



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 04:01 PM EDT

PDB ID : 7BZ3  
Title : The mutant variant of PNGM-1. H257 was substituted for alanine to study substrate binding.  
Authors : Park, Y.S.; Kang, L.W.; Lee, J.H.  
Deposited on : 2020-04-26  
Resolution : 2.00 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

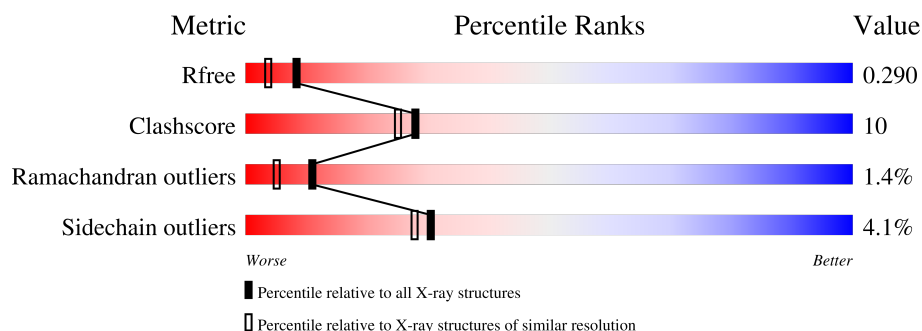
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	372	
1	B	372	
1	C	372	
1	D	372	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11589 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 Metallo-beta-lactamase PNGM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2710	1717	466	508	19			
1	B	344	Total	C	N	O	S	0	0	0
			2718	1721	468	510	19			
1	C	335	Total	C	N	O	S	0	0	0
			2642	1675	453	497	17			
1	D	324	Total	C	N	O	S	0	0	0
			2570	1631	442	480	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
B	257	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
C	257	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
D	257	ALA	HIS	engineered mutation	UNP A0A2U8UYM6

- Molecule 2 is ZINC ION (three-letter code: 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		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

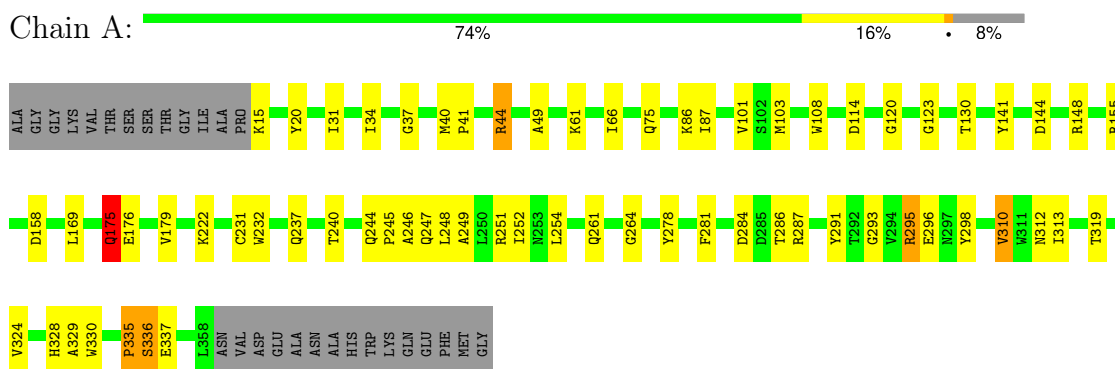
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	237	Total 237	O 237	0	0
3	B	247	Total 247	O 247	0	0
3	C	227	Total 227	O 227	0	0
3	D	230	Total 230	O 230	0	0

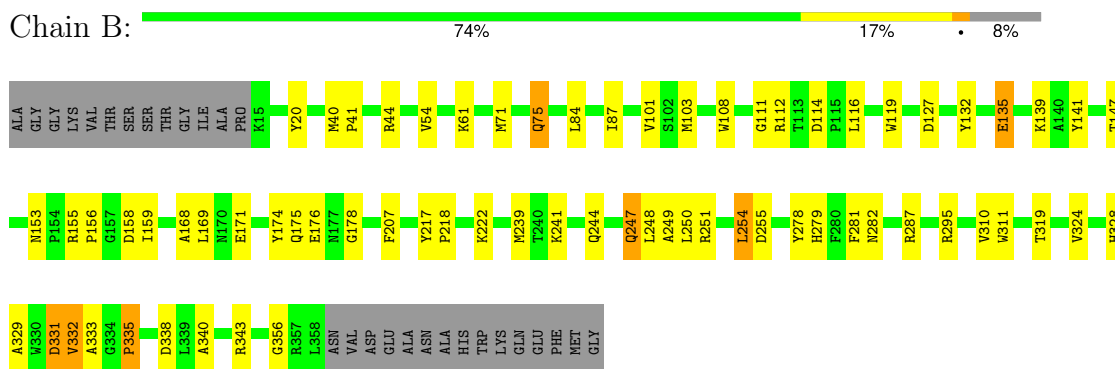
### 3 Residue-property plots

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.

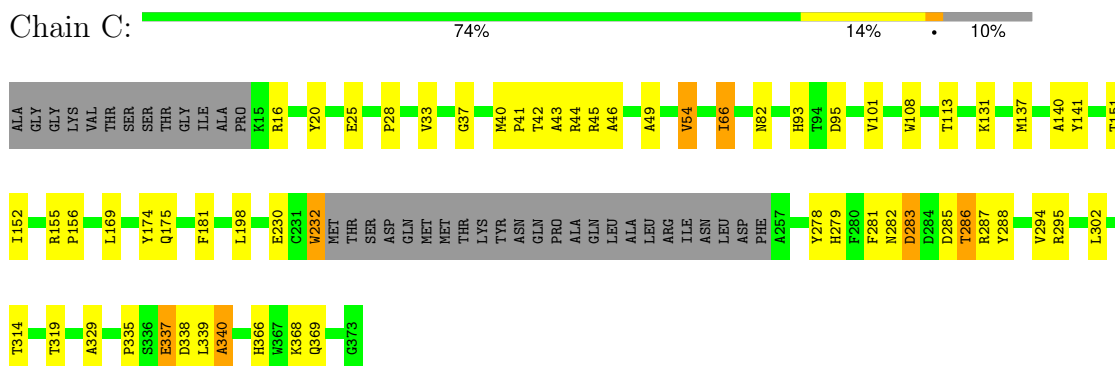
#### • Molecule 1: Metallo-beta-lactamase PNGM-1



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● Molecule 1: Metallo-beta-lactamase PNGM-1

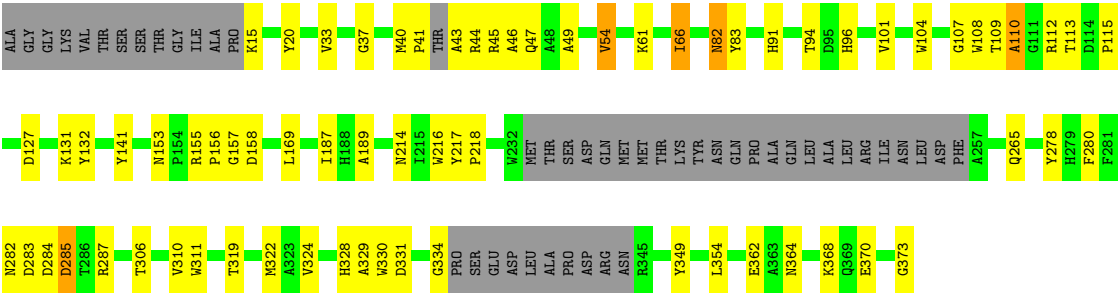
Chain D: 

