



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:17 AM UTC

PDB ID : 7BZ3 / pdb_00007bz3
Title : The mutant variant of PNGM-1. H257 was substituted for alanine to study substrate binding.
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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

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 Phenix2.0
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

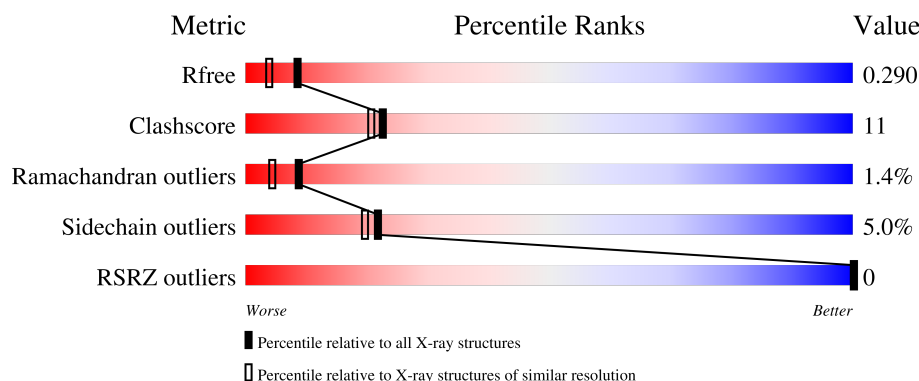
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 ≥ 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	372	 71% 19% • 8%
1	B	372	 72% 18% •• 8%
1	C	372	 72% 15% • 10%
1	D	372	 66% 19% • 13%

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 (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		
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		

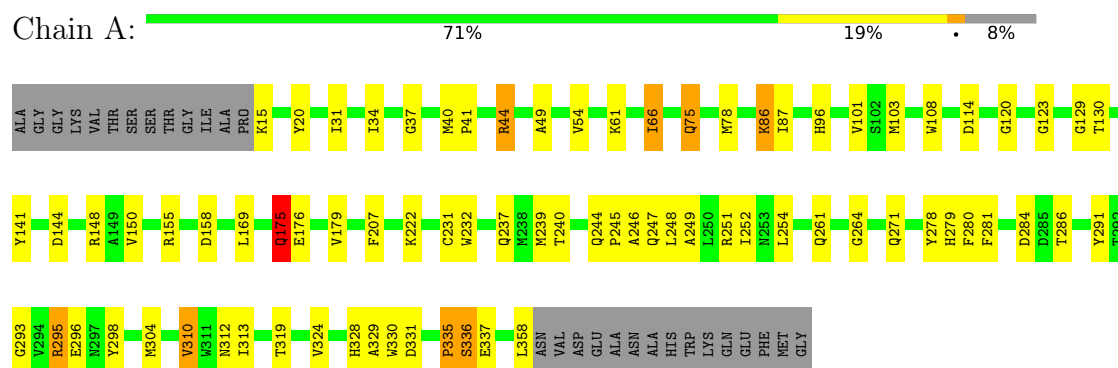
- Molecule 3 is water.

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

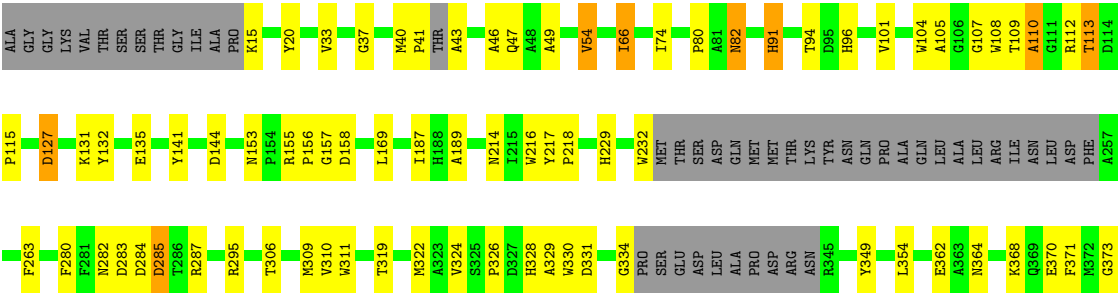
3 Residue-property plots [i](#)

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: Metallo-beta-lactamase PNGM-1



