



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 9KOV / pdb\_00009kov  
Title : Crystal structure of an amidohydrolase mutant from Thermonema  
Authors : Xu, N.N.; Jian, G.; Wei, H.L.; Chen, Y.Y.; Wu, P.; Han, X.; Liu, W.  
Deposited on : 2024-11-21  
Resolution : 2.56 Å(reported)

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

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<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

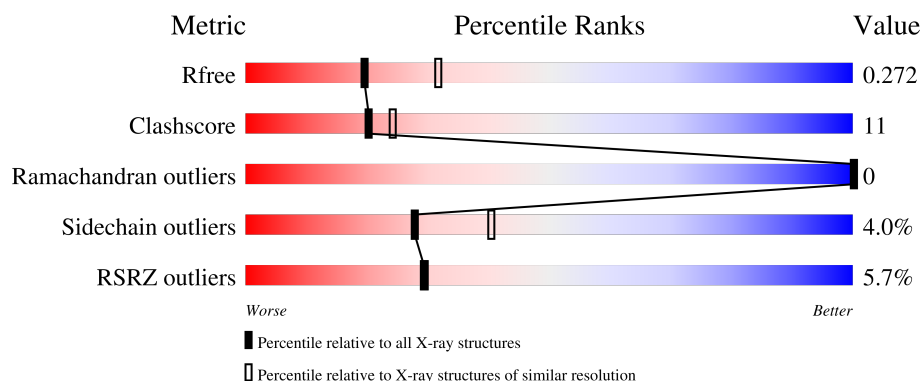
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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))
$R_{free}$	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	422	 4% 68% 24% • 8%
1	B	422	 5% 63% 24% • 11%
1	C	422	 4% 64% 23% • 12%
1	D	422	 4% 69% 19% 12%
1	E	422	 7% 68% 23% • 8%

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Mol	Chain	Length	Quality of chain
1	F	422	<div><div></div><div>5%</div><div>62%</div><div>27%</div><div>10%</div></div>
1	G	422	<div><div></div><div>3%</div><div>69%</div><div>20%</div><div>10%</div></div>
1	H	422	<div><div></div><div>10%</div><div>66%</div><div>21%</div><div>11%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22609 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 trum-mut.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2903	1832	512	546	13			
1	B	375	Total	C	N	O	S	0	0	0
			2811	1769	496	533	13			
1	C	373	Total	C	N	O	S	0	0	0
			2777	1749	492	523	13			
1	D	372	Total	C	N	O	S	0	0	0
			2748	1731	483	521	13			
1	E	389	Total	C	N	O	S	0	0	0
			2838	1796	495	534	13			
1	F	378	Total	C	N	O	S	0	0	0
			2768	1746	485	524	13			
1	G	379	Total	C	N	O	S	0	0	0
			2796	1758	488	537	13			
1	H	376	Total	C	N	O	S	0	0	0
			2745	1729	480	523	13			

- 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	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	35	Total	O	0	0
			35	35		