68%

18%

•

13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.79Å 143.74Å 79.76Å 90.00° 111.82° 90.00°	Depositor
Resolution (Å)	48.69 – 2.00 48.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.69-2.00) 97.2 (48.64-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.229 , 0.286 0.234 , 0.290	Depositor DCC
$R_{free}$ test set	5529 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 20.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.447 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.14% 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	0.77	1/2788 (0.0%)	0.97	4/3802 (0.1%)
1	B	0.78	0/2797	0.94	4/3814 (0.1%)
1	C	0.75	0/2722	0.95	3/3713 (0.1%)
1	D	0.77	0/2646	0.93	1/3603 (0.0%)
All	All	0.77	1/10953 (0.0%)	0.95	12/14932 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLY	C-O	5.16	1.31	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	45	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	C	295	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	287	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	295	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	295	ARG	NE-CZ-NH1	5.56	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	175	GLN	CB-CA-C	5.22	120.85	110.40
1	A	295	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	335	PRO	N-CA-CB	5.17	109.50	103.30
1	C	45	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	135	GLU	CB-CA-C	5.09	120.58	110.40
1	A	287	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	SER	Peptide
1	C	46	ALA	Peptide
1	D	46	ALA	Peptide

## 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	2710	0	2543	60	0
1	B	2718	0	2550	52	0
1	C	2642	0	2456	48	0
1	D	2570	0	2396	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	237	0	0	25	1
3	B	247	0	0	15	1
3	C	227	0	0	14	1
3	D	230	0	0	23	1
All	All	11589	0	9945	204	2

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 10.