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.79Å 143.74Å 79.76Å 90.00° 111.82° 90.00°	Depositor
Resolution (Å)	48.69 – 2.00 48.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.69-2.00) 97.3 (48.69-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.447 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11589	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	1.16	5/2788 (0.2%)	1.45	9/3802 (0.2%)
1	B	1.15	0/2797	1.42	8/3814 (0.2%)
1	C	1.14	2/2722 (0.1%)	1.44	7/3713 (0.2%)
1	D	1.15	2/2646 (0.1%)	1.43	10/3603 (0.3%)
All	All	1.15	9/10953 (0.1%)	1.44	34/14932 (0.2%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	91	HIS	CE1-NE2	6.04	1.38	1.32
1	A	123	GLY	C-O	5.92	1.31	1.23
1	A	96	HIS	CE1-NE2	5.62	1.38	1.32
1	A	271	GLN	N-CA	5.33	1.50	1.46
1	A	279	HIS	CE1-NE2	5.28	1.37	1.32
1	A	129	GLY	C-O	5.23	1.30	1.23
1	C	291	TYR	C-O	5.13	1.29	1.24
1	D	91	HIS	CE1-NE2	5.02	1.37	1.32
1	D	229	HIS	CE1-NE2	5.00	1.37	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	GLN	CB-CA-C	7.59	120.85	111.43
1	D	144	ASP	CA-CB-CG	6.78	119.38	112.60
1	D	105	ALA	CA-C-N	6.71	127.38	120.00
1	D	105	ALA	C-N-CA	6.71	127.38	120.00
1	A	66	ILE	CA-C-N	6.67	126.44	120.10
1	A	66	ILE	C-N-CA	6.67	126.44	120.10
1	C	292	THR	CA-C-N	6.30	126.97	119.98
1	C	292	THR	C-N-CA	6.30	126.97	119.98
1	B	135	GLU	CB-CA-C	6.10	120.58	110.81
1	A	335	PRO	N-CA-CB	5.95	109.50	103.25
1	B	176	GLU	CB-CG-CD	5.93	122.69	112.60
1	D	74	ILE	CA-C-O	-5.86	114.86	120.95
1	B	66	ILE	CA-C-N	5.82	125.63	120.10
1	B	66	ILE	C-N-CA	5.82	125.63	120.10
1	D	326	PRO	CB-CA-C	-5.61	105.45	111.56
1	B	331	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	331	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	207	PHE	CA-C-N	5.47	126.98	120.14
1	C	207	PHE	C-N-CA	5.47	126.98	120.14
1	B	75	GLN	CB-CG-CD	-5.36	103.49	112.60
1	B	335	PRO	N-CA-CB	5.36	108.88	103.25
1	A	358	LEU	CA-C-O	-5.33	111.74	120.80
1	A	75	GLN	N-CA-CB	-5.32	102.03	110.28
1	D	127	ASP	N-CA-C	-5.30	106.85	113.15
1	B	175	GLN	CB-CA-C	5.24	117.92	111.43
1	C	127	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	150	VAL	CA-C-O	-5.16	115.38	120.85
1	A	207	PHE	CA-C-O	-5.11	115.33	120.84
1	D	326	PRO	CA-C-N	5.08	127.60	120.28
1	D	326	PRO	C-N-CA	5.08	127.60	120.28
1	D	80	PRO	CA-C-N	5.02	127.26	120.38
1	D	80	PRO	C-N-CA	5.02	127.26	120.38
1	C	139	LYS	CA-C-N	5.01	127.25	120.38
1	C	139	LYS	C-N-CA	5.01	127.25	120.38

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	65	0
1	B	2718	0	2550	59	0
1	C	2642	0	2456	48	0
1	D	2570	0	2396	60	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	217	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 11.

All (217) 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:D:334:GLY:C	3:D:555:HOH:O	1.96	1.06
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:40:MET:HE1	1:D:232:TRP:CZ2	2.29	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
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:C:198:LEU:C	1:C:198:LEU:HD23	2.25	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TRP:CD1	1:C:108:TRP:O	2.55	0.59
1:A:284:ASP:CG	3:A:536:HOH:O	2.45	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:335:PRO:HB3	1:C:337:GLU:OE1	2.05	0.57
1:B:239:MET:HE3	1:B:244:GLN:O	2.04	0.56
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:B:290:ILE:HG22	1:B:304:MET:HE1	1.86	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:231:CYS:C	3:A:504:HOH:O	2.49	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: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:71:MET:HE2	1:B:75:GLN:HE22	1.73	0.53
1:A:280:PHE:CZ	1:A:304:MET:HE3	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:MET:HE3	1:A:244:GLN:O	2.12	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:78:MET:HE1	1:B:17:TYR:CE1	2.46	0.50
1:C:93:HIS:HB3	1:C:95:ASP:OD1	2.11	0.50
1:D:306:THR:HG23	1:D:322:MET:HE1	1.94	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:D:306:THR:HG22	1:D:309:MET:HE3	1.94	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:HE21	1:A:330:TRP:CG	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:198:LEU:C	1:B:198:LEU:HD23	2.42	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
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:A:78:MET:HE1	1:B:17:TYR:CD1	2.54	0.43
1:B:263:PHE:CD1	1:B:263:PHE:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:371:PHE:CD1	1:D:371:PHE:C	2.97	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:D:263:PHE:CD1	1:D:263:PHE:C	2.99	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:B:342:ASP:OD1	1:B:342:ASP:C	2.65	0.40
1:B:127:ASP:HA	1:B:132:TYR:CG	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry 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%)	8	4
1	B	342/372 (92%)	321 (94%)	16 (5%)	5 (2%)	8	4
1	C	331/372 (89%)	301 (91%)	25 (8%)	5 (2%)	8	4
1	D	316/372 (85%)	296 (94%)	17 (5%)	3 (1%)	14	9
All	All	1331/1488 (89%)	1235 (93%)	78 (6%)	18 (1%)	9	4

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
1	A	336	SER

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Mol	Chain	Res	Type
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%)	263 (95%)	13 (5%)	23	22
1	B	278/301 (92%)	261 (94%)	17 (6%)	17	14
1	C	268/301 (89%)	255 (95%)	13 (5%)	22	20
1	D	261/301 (87%)	250 (96%)	11 (4%)	26	25
All	All	1083/1204 (90%)	1029 (95%)	54 (5%)	22	20

