



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2025 – 04:08 PM JST

PDB ID : 9LHU / pdb_00009lhu
Title : Crystal structure of an agose isomerase mutant 5 (TsT4Ease M5) from Thermotoga bacterium with Zn
Authors : Wei, H.L.; Wang, Y.X.; Liu, W.D.; Zhu, L.L.
Deposited on : 2025-01-13
Resolution : 2.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

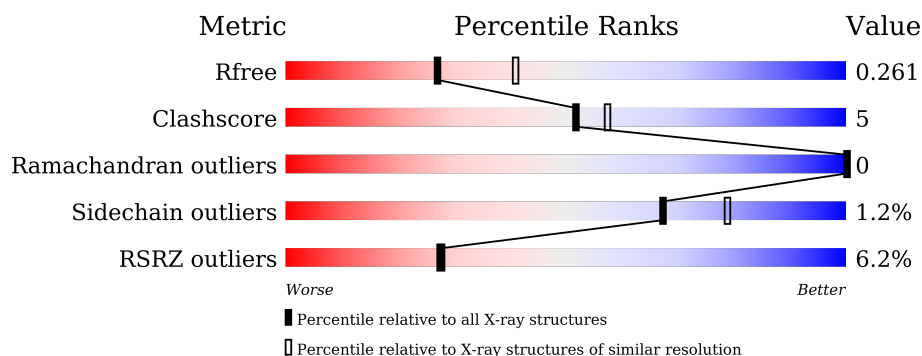
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	507	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4061 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 Tagaturonate/fructuronate epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	P	S	0	0	0
			3985	2535	680	762	1	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A3D6D9W2
A	-4	HIS	-	expression tag	UNP A0A3D6D9W2
A	-3	HIS	-	expression tag	UNP A0A3D6D9W2
A	-2	HIS	-	expression tag	UNP A0A3D6D9W2
A	-1	HIS	-	expression tag	UNP A0A3D6D9W2
A	0	HIS	-	expression tag	UNP A0A3D6D9W2
A	1	HIS	-	expression tag	UNP A0A3D6D9W2
A	138	ALA	SER	conflict	UNP A0A3D6D9W2
A	149	ALA	TRP	conflict	UNP A0A3D6D9W2
A	150	ARG	LEU	conflict	UNP A0A3D6D9W2
A	173	VAL	ALA	conflict	UNP A0A3D6D9W2
A	323	GLY	ALA	conflict	UNP A0A3D6D9W2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

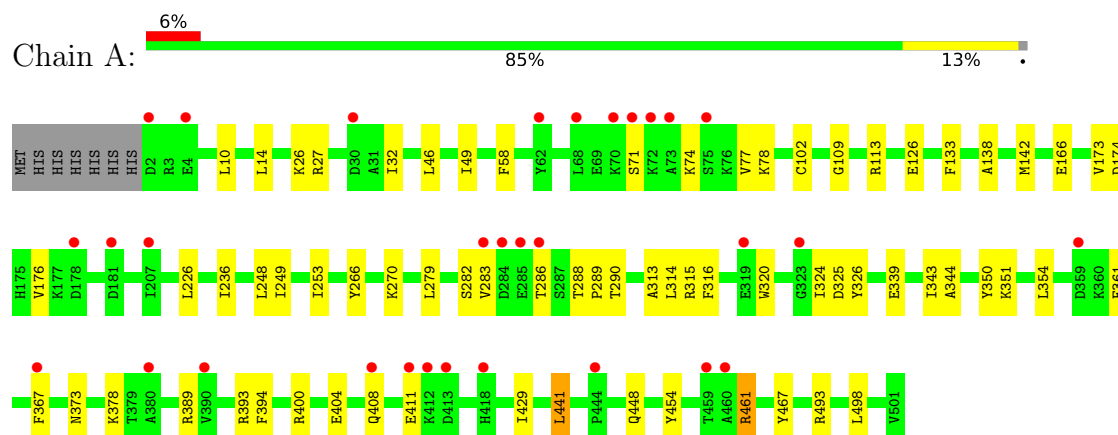
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		

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: Tagaturonate/fructuronate epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.78Å 85.53Å 108.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.88 – 2.43 56.88 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.88-2.43) 99.7 (56.88-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.218 , 0.259 0.234 , 0.261	Depositor DCC
R_{free} test set	22867 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.2	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	0.94	EDS
Total number of atoms	4061	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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

5.1 Standard geometry

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

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	0.27	0/4063	0.45	0/5494

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

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	3985	0	3871	39	0
2	A	2	0	0	0	0
3	A	74	0	0	1	0
All	All	4061	0	3871	39	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 5.