All (204) 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:244:GLN:HB3	3:A:529:HOH:O	1.42	1.12
1:A:328:HIS:CB	3:A:671:HOH:O	2.02	1.06
1:A:319:THR:HB	3:A:533:HOH:O	1.56	1.05
1:D:334:GLY:C	3:D:555:HOH:O	1.96	1.03
1:A:86:LYS:HE2	3:A:635:HOH:O	1.58	1.00
1:B:249:ALA:HA	3:B:703:HOH:O	1.60	1.00
1:C:40:MET:SD	3:C:687:HOH:O	2.21	0.98
1:B:282:ASN:OD1	3:B:501:HOH:O	1.81	0.98
1:A:328:HIS:CB	3:B:662:HOH:O	2.12	0.97
1:B:44:ARG:HD2	1:D:329:ALA:O	1.66	0.95
1:D:331:ASP:HB2	3:D:629:HOH:O	1.66	0.94
1:A:44:ARG:HD2	1:C:329:ALA:O	1.68	0.93
1:D:43:ALA:HB1	3:D:679:HOH:O	1.68	0.93
1:D:373:GLY:O	3:D:501:HOH:O	1.85	0.91
1:C:40:MET:HB3	1:C:41:PRO:HD2	1.55	0.87
1:C:232:TRP:CH2	3:C:530:HOH:O	2.32	0.81
1:C:285:ASP:O	1:C:286:THR:HG23	1.83	0.79
1:A:312:ASN:HB2	3:A:533:HOH:O	1.83	0.78
1:A:114:ASP:OD1	1:A:155:ARG:NH2	2.16	0.77
1:B:249:ALA:HA	3:B:507:HOH:O	1.86	0.75
1:D:368:LYS:HE3	3:D:655:HOH:O	1.84	0.75
1:D:368:LYS:CE	3:D:655:HOH:O	2.34	0.74
1:A:75:GLN:NE2	1:A:330:TRP:H	1.84	0.74
1:A:244:GLN:HA	3:A:545:HOH:O	1.86	0.73
1:C:175:GLN:NE2	3:C:501:HOH:O	2.12	0.73
1:A:293:GLY:O	3:A:502:HOH:O	2.06	0.73
1:D:115:PRO:HB3	1:D:158:ASP:HB2	1.70	0.73
1:B:332:VAL:HG13	1:B:332:VAL:O	1.89	0.73
1:B:44:ARG:HD3	1:B:281:PHE:CZ	2.25	0.70
1:A:245:PRO:HD2	3:A:529:HOH:O	1.90	0.70
1:D:43:ALA:CB	3:D:679:HOH:O	2.34	0.68
1:B:75:GLN:HG2	1:B:329:ALA:HA	1.77	0.67
1:A:319:THR:HG21	3:A:691:HOH:O	1.95	0.66
1:D:283:ASP:O	1:D:285:ASP:N	2.29	0.64
1:C:25:GLU:HG3	3:C:688:HOH:O	1.97	0.64
1:A:75:GLN:HE21	1:A:330:TRP:N	1.95	0.64
1:A:244:GLN:CB	3:A:529:HOH:O	2.16	0.63
1:D:331:ASP:CB	3:D:629:HOH:O	2.33	0.63
1:B:331:ASP:HA	3:B:634:HOH:O	1.98	0.63
1:A:75:GLN:HG2	1:A:328:HIS:O	1.99	0.63
1:C:366:HIS:HB2	3:C:520:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:HG22	1:D:54:VAL:HG13	1.82	0.62
1:C:82:ASN:HD22	1:C:335:PRO:HG2	1.64	0.62
1:A:264:GLY:HA3	3:A:530:HOH:O	1.99	0.61
1:B:54:VAL:HG21	1:B:207:PHE:CZ	2.36	0.60
1:A:291:TYR:CZ	1:A:295:ARG:HD2	2.36	0.60
1:D:280:PHE:O	3:D:502:HOH:O	2.16	0.60
1:D:43:ALA:CA	3:D:679:HOH:O	2.50	0.60
1:D:47:GLN:NE2	3:D:502:HOH:O	2.35	0.60
1:B:40:MET:HB3	1:B:41:PRO:HD2	1.84	0.60
1:B:75:GLN:HE21	1:B:75:GLN:CA	2.15	0.59
1:A:75:GLN:HG2	1:A:329:ALA:HA	1.83	0.59
1:C:20:TYR:CD2	1:D:20:TYR:HB3	2.37	0.59
1:A:248:LEU:O	1:A:252:ILE:HG13	2.01	0.59
1:C:108:TRP:CD1	1:C:108:TRP:O	2.55	0.59
1:D:37:GLY:HA3	1:D:49:ALA:O	2.02	0.59
1:B:114:ASP:OD1	1:B:155:ARG:NH2	2.35	0.58
1:C:42:THR:OG1	1:C:43:ALA:O	2.21	0.58
1:B:332:VAL:O	1:B:332:VAL:CG1	2.53	0.57
1:C:155:ARG:HB3	1:C:155:ARG:CZ	2.34	0.57
1:C:198:LEU:C	1:C:198:LEU:HD23	2.25	0.57
1:C:335:PRO:HB3	1:C:337:GLU:OE1	2.05	0.57
1:A:179:VAL:CG2	3:A:503:HOH:O	2.53	0.56
1:B:153:ASN:HB2	1:B:340:ALA:O	2.06	0.56
1:B:54:VAL:HG21	1:B:207:PHE:HZ	1.69	0.55
1:B:249:ALA:CB	3:B:703:HOH:O	2.53	0.55
1:C:181:PHE:CZ	1:C:198:LEU:HD12	2.41	0.55
1:C:40:MET:HB3	1:C:41:PRO:CD	2.32	0.55
1:A:34:ILE:HG13	1:A:310:VAL:HB	1.89	0.55
1:B:101:VAL:HG22	1:D:94:THR:HG21	1.89	0.54
1:A:296:GLU:HB2	3:A:502:HOH:O	2.07	0.54
1:A:61:LYS:NZ	3:A:507:HOH:O	2.39	0.54
1:B:178:GLY:HA2	3:B:705:HOH:O	2.08	0.54
1:B:241:LYS:HG3	1:D:330:TRP:CZ3	2.42	0.54
1:A:284:ASP:CG	3:A:536:HOH:O	2.45	0.53
1:D:66:ILE:HG23	1:D:66:ILE:O	2.08	0.53
1:A:232:TRP:HA	3:A:504:HOH:O	2.09	0.53
1:A:87:ILE:HD11	1:A:103:MET:HG2	1.91	0.53
1:B:247:GLN:HG3	1:B:248:LEU:N	2.23	0.52
1:C:232:TRP:HH2	3:C:530:HOH:O	1.82	0.52
1:B:249:ALA:CA	3:B:703:HOH:O	2.36	0.52
1:B:251:ARG:HD2	3:B:632:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ARG:HA	3:C:605:HOH:O	2.10	0.52
1:D:40:MET:HB3	1:D:41:PRO:HD2	1.91	0.52
1:C:319:THR:HG22	3:C:542:HOH:O	2.09	0.52
1:D:127:ASP:HA	1:D:132:TYR:CG	2.45	0.52
1:C:279:HIS:CE1	3:C:530:HOH:O	2.62	0.51
1:C:43:ALA:HB1	3:C:633:HOH:O	2.11	0.51
1:B:331:ASP:O	1:B:332:VAL:HB	2.09	0.51
1:A:284:ASP:OD2	1:D:306:THR:HG21	2.10	0.51
1:B:139:LYS:HE3	3:B:552:HOH:O	2.10	0.51
1:A:108:TRP:CE3	1:A:148:ARG:HD2	2.45	0.51
1:B:116:LEU:HB2	1:B:159:ILE:HG12	1.93	0.51
1:D:364:ASN:O	1:D:368:LYS:HB2	2.11	0.51
1:A:144:ASP:OD1	1:A:148:ARG:NH1	2.45	0.50
1:B:217:TYR:HB3	1:B:218:PRO:HD3	1.94	0.50
1:B:251:ARG:HD3	1:B:255:ASP:OD2	2.11	0.50
1:B:328:HIS:CE1	3:B:604:HOH:O	2.63	0.50
1:A:44:ARG:HD3	1:A:281:PHE:CZ	2.46	0.50
1:A:245:PRO:CD	3:A:545:HOH:O	2.59	0.50
1:B:217:TYR:N	1:B:218:PRO:CD	2.74	0.50
1:B:139:LYS:CE	3:B:552:HOH:O	2.58	0.50
1:B:356:GLY:HA3	1:D:216:TRP:CH2	2.46	0.50
1:D:110:ALA:HB1	1:D:331:ASP:OD1	2.11	0.50
1:A:231:CYS:C	3:A:504:HOH:O	2.49	0.50
1:C:93:HIS:HB3	1:C:95:ASP:OD1	2.11	0.50
1:D:131:LYS:HE2	3:D:681:HOH:O	2.11	0.49
1:B:75:GLN:HG2	1:B:328:HIS:O	2.12	0.49
1:C:314:THR:HB	3:C:573:HOH:O	2.11	0.49
1:C:113:THR:O	1:C:155:ARG:NH2	2.45	0.49
1:B:75:GLN:HE21	1:B:75:GLN:HA	1.78	0.48
1:B:335:PRO:CB	3:B:554:HOH:O	2.61	0.48
1:C:66:ILE:HG23	1:C:66:ILE:O	2.13	0.48
1:A:75:GLN:NE2	1:A:330:TRP:N	2.52	0.48
1:C:151:THR:OG1	1:C:152:ILE:HD12	2.12	0.48
1:D:370:GLU:HB3	3:D:541:HOH:O	2.12	0.48
1:A:120:GLY:HA3	1:A:130:THR:HG21	1.96	0.47
1:B:250:LEU:O	1:B:254:LEU:HB2	2.15	0.47
1:D:43:ALA:HA	3:D:679:HOH:O	2.14	0.47
1:A:245:PRO:O	1:A:247:GLN:N	2.46	0.47
1:A:264:GLY:O	1:A:298:TYR:HB2	2.15	0.47
1:A:291:TYR:OH	1:A:295:ARG:HD2	2.15	0.46
1:B:311:TRP:HA	1:B:319:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:TYR:CG	1:D:354:LEU:HD21	2.51	0.46
1:D:131:LYS:CD	3:D:681:HOH:O	2.64	0.46
1:D:373:GLY:HA2	3:D:524:HOH:O	2.15	0.46
1:D:107:GLY:HA3	1:D:112:ARG:NH1	2.30	0.46
1:A:261:GLN:HA	3:A:530:HOH:O	2.15	0.46
1:D:187:ILE:HD12	1:D:214:ASN:HB3	1.97	0.46
1:A:247:GLN:HE21	1:A:248:LEU:HD12	1.81	0.46
1:C:287:ARG:HG3	1:C:288:TYR:N	2.31	0.46
1:D:324:VAL:HA	3:D:590:HOH:O	2.15	0.46
1:B:251:ARG:NE	1:B:251:ARG:HA	2.30	0.46
1:A:101:VAL:HG21	1:A:141:TYR:CZ	2.51	0.46
1:B:71:MET:HE2	1:B:75:GLN:HE22	1.81	0.46
1:C:175:GLN:O	1:C:175:GLN:HG3	2.16	0.46
1:A:240:THR:CG2	3:A:684:HOH:O	2.64	0.45
1:D:40:MET:O	1:D:43:ALA:N	2.50	0.45
1:A:175:GLN:HE21	1:A:175:GLN:HA	1.82	0.45
1:A:179:VAL:HG23	3:A:503:HOH:O	2.16	0.45
1:C:37:GLY:HA3	1:C:49:ALA:O	2.15	0.45
1:A:247:GLN:HE21	1:A:248:LEU:CD1	2.29	0.45
1:A:75:GLN:NE2	1:A:330:TRP:CG	2.85	0.45
1:A:44:ARG:CD	1:C:329:ALA:O	2.54	0.45
1:C:40:MET:HA	3:C:687:HOH:O	2.17	0.45
1:A:31:ILE:HB	1:A:313:ILE:HB	1.99	0.45
1:D:282:ASN:HB3	3:D:587:HOH:O	2.17	0.45
1:B:141:TYR:CD1	1:D:94:THR:HG22	2.53	0.44
1:A:20:TYR:CD1	1:B:20:TYR:CD1	3.05	0.44
1:B:108:TRP:CD1	1:B:156:PRO:HB2	2.51	0.44
1:B:111:GLY:CA	1:B:333:ALA:HB2	2.47	0.44
1:B:112:ARG:O	1:B:156:PRO:HB3	2.18	0.44
1:C:174:TYR:HB3	1:C:181:PHE:HB2	1.98	0.44
1:B:61:LYS:HE3	3:B:598:HOH:O	2.17	0.44
1:B:119:TRP:CZ2	1:B:174:TYR:HD2	2.35	0.44
1:D:91:HIS:CE1	1:D:96:HIS:CD2	3.06	0.44
1:C:281:PHE:HB3	1:C:283:ASP:OD1	2.18	0.43
1:C:294:VAL:HG11	1:C:302:LEU:CD2	2.48	0.43
1:B:84:LEU:HA	3:B:584:HOH:O	2.19	0.43
1:D:328:HIS:HD2	3:D:673:HOH:O	2.01	0.43
1:C:33:VAL:HG22	1:C:54:VAL:HG13	2.01	0.43
1:C:44:ARG:HD3	1:C:281:PHE:CE1	2.53	0.43
1:C:101:VAL:HG21	1:C:141:TYR:CZ	2.54	0.43
1:C:369:GLN:HA	3:C:686:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG21	1:D:141:TYR:CZ	2.54	0.43
1:D:108:TRP:O	1:D:108:TRP:CD1	2.72	0.43
1:D:331:ASP:CA	3:D:629:HOH:O	2.64	0.43
1:C:294:VAL:HG11	1:C:302:LEU:HD22	2.00	0.43
1:C:366:HIS:CD2	1:C:369:GLN:HE22	2.36	0.43
1:D:101:VAL:HG21	1:D:141:TYR:CE1	2.54	0.43
1:D:109:THR:CG2	3:D:594:HOH:O	2.67	0.42
1:A:319:THR:CA	3:A:533:HOH:O	2.64	0.42
1:A:244:GLN:HB2	1:A:249:ALA:HB2	2.00	0.42
1:D:217:TYR:N	1:D:218:PRO:CD	2.82	0.42
1:D:104:TRP:NE1	1:D:157:GLY:O	2.39	0.42
1:D:155:ARG:N	1:D:156:PRO:CD	2.82	0.42
1:D:368:LYS:HE2	3:D:655:HOH:O	2.08	0.42
1:C:155:ARG:HB2	1:C:156:PRO:HD3	2.02	0.42
1:A:40:MET:HB3	1:A:41:PRO:HD2	2.01	0.42
1:B:168:ALA:HB1	1:B:171:GLU:CG	2.49	0.42
1:A:37:GLY:HA3	1:A:49:ALA:O	2.20	0.42
1:A:237:GLN:NE2	1:A:286:THR:HA	2.34	0.42
1:C:339:LEU:O	1:C:340:ALA:HB3	2.20	0.42
1:A:245:PRO:HD2	3:A:545:HOH:O	2.18	0.42
1:D:82:ASN:OD1	1:D:113:THR:N	2.50	0.42
1:D:217:TYR:HB3	1:D:218:PRO:HD3	2.02	0.41
1:A:251:ARG:NE	1:A:251:ARG:HA	2.35	0.41
1:B:147:THR:HB	1:D:189:ALA:HB1	2.02	0.41
1:C:285:ASP:O	1:C:286:THR:CG2	2.62	0.41
1:A:245:PRO:CD	3:A:529:HOH:O	2.59	0.41
1:D:15:LYS:NZ	3:D:515:HOH:O	2.47	0.41
1:D:311:TRP:HA	1:D:319:THR:O	2.20	0.41
1:C:281:PHE:HD1	1:C:281:PHE:HA	1.82	0.41
1:A:324:VAL:HG12	1:B:324:VAL:HG12	2.02	0.41
1:C:137:MET:O	1:C:140:ALA:HB3	2.21	0.41
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.86	0.41
1:C:20:TYR:CD1	1:D:20:TYR:CD1	3.09	0.41
1:A:245:PRO:HD3	3:A:545:HOH:O	2.19	0.41
1:B:87:ILE:HD11	1:B:103:MET:HG2	2.03	0.40
1:C:28:PRO:HD3	3:C:617:HOH:O	2.19	0.40
1:A:34:ILE:HD12	1:A:34:ILE:N	2.37	0.40
1:D:322:MET:HB3	1:D:322:MET:HE3	2.01	0.40
1:B:127:ASP:HA	1:B:132:TYR:CG	2.56	0.40
1:D:61:LYS:HZ2	1:D:83:TYR:HD2	1.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:584:HOH:O	3:D:506:HOH:O[2_556]	1.74	0.46
3:B:637:HOH:O	3:C:501:HOH:O[1_455]	2.11	0.09

