



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2024 – 03:01 PM JST

PDB ID : 8WWD
Title : Crystal structure of (S)-DHPS dehydrogenase HpsP from *Dinoroseobacter shibae* DFL 12
Authors : Liu, L.; Tang, K.
Deposited on : 2023-10-25
Resolution : 2.30 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

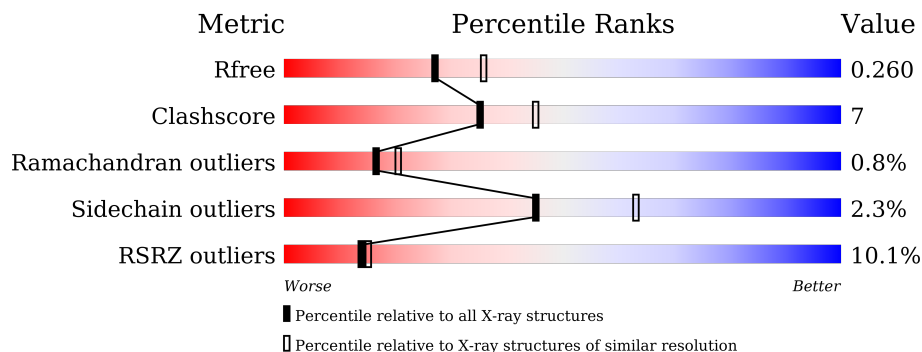
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	337	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">2% 87% 11% .</p>
1	B	337	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">3% 89% 9% ..</p>
1	C	337	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">13% 80% 17% ..</p>
1	D	337	<div style="display: flex; align-items: center;"> <div style="width: 22%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">22% 79% 20% .</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10736 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 Zinc-containing alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2559	1594	477	475	13	0	10	0
1	B	336	2524	1573	471	467	13	0	7	0
1	C	329	2491	1553	460	465	13	0	10	0
1	D	336	2553	1589	477	474	13	0	10	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP A8LPS1
A	-9	HIS	-	expression tag	UNP A8LPS1
A	-8	HIS	-	expression tag	UNP A8LPS1
A	-6	HIS	-	expression tag	UNP A8LPS1
A	-5	HIS	-	expression tag	UNP A8LPS1
A	-4	HIS	-	expression tag	UNP A8LPS1
A	-3	SER	-	expression tag	UNP A8LPS1
A	-2	SER	-	expression tag	UNP A8LPS1
A	-1	GLY	-	expression tag	UNP A8LPS1
A	0	GLY	-	expression tag	UNP A8LPS1
B	-10	HIS	-	expression tag	UNP A8LPS1
B	-9	HIS	-	expression tag	UNP A8LPS1
B	-8	HIS	-	expression tag	UNP A8LPS1
B	-6	HIS	-	expression tag	UNP A8LPS1
B	-5	HIS	-	expression tag	UNP A8LPS1
B	-4	HIS	-	expression tag	UNP A8LPS1
B	-3	SER	-	expression tag	UNP A8LPS1
B	-2	SER	-	expression tag	UNP A8LPS1
B	-1	GLY	-	expression tag	UNP A8LPS1
B	0	GLY	-	expression tag	UNP A8LPS1
C	-9	HIS	-	expression tag	UNP A8LPS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	HIS	-	expression tag	UNP A8LPS1
C	-7	HIS	-	expression tag	UNP A8LPS1
C	-6	HIS	-	expression tag	UNP A8LPS1
C	-5	HIS	-	expression tag	UNP A8LPS1
C	-4	HIS	-	expression tag	UNP A8LPS1
C	-3	SER	-	expression tag	UNP A8LPS1
C	-2	SER	-	expression tag	UNP A8LPS1
C	-1	GLY	-	expression tag	UNP A8LPS1
C	0	GLY	-	expression tag	UNP A8LPS1
D	-10	HIS	-	expression tag	UNP A8LPS1
D	-9	HIS	-	expression tag	UNP A8LPS1
D	-8	HIS	-	expression tag	UNP A8LPS1
D	-6	HIS	-	expression tag	UNP A8LPS1
D	-5	HIS	-	expression tag	UNP A8LPS1
D	-4	HIS	-	expression tag	UNP A8LPS1
D	-3	SER	-	expression tag	UNP A8LPS1
D	-2	SER	-	expression tag	UNP A8LPS1
D	-1	GLY	-	expression tag	UNP A8LPS1
D	0	GLY	-	expression tag	UNP A8LPS1

- 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	3	Total Zn 3 3	0	0
2	B	3	Total Zn 3 3	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	238	Total O 238 238	0	0
3	B	254	Total O 254 254	0	0
3	C	53	Total O 53 53	0	0

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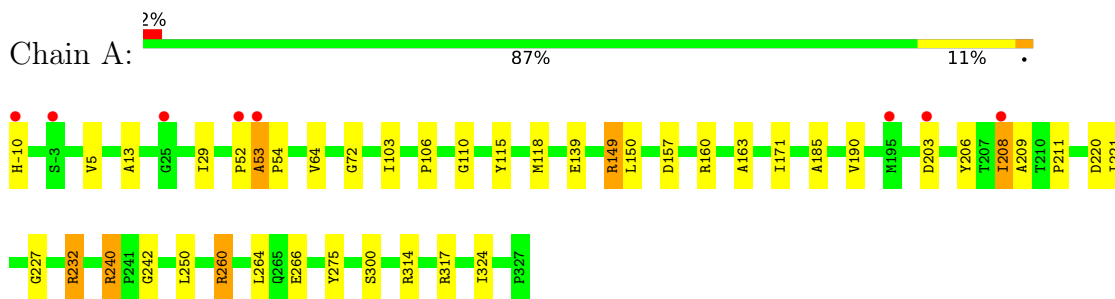
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	54	Total	O	0	0
			54	54		

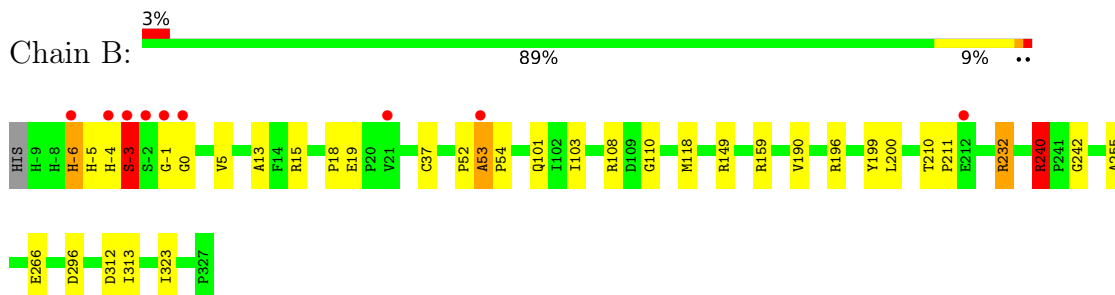
3 Residue-property plots [i](#)

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.

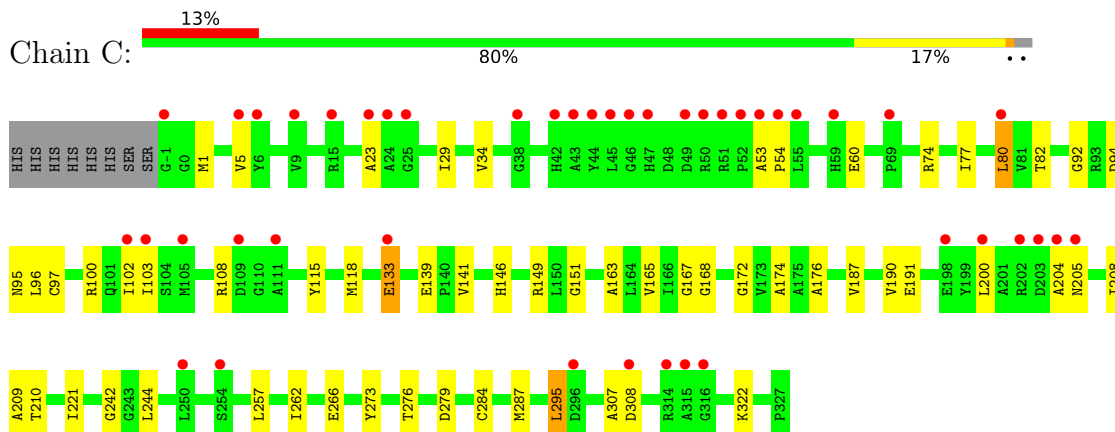
- Molecule 1: Zinc-containing alcohol dehydrogenase



