



## wwPDB EM Validation Summary Report ⓘ

May 17, 2026 – 10:34 PM JST

PDB ID : 9VIM / pdb\_00009vim  
EMDB ID : EMD-65093  
Title : Zea mays URE transporter DUR3 - URE bound  
Authors : Wang, Y.L.; Lin, H.J.; Zhang, J.R.; Fan, M.R.  
Deposited on : 2025-06-18  
Resolution : 3.41 Å(reported)

This is a wwPDB EM Validation Summary 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 Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

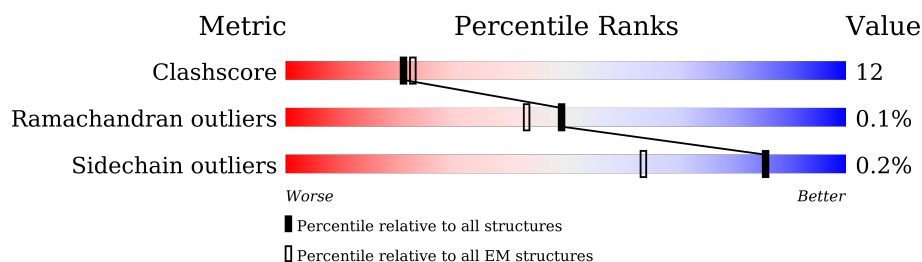
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.41 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	773	66% 18% 15%
1	B	773	53% 26% 21%
1	C	773	58% 20% 22%
1	D	773	56% 22% 22%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18404 atoms, of which 0 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 Urea-proton symporter DUR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	659	Total	C	N	O	S	0	0
			4931	3231	817	855	28		
1	B	613	Total	C	N	O	S	0	0
			4551	2976	752	795	28		
1	C	601	Total	C	N	O	S	0	0
			4459	2917	734	781	27		
1	D	601	Total	C	N	O	S	0	0
			4459	2917	734	781	27		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	732	VAL	-	expression tag	UNP A0A0A0US36
A	733	ASP	-	expression tag	UNP A0A0A0US36
A	734	GLU	-	expression tag	UNP A0A0A0US36
A	735	LEU	-	expression tag	UNP A0A0A0US36
A	736	THR	-	expression tag	UNP A0A0A0US36
A	737	SER	-	expression tag	UNP A0A0A0US36
A	738	ARG	-	expression tag	UNP A0A0A0US36
A	739	GLY	-	expression tag	UNP A0A0A0US36
A	740	ARG	-	expression tag	UNP A0A0A0US36
A	741	ASP	-	expression tag	UNP A0A0A0US36
A	742	TYR	-	expression tag	UNP A0A0A0US36
A	743	LYS	-	expression tag	UNP A0A0A0US36
A	744	ASP	-	expression tag	UNP A0A0A0US36
A	745	ASP	-	expression tag	UNP A0A0A0US36
A	746	ASP	-	expression tag	UNP A0A0A0US36
A	747	ASP	-	expression tag	UNP A0A0A0US36
A	748	LYS	-	expression tag	UNP A0A0A0US36
A	749	TRP	-	expression tag	UNP A0A0A0US36
A	750	SER	-	expression tag	UNP A0A0A0US36
A	751	HIS	-	expression tag	UNP A0A0A0US36
A	752	PRO	-	expression tag	UNP A0A0A0US36
A	753	GLN	-	expression tag	UNP A0A0A0US36