## 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	342/372 (92%)	317 (93%)	20 (6%)	5 (2%)	10	4
1	B	342/372 (92%)	321 (94%)	16 (5%)	5 (2%)	10	4
1	C	331/372 (89%)	301 (91%)	25 (8%)	5 (2%)	10	4
1	D	316/372 (85%)	296 (94%)	17 (5%)	3 (1%)	17	11
All	All	1331/1488 (89%)	1235 (93%)	78 (6%)	18 (1%)	11	5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	ASP
1	B	332	VAL
1	B	335	PRO
1	C	338	ASP
1	D	284	ASP
1	A	246	ALA
1	A	335	PRO
1	B	247	GLN
1	D	110	ALA
1	C	66	ILE
1	C	286	THR
1	C	368	LYS
1	A	66	ILE
1	A	337	GLU
1	B	279	HIS

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Mol	Chain	Res	Type
1	A	336	SER
1	C	340	ALA
1	D	66	ILE

### 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	276/301 (92%)	266 (96%)	10 (4%)	35	34
1	B	278/301 (92%)	264 (95%)	14 (5%)	24	20
1	C	268/301 (89%)	259 (97%)	9 (3%)	37	36
1	D	261/301 (87%)	250 (96%)	11 (4%)	30	27
All	All	1083/1204 (90%)	1039 (96%)	44 (4%)	30	28

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	44	ARG
1	A	158	ASP
1	A	169	LEU
1	A	175	GLN
1	A	176	GLU
1	A	222	LYS
1	A	254	LEU
1	A	278	TYR
1	A	310	VAL
1	B	75	GLN
1	B	135	GLU
1	B	158	ASP
1	B	169	LEU
1	B	175	GLN
1	B	176	GLU
1	B	222	LYS
1	B	239	MET

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Mol	Chain	Res	Type
1	B	244	GLN
1	B	254	LEU
1	B	278	TYR
1	B	310	VAL
1	B	338	ASP
1	B	343	ARG
1	C	54	VAL
1	C	131	LYS
1	C	169	LEU
1	C	230	GLU
1	C	232	TRP
1	C	278	TYR
1	C	282	ASN
1	C	283	ASP
1	C	337	GLU
1	D	44	ARG
1	D	54	VAL
1	D	82	ASN
1	D	153	ASN
1	D	169	LEU
1	D	265	GLN
1	D	278	TYR
1	D	285	ASP
1	D	287	ARG
1	D	310	VAL
1	D	362	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	175	GLN
1	A	247	GLN
1	A	344	ASN
1	B	75	GLN
1	B	175	GLN
1	B	244	GLN
1	B	328	HIS
1	B	344	ASN
1	C	75	GLN
1	C	359	ASN
1	C	366	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