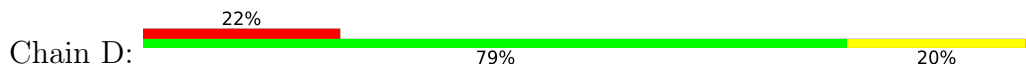
- Molecule 1: Zinc-containing alcohol dehydrogenase

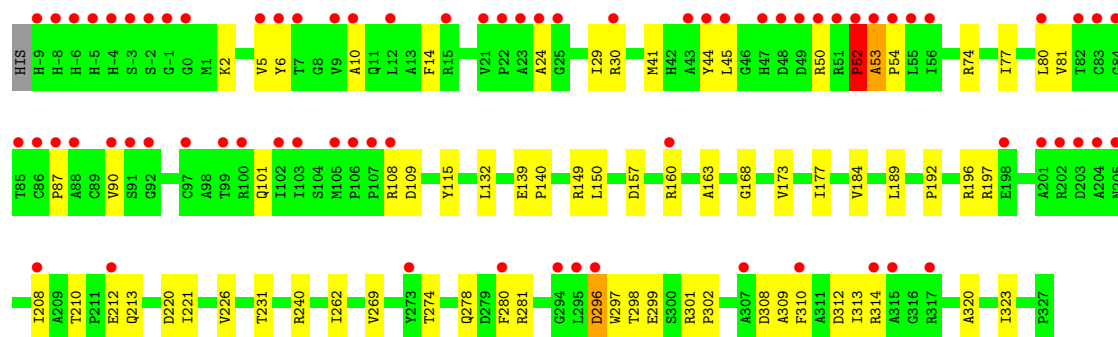


- Molecule 1: Zinc-containing alcohol dehydrogenase



- Molecule 1: Zinc-containing alcohol dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.18Å 290.54Å 54.28Å 90.00° 98.38° 90.00°	Depositor
Resolution (Å)	48.47 – 2.30 48.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.47-2.30) 99.2 (48.47-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.258 0.212 , 0.260	Depositor DCC
R_{free} test set	2797 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10736	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.73	0/2609	0.86	2/3553 (0.1%)
1	B	0.72	0/2573	0.87	5/3503 (0.1%)
1	C	0.68	0/2535	0.83	1/3451 (0.0%)
1	D	0.70	0/2602	0.83	1/3542 (0.0%)
All	All	0.71	0/10319	0.85	9/14049 (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	C	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	B	240	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	A	160	ARG	CB-CA-C	-7.08	96.25	110.40
1	C	133	GLU	CB-CA-C	-5.55	99.31	110.40
1	A	232	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	312	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	232	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	240	ARG	CD-NE-CZ	5.09	130.73	123.60
1	D	52	PRO	N-CA-CB	-5.04	97.06	102.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	295	LEU	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	2559	0	2546	29	0
1	B	2524	0	2520	33	0
1	C	2491	0	2498	43	0
1	D	2553	0	2543	45	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	238	0	0	5	0
3	B	254	0	0	5	0
3	C	53	0	0	4	0
3	D	54	0	0	0	0
All	All	10736	0	10107	149	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 7.