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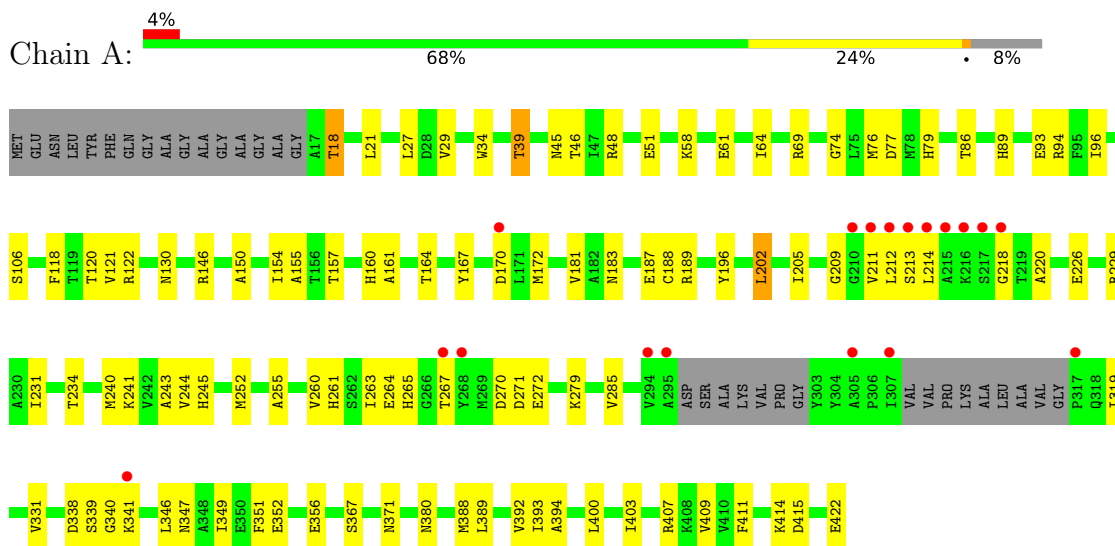
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	28	Total 28	O 28	0	0
3	D	28	Total 28	O 28	0	0
3	E	22	Total 22	O 22	0	0
3	F	23	Total 23	O 23	0	0
3	G	35	Total 35	O 35	0	0
3	H	20	Total 20	O 20	0	0

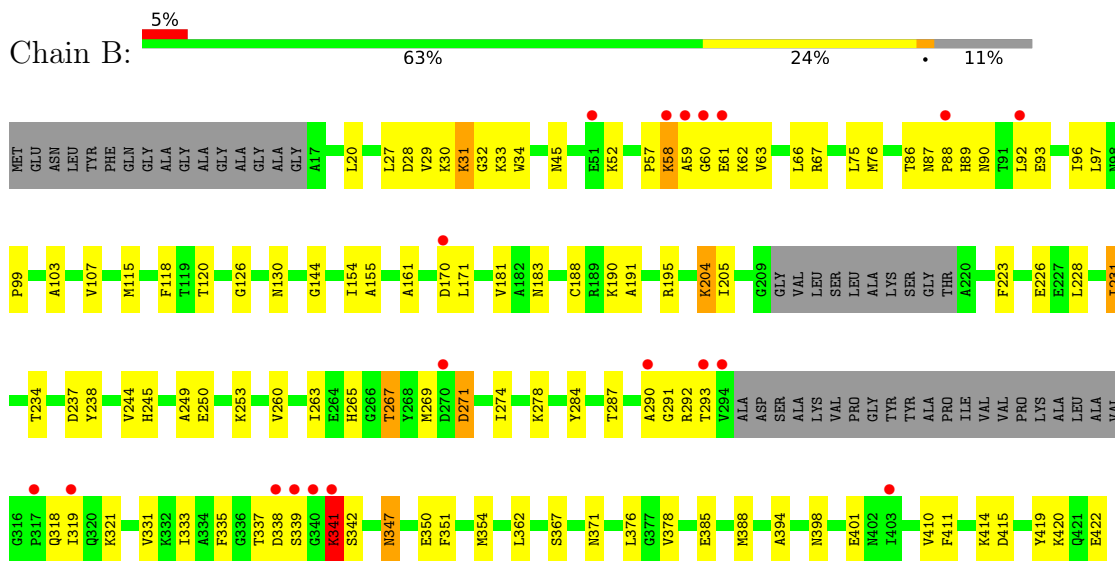
### 3 Residue-property plots [i](#)