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Chain	Residue	Modelled	Actual	Comment	Reference
A	754	PHE	-	expression tag	UNP A0A0A0US36
A	755	GLU	-	expression tag	UNP A0A0A0US36
A	756	LYS	-	expression tag	UNP A0A0A0US36
A	757	GLY	-	expression tag	UNP A0A0A0US36
A	758	GLY	-	expression tag	UNP A0A0A0US36
A	759	GLY	-	expression tag	UNP A0A0A0US36
A	760	GLY	-	expression tag	UNP A0A0A0US36
A	761	SER	-	expression tag	UNP A0A0A0US36
A	762	GLY	-	expression tag	UNP A0A0A0US36
A	763	GLY	-	expression tag	UNP A0A0A0US36
A	764	SER	-	expression tag	UNP A0A0A0US36
A	765	ALA	-	expression tag	UNP A0A0A0US36
A	766	TRP	-	expression tag	UNP A0A0A0US36
A	767	SER	-	expression tag	UNP A0A0A0US36
A	768	HIS	-	expression tag	UNP A0A0A0US36
A	769	PRO	-	expression tag	UNP A0A0A0US36
A	770	GLN	-	expression tag	UNP A0A0A0US36
A	771	PHE	-	expression tag	UNP A0A0A0US36
A	772	GLU	-	expression tag	UNP A0A0A0US36
A	773	LYS	-	expression tag	UNP A0A0A0US36
B	732	VAL	-	expression tag	UNP A0A0A0US36
B	733	ASP	-	expression tag	UNP A0A0A0US36
B	734	GLU	-	expression tag	UNP A0A0A0US36
B	735	LEU	-	expression tag	UNP A0A0A0US36
B	736	THR	-	expression tag	UNP A0A0A0US36
B	737	SER	-	expression tag	UNP A0A0A0US36
B	738	ARG	-	expression tag	UNP A0A0A0US36
B	739	GLY	-	expression tag	UNP A0A0A0US36
B	740	ARG	-	expression tag	UNP A0A0A0US36
B	741	ASP	-	expression tag	UNP A0A0A0US36
B	742	TYR	-	expression tag	UNP A0A0A0US36
B	743	LYS	-	expression tag	UNP A0A0A0US36
B	744	ASP	-	expression tag	UNP A0A0A0US36
B	745	ASP	-	expression tag	UNP A0A0A0US36
B	746	ASP	-	expression tag	UNP A0A0A0US36
B	747	ASP	-	expression tag	UNP A0A0A0US36
B	748	LYS	-	expression tag	UNP A0A0A0US36
B	749	TRP	-	expression tag	UNP A0A0A0US36
B	750	SER	-	expression tag	UNP A0A0A0US36
B	751	HIS	-	expression tag	UNP A0A0A0US36
B	752	PRO	-	expression tag	UNP A0A0A0US36
B	753	GLN	-	expression tag	UNP A0A0A0US36

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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	PHE	-	expression tag	UNP A0A0A0US36
B	755	GLU	-	expression tag	UNP A0A0A0US36
B	756	LYS	-	expression tag	UNP A0A0A0US36
B	757	GLY	-	expression tag	UNP A0A0A0US36
B	758	GLY	-	expression tag	UNP A0A0A0US36
B	759	GLY	-	expression tag	UNP A0A0A0US36
B	760	GLY	-	expression tag	UNP A0A0A0US36
B	761	SER	-	expression tag	UNP A0A0A0US36
B	762	GLY	-	expression tag	UNP A0A0A0US36
B	763	GLY	-	expression tag	UNP A0A0A0US36
B	764	SER	-	expression tag	UNP A0A0A0US36
B	765	ALA	-	expression tag	UNP A0A0A0US36
B	766	TRP	-	expression tag	UNP A0A0A0US36
B	767	SER	-	expression tag	UNP A0A0A0US36
B	768	HIS	-	expression tag	UNP A0A0A0US36
B	769	PRO	-	expression tag	UNP A0A0A0US36
B	770	GLN	-	expression tag	UNP A0A0A0US36
B	771	PHE	-	expression tag	UNP A0A0A0US36
B	772	GLU	-	expression tag	UNP A0A0A0US36
B	773	LYS	-	expression tag	UNP A0A0A0US36
C	732	VAL	-	expression tag	UNP A0A0A0US36
C	733	ASP	-	expression tag	UNP A0A0A0US36
C	734	GLU	-	expression tag	UNP A0A0A0US36
C	735	LEU	-	expression tag	UNP A0A0A0US36
C	736	THR	-	expression tag	UNP A0A0A0US36
C	737	SER	-	expression tag	UNP A0A0A0US36
C	738	ARG	-	expression tag	UNP A0A0A0US36
C	739	GLY	-	expression tag	UNP A0A0A0US36
C	740	ARG	-	expression tag	UNP A0A0A0US36
C	741	ASP	-	expression tag	UNP A0A0A0US36
C	742	TYR	-	expression tag	UNP A0A0A0US36
C	743	LYS	-	expression tag	UNP A0A0A0US36
C	744	ASP	-	expression tag	UNP A0A0A0US36
C	745	ASP	-	expression tag	UNP A0A0A0US36
C	746	ASP	-	expression tag	UNP A0A0A0US36
C	747	ASP	-	expression tag	UNP A0A0A0US36
C	748	LYS	-	expression tag	UNP A0A0A0US36
C	749	TRP	-	expression tag	UNP A0A0A0US36
C	750	SER	-	expression tag	UNP A0A0A0US36
C	751	HIS	-	expression tag	UNP A0A0A0US36
C	752	PRO	-	expression tag	UNP A0A0A0US36
C	753	GLN	-	expression tag	UNP A0A0A0US36