All (149) 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:D:309:ALA:O	1:D:313:ILE:HD12	1.65	0.97
1:B:53:ALA:HB1	1:B:54:PRO:HD2	1.45	0.95
1:C:95:ASN:OD1	3:C:501:HOH:O	1.90	0.88
1:D:197:ARG:HA	1:D:208:ILE:HD11	1.54	0.87
1:C:103:ILE:HG13	1:C:118:MET:CE	2.09	0.82
1:D:53:ALA:HB1	1:D:54:PRO:HD2	1.61	0.81
1:C:103:ILE:HG13	1:C:118:MET:HE2	1.62	0.80
1:D:160:ARG:HG2	1:D:184:VAL:HG22	1.70	0.73
1:B:190:VAL:HG21	1:B:211:PRO:HA	1.71	0.73
1:D:296:ASP:O	1:D:298:THR:N	2.22	0.68
1:C:200:LEU:HB3	1:C:208:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:HD11	1:B:118:MET:SD	2.35	0.67
1:C:284:CYS:HA	1:C:287:MET:HE2	1.77	0.66
1:B:53:ALA:CB	1:B:54:PRO:HD2	2.22	0.66
1:D:197:ARG:HA	1:D:208:ILE:CD1	2.25	0.66
1:B:15[B]:ARG:NH2	3:B:504:HOH:O	2.29	0.65
1:A:5[A]:VAL:HG12	1:A:13:ALA:O	1.96	0.64
1:B:266:GLU:OE1	3:B:501:HOH:O	2.15	0.64
1:B:101:GLN:HE21	1:B:108[A]:ARG:HE	1.44	0.63
1:B:37:CYS:SG	3:B:724:HOH:O	2.55	0.63
1:D:30:ARG:NH2	1:D:115:TYR:OH	2.32	0.62
1:C:103:ILE:HG13	1:C:118:MET:HE1	1.82	0.61
1:A:53:ALA:HB1	1:A:54:PRO:HD2	1.81	0.61
1:D:313:ILE:HD11	1:D:323:ILE:HD12	1.82	0.60
1:C:53:ALA:HB3	1:C:54:PRO:HD3	1.82	0.60
1:D:44:TYR:HD1	1:D:45:LEU:HD12	1.67	0.59
1:A:157:ASP:OD2	1:A:240:ARG:NH2	2.36	0.59
1:B:159:ARG:HB2	1:B:240:ARG:HH22	1.67	0.58
1:C:103:ILE:CG1	1:C:118:MET:HE1	2.34	0.57
1:B:53:ALA:HB1	1:B:54:PRO:CD	2.30	0.57
1:C:200:LEU:O	1:C:204:ALA:HB2	2.04	0.56
1:D:50:ARG:O	1:D:52:PRO:HD3	2.05	0.56
1:A:103:ILE:HG22	1:A:110:GLY:HA2	1.88	0.55
1:A:190:VAL:HG21	1:A:211:PRO:HA	1.88	0.55
1:D:87:PRO:HA	1:D:90:VAL:HG22	1.89	0.54
1:A:227:GLY:O	1:A:232:ARG:NH2	2.41	0.54
1:B:199:TYR:HD2	1:B:200:LEU:HD12	1.73	0.53
1:C:287:MET:HG2	1:C:295:LEU:HD11	1.90	0.53
1:C:77:ILE:CG2	1:C:118:MET:HE3	2.38	0.53
1:B:159:ARG:HB2	1:B:240:ARG:NH2	2.23	0.53
1:C:95:ASN:ND2	1:C:273:TYR:O	2.42	0.53
1:C:95:ASN:OD1	1:C:96:LEU:HG	2.09	0.53
1:A:190:VAL:HA	1:A:209:ALA:O	2.09	0.53
1:D:139[B]:GLU:H	1:D:139[B]:GLU:CD	2.12	0.52
1:B:103:ILE:HG22	1:B:110:GLY:HA2	1.91	0.52
1:D:81:VAL:CG2	1:D:101:GLN:HB2	2.40	0.52
1:D:81:VAL:HG21	1:D:108[A]:ARG:CZ	2.39	0.52
1:C:95:ASN:CG	3:C:501:HOH:O	2.41	0.51
1:A:139[B]:GLU:H	1:A:139[B]:GLU:CD	2.14	0.51
1:A:103:ILE:HD11	1:A:118:MET:SD	2.51	0.51
1:A:220:ASP:OD1	1:A:240:ARG:HD3	2.10	0.51
1:C:139[B]:GLU:H	1:C:139[B]:GLU:CD	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:MET:HE1	1:D:310:PHE:HD2	1.76	0.51
1:A:250:LEU:HA	3:A:549:HOH:O	2.11	0.50
1:B:5[A]:VAL:HG12	1:B:13:ALA:O	2.12	0.50
1:C:257:LEU:HD22	1:C:262:ILE:HD11	1.93	0.49
1:D:278:GLN:OE1	1:D:281:ARG:NH2	2.43	0.49
1:B:196:ARG:HD3	1:B:200:LEU:HD13	1.93	0.49
1:C:103:ILE:CG1	1:C:118:MET:CE	2.85	0.49
1:D:149[B]:ARG:HG3	1:D:150:LEU:N	2.27	0.49
1:C:34:VAL:HA	1:C:60:GLU:O	2.13	0.49
1:C:200:LEU:HB3	1:C:208:ILE:CD1	2.42	0.49
1:C:77:ILE:HG21	1:C:118:MET:HE3	1.95	0.48
1:C:108[B]:ARG:HA	1:C:108[B]:ARG:CZ	2.43	0.48
1:C:168:GLY:N	1:C:191:GLU:OE1	2.38	0.48
1:D:220:ASP:HA	1:D:240:ARG:HG2	1.95	0.48
1:D:197:ARG:CZ	1:D:210:THR:HG22	2.43	0.48
1:A:149[B]:ARG:HG3	1:A:150:LEU:N	2.27	0.48
1:C:146:HIS:ND1	1:C:279:ASP:OD2	2.39	0.48
1:A:208:ILE:HG22	1:A:208:ILE:O	2.12	0.47
1:B:232:ARG:HD2	1:B:255:ALA:O	2.14	0.47
1:D:44:TYR:CD1	1:D:45:LEU:HD12	2.48	0.47
1:A:220:ASP:HA	1:A:240:ARG:HG2	1.97	0.47
1:C:97:CYS:HB3	1:C:100:ARG:HB3	1.97	0.47
1:D:301:ARG:HD3	1:D:309:ALA:HB2	1.97	0.46
1:B:53:ALA:CB	1:B:54:PRO:CD	2.93	0.46
1:B:190:VAL:CG2	1:B:211:PRO:HA	2.44	0.46
1:D:210:THR:H	1:D:213:GLN:NE2	2.13	0.46
1:A:185:ALA:N	3:A:510:HOH:O	2.45	0.46
1:C:190:VAL:HA	1:C:209:ALA:O	2.16	0.46
1:D:299[B]:GLU:HG2	1:D:320:ALA:HB2	1.97	0.46
1:A:103:ILE:CG2	1:A:110:GLY:HA2	2.45	0.46
1:A:260:ARG:O	1:A:264:LEU:HG	2.16	0.45
1:D:262:ILE:HD13	1:D:269:VAL:HG21	1.98	0.45
1:C:284:CYS:HA	1:C:287:MET:CE	2.45	0.45
1:C:74:ARG:CZ	1:D:302:PRO:HG3	2.47	0.45
1:C:307:ALA:HB3	3:C:528:HOH:O	2.15	0.45
1:B:5[A]:VAL:HG13	1:B:13:ALA:HB3	1.98	0.45
1:D:168:GLY:HA2	1:D:189:LEU:HD21	1.99	0.45
1:C:92:GLY:HA2	3:C:540:HOH:O	2.17	0.44
1:C:94:ASP:OD1	1:C:276:THR:HA	2.18	0.44
1:D:2:LYS:HD2	1:D:14:PHE:CE2	2.51	0.44
1:D:74:ARG:HB3	1:D:132:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5[A]:VAL:HG11	1:B:15[A]:ARG:NE	2.32	0.44
1:B:240:ARG:HH11	1:B:242:GLY:C	2.21	0.44
1:C:29:ILE:HG21	1:C:77:ILE:HD11	1.99	0.44
1:C:80:LEU:CD2	1:C:102:ILE:HD12	2.46	0.44
1:B:-1:GLY:HA2	1:B:18:PRO:HA	1.99	0.44
1:B:190:VAL:HG21	1:B:211:PRO:CA	2.45	0.44
1:C:165:VAL:HG11	1:C:172:GLY:O	2.18	0.44
1:B:313:ILE:HD11	1:B:323:ILE:HD12	1.99	0.44
1:C:242:GLY:HA2	1:C:266:GLU:O	2.18	0.44
1:D:139[B]:GLU:HG3	1:D:280:PHE:HE2	1.81	0.44
1:C:163:ALA:HA	1:C:221:ILE:O	2.18	0.43
1:A:29:ILE:O	1:A:115:TYR:HA	2.17	0.43
1:D:173:VAL:O	1:D:177:ILE:HG12	2.19	0.43
1:D:210:THR:OG1	1:D:213:GLN:HG3	2.19	0.43
1:B:-5:HIS:HD2	1:B:19:GLU:OE2	2.01	0.43
1:D:80:LEU:HD11	1:D:274:THR:HG21	2.00	0.43
1:A:206:TYR:CE1	1:A:208:ILE:CD1	3.02	0.43
1:B:19:GLU:HG2	3:B:529:HOH:O	2.19	0.43
1:C:151:GLY:HA3	1:C:244:LEU:HD21	2.01	0.43
1:C:141:VAL:HA	1:C:174:ALA:HB1	2.00	0.43
1:B:-6:HIS:CE1	1:B:-4:HIS:CD2	3.07	0.42
1:D:81:VAL:HG22	1:D:101:GLN:HB2	2.01	0.42
1:D:10:ALA:HA	1:D:44:TYR:CZ	2.54	0.42
1:A:314:ARG:HD2	1:A:314:ARG:HA	1.90	0.42
1:B:-5:HIS:CD2	1:B:19:GLU:OE2	2.72	0.42
1:B:103:ILE:CG2	1:B:110:GLY:HA2	2.50	0.42
1:B:196:ARG:HD3	1:B:200:LEU:CD1	2.50	0.42
1:C:176:ALA:HA	1:C:187:VAL:HG11	2.01	0.42
1:B:296:ASP:HB2	3:B:637:HOH:O	2.19	0.42
1:D:168:GLY:O	1:D:196:ARG:HD2	2.20	0.42
1:A:163:ALA:HA	1:A:221:ILE:O	2.20	0.41
1:D:45:LEU:HD11	1:D:314:ARG:HD3	2.02	0.41
1:A:106:PRO:HG2	3:A:563:HOH:O	2.20	0.41
1:A:171:ILE:HD11	3:A:718:HOH:O	2.18	0.41
1:C:167:GLY:O	1:C:172:GLY:HA3	2.20	0.41
1:C:190:VAL:HG23	1:C:210:THR:C	2.40	0.41
1:B:190:VAL:HG23	1:B:210:THR:C	2.41	0.41
1:A:242:GLY:HA2	1:A:266:GLU:O	2.21	0.41
1:C:1:MET:SD	1:C:115:TYR:HB2	2.61	0.41
1:D:2:LYS:HD2	1:D:14:PHE:CZ	2.56	0.41
1:D:163:ALA:HA	1:D:221:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLU:OE1	1:C:322:LYS:NZ	2.43	0.41
1:D:301:ARG:NH1	1:D:312:ASP:OD2	2.49	0.41
1:A:103:ILE:HD11	3:A:644:HOH:O	2.20	0.41
1:D:6:TYR:CE1	1:D:44:TYR:HA	2.56	0.41
1:D:29:ILE:HG21	1:D:77:ILE:HD11	2.03	0.41
1:D:192:PRO:O	1:D:197:ARG:NH1	2.53	0.41
1:A:64[A]:VAL:CG2	1:A:72:GLY:HA2	2.51	0.41
1:A:171:ILE:HD13	1:A:171:ILE:HA	1.89	0.40
1:D:157:ASP:OD1	1:D:240:ARG:NH1	2.53	0.40
1:D:139[B]:GLU:N	1:D:140:PRO:HD2	2.36	0.40
1:D:226:VAL:HB	1:D:231:THR:HG21	2.03	0.40
1:A:300:SER:HA	1:A:324:ILE:O	2.21	0.40
1:C:82:THR:HG21	1:C:94:ASP:HB2	2.03	0.40
1:A:317:ARG:NE	1:A:317:ARG:HA	2.36	0.40
1:B:-3:SER:OG	1:B:-1:GLY:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/337 (102%)	330 (96%)	12 (4%)	2 (1%)	22	27
1	B	340/337 (101%)	325 (96%)	11 (3%)	4 (1%)	11	12
1	C	336/337 (100%)	317 (94%)	18 (5%)	1 (0%)	37	47
1	D	343/337 (102%)	326 (95%)	13 (4%)	4 (1%)	11	12
All	All	1363/1348 (101%)	1298 (95%)	54 (4%)	11 (1%)	16	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	PRO
1	B	53	ALA
1	A	53	ALA
1	D	53	ALA
1	B	-3	SER
1	C	23	ALA
1	D	52	PRO
1	B	0	GLY
1	D	24	ALA
1	D	297	TRP
1	A	52	PRO

5.3.2 Protein sidechains [i](#)

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	259/249 (104%)	251 (97%)	8 (3%)	35 51
1	B	255/249 (102%)	250 (98%)	5 (2%)	50 68
1	C	251/249 (101%)	243 (97%)	8 (3%)	34 50
1	D	258/249 (104%)	251 (97%)	7 (3%)	40 57
All	All	1023/996 (103%)	995 (97%)	28 (3%)	45 57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-10	HIS
1	A	149[A]	ARG
1	A	149[B]	ARG
1	A	203	ASP
1	A	208	ILE
1	A	240	ARG
1	A	260	ARG
1	A	275	TYR
1	B	-6	HIS
1	B	-3	SER
1	B	149[A]	ARG