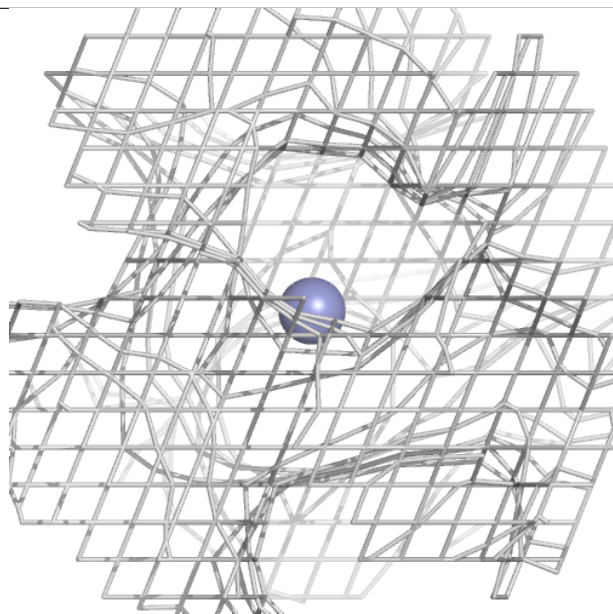
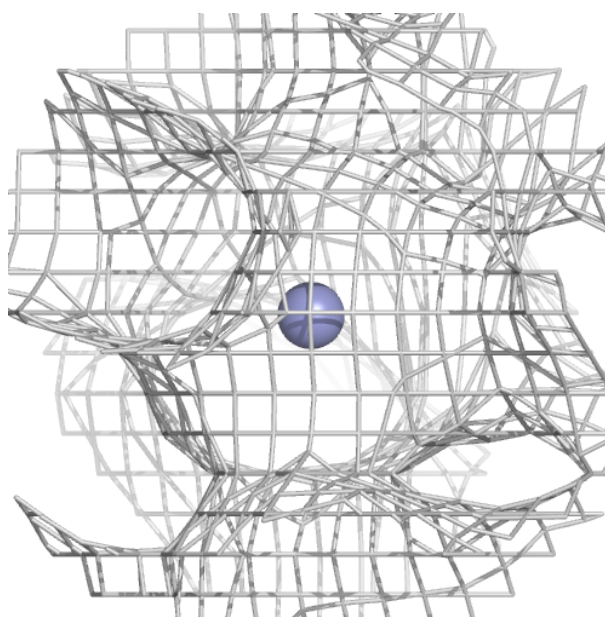
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

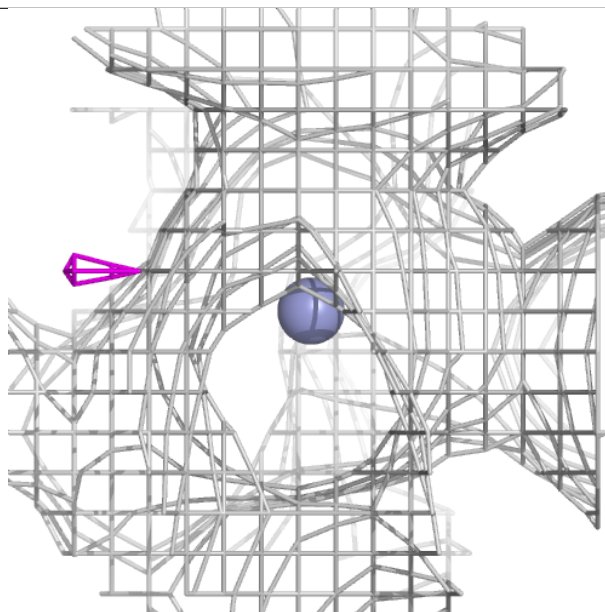
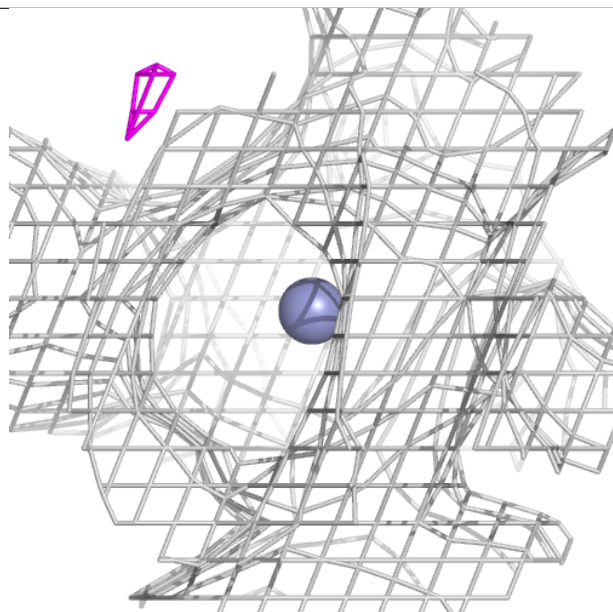
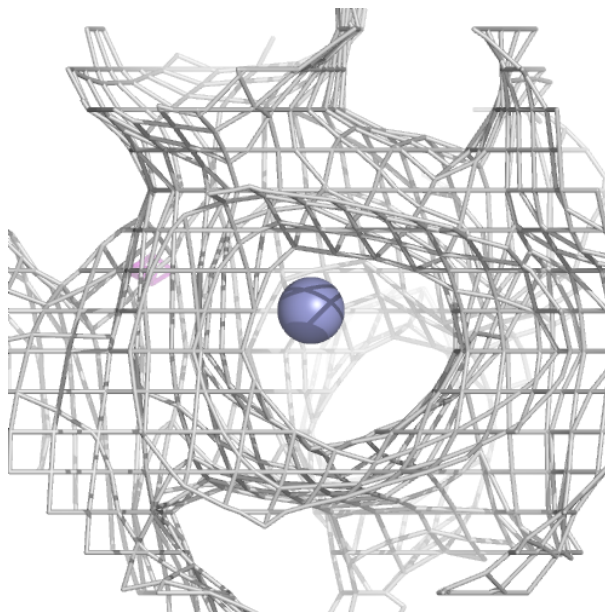
**Electron density around ZN A 401:**