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	44	ARG
1	A	54	VAL
1	A	86	LYS
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	295	ARG
1	A	310	VAL
1	B	44	ARG
1	B	75	GLN
1	B	135	GLU
1	B	158	ASP
1	B	169	LEU
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	176	GLU
1	B	215	ILE
1	B	219	GLU
1	B	222	LYS
1	B	230	GLU
1	B	239	MET
1	B	254	LEU
1	B	295	ARG
1	B	310	VAL
1	B	338	ASP
1	B	343	ARG
1	C	45	ARG
1	C	54	VAL
1	C	131	LYS
1	C	152	ILE
1	C	155	ARG
1	C	169	LEU
1	C	230	GLU
1	C	282	ASN
1	C	283	ASP
1	C	295	ARG
1	C	319	THR
1	C	362	GLU
1	C	369	GLN
1	D	54	VAL
1	D	82	ASN
1	D	113	THR
1	D	135	GLU
1	D	153	ASN
1	D	169	LEU
1	D	285	ASP
1	D	287	ARG
1	D	295	ARG
1	D	310	VAL
1	D	362	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	175	GLN
1	A	247	GLN

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Mol	Chain	Res	Type
1	A	253	ASN
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
1	D	170	ASN
1	D	268	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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, 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	344/372 (92%)	-1.15	0 100 100	13, 21, 50, 82	0
1	B	344/372 (92%)	-1.14	0 100 100	13, 22, 51, 82	0
1	C	335/372 (90%)	-1.02	0 100 100	16, 25, 58, 104	0
1	D	324/372 (87%)	-1.07	0 100 100	15, 24, 45, 72	0
All	All	1347/1488 (90%)	-1.10	0 100 100	13, 23, 52, 104	0

There are no RSRZ outliers to report.

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, 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	401	1/1	1.00	0.03	17,17,17,17	0
2	ZN	A	402	1/1	1.00	0.01	16,16,16,16	0
2	ZN	B	401	1/1	1.00	0.01	17,17,17,17	0
2	ZN	B	402	1/1	1.00	0.01	18,18,18,18	0

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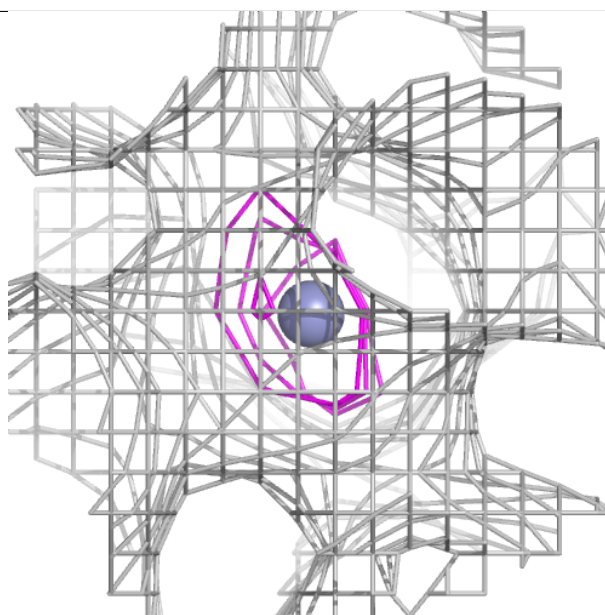
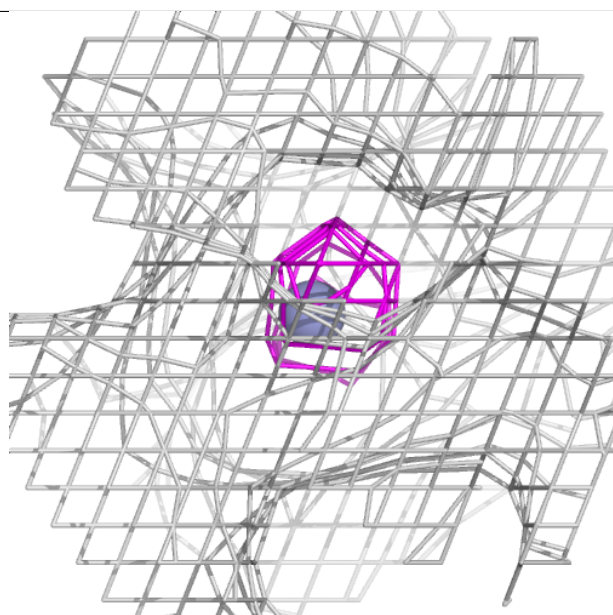
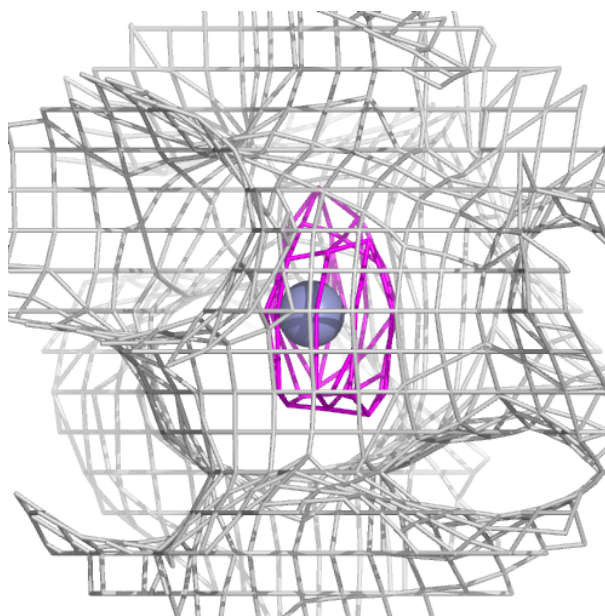
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	401	1/1	1.00	0.02	22,22,22,22	0
2	ZN	C	402	1/1	1.00	0.01	19,19,19,19	0
2	ZN	D	401	1/1	1.00	0.01	24,24,24,24	0
2	ZN	D	402	1/1	1.00	0.01	20,20,20,20	0

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.

