



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2025 – 08:06 AM EST

PDB ID : 9PTD / pdb\_00009ptd  
Title : Crystal structure of C. elegans PUF-3  
Authors : Zhang, Y.; Hall, T.M.T.  
Deposited on : 2025-07-28  
Resolution : 3.14 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.47

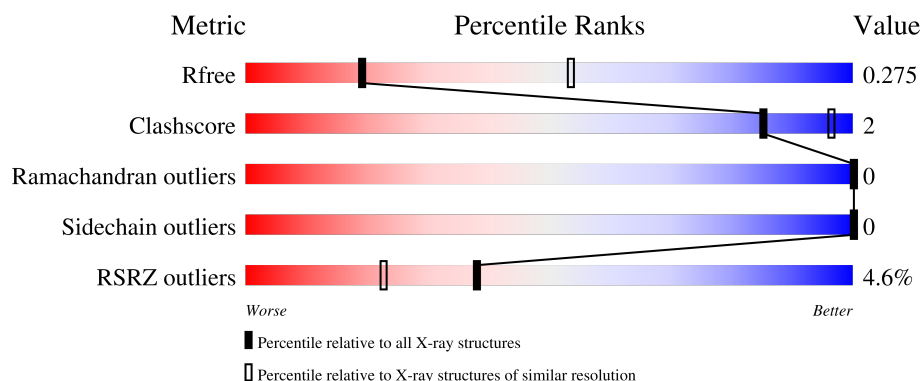
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (3.18-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	379	<div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	B	379	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	C	379	<div> <div>3%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	D	379	<div> <div>6%</div> <div>90%</div> <div>.</div> <div>7%</div> </div>
1	E	379	<div> <div>10%</div> <div>65%</div> <div>.</div> <div>31%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12805 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 PUM-HD domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2847	1791	497	537	22			
1	B	364	Total	C	N	O	S	0	0	0
			2850	1791	495	541	23			
1	C	350	Total	C	N	O	S	0	0	0
			2641	1658	459	504	20			
1	D	352	Total	C	N	O	S	0	0	0
			2547	1604	443	480	20			
1	E	261	Total	C	N	O	S	0	0	0
			1813	1128	316	351	18			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	SER	-	expression tag	UNP Q9U2G4
B	124	SER	-	expression tag	UNP Q9U2G4
C	124	SER	-	expression tag	UNP Q9U2G4
D	124	SER	-	expression tag	UNP Q9U2G4
E	124	SER	-	expression tag	UNP Q9U2G4

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		

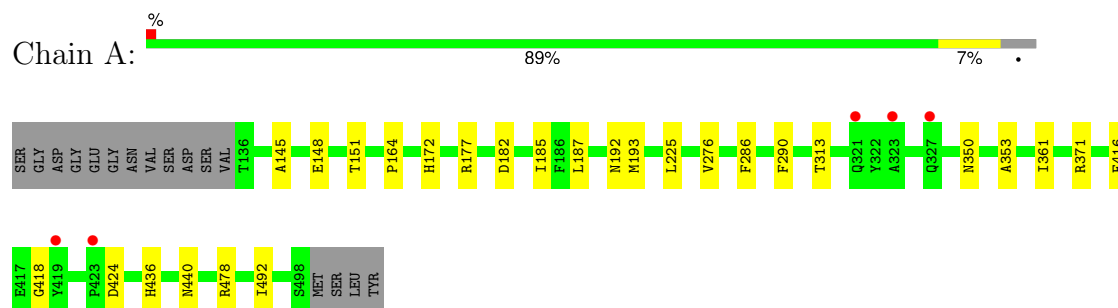
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	32	Total	O	0	0
			32	32		
3	C	16	Total	O	0	0
			16	16		
3	D	7	Total	O	0	0
			7	7		
3	E	6	Total	O	0	0
			6	6		