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



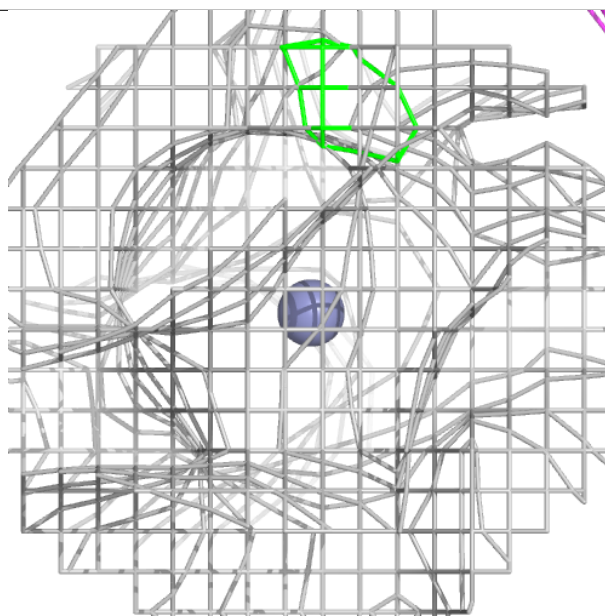
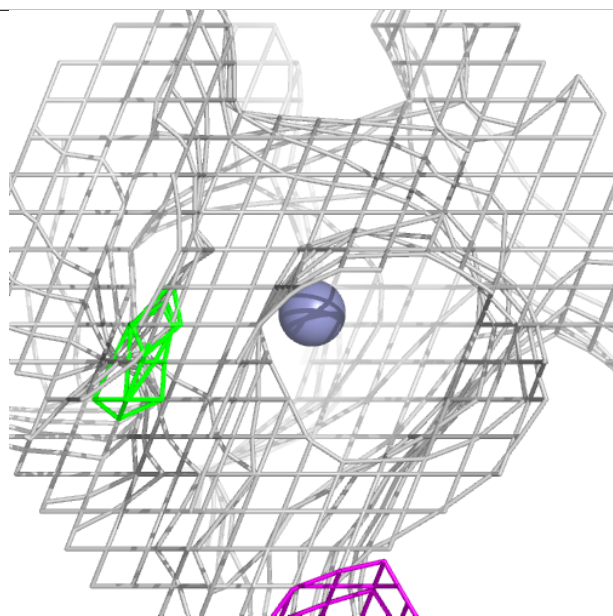
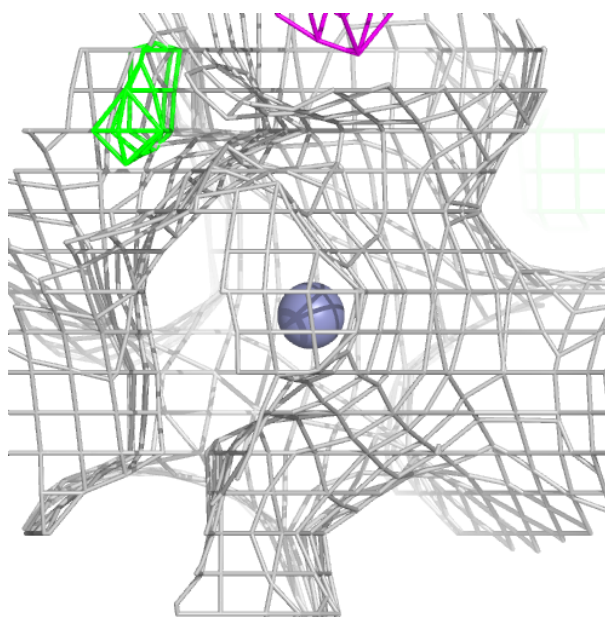
**Electron density around ZN A 402:**

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



**Electron density around ZN B 401:**

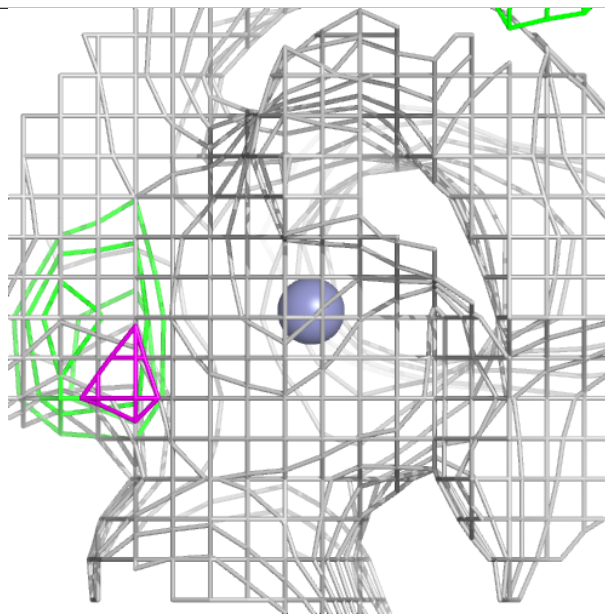
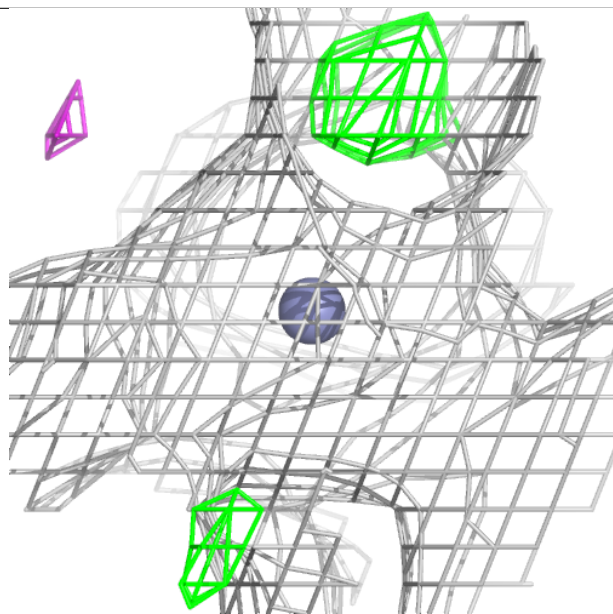
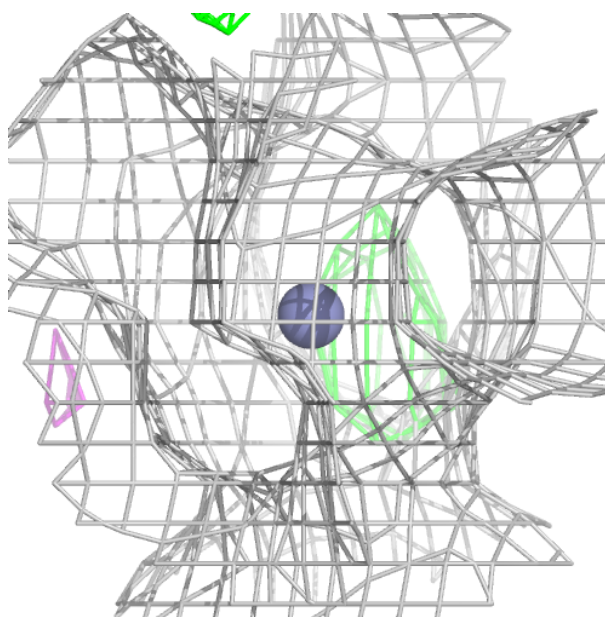
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