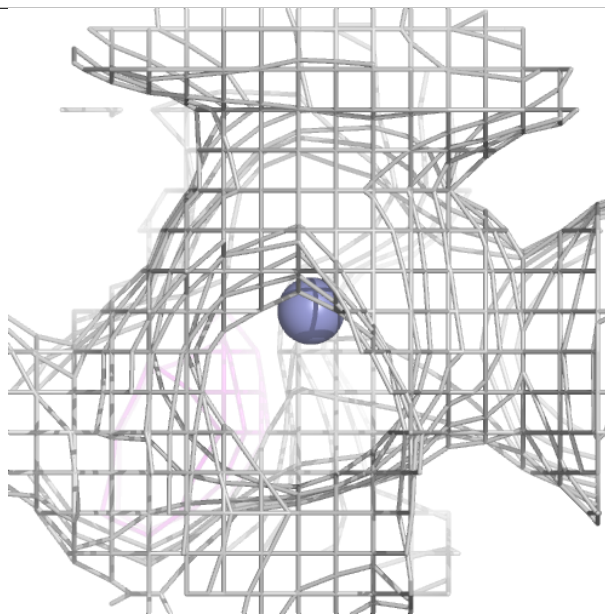
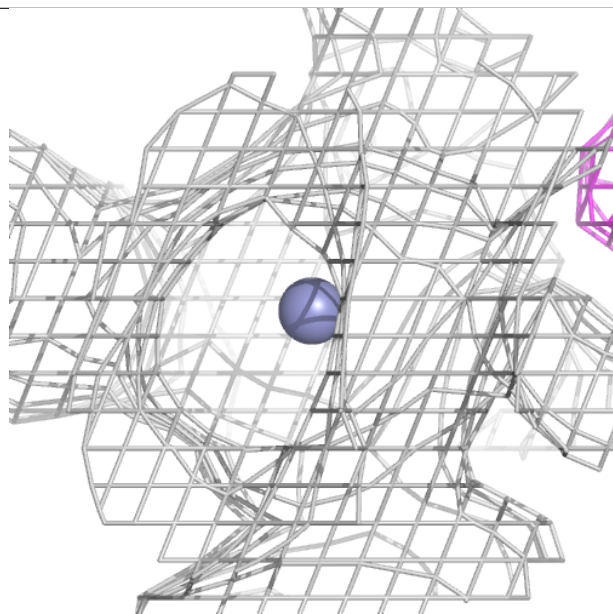
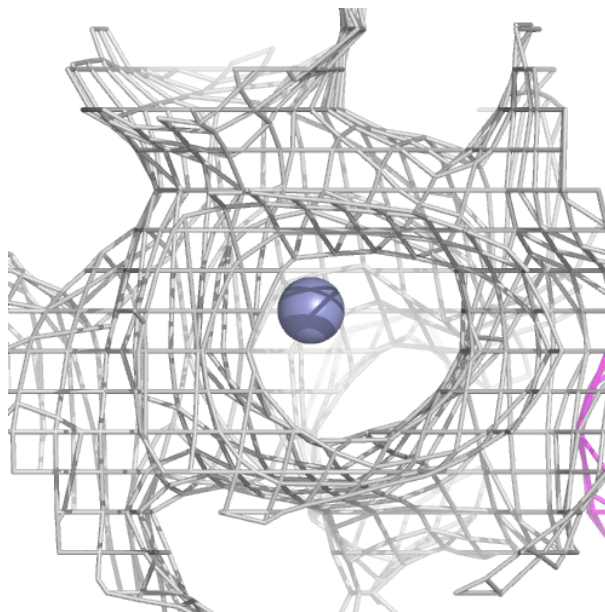
Electron density around ZN A 401:

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



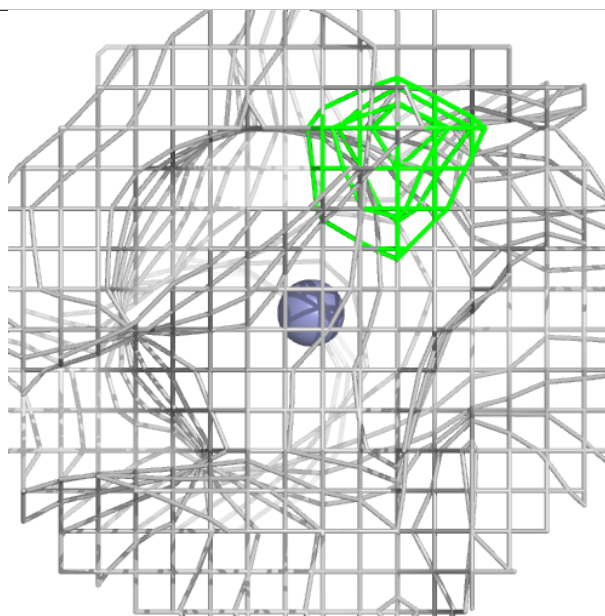
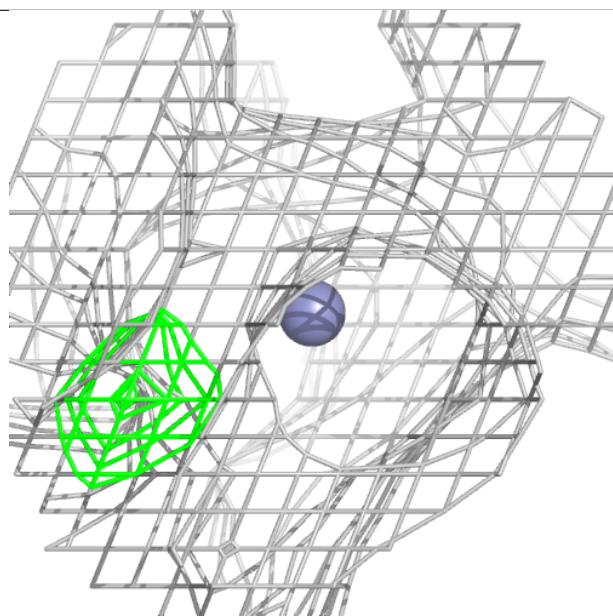
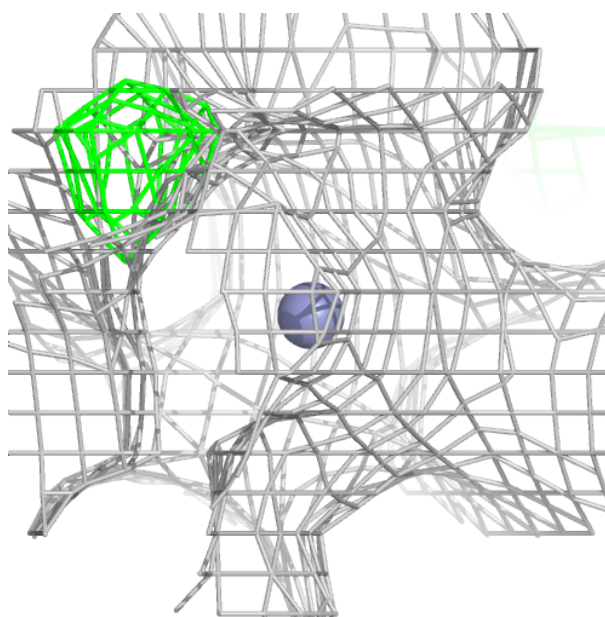
Electron density around ZN A 402:

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



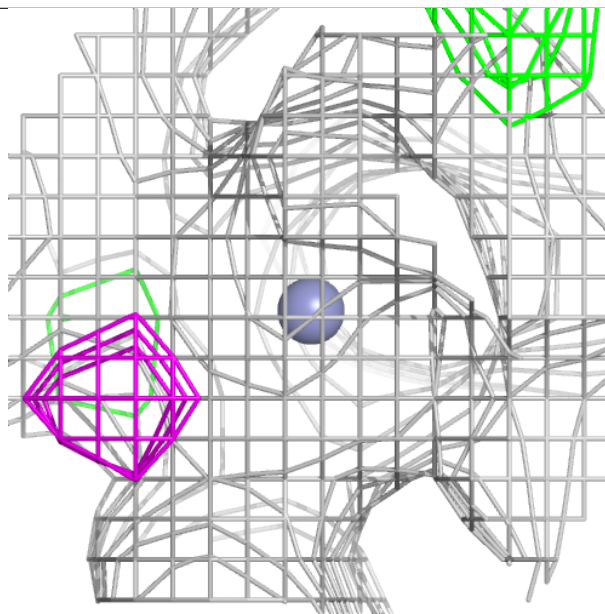
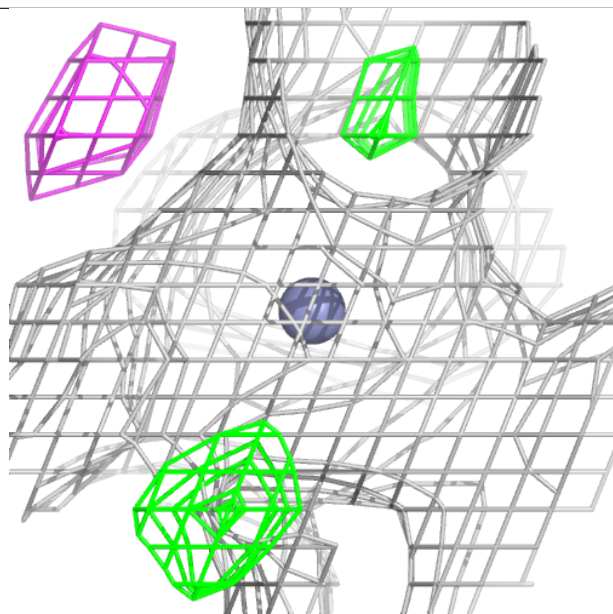
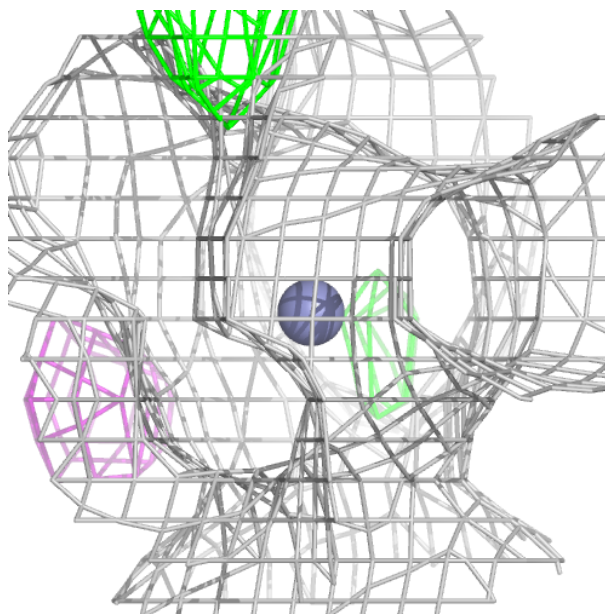
Electron density around ZN B 401:

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



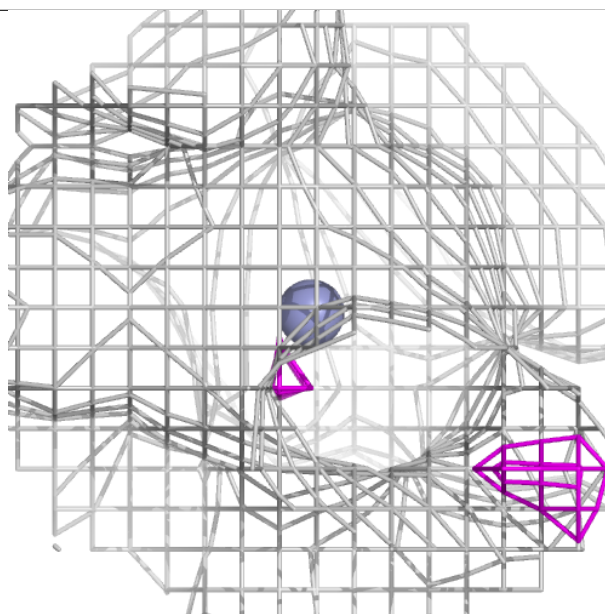
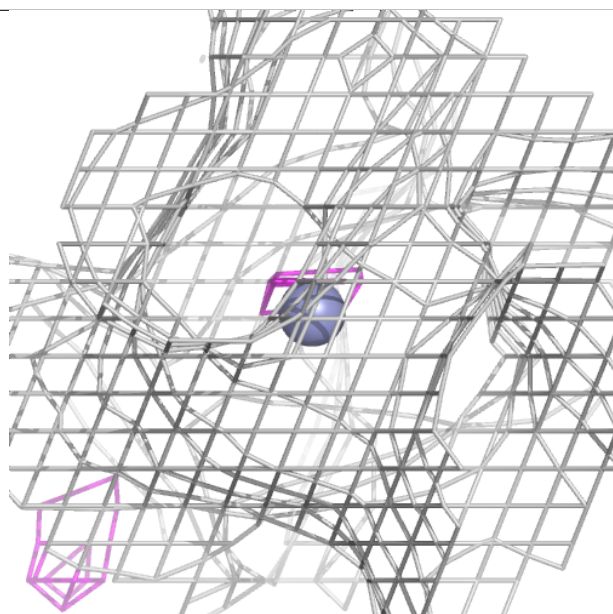
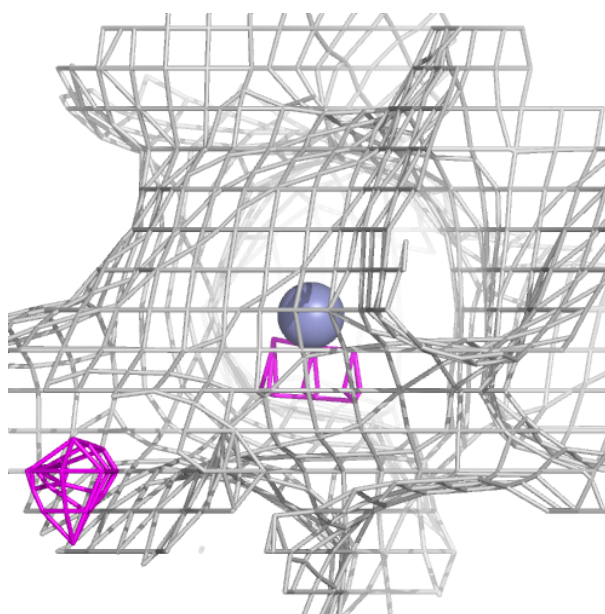
Electron density around ZN B 402:

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



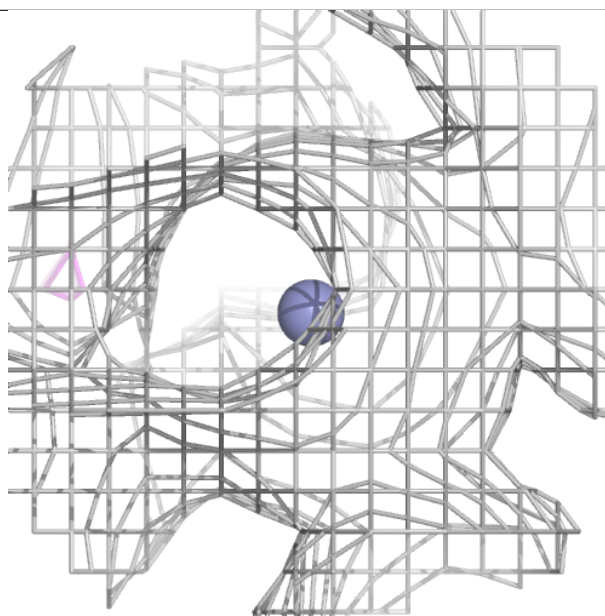
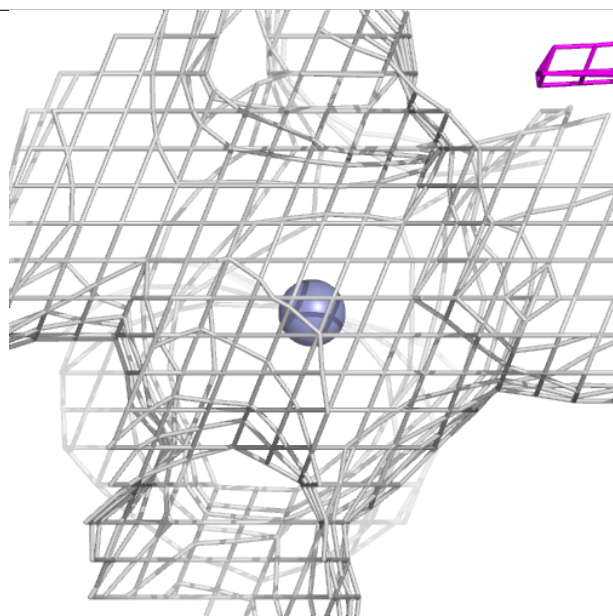
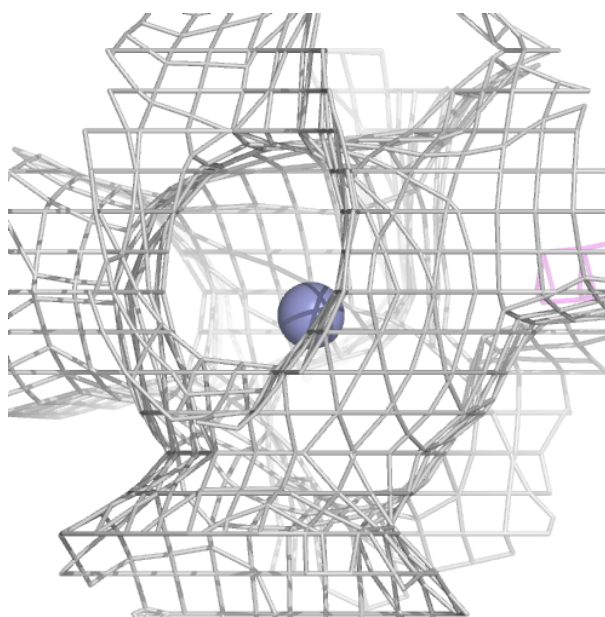
Electron density around ZN C 401:

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



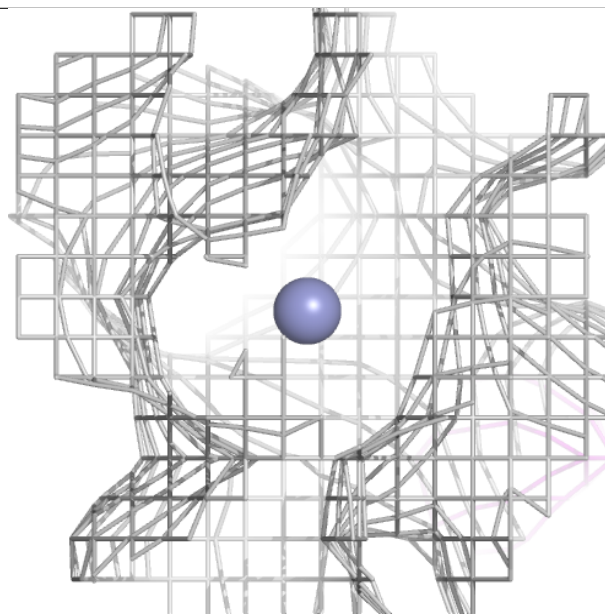
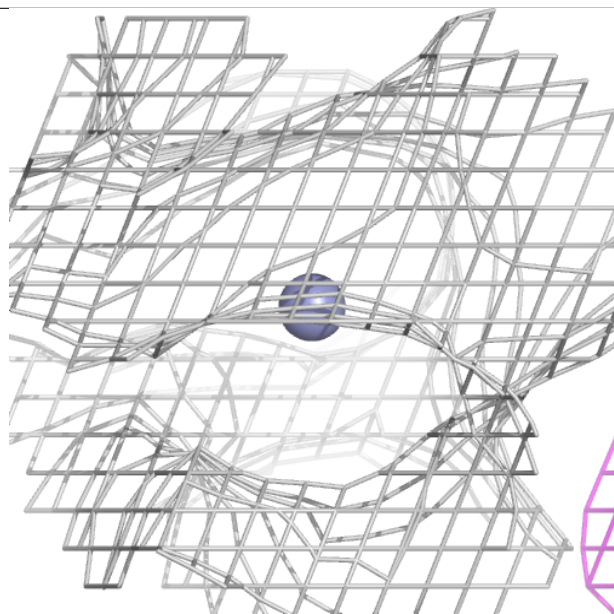
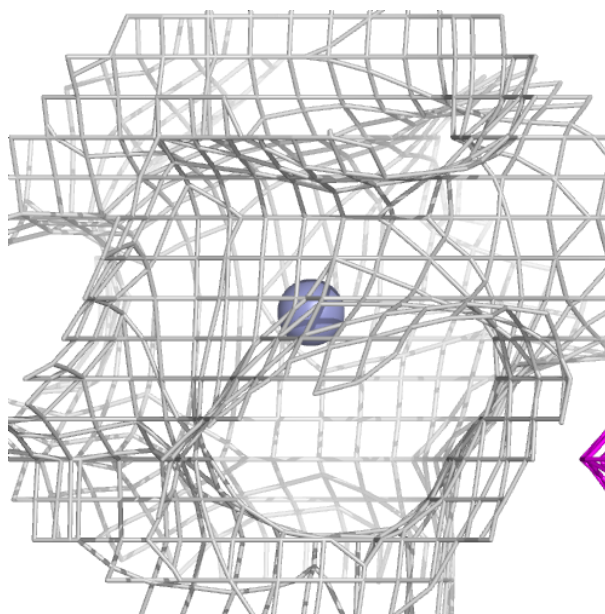
Electron density around ZN C 402:

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



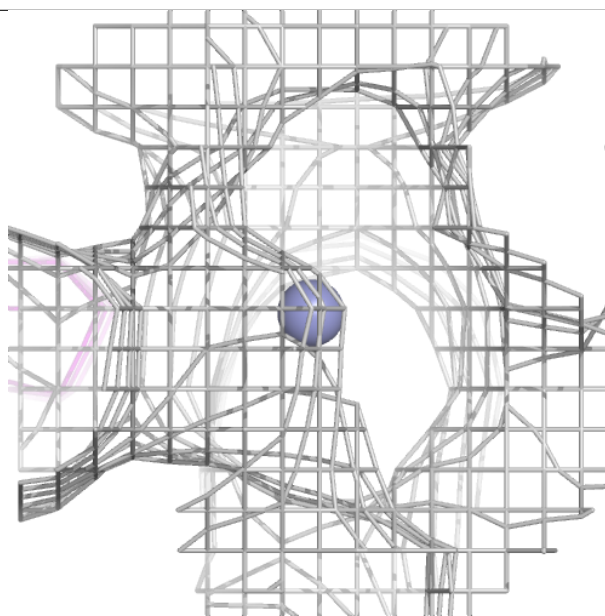
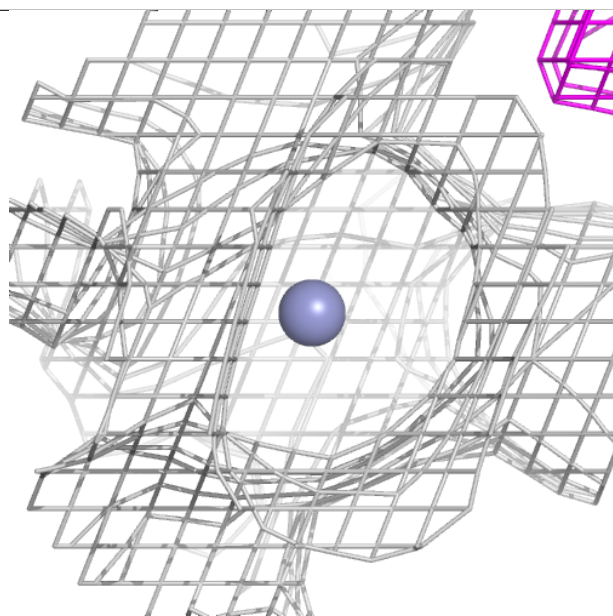
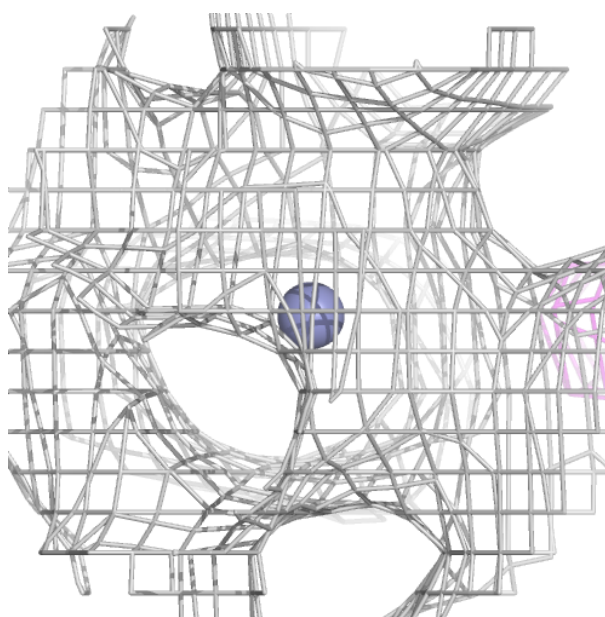
Electron density around ZN D 401:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.