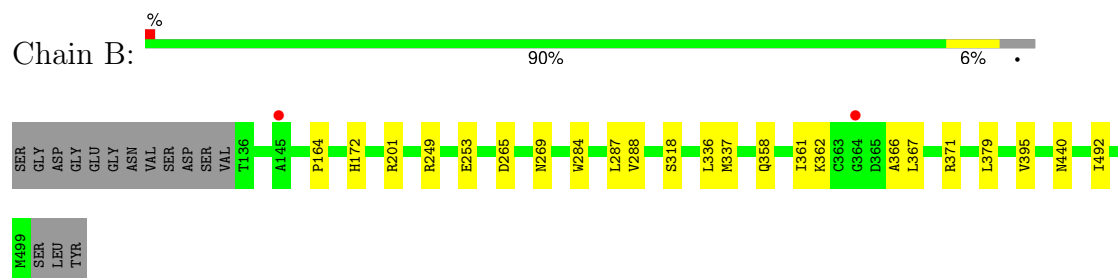
### 3 Residue-property plots [i](#)

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

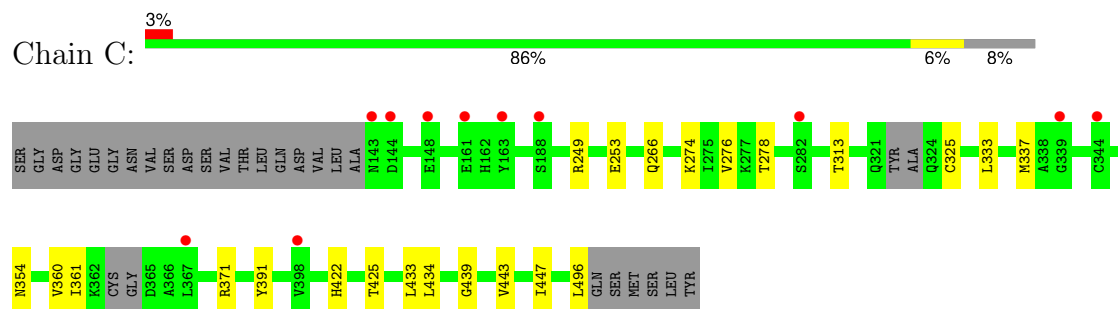
- Molecule 1: PUM-HD domain-containing protein



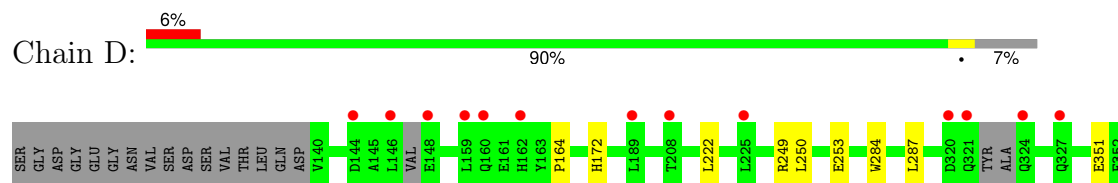
- Molecule 1: PUM-HD domain-containing protein

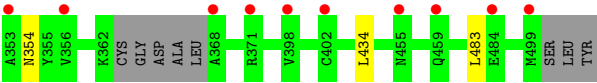


- Molecule 1: PUM-HD domain-containing protein

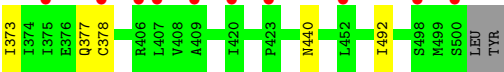
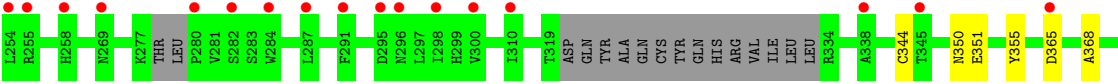
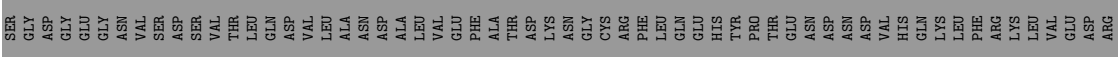