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: trum-mut

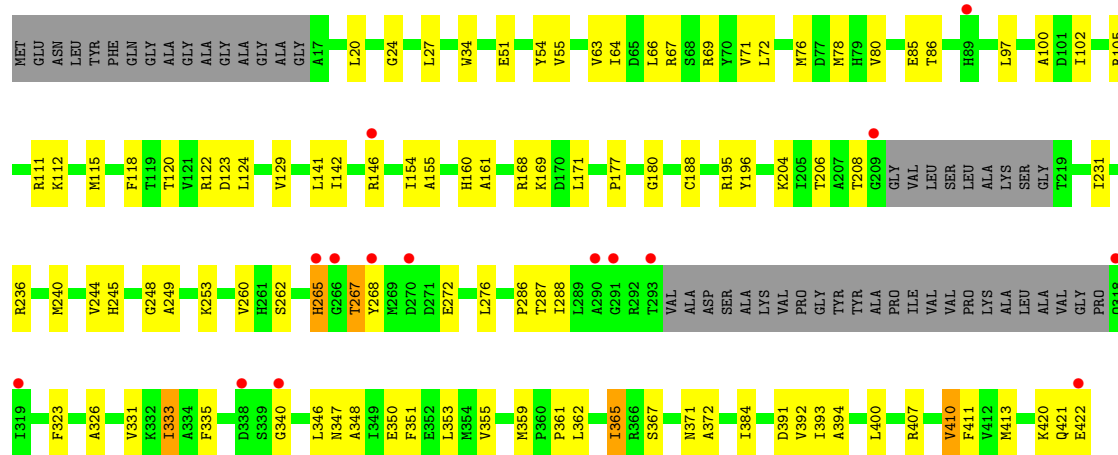


- Molecule 1: trum-mut

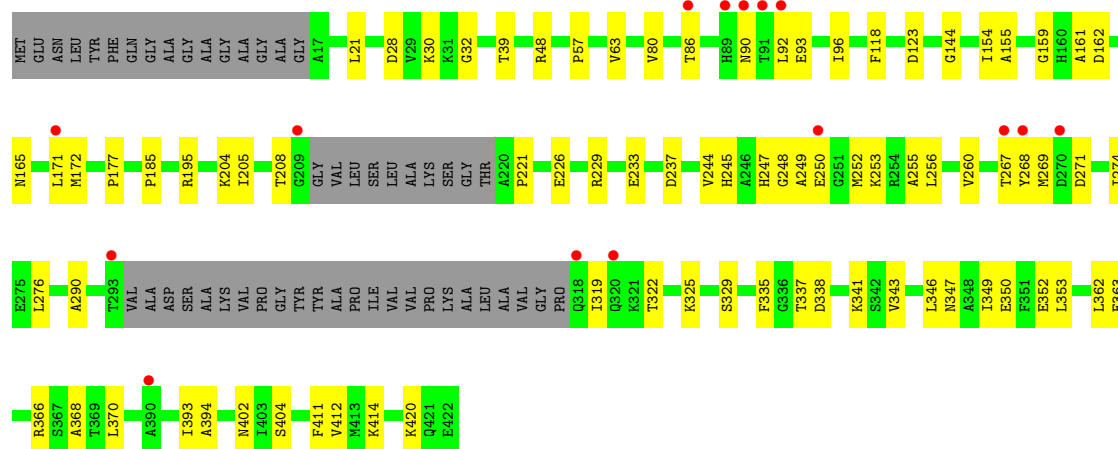


- Molecule 1: trum-mut

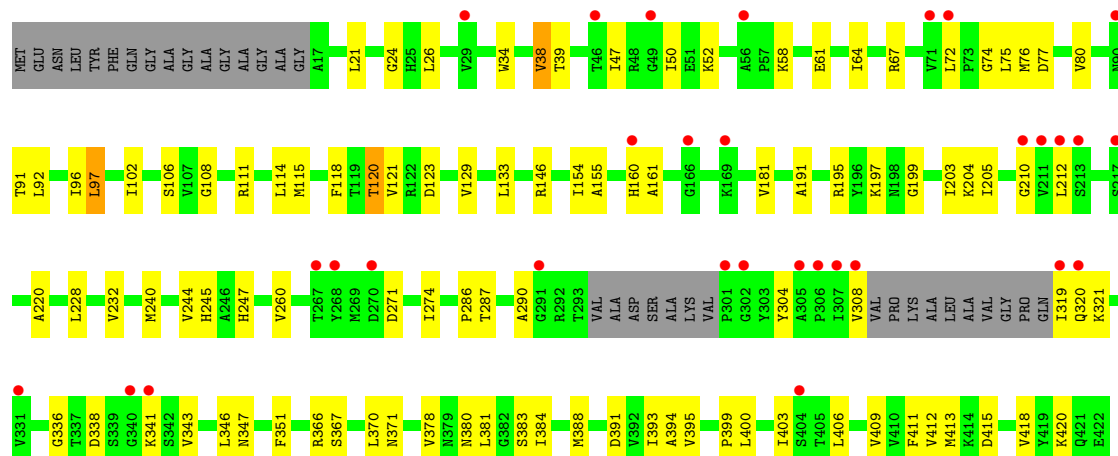




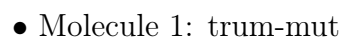
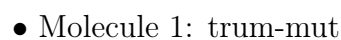
• Molecule 1: trum-mut



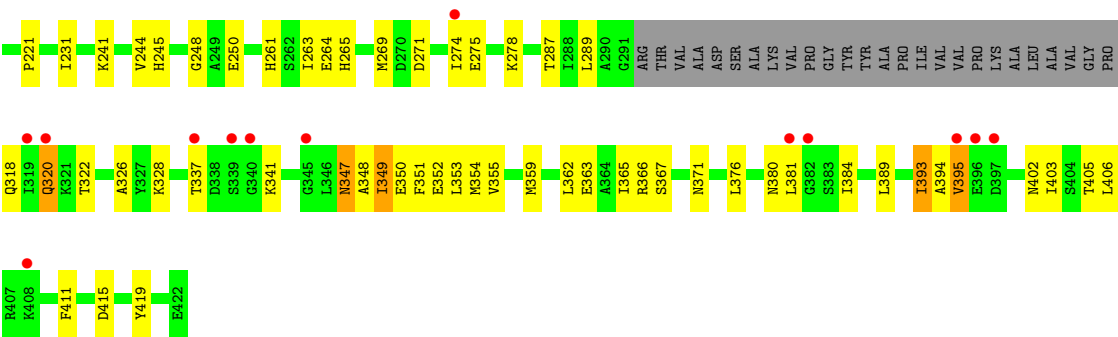
• Molecule 1: trum-mut



• Molecule 1: trum-mut







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.64Å 205.75Å 105.27Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	49.92 – 2.56 49.92 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.92-2.56) 99.5 (49.92-2.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, $R_{free}$	0.222 , 0.264 0.242 , 0.272	Depositor DCC
$R_{free}$ test set	5000 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	22609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/2953	0.59	2/3998 (0.1%)