All (39) 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:325:ASP:OD1	1:A:326:TYR:N	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ARG:HA	1:A:441:LEU:HD13	1.75	0.69
1:A:27:ARG:HG2	1:A:32:ILE:HG13	1.84	0.60
1:A:266:TYR:HD1	1:A:279:LEU:HD13	1.71	0.56
1:A:393:ARG:HG2	1:A:394:PHE:CE2	2.42	0.55
1:A:461:ARG:HA	1:A:467:TYR:HA	1.91	0.52
1:A:249:ILE:O	1:A:253:ILE:HG13	2.09	0.52
1:A:400:ARG:HA	1:A:429:ILE:HD11	1.92	0.50
1:A:290:THR:HG21	1:A:314:LEU:HD22	1.95	0.49
1:A:286:THR:HG22	1:A:288:THR:H	1.78	0.48
1:A:324:ILE:HD13	1:A:448:GLN:NE2	2.28	0.48
1:A:174:ASP:OD1	1:A:378:LYS:NZ	2.47	0.48
1:A:226:LEU:HD23	1:A:248:LEU:HD23	1.94	0.48
1:A:102:CYS:SG	1:A:351:LYS:NZ	2.86	0.48
1:A:138:ALA:O	1:A:142:MET:HG3	2.14	0.48
1:A:289:PRO:HA	1:A:315:ARG:HG3	1.96	0.48
1:A:126:GLU:O	1:A:493:ARG:NH2	2.26	0.47
1:A:282:SER:HA	1:A:313:ALA:HB3	1.96	0.47
1:A:354:LEU:HB2	1:A:367:PHE:CZ	2.51	0.46
1:A:26:LYS:NZ	1:A:166:GLU:OE2	2.45	0.46
1:A:316:PHE:HA	3:A:717:HOH:O	2.16	0.46
1:A:236:ILE:HG21	1:A:343:ILE:HA	1.99	0.44
1:A:339:GLU:O	1:A:343:ILE:HG13	2.18	0.44
1:A:49:ILE:HG12	1:A:77:VAL:HG13	1.99	0.44
1:A:411:GLU:H	1:A:411:GLU:CD	2.26	0.44
1:A:344:ALA:HA	1:A:350:TYR:CZ	2.54	0.43
1:A:58:PHE:O	1:A:78:LYS:NZ	2.47	0.43
1:A:404:GLU:O	1:A:408:GLN:HG2	2.19	0.43
1:A:109:GLY:HA2	1:A:133:PHE:HB2	2.01	0.42
1:A:270:LYS:HB3	1:A:270:LYS:HE2	1.93	0.42
1:A:411:GLU:OE2	1:A:411:GLU:N	2.43	0.42
1:A:283:VAL:O	1:A:283:VAL:HG12	2.20	0.42
1:A:320:TRP:CZ3	1:A:354:LEU:HD11	2.55	0.42
1:A:373:ASN:OD1	1:A:373:ASN:N	2.50	0.41
1:A:173:VAL:HG22	1:A:176:VAL:HG22	2.03	0.41
1:A:10:LEU:O	1:A:14:LEU:HD12	2.21	0.41
1:A:361:PHE:CD1	1:A:498:LEU:HD12	2.57	0.40
1:A:113:ARG:HD3	1:A:454:TYR:CD2	2.56	0.40
1:A:411:GLU:CD	1:A:411:GLU:N	2.79	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	497/507 (98%)	481 (97%)	16 (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	423/440 (96%)	418 (99%)	5 (1%)	67	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	71	SER
1	A	74	LYS
1	A	441	LEU
1	A	461	ARG

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	137	GLN
1	A	408	GLN
1	A	462	ASN