- Molecule 1: PUM-HD domain-containing protein





● Molecule 1: PUM-HD domain-containing protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	251.55Å 251.55Å 39.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.47 – 3.14 44.47 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.47-3.14) 97.7 (44.47-3.15)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.241 , 0.275 0.241 , 0.275	Depositor DCC
$R_{free}$ test set	1991 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 72.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.21	0/2894	0.46	0/3928
1	B	0.20	0/2895	0.45	0/3927
1	C	0.18	0/2683	0.41	0/3655
1	D	0.19	0/2584	0.42	0/3529
1	E	0.21	0/1835	0.47	0/2501
All	All	0.20	0/12891	0.44	0/17540

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	2847	0	2754	16	0
1	B	2850	0	2758	12	0
1	C	2641	0	2448	13	0
1	D	2547	0	2311	6	0
1	E	1813	0	1565	7	0
2	A	7	0	2	0	0
2	B	7	0	2	0	0
3	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	0	1	0
3	C	16	0	0	1	0
3	D	7	0	0	0	0
3	E	6	0	0	0	0
All	All	12805	0	11840	52	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 2.

All (52) 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:265:ASP:O	1:B:269:ASN:ND2	2.34	0.56
1:A:164:PRO:HB2	1:A:172:HIS:HB2	1.87	0.55
1:E:440:ASN:HB2	1:E:492:ILE:HD11	1.89	0.55
1:A:182:ASP:HB3	1:A:185:ILE:HB	1.92	0.51
1:B:337:MET:HE3	1:B:367:LEU:HD22	1.93	0.51
1:A:361:ILE:HG23	1:A:371:ARG:HG3	1.92	0.51
1:C:433:LEU:HD22	1:C:439:GLY:HA3	1.92	0.51
1:A:145:ALA:HB1	1:A:148:GLU:HB3	1.94	0.50
1:B:249:ARG:NH1	1:B:253:GLU:OE2	2.45	0.50
1:C:447:ILE:HD12	1:C:496:LEU:HD21	1.94	0.50
1:D:164:PRO:HB2	1:D:172:HIS:HB2	1.92	0.50
1:E:350:ASN:OD1	1:E:351:GLU:N	2.45	0.49
1:C:337:MET:HE2	1:C:360:VAL:HG22	1.95	0.49
1:B:284:TRP:HB2	1:B:287:LEU:HD12	1.93	0.49
1:C:266:GLN:NE2	3:C:601:HOH:O	2.43	0.48
1:D:249:ARG:NH1	1:D:253:GLU:OE2	2.46	0.48
1:A:286:PHE:O	1:A:290:PHE:N	2.46	0.48
1:C:361:ILE:HG23	1:C:371:ARG:HG3	1.95	0.48
1:E:365:ASP:H	1:E:368:ALA:HB2	1.79	0.48
1:C:354:ASN:HD22	1:C:391:TYR:HB3	1.78	0.47
1:C:249:ARG:NH1	1:C:253:GLU:OE2	2.47	0.47
1:A:478:ARG:NE	1:E:355:TYR:OH	2.46	0.47
1:C:434:LEU:HD23	1:C:443:VAL:HG11	1.96	0.47
1:B:358:GLN:O	1:B:362:LYS:HB2	2.16	0.46
1:B:164:PRO:HB2	1:B:172:HIS:HB2	1.96	0.46
1:B:440:ASN:HB2	1:B:492:ILE:HD11	1.97	0.45
1:B:201:ARG:NH2	3:B:702:HOH:O	2.49	0.45
1:A:276:VAL:HG11	1:A:313:THR:HA	1.97	0.45
1:D:434:LEU:HB3	1:D:483:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:NH2	1:C:325:CYS:O	2.47	0.44
1:A:192:ASN:OD1	1:A:193:MET:N	2.50	0.44