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Mol	Chain	Res	Type
1	B	149[B]	ARG
1	B	240	ARG
1	C	5[A]	VAL
1	C	5[B]	VAL
1	C	80	LEU
1	C	133	GLU
1	C	149[A]	ARG
1	C	149[B]	ARG
1	C	205	ASN
1	C	308	ASP
1	D	5[A]	VAL
1	D	5[B]	VAL
1	D	52	PRO
1	D	109	ASP
1	D	212	GLU
1	D	296	ASP
1	D	308	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	-6	HIS
1	B	-5	HIS
1	B	-4	HIS
1	B	47	HIS
1	B	101	GLN
1	D	114	GLN
1	D	213	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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	337/337 (100%)	-0.11	8 (2%) 59 61	3, 16, 35, 51	10 (2%)
1	B	336/337 (99%)	-0.08	9 (2%) 56 57	4, 18, 39, 83	7 (2%)
1	C	329/337 (97%)	0.87	44 (13%) 8 9	13, 35, 64, 91	10 (3%)
1	D	336/337 (99%)	1.19	74 (22%) 3 3	17, 41, 81, 160	10 (2%)
All	All	1338/1348 (99%)	0.46	135 (10%) 14 15	3, 28, 63, 160	37 (2%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	6.9
1	B	-2	SER	5.4
1	A	53	ALA	5.2
1	D	-5	HIS	5.1
1	D	-8	HIS	4.7
1	C	-1	GLY	4.5
1	D	-1	GLY	4.5
1	C	53	ALA	4.4
1	D	24	ALA	4.3
1	D	-6	HIS	4.3
1	D	90	VAL	4.3
1	D	-3	SER	4.2
1	D	-4	HIS	4.1
1	C	45	LEU	4.0
1	D	-9	HIS	4.0
1	C	202	ARG	4.0
1	C	103	ILE	3.9
1	C	52	PRO	3.9
1	D	-2	SER	3.8
1	B	53	ALA	3.8
1	D	56	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	109	ASP	3.7
1	D	21	VAL	3.7
1	D	45	LEU	3.7
1	D	25	GLY	3.7
1	D	106	PRO	3.6
1	D	108[A]	ARG	3.6
1	D	23	ALA	3.5
1	C	54	PRO	3.5
1	C	250	LEU	3.5
1	D	296	ASP	3.4
1	C	314	ARG	3.4
1	D	294	GLY	3.4
1	D	315	ALA	3.4
1	C	55	LEU	3.3
1	D	44	TYR	3.3
1	B	-3	SER	3.3
1	D	105	MET	3.3
1	D	51	ARG	3.3
1	C	9	VAL	3.2
1	C	43	ALA	3.2
1	D	86	CYS	3.2
1	D	107	PRO	3.2
1	D	202	ARG	3.2
1	C	315	ALA	3.1
1	D	15[A]	ARG	3.1
1	D	203	ASP	3.1
1	C	38	GLY	3.1
1	C	47	HIS	3.1
1	D	55	LEU	3.1
1	D	83	CYS	3.0
1	C	49	ASP	3.0
1	D	6	TYR	3.0
1	C	133	GLU	3.0
1	C	203	ASP	3.0
1	C	50	ARG	2.9
1	C	44	TYR	2.9
1	D	314	ARG	2.9
1	D	9	VAL	2.9
1	D	52	PRO	2.9
1	C	200	LEU	2.9
1	D	92	GLY	2.8
1	D	85	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	47	HIS	2.8
1	D	273	TYR	2.8
1	D	82	THR	2.8
1	A	-3	SER	2.7
1	C	254	SER	2.7
1	D	5[A]	VAL	2.7
1	D	0	GLY	2.6
1	D	7	THR	2.6
1	C	205	ASN	2.6
1	D	205	ASN	2.6
1	C	102	ILE	2.6
1	A	203	ASP	2.6
1	C	105	MET	2.6
1	D	317	ARG	2.6
1	C	59	HIS	2.6
1	D	22	PRO	2.6
1	D	54	PRO	2.6
1	C	308	ASP	2.6
1	A	25	GLY	2.5
1	A	195	MET	2.5
1	B	-6	HIS	2.5
1	D	91	SER	2.5
1	B	0	GLY	2.5
1	A	52	PRO	2.5
1	D	212	GLU	2.5
1	C	204	ALA	2.5
1	B	-4	HIS	2.5
1	C	51	ARG	2.5
1	C	5[A]	VAL	2.4
1	D	88	ALA	2.4
1	C	42	HIS	2.4
1	D	100	ARG	2.4
1	D	12	LEU	2.4
1	D	50	ARG	2.4
1	C	15[A]	ARG	2.4
1	D	204	ALA	2.4
1	D	10	ALA	2.3
1	B	21	VAL	2.3
1	D	48	ASP	2.3
1	A	-10	HIS	2.3
1	D	97	CYS	2.3
1	D	99	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	201	ALA	2.3
1	D	30	ARG	2.3
1	D	160	ARG	2.3
1	D	103	ILE	2.2
1	C	316	GLY	2.2
1	D	53	ALA	2.2
1	C	296	ASP	2.2
1	D	84	GLY	2.2
1	C	6	TYR	2.2
1	C	23	ALA	2.2
1	D	43	ALA	2.2
1	D	102	ILE	2.1
1	D	208	ILE	2.1
1	C	80	LEU	2.1
1	B	212	GLU	2.1
1	D	295	LEU	2.1
1	D	198	GLU	2.1
1	D	280	PHE	2.1
1	D	80	LEU	2.1
1	C	25	GLY	2.1
1	C	24	ALA	2.1
1	C	111	ALA	2.1
1	D	310	PHE	2.0
1	C	46	GLY	2.0
1	A	208	ILE	2.0
1	C	69	PRO	2.0
1	C	198	GLU	2.0
1	D	307	ALA	2.0
1	D	49	ASP	2.0
1	D	87	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

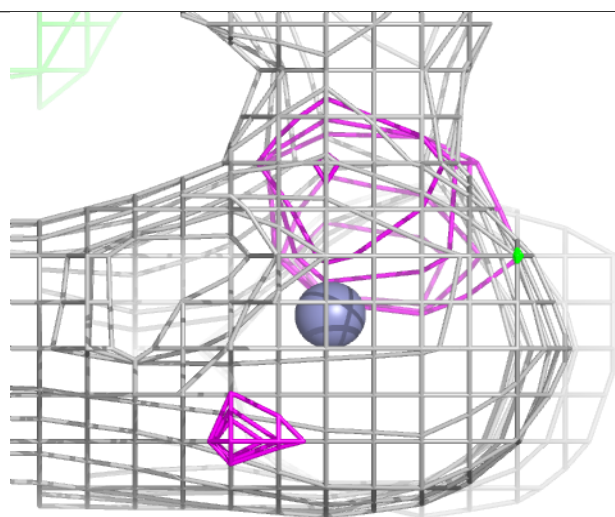
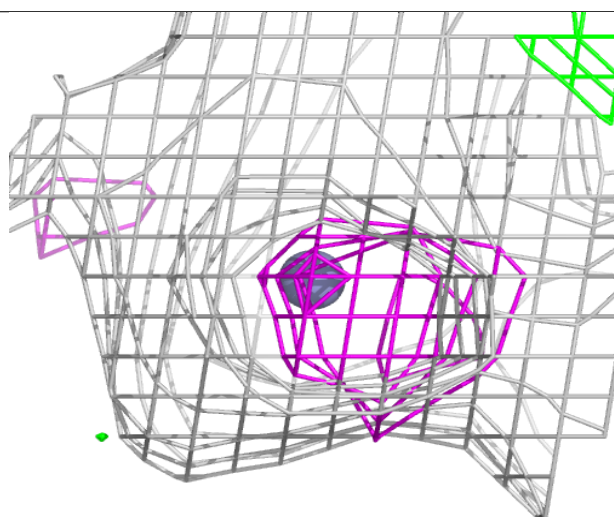
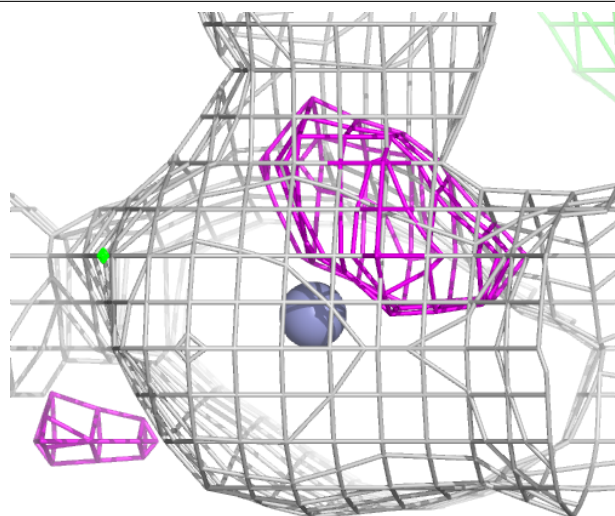
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	402	1/1	0.90	0.12	62,62,62,62	0
2	ZN	D	401	1/1	0.92	0.08	47,47,47,47	0
2	ZN	C	402	1/1	0.93	0.09	64,64,64,64	0
2	ZN	A	403	1/1	0.95	0.08	34,34,34,34	0
2	ZN	C	401	1/1	0.97	0.04	34,34,34,34	0
2	ZN	A	402	1/1	0.97	0.08	32,32,32,32	0
2	ZN	B	401	1/1	0.98	0.03	16,16,16,16	0
2	ZN	B	403	1/1	0.98	0.12	32,32,32,32	0
2	ZN	B	402	1/1	0.99	0.02	26,26,26,26	0
2	ZN	A	401	1/1	0.99	0.01	23,23,23,23	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.