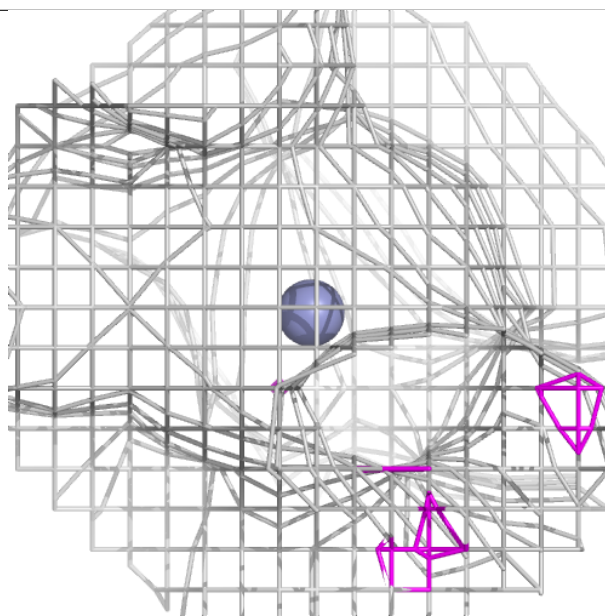
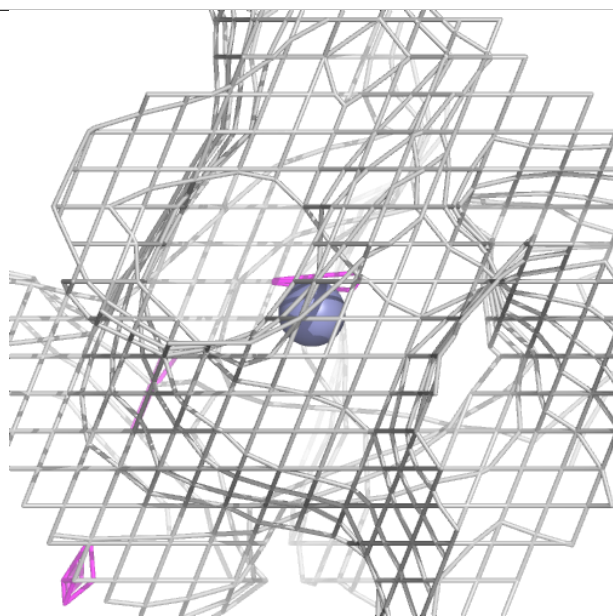
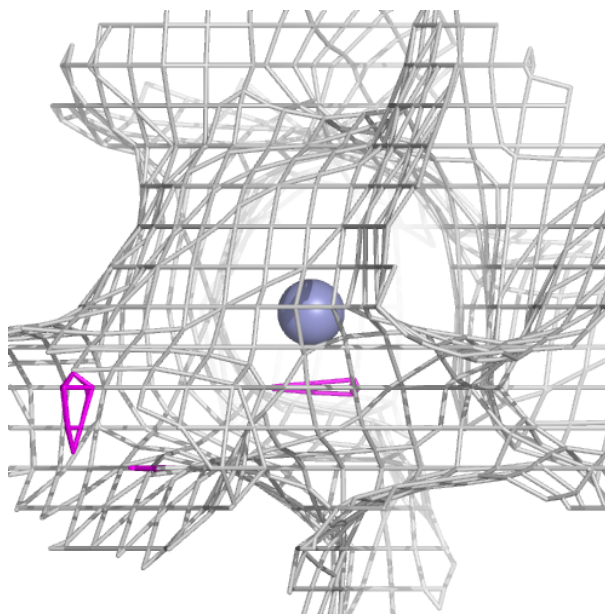
**Electron density around ZN B 402:**

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



**Electron density around ZN C 401:**

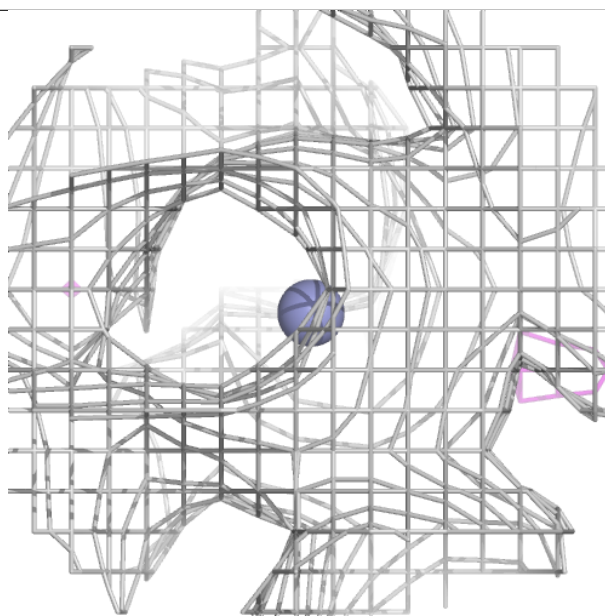
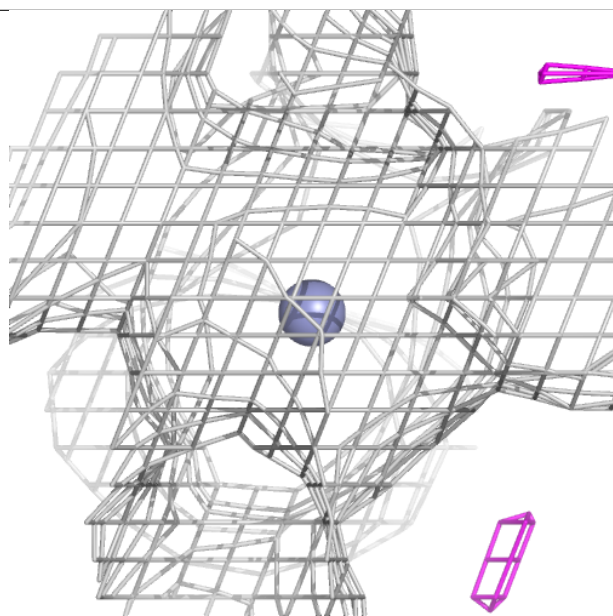
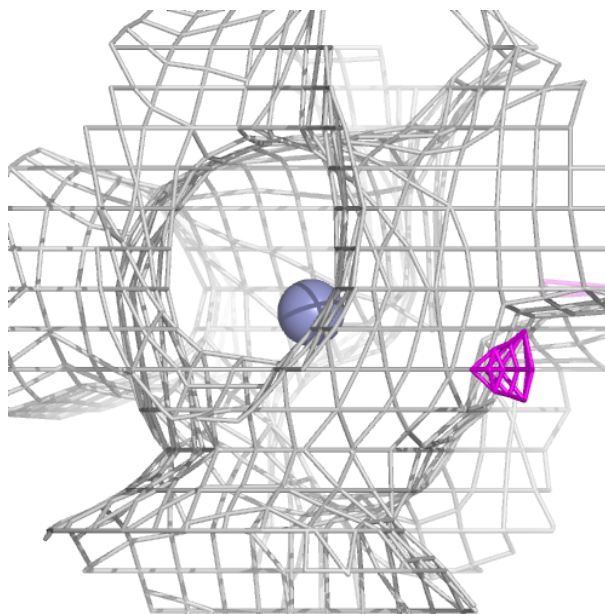
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