1:A:187:LEU:HD22	1:A:225:LEU:HD11	2.00	0.44
1:B:361:ILE:HG23	1:B:371:ARG:HG3	1.98	0.44
1:E:344:CYS:HB3	1:E:378:CYS:HB3	1.82	0.44
1:E:373:ILE:O	1:E:377:GLN:CB	2.67	0.43
1:A:440:ASN:HB2	1:A:492:ILE:HD11	1.99	0.43
1:B:288:VAL:HG13	1:B:336:LEU:HD13	2.00	0.43
1:A:436:HIS:O	1:A:440:ASN:ND2	2.50	0.43
1:C:276:VAL:HG11	1:C:313:THR:HA	2.00	0.43
1:B:379:LEU:HD21	1:B:395:VAL:HG12	2.01	0.43
1:D:351:GLU:O	1:D:354:ASN:ND2	2.52	0.43
1:C:422:HIS:HB3	1:C:425:THR:HB	2.01	0.42
1:A:416:PHE:O	1:A:418:GLY:N	2.54	0.41
1:E:235:ILE:O	1:E:239:ILE:HG12	2.21	0.41
1:D:222:LEU:HD13	1:D:250:LEU:HD22	2.02	0.41
1:A:350:ASN:HB3	1:A:353:ALA:HB3	2.02	0.41
1:B:318:SER:HB2	1:B:366:ALA:HB3	2.03	0.41
1:C:274:LYS:O	1:C:278:THR:HB	2.20	0.41
1:C:333:LEU:HD11	1:C:337:MET:HE3	2.02	0.41
1:D:284:TRP:HB2	1:D:287:LEU:HD12	2.03	0.41
1:A:424:ASP:OD1	1:A:424:ASP:N	2.53	0.41
1:A:151:THR:HG22	1:A:192:ASN:ND2	2.36	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 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	361/379 (95%)	348 (96%)	13 (4%)	0	100	100
1	B	362/379 (96%)	356 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	344/379 (91%)	341 (99%)	3 (1%)	0	100	100
1	D	344/379 (91%)	335 (97%)	9 (3%)	0	100	100
1	E	253/379 (67%)	240 (95%)	13 (5%)	0	100	100
All	All	1664/1895 (88%)	1620 (97%)	44 (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 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	309/341 (91%)	309 (100%)	0	100	100
1	B	309/341 (91%)	309 (100%)	0	100	100
1	C	272/341 (80%)	272 (100%)	0	100	100
1	D	247/341 (72%)	247 (100%)	0	100	100
1	E	163/341 (48%)	163 (100%)	0	100	100
All	All	1300/1705 (76%)	1300 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	169	ASN
1	A	328	HIS
1	A	358	GLN
1	B	143	ASN
1	B	236	GLN
1	B	350	ASN
1	B	445	GLN
1	B	473	HIS

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Mol	Chain	Res	Type
1	C	299	HIS
1	C	343	ASN
1	C	444	GLN
1	C	445	GLN
1	D	302	GLN
1	D	343	ASN
1	D	346	GLN
1	D	354	ASN
1	E	267	ASN
1	E	359	HIS
1	E	444	GLN
1	E	454	GLN

### 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](#)

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	MLI	A	601	-	6,6,6	1.58	1 (16%)	7,7,7	1.22	1 (14%)
2	MLI	B	601	-	6,6,6	1.43	0	7,7,7	1.41	1 (14%)

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	MLI	A	601	-	-	0/4/4/4	-
2	MLI	B	601	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	MLI	C1-C3	2.37	1.54	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	MLI	O6-C2-C1	-2.46	115.12	122.11
2	A	601	MLI	O6-C2-C1	-2.09	116.16	122.11

There are no chirality outliers.