1	B	0.37	0/2858	0.70	5/3865 (0.1%)
1	C	0.36	0/2823	0.65	0/3820
1	D	0.31	0/2793	0.67	2/3784 (0.1%)
1	E	0.23	0/2888	0.52	0/3920
1	F	0.34	0/2815	0.65	2/3814 (0.1%)
1	G	0.30	0/2842	0.60	2/3852 (0.1%)
1	H	0.32	0/2791	0.61	1/3786 (0.0%)
All	All	0.32	0/22763	0.63	14/30839 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LYS	N-CA-C	-10.20	100.24	111.36
1	A	340	GLY	N-CA-C	-9.33	103.59	114.69
1	B	341	LYS	N-CA-C	-8.07	102.48	111.28
1	B	292	ARG	N-CA-C	-8.00	102.64	111.36
1	H	341	LYS	N-CA-C	-7.26	103.37	111.28

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	2903	0	2902	60	0
1	B	2811	0	2813	72	0
1	C	2777	0	2770	63	0
1	D	2748	0	2716	48	0
1	E	2838	0	2797	67	0
1	F	2768	0	2734	81	0
1	G	2796	0	2752	54	0
1	H	2745	0	2686	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	0	0	0
3	B	35	0	0	1	0
3	C	28	0	0	2	0
3	D	28	0	0	0	0
3	E	22	0	0	0	0
3	F	23	0	0	2	0
3	G	35	0	0	0	0
3	H	20	0	0	2	0
All	All	22609	0	22170	505	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 11.