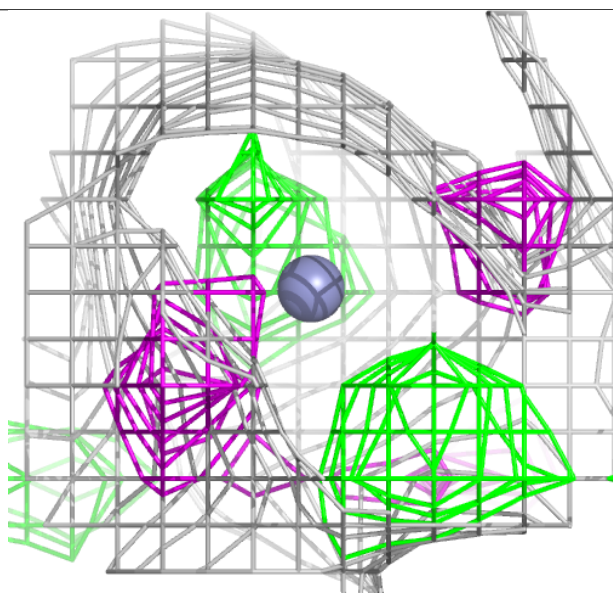
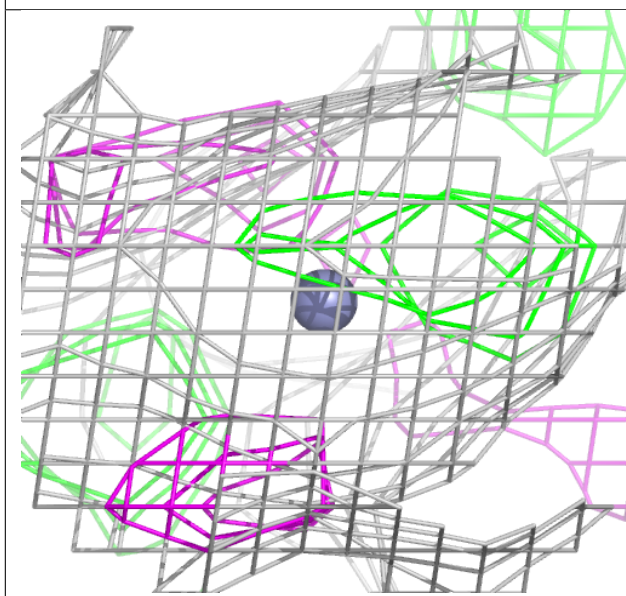
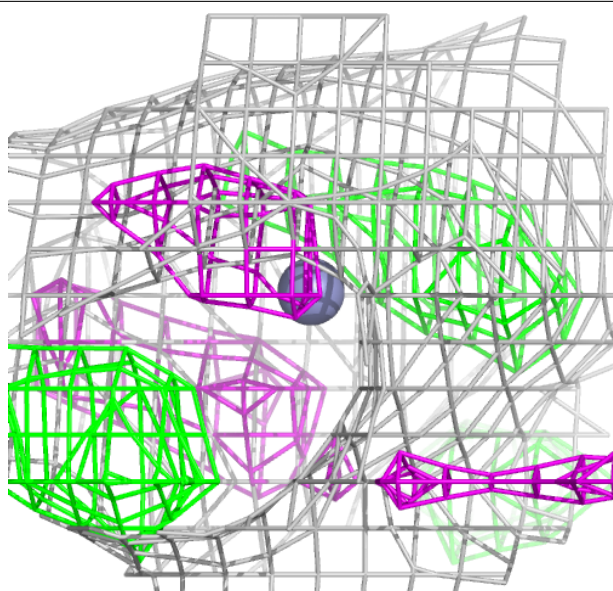
Electron density around ZN D 402:

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



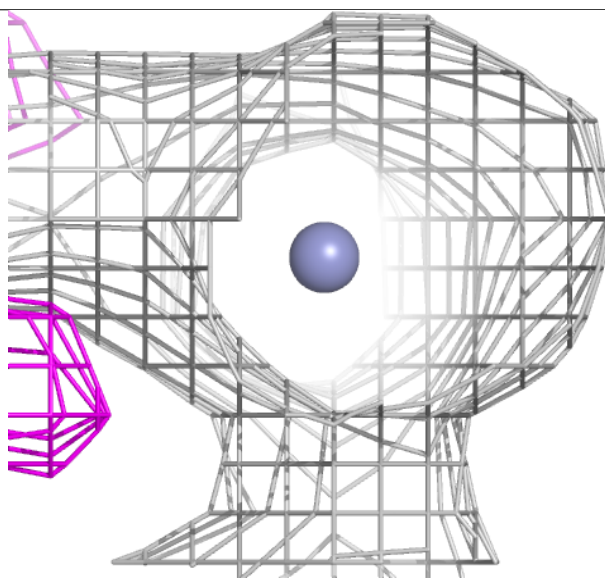
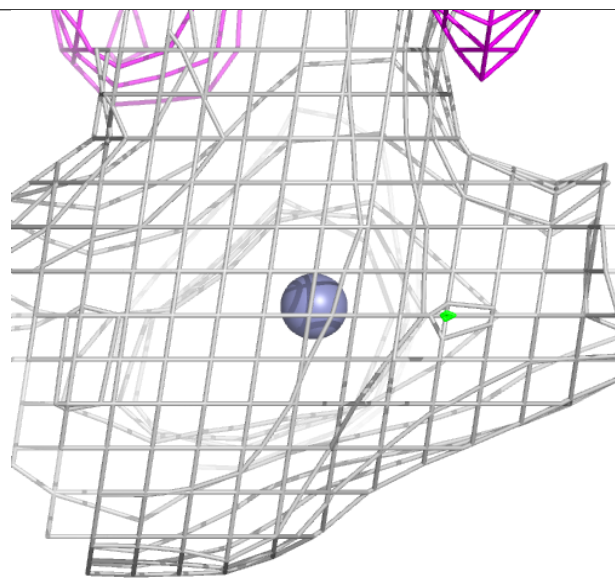
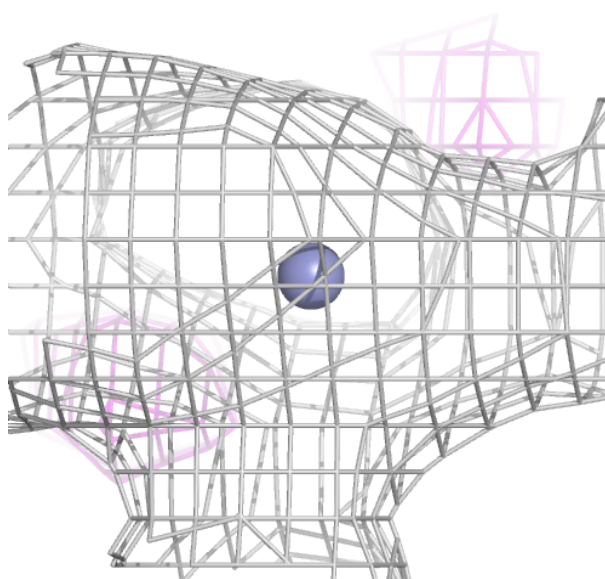
Electron density around ZN D 401:

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



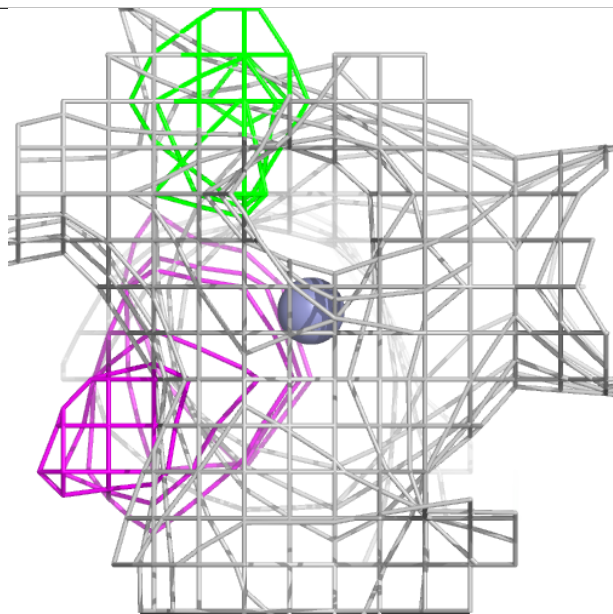
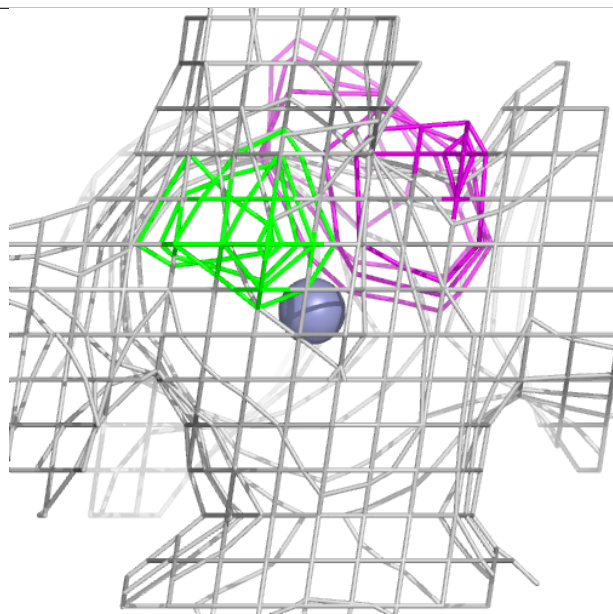
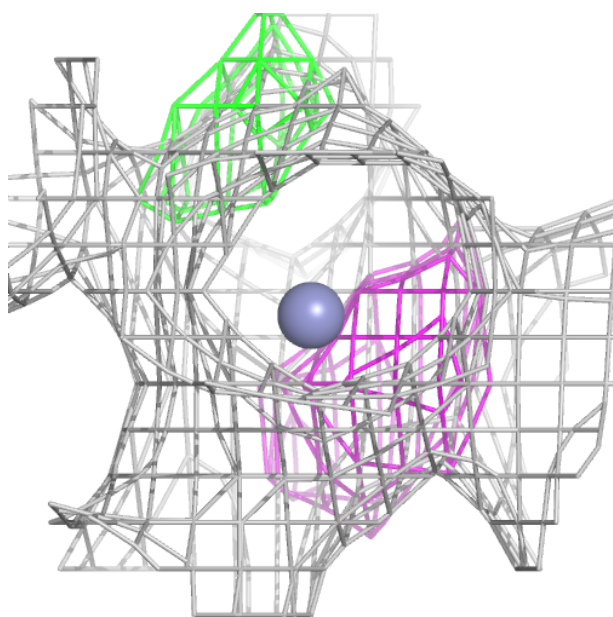
Electron density around ZN C 402:

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



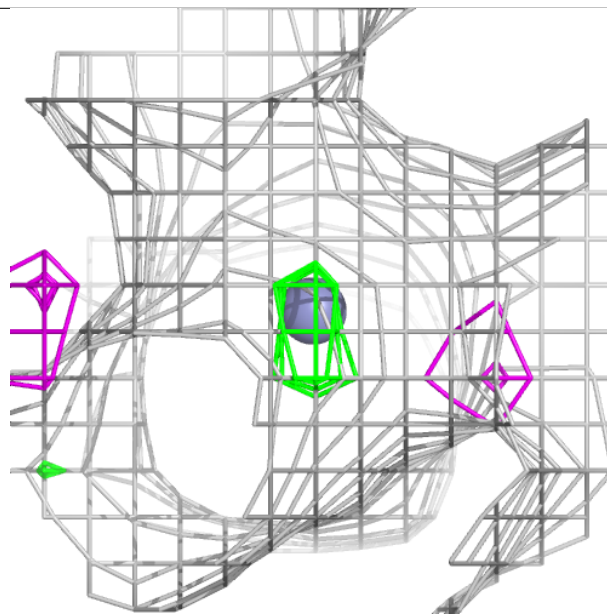
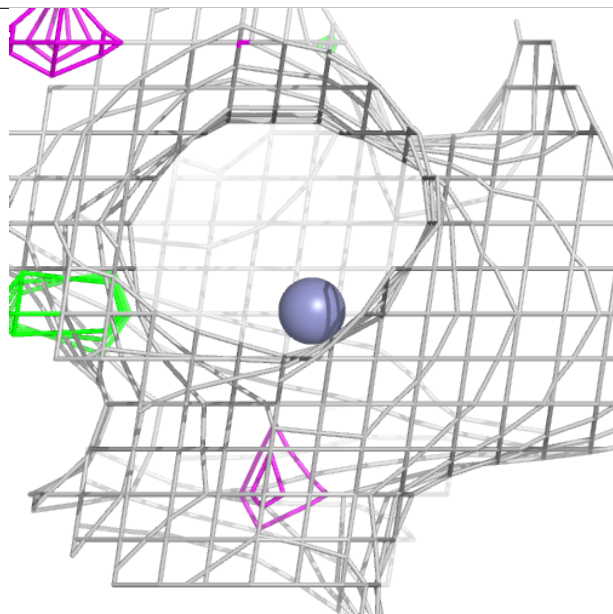
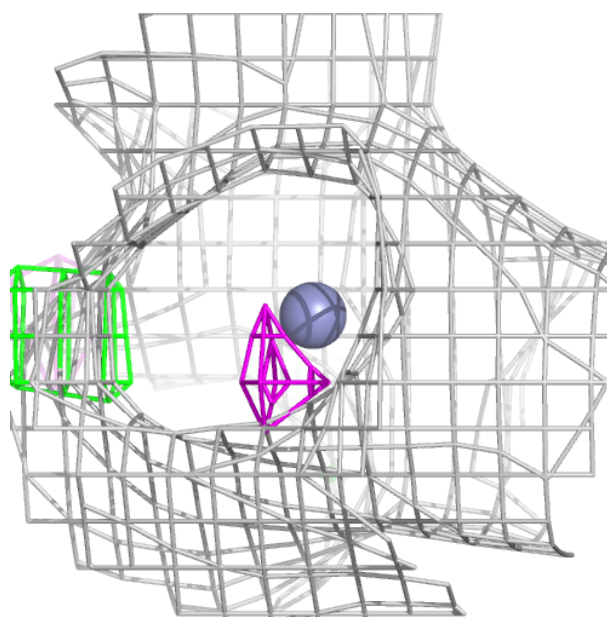
Electron density around ZN A 403:

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



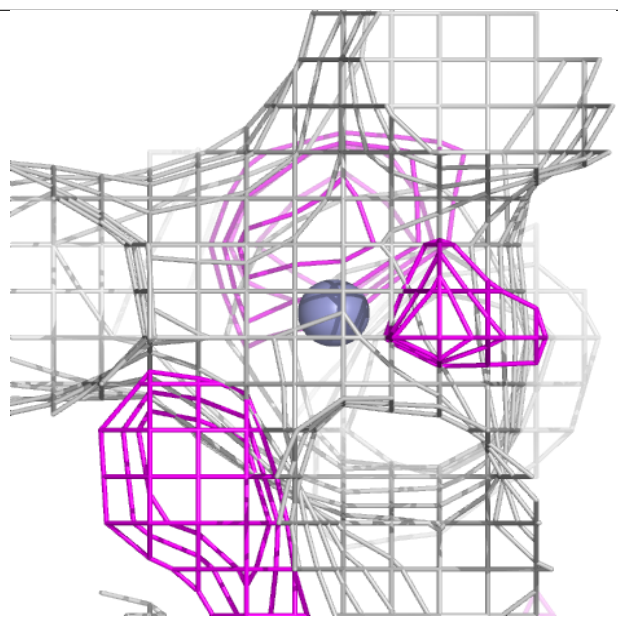
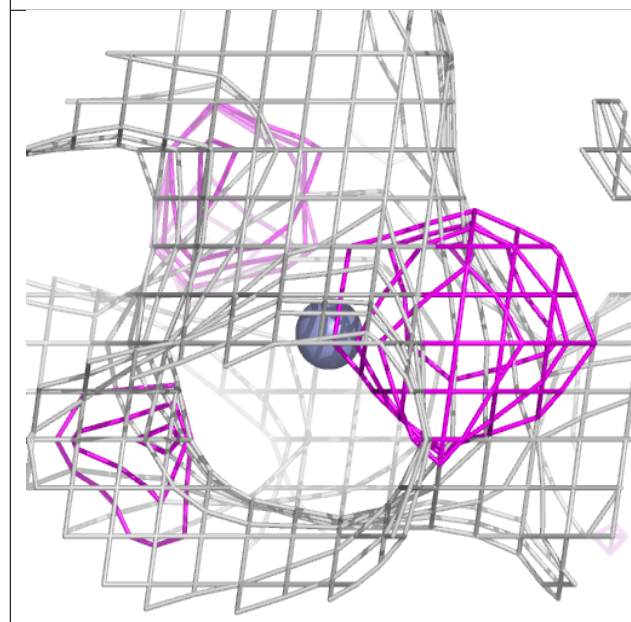
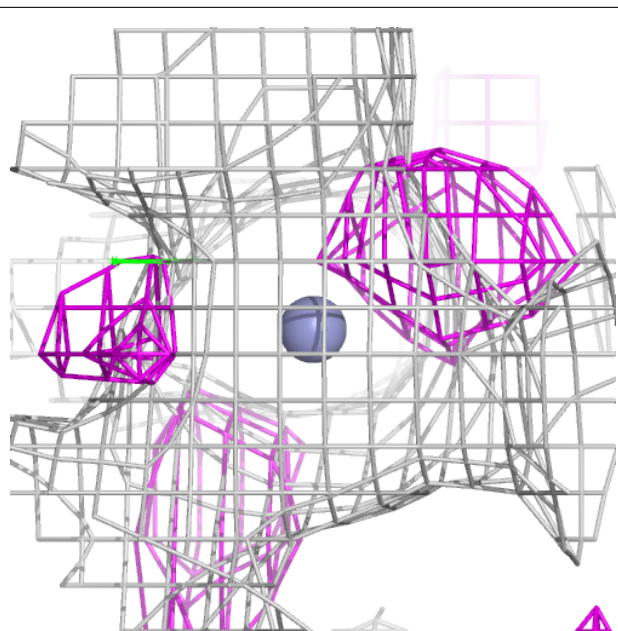
Electron density around ZN C 401:

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



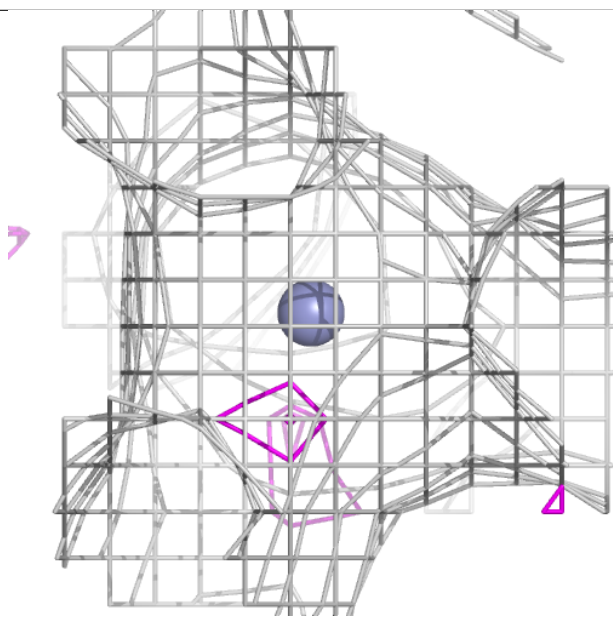
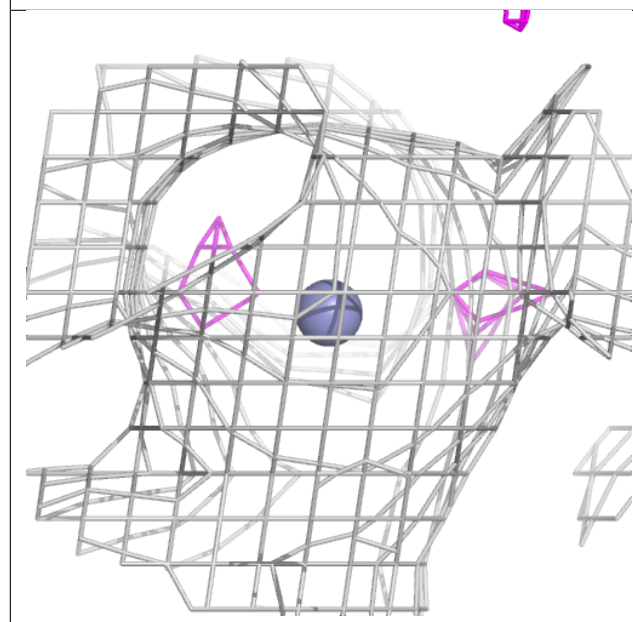
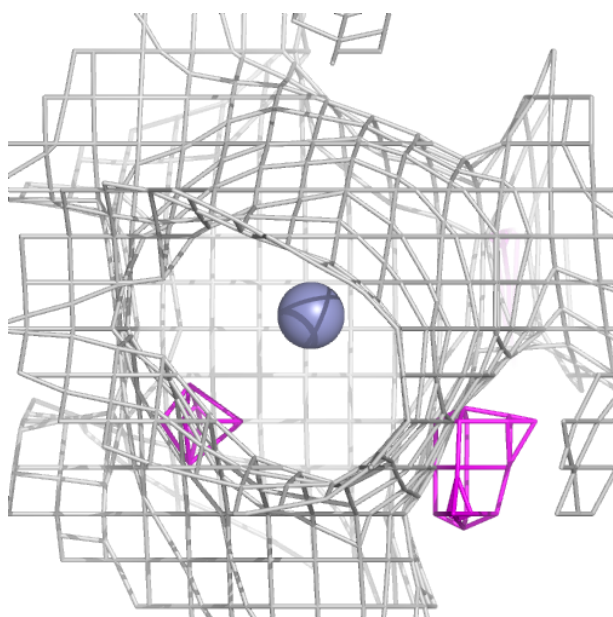
Electron density around ZN A 402:

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



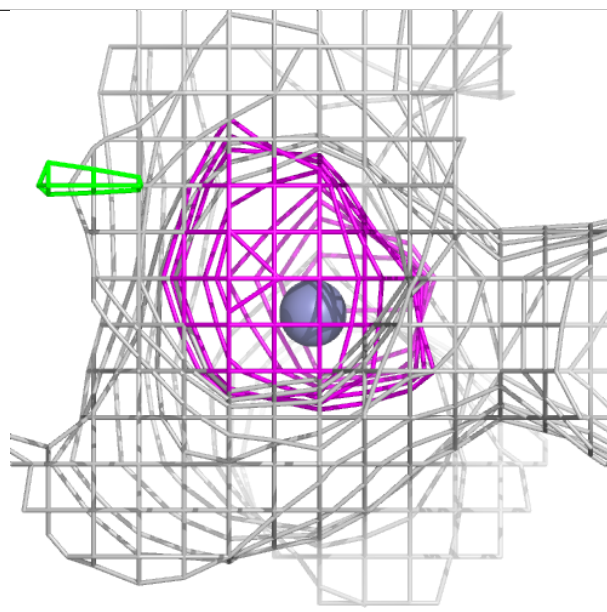
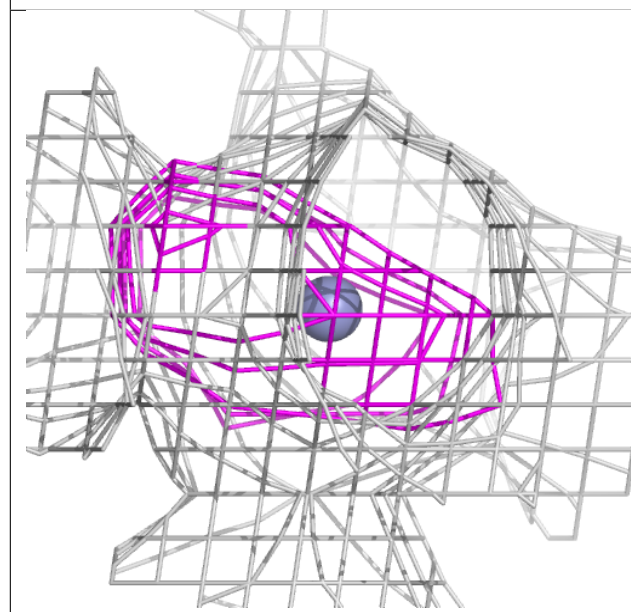
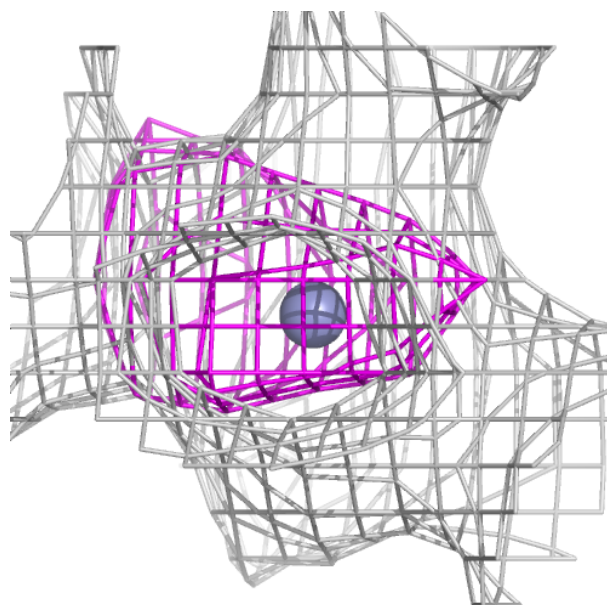
Electron density around ZN B 401:

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



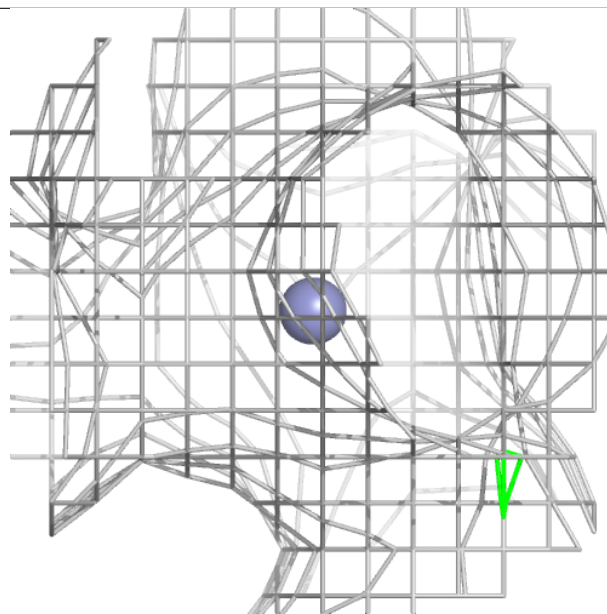
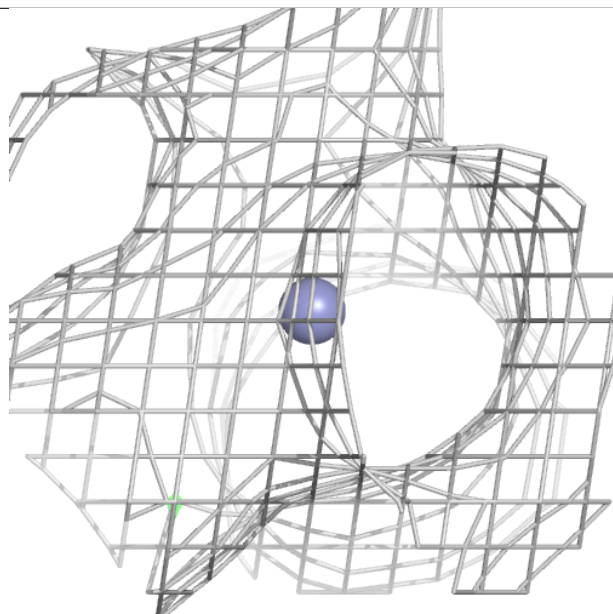
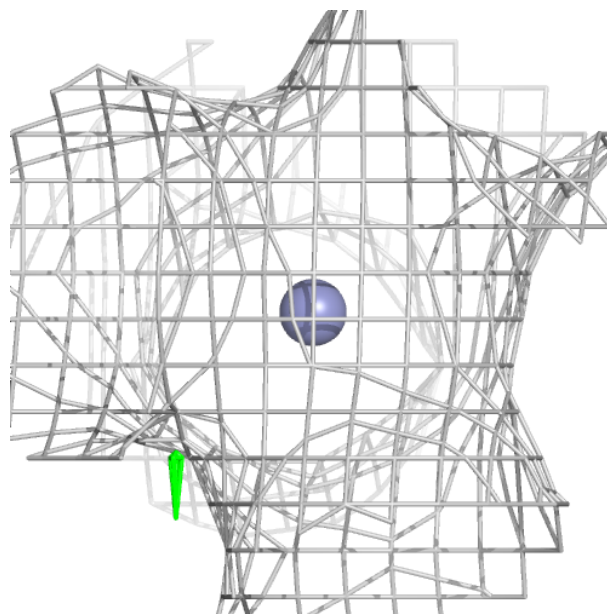
Electron density around ZN B 403:

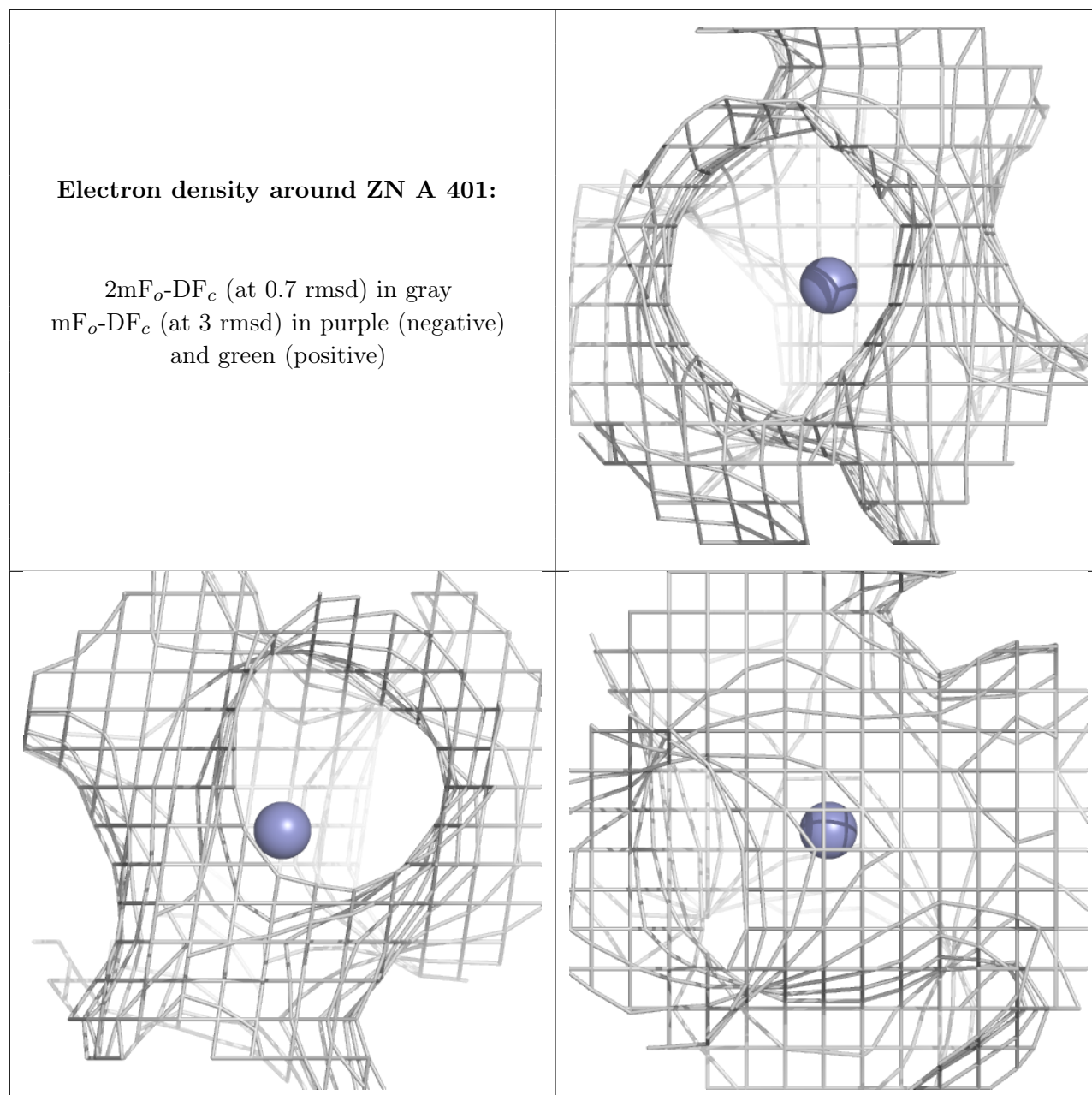
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 402:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.