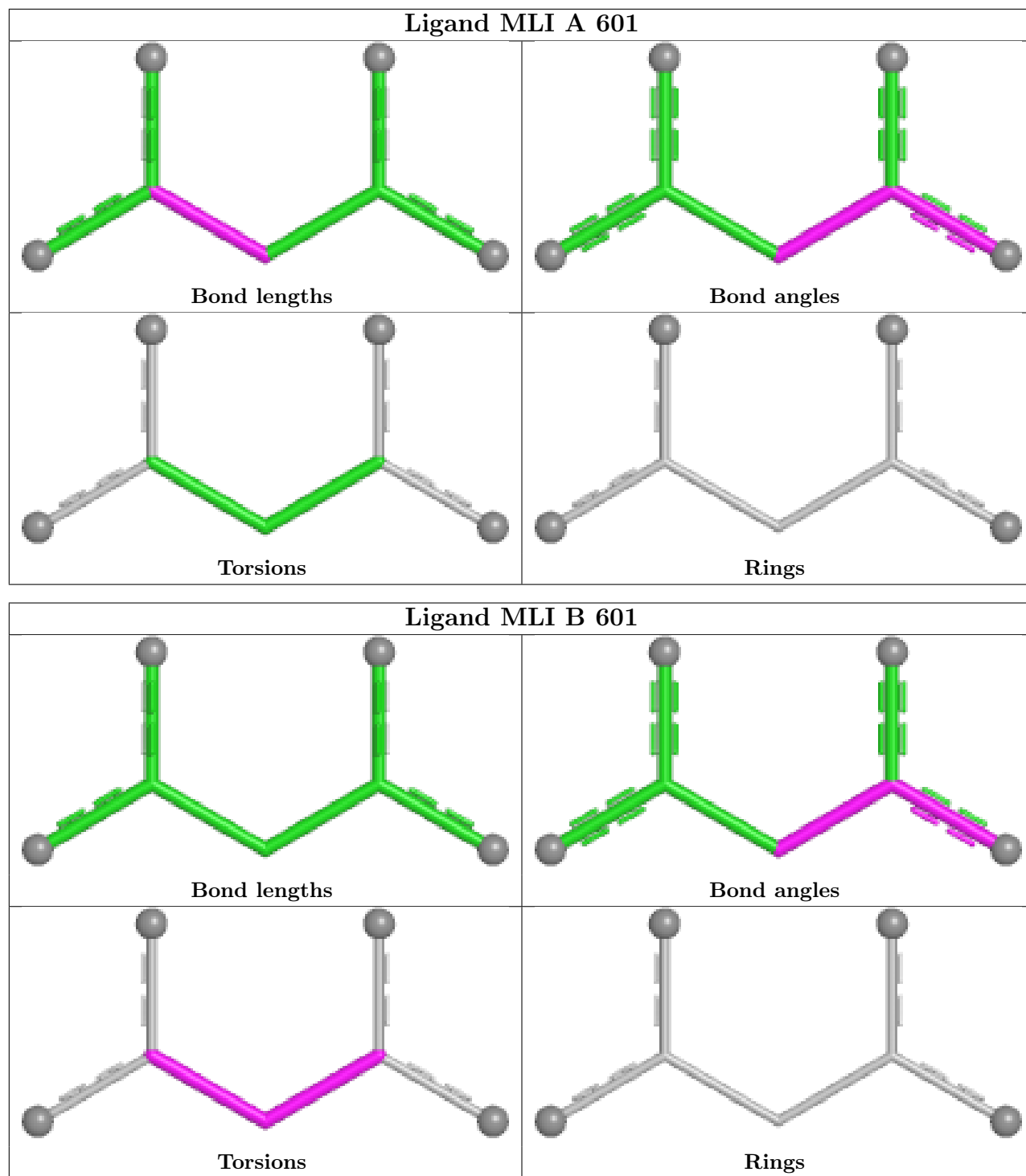
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	MLI	C3-C1-C2-O6
2	B	601	MLI	C3-C1-C2-O7
2	B	601	MLI	C2-C1-C3-O8
2	B	601	MLI	C2-C1-C3-O9