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Mol	Chain	Res	Type
1	A	487	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	SEP	A	358	1	8,9,10	0.70	0	8,12,14	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	358	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	358	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	499/507 (98%)	0.63	31 (6%) 28 27	44, 63, 89, 122	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	LYS	3.2
1	A	284	ASP	2.9
1	A	73	ALA	2.9
1	A	68	LEU	2.8
1	A	413	ASP	2.8
1	A	70	LYS	2.7
1	A	71	SER	2.7
1	A	2	ASP	2.6
1	A	286	THR	2.6
1	A	444	PRO	2.5
1	A	411	GLU	2.5
1	A	207	ILE	2.4
1	A	30	ASP	2.4
1	A	412	LYS	2.4
1	A	178	ASP	2.4
1	A	181	ASP	2.4
1	A	367	PHE	2.4
1	A	283	VAL	2.4
1	A	380	ALA	2.4
1	A	459	THR	2.4
1	A	359	ASP	2.3
1	A	408	GLN	2.3
1	A	323	GLY	2.3
1	A	390	VAL	2.2
1	A	62	TYR	2.1
1	A	285	GLU	2.1
1	A	460	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	319	GLU	2.1
1	A	75	SER	2.0
1	A	418	HIS	2.0
1	A	4	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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(Å ²)	Q<0.9
1	SEP	A	358	10/11	0.71	0.34	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

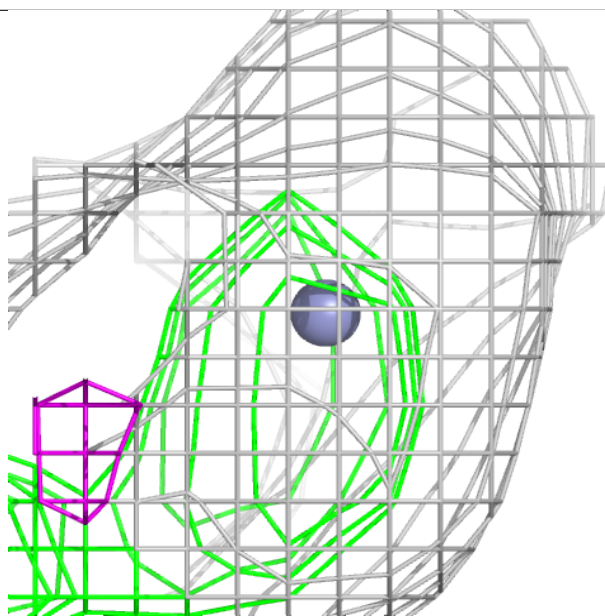
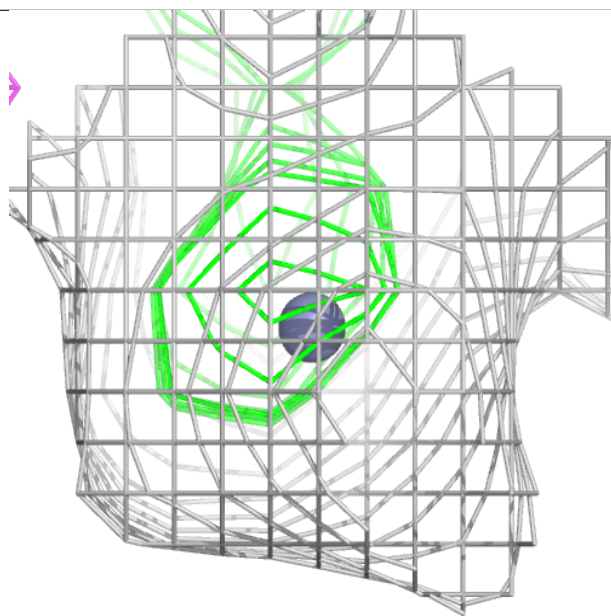
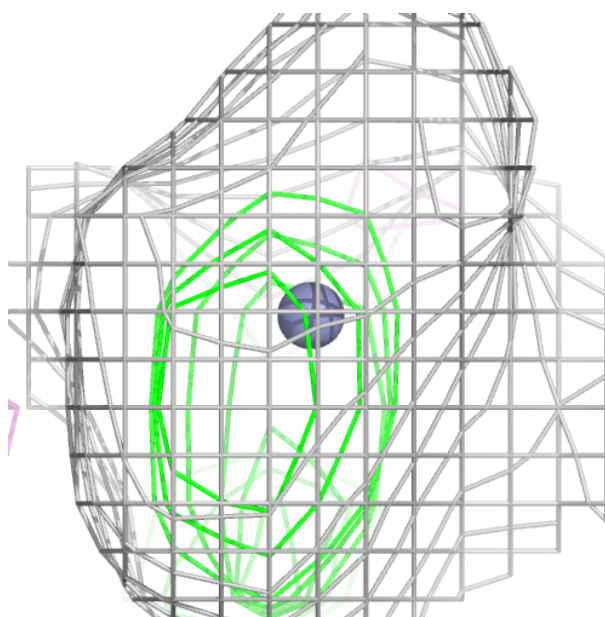
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	601	1/1	0.89	0.17	147,147,147,147	0
2	ZN	A	602	1/1	0.95	0.06	75,75,75,75	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.

