-C10-N2	-3.55	119.85	125.42
2	D	401	L1U	N3-C10-N2	-3.54	119.87	125.42
2	C	401	L1U	N3-C10-N2	-3.52	119.89	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	L1U	N4-C11-N3	-3.41	120.06	125.42
2	C	401	L1U	N4-C11-N3	-3.41	120.07	125.42
2	B	401	L1U	N4-C11-N3	-3.40	120.09	125.42
2	D	401	L1U	N4-C11-N3	-3.35	120.17	125.42
2	A	401	L1U	C11-N3-C10	2.89	119.72	114.83
2	B	401	L1U	C11-N3-C10	2.88	119.70	114.83
2	C	401	L1U	C11-N3-C10	2.87	119.69	114.83
2	D	401	L1U	C11-N3-C10	2.84	119.63	114.83
2	C	401	L1U	N1-C9-N4	2.25	124.54	116.92
2	B	401	L1U	N1-C9-N4	2.24	124.52	116.92
2	D	401	L1U	N1-C9-N4	2.24	124.50	116.92
2	A	401	L1U	N1-C9-N4	2.23	124.47	116.92

There are no chirality outliers.

All (20) torsion outliers are listed below:

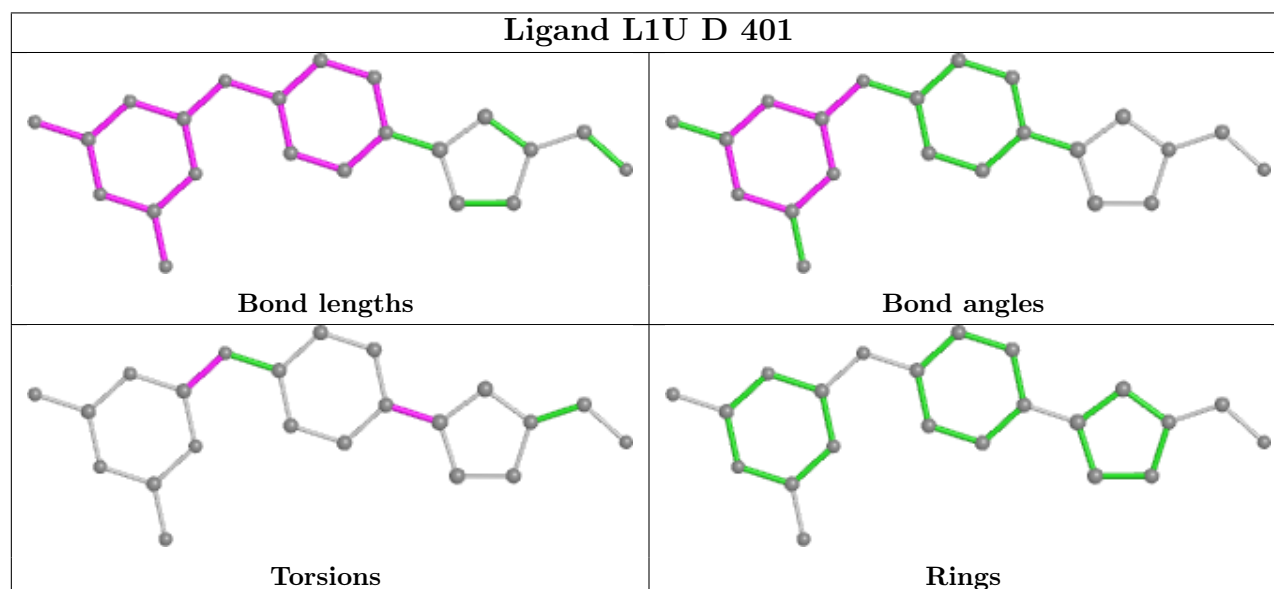
Mol	Chain	Res	Type	Atoms
2	A	401	L1U	N4-C9-N1-C6
2	B	401	L1U	N4-C9-N1-C6
2	C	401	L1U	N4-C9-N1-C6
2	D	401	L1U	N4-C9-N1-C6
2	A	401	L1U	S1-AS-C3-C8
2	A	401	L1U	S2-AS-C3-C8
2	A	401	L1U	S2-AS-C3-C4
2	B	401	L1U	S1-AS-C3-C8
2	B	401	L1U	S2-AS-C3-C8
2	B	401	L1U	S2-AS-C3-C4
2	C	401	L1U	S1-AS-C3-C8
2	C	401	L1U	S2-AS-C3-C8
2	C	401	L1U	S2-AS-C3-C4
2	D	401	L1U	S1-AS-C3-C8
2	D	401	L1U	S2-AS-C3-C8
2	D	401	L1U	S2-AS-C3-C4
2	A	401	L1U	N2-C9-N1-C6
2	B	401	L1U	N2-C9-N1-C6
2	C	401	L1U	N2-C9-N1-C6
2	D	401	L1U	N2-C9-N1-C6