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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	363/379 (95%)	-0.15	5 (1%) 73 56	20, 41, 78, 114	0
1	B	364/379 (96%)	0.14	2 (0%) 87 75	24, 52, 87, 109	0
1	C	350/379 (92%)	0.48	11 (3%) 51 33	36, 63, 95, 111	0
1	D	352/379 (92%)	0.69	23 (6%) 26 16	43, 76, 103, 117	0
1	E	261/379 (68%)	0.97	37 (14%) 7 4	26, 86, 113, 130	0
All	All	1690/1895 (89%)	0.39	78 (4%) 38 23	20, 62, 102, 130	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	284	TRP	5.6
1	E	291	PHE	3.9
1	E	241	LYS	3.5
1	D	356	VAL	3.4
1	C	144	ASP	3.3
1	E	269	ASN	3.2
1	E	230	SER	3.1
1	D	402	CYS	3.1
1	D	148	GLU	3.0
1	E	406	ARG	2.9
1	A	423	PRO	2.9
1	E	423	PRO	2.8
1	E	500	SER	2.8
1	D	324	GLN	2.8
1	D	459	GLN	2.7
1	B	364	GLY	2.7
1	E	407	LEU	2.7
1	A	419	TYR	2.7
1	E	258	HIS	2.6
1	E	254	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	353	ALA	2.6
1	A	327	GLN	2.6
1	D	321	GLN	2.6
1	E	238	ALA	2.6
1	E	296	ASN	2.6
1	E	345	THR	2.6
1	E	420	ILE	2.5
1	C	282	SER	2.5
1	A	321	GLN	2.5
1	D	160	GLN	2.5
1	D	146	LEU	2.5
1	C	143	ASN	2.5
1	E	247	ALA	2.5
1	C	148	GLU	2.4
1	E	251	SER	2.4
1	D	162	HIS	2.3
1	D	327	GLN	2.3
1	E	239	ILE	2.3
1	E	232	CYS	2.3
1	E	298	ILE	2.3
1	C	161	GLU	2.3
1	E	365	ASP	2.3
1	D	398	VAL	2.3
1	E	300	VAL	2.3
1	D	189	LEU	2.3
1	C	163	TYR	2.3
1	E	223	TYR	2.3
1	D	371	ARG	2.3
1	D	499	MET	2.3
1	A	323	ALA	2.3
1	E	253	GLU	2.2
1	B	145	ALA	2.2
1	E	282	SER	2.2
1	E	310	ILE	2.2
1	C	398	VAL	2.2
1	E	234	VAL	2.2
1	E	287	LEU	2.2
1	D	455	ASN	2.2
1	D	208	THR	2.2
1	E	295	ASP	2.2
1	C	339	GLY	2.1
1	C	344	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	367	LEU	2.1
1	D	368	ALA	2.1
1	E	409	ALA	2.1
1	E	255	ARG	2.1
1	D	159	LEU	2.1
1	D	225	LEU	2.1
1	D	144	ASP	2.1
1	E	375	ILE	2.0
1	E	378	CYS	2.0
1	C	188	SER	2.0
1	E	452	LEU	2.0
1	E	498	SER	2.0
1	D	320	ASP	2.0
1	E	280	PRO	2.0
1	D	484	GLU	2.0
1	E	338	ALA	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