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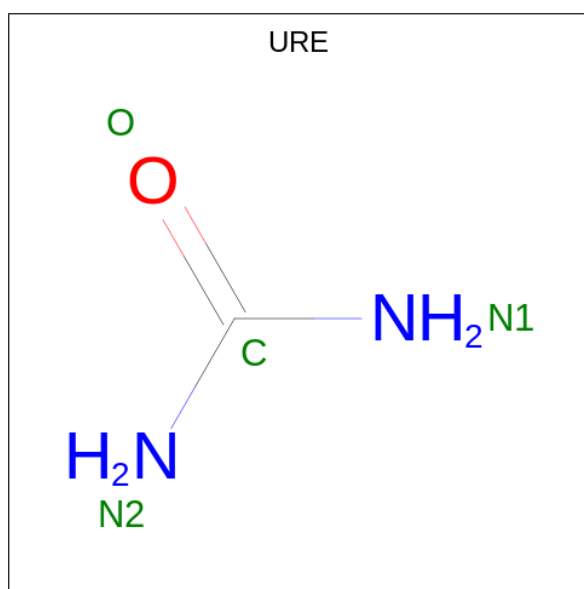
Chain	Residue	Modelled	Actual	Comment	Reference
C	754	PHE	-	expression tag	UNP A0A0A0US36
C	755	GLU	-	expression tag	UNP A0A0A0US36
C	756	LYS	-	expression tag	UNP A0A0A0US36
C	757	GLY	-	expression tag	UNP A0A0A0US36
C	758	GLY	-	expression tag	UNP A0A0A0US36
C	759	GLY	-	expression tag	UNP A0A0A0US36
C	760	GLY	-	expression tag	UNP A0A0A0US36
C	761	SER	-	expression tag	UNP A0A0A0US36
C	762	GLY	-	expression tag	UNP A0A0A0US36
C	763	GLY	-	expression tag	UNP A0A0A0US36
C	764	SER	-	expression tag	UNP A0A0A0US36
C	765	ALA	-	expression tag	UNP A0A0A0US36
C	766	TRP	-	expression tag	UNP A0A0A0US36
C	767	SER	-	expression tag	UNP A0A0A0US36
C	768	HIS	-	expression tag	UNP A0A0A0US36
C	769	PRO	-	expression tag	UNP A0A0A0US36
C	770	GLN	-	expression tag	UNP A0A0A0US36
C	771	PHE	-	expression tag	UNP A0A0A0US36
C	772	GLU	-	expression tag	UNP A0A0A0US36
C	773	LYS	-	expression tag	UNP A0A0A0US36
D	732	VAL	-	expression tag	UNP A0A0A0US36
D	733	ASP	-	expression tag	UNP A0A0A0US36
D	734	GLU	-	expression tag	UNP A0A0A0US36
D	735	LEU	-	expression tag	UNP A0A0A0US36
D	736	THR	-	expression tag	UNP A0A0A0US36
D	737	SER	-	expression tag	UNP A0A0A0US36
D	738	ARG	-	expression tag	UNP A0A0A0US36
D	739	GLY	-	expression tag	UNP A0A0A0US36
D	740	ARG	-	expression tag	UNP A0A0A0US36
D	741	ASP	-	expression tag	UNP A0A0A0US36
D	742	TYR	-	expression tag	UNP A0A0A0US36
D	743	LYS	-	expression tag	UNP A0A0A0US36
D	744	ASP	-	expression tag	UNP A0A0A0US36
D	745	ASP	-	expression tag	UNP A0A0A0US36
D	746	ASP	-	expression tag	UNP A0A0A0US36
D	747	ASP	-	expression tag	UNP A0A0A0US36
D	748	LYS	-	expression tag	UNP A0A0A0US36
D	749	TRP	-	expression tag	UNP A0A0A0US36
D	750	SER	-	expression tag	UNP A0A0A0US36
D	751	HIS	-	expression tag	UNP A0A0A0US36
D	752	PRO	-	expression tag	UNP A0A0A0US36
D	753	GLN	-	expression tag	UNP A0A0A0US36