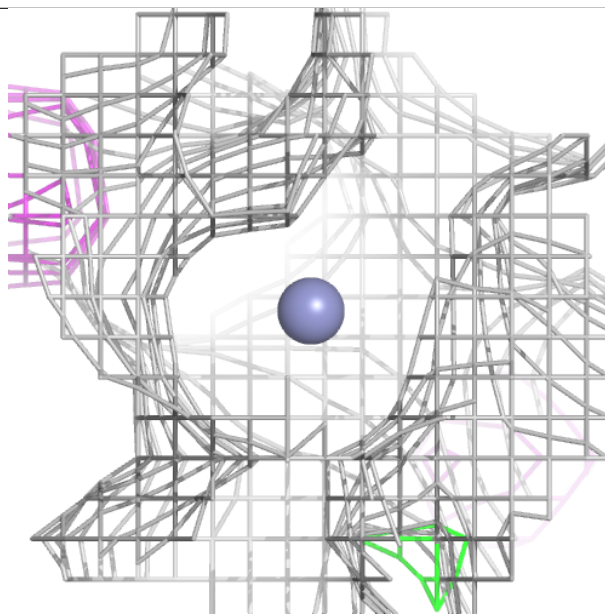
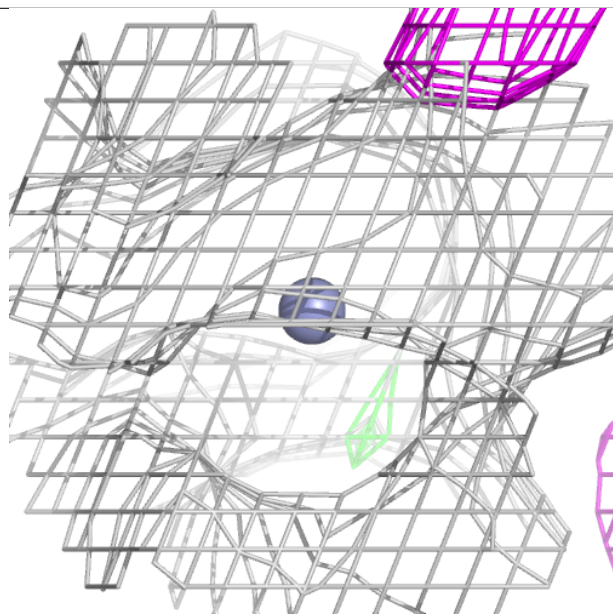
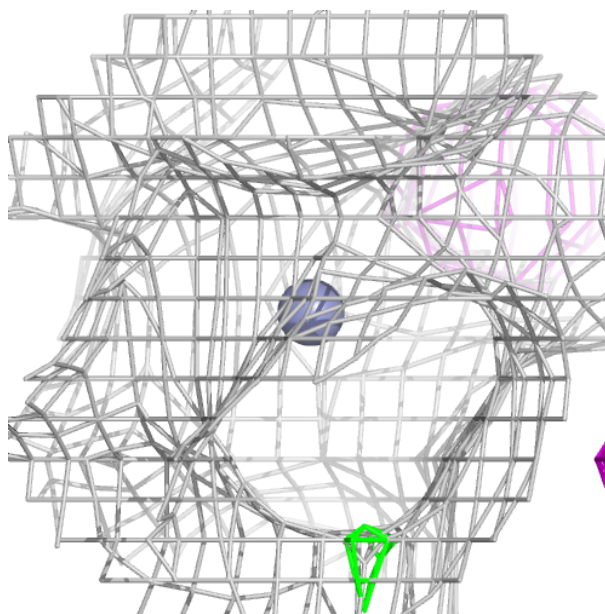
**Electron density around ZN C 402:**

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



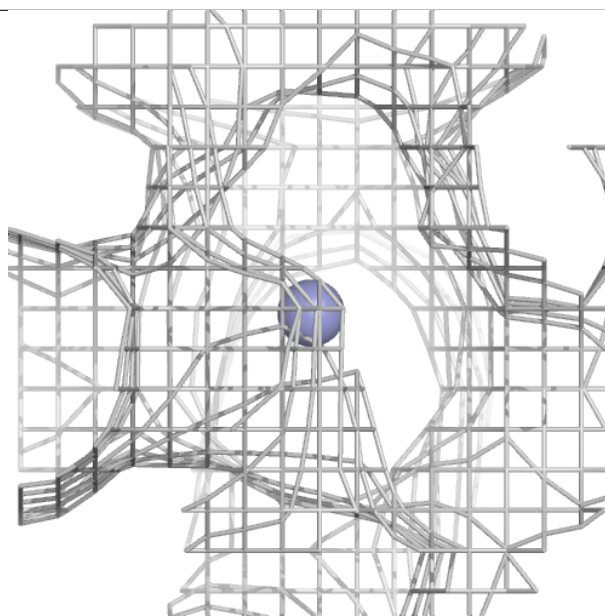
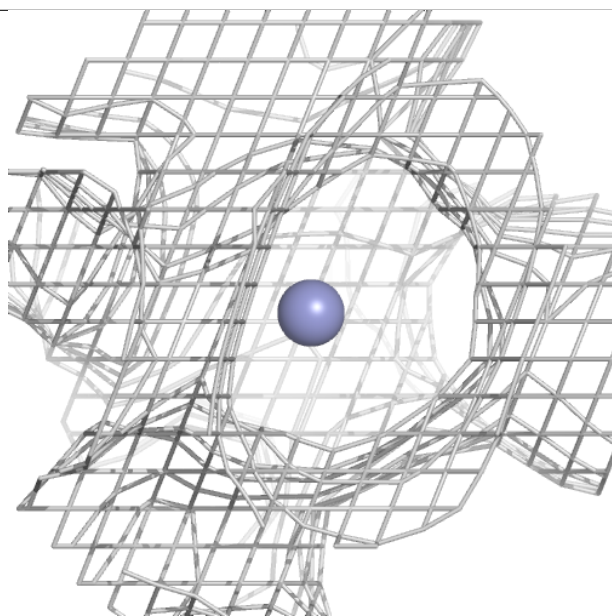
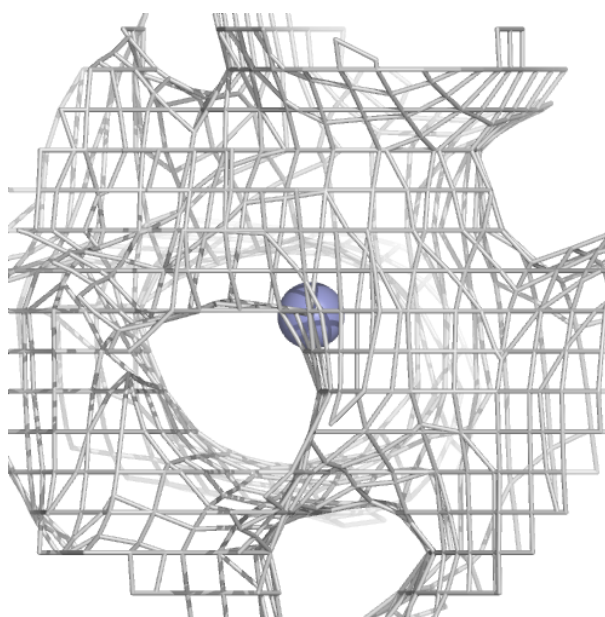
**Electron density around ZN D 401:**

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



**Electron density around ZN D 402:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.