The worst 5 of 505 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:E:38:VAL:HB	1:E:50:ILE:HD11	1.50	0.92
1:H:289:LEU:HD23	1:H:337:THR:HG23	1.52	0.92
1:F:76:MET:HG2	1:F:120:THR:HB	1.48	0.92
1:D:86:THR:HA	1:D:90:ASN:HD21	1.40	0.87
1:A:394:ALA:HB3	1:A:411:PHE:HB3	1.58	0.84

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	384/422 (91%)	372 (97%)	12 (3%)	0	100	100
1	B	369/422 (87%)	357 (97%)	12 (3%)	0	100	100
1	C	367/422 (87%)	361 (98%)	6 (2%)	0	100	100
1	D	366/422 (87%)	360 (98%)	6 (2%)	0	100	100
1	E	383/422 (91%)	368 (96%)	15 (4%)	0	100	100
1	F	372/422 (88%)	361 (97%)	11 (3%)	0	100	100
1	G	373/422 (88%)	363 (97%)	10 (3%)	0	100	100
1	H	370/422 (88%)	360 (97%)	10 (3%)	0	100	100
All	All	2984/3376 (88%)	2902 (97%)	82 (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	294/323 (91%)	281 (96%)	13 (4%)	25	37
1	B	288/323 (89%)	266 (92%)	22 (8%)	12	17
1	C	281/323 (87%)	270 (96%)	11 (4%)	28	41
1	D	275/323 (85%)	270 (98%)	5 (2%)	51	67
1	E	281/323 (87%)	274 (98%)	7 (2%)	42	58
1	F	276/323 (85%)	264 (96%)	12 (4%)	26	38
1	G	281/323 (87%)	271 (96%)	10 (4%)	31	44
1	H	272/323 (84%)	261 (96%)	11 (4%)	28	40
All	All	2248/2584 (87%)	2157 (96%)	91 (4%)	28	40

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	415	ASP
1	G	36	GLU
1	F	62	LYS
1	F	288	ILE
1	G	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	344	HIS
1	H	25	HIS
1	H	347	ASN
1	C	421	GLN
1	C	245	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](#)

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 [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, 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	390/422 (92%)	0.51	18 (4%) 37 38	13, 33, 68, 109	0
1	B	375/422 (88%)	0.52	19 (5%) 33 34	17, 33, 61, 86	0
1	C	373/422 (88%)	0.50	15 (4%) 42 43	21, 35, 59, 89	0
1	D	372/422 (88%)	0.48	15 (4%) 42 43	14, 31, 62, 116	0
1	E	389/422 (92%)	0.76	31 (7%) 18 18	21, 42, 66, 114	0
1	F	378/422 (89%)	0.74	22 (5%) 29 29	19, 44, 65, 87	0
1	G	379/422 (89%)	0.41	11 (2%) 53 55	15, 30, 61, 101	0
1	H	376/422 (89%)	0.90	41 (10%) 10 10	21, 47, 82, 102	0
All	All	3032/3376 (89%)	0.60	172 (5%) 29 29	13, 36, 69, 116	0

The worst 5 of 172 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	VAL	5.5
1	H	397	ASP	5.3
1	A	215	ALA	4.9
1	B	340	GLY	4.7
1	E	267	THR	4.7