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Chain	Residue	Modelled	Actual	Comment	Reference
D	754	PHE	-	expression tag	UNP A0A0A0US36
D	755	GLU	-	expression tag	UNP A0A0A0US36
D	756	LYS	-	expression tag	UNP A0A0A0US36
D	757	GLY	-	expression tag	UNP A0A0A0US36
D	758	GLY	-	expression tag	UNP A0A0A0US36
D	759	GLY	-	expression tag	UNP A0A0A0US36
D	760	GLY	-	expression tag	UNP A0A0A0US36
D	761	SER	-	expression tag	UNP A0A0A0US36
D	762	GLY	-	expression tag	UNP A0A0A0US36
D	763	GLY	-	expression tag	UNP A0A0A0US36
D	764	SER	-	expression tag	UNP A0A0A0US36
D	765	ALA	-	expression tag	UNP A0A0A0US36
D	766	TRP	-	expression tag	UNP A0A0A0US36
D	767	SER	-	expression tag	UNP A0A0A0US36
D	768	HIS	-	expression tag	UNP A0A0A0US36
D	769	PRO	-	expression tag	UNP A0A0A0US36
D	770	GLN	-	expression tag	UNP A0A0A0US36
D	771	PHE	-	expression tag	UNP A0A0A0US36
D	772	GLU	-	expression tag	UNP A0A0A0US36
D	773	LYS	-	expression tag	UNP A0A0A0US36

- Molecule 2 is UREA (CCD ID: URE) (formula:  $\text{CH}_4\text{N}_2\text{O}$ ) (labeled as "Ligand of Interest" by depositor).