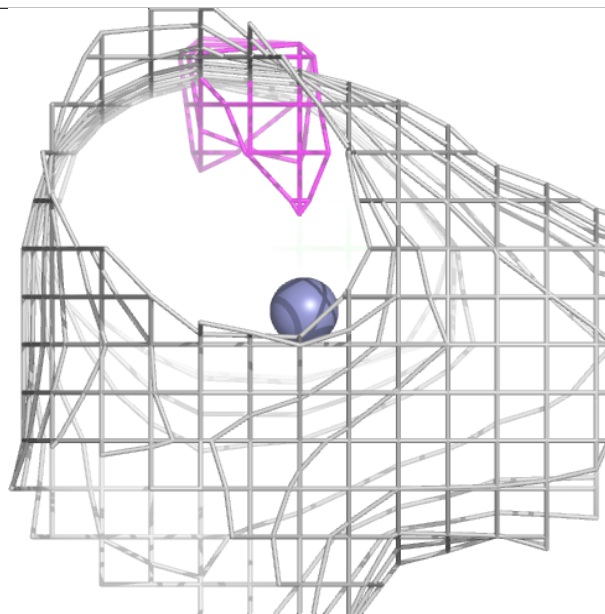
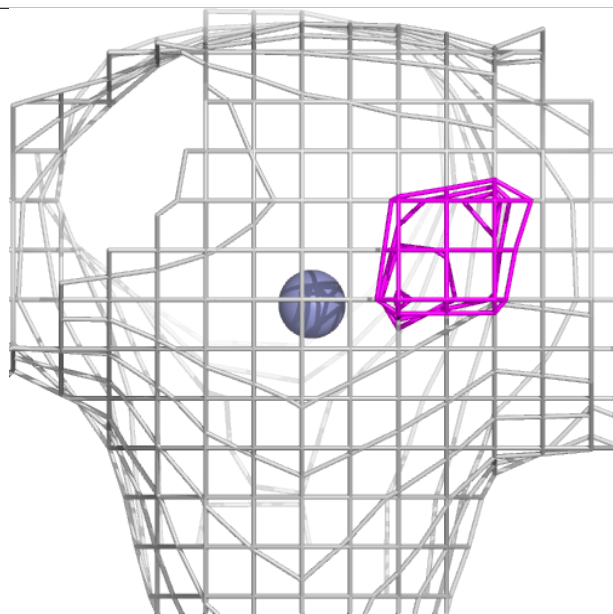
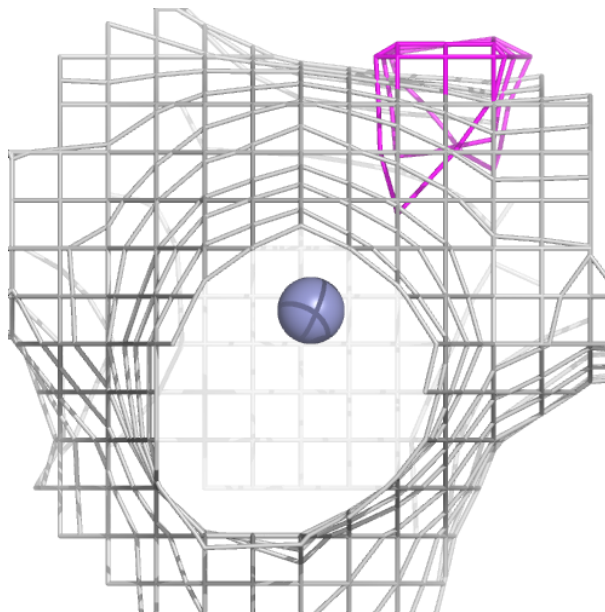
Electron density around ZN A 601:

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



Electron density around ZN A 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.