### 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

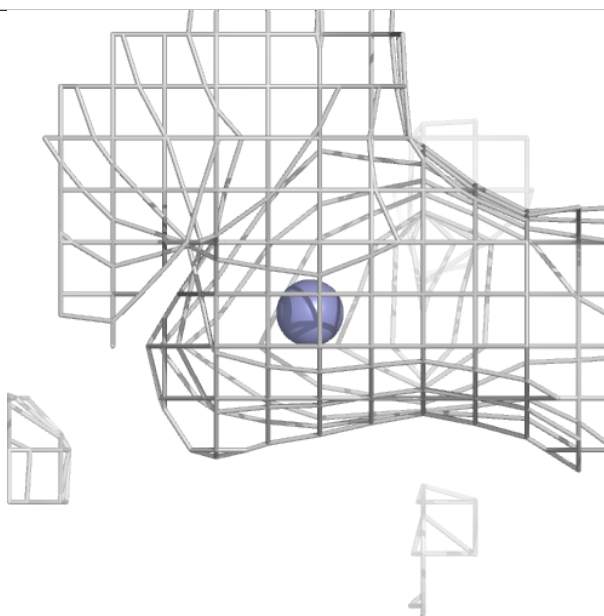
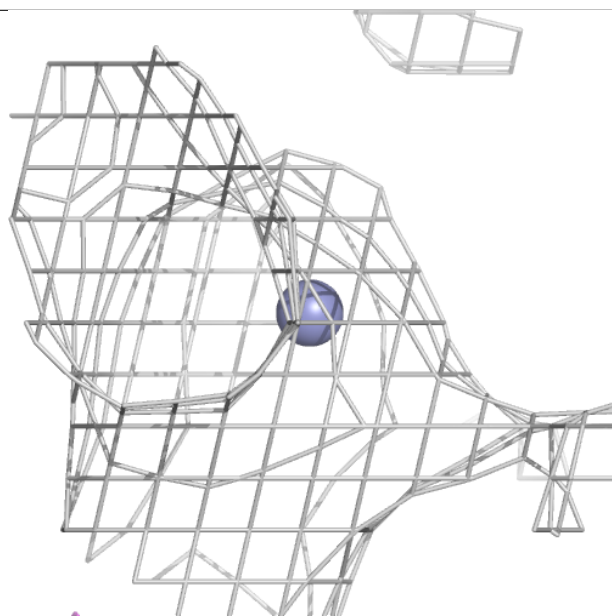
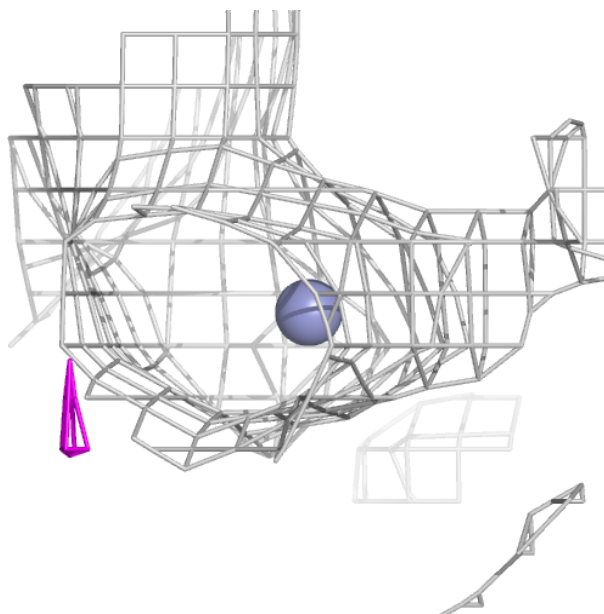
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