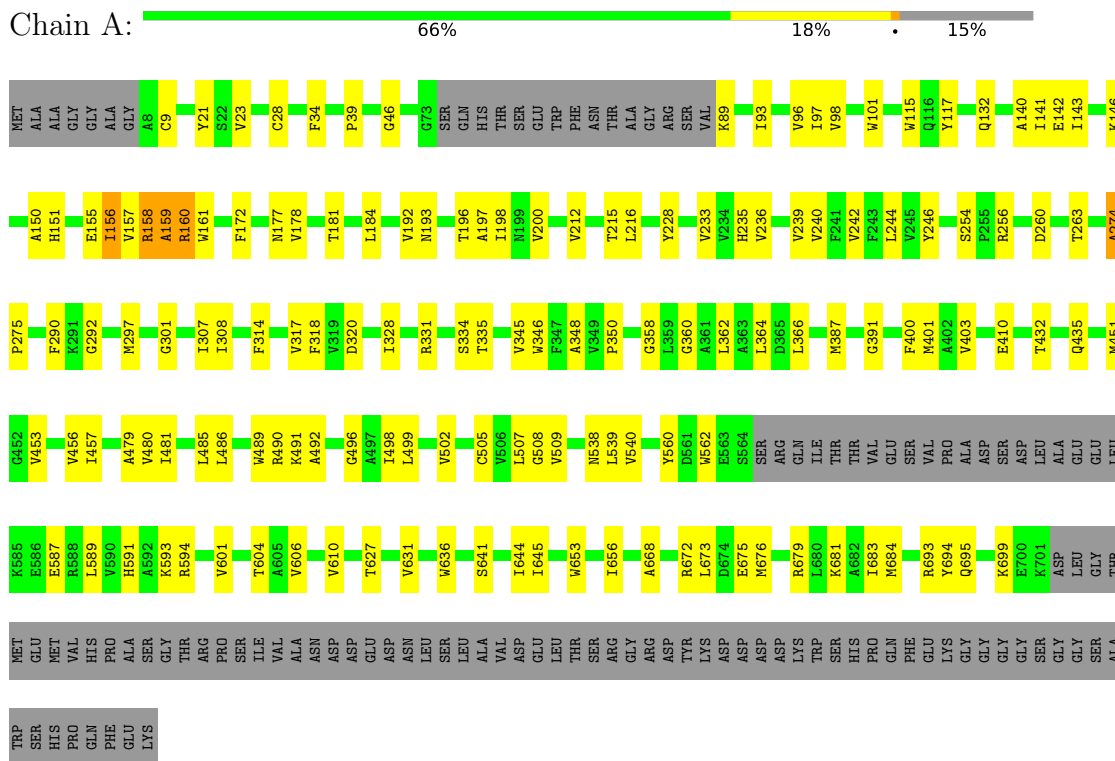


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			4	1	2	1	

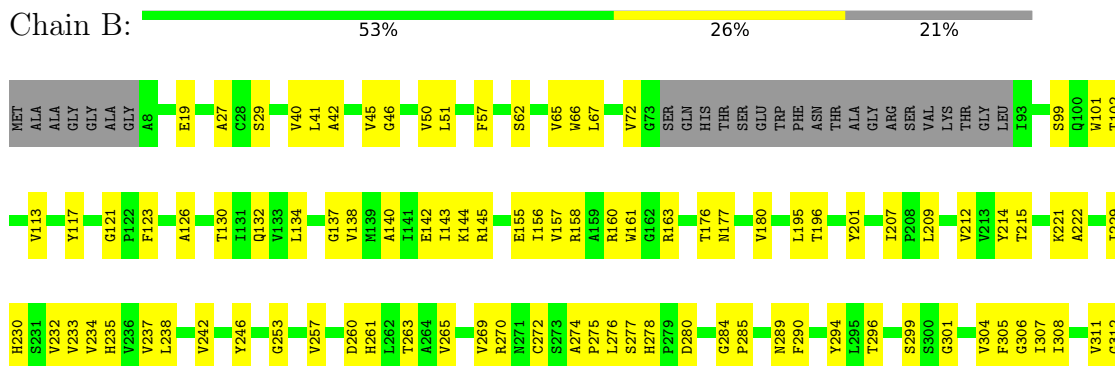
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Urea-proton symporter DUR3



#### • Molecule 1: Urea-proton symporter DUR3







WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: URE

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	0.23	1/5052 (0.0%)	0.44	2/6897 (0.0%)
1	B	0.20	0/4658	0.45	2/6358 (0.0%)
1	C	0.20	0/4561	0.42	2/6223 (0.0%)
1	D	0.23	1/4561 (0.0%)	0.41	1/6223 (0.0%)
All	All	0.22	2/18832 (0.0%)	0.43	7/25701 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ARG	CA-C	-6.05	1.45	1.52
1	D	661	GLU	CA-C	-5.85	1.45	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	N-CA-C	-8.69	101.39	111.03
1	B	663	MET	N-CA-C	8.64	122.39	111.24
1	D	663	MET	N-CA-C	8.39	122.81	112.23
1	A	159	ALA	N-CA-C	-7.42	98.91	109.96
1	C	663	MET	N-CA-C	6.65	121.14	112.89

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	4931	0	5041	100	0
1	B	4551	0	4651	134	0
1	C	4459	0	4567	102	0
1	D	4459	0	4567	113	0
2	A	4	0	4	1	0
All	All	18404	0	18830	443	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 12.

The worst 5 of 443 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:400:PHE:HA	1:A:403:VAL:HG12	1.65	0.79
1:D:200:VAL:HG22	1:D:459:ASN:HD21	1.48	0.78
1:A:159:ALA:O	1:A:160:ARG:HB2	1.85	0.77
1:A:160:ARG:HH12	1:A:492:ALA:HB3	1.48	0.76
1:B:40:VAL:O	1:B:389:LYS:NZ	2.20	0.74

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 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	653/773 (84%)	591 (90%)	60 (9%)	2 (0%)	36	65
1	B	607/773 (78%)	541 (89%)	66 (11%)	0	100	100
1	C	595/773 (77%)	538 (90%)	57 (10%)	0	100	100
1	D	595/773 (77%)	536 (90%)	59 (10%)	0	100	100
All	All	2450/3092 (79%)	2206 (90%)	242 (10%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	ALA
1	A	160	ARG