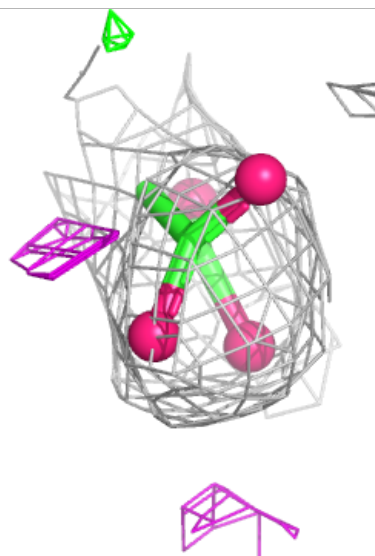
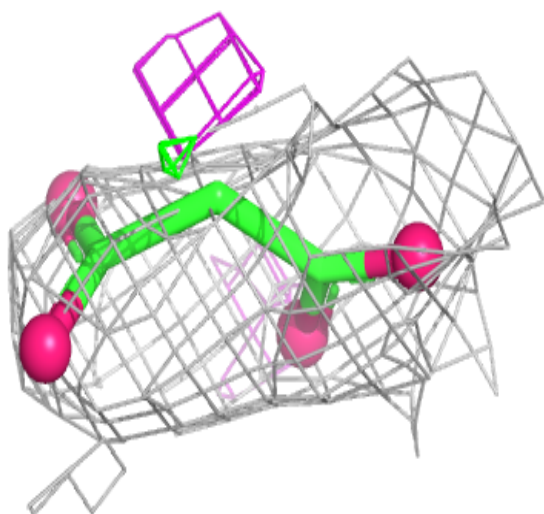
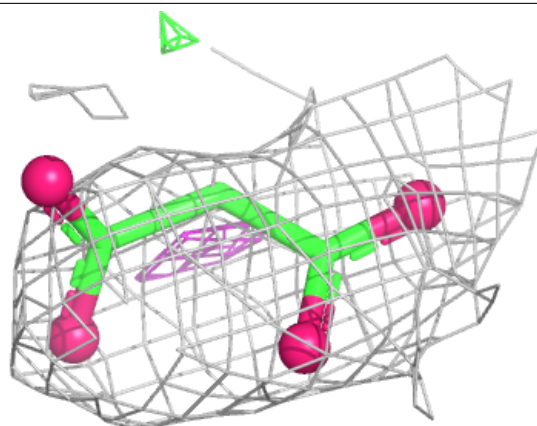
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLI	A	601	7/7	0.82	0.22	48,64,83,97	0
2	MLI	B	601	7/7	0.92	0.16	27,33,59,71	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.

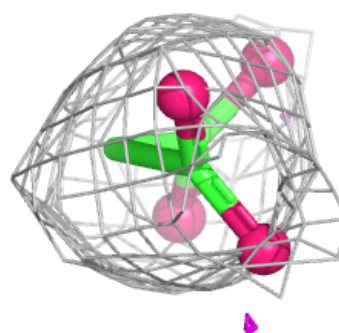
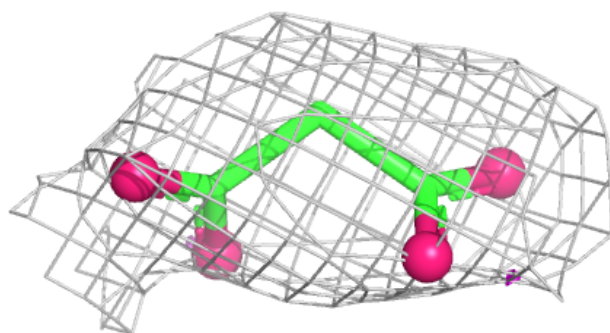
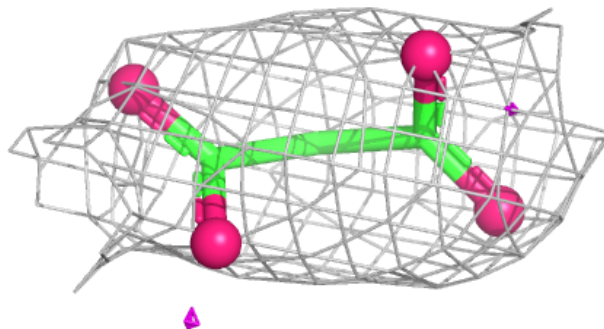
**Electron density around MLI A 601:**

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



**Electron density around MLI B 601:**

$2mF_o-DF_c$  (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.