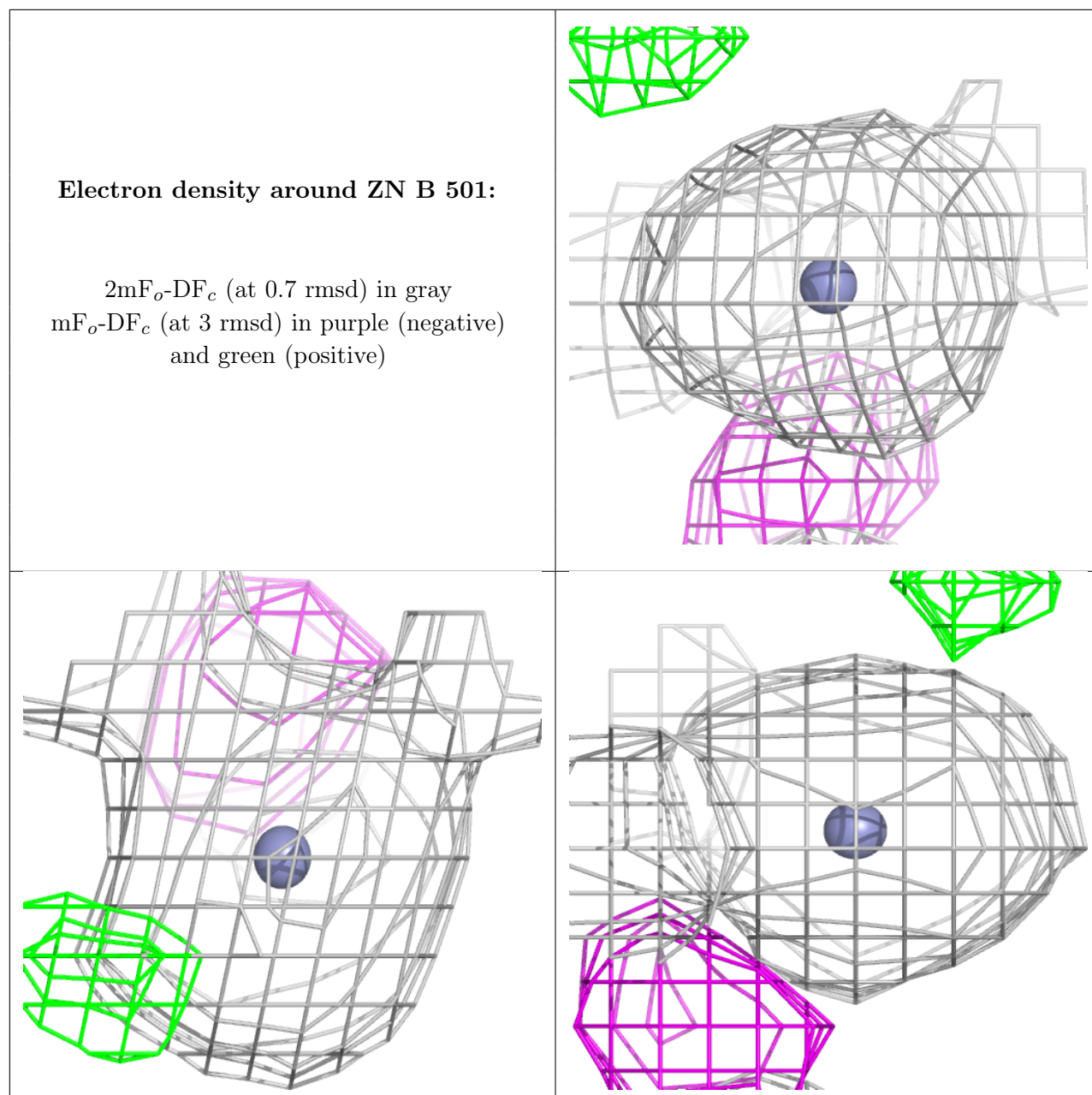
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	501	1/1	0.85	0.22	172,172,172,172	0
2	ZN	B	501	1/1	0.88	0.11	102,102,102,102	0

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 501:**

$2mF_o-DF_c$  (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.