### 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	508/599 (85%)	507 (100%)	1 (0%)	87	85
1	B	470/599 (78%)	470 (100%)	0	100	100
1	C	461/599 (77%)	460 (100%)	1 (0%)	87	85
1	D	461/599 (77%)	459 (100%)	2 (0%)	84	82
All	All	1900/2396 (79%)	1896 (100%)	4 (0%)	85	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ILE
1	C	663	MET
1	D	659	VAL
1	D	663	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	459	ASN
1	D	309	ASN
1	D	199	ASN
1	C	695	GLN
1	D	230	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	URE	A	801	-	3,3,3	0.85	0	3,3,3	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

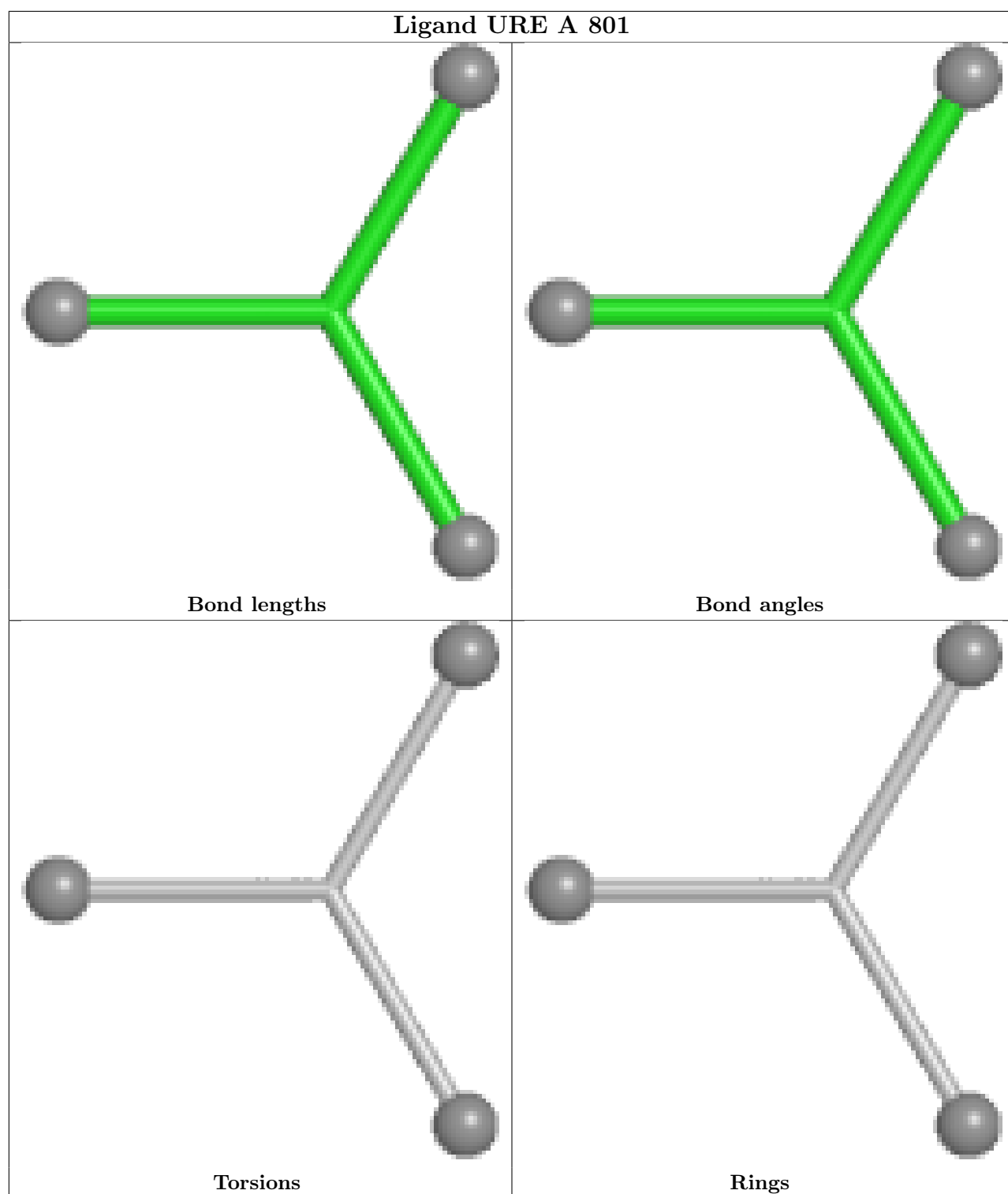
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	URE	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 ⓘ

There are no chain breaks in this entry.