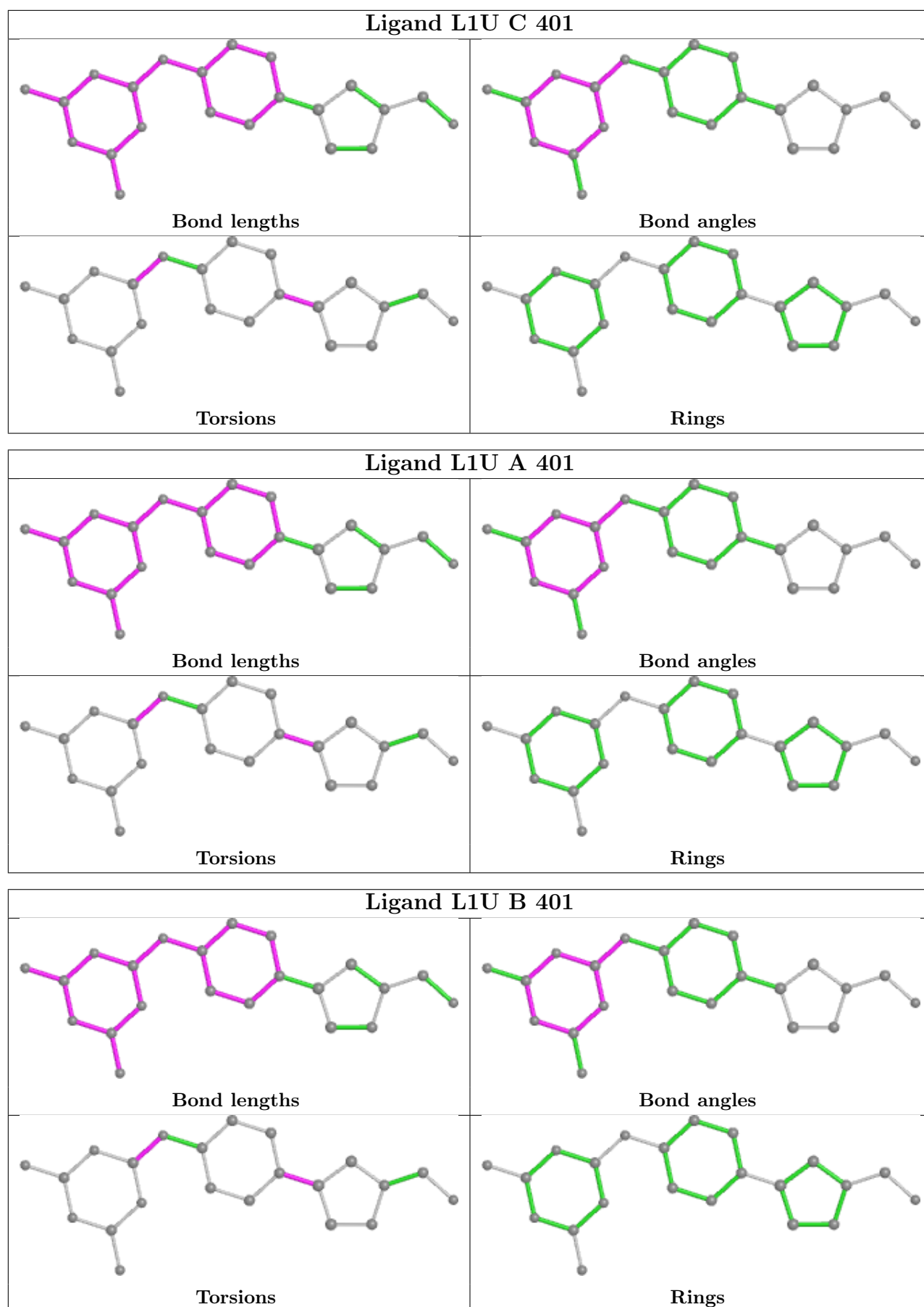
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	L1U	1	0
2	C	401	L1U	1	0
2	A	401	L1U	1	0
2	B	401	L1U	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.