



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 03:24 AM EST

PDB ID : 6VBS
Title : The C2 Crystal form of SodCI Superoxide Dismutase at 1.7 Å resolution with 6 molecules in the asymmetric unit.
Authors : Satyshur, K.A.; Forest, K.T.; Newhouse, P.W.
Deposited on : 2019-12-19
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

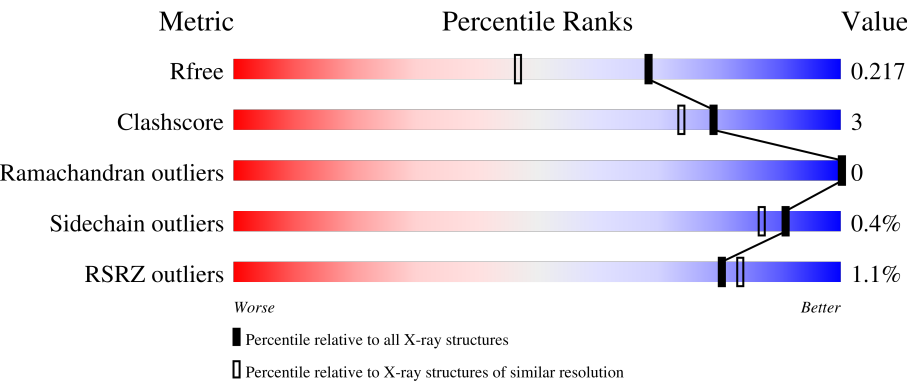
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	165	<div><div>%</div><div>90% . . 5%</div></div>
1	B	165	<div><div>%</div><div>89% 5% 6%</div></div>
1	C	165	<div><div></div><div>88% 6% 5%</div></div>
1	D	165	<div><div>%</div><div>93% . .</div></div>
1	E	165	<div><div>%</div><div>88% 6% 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	165	<div><div></div><div>3%</div><div>86%</div><div>6%</div><div>8%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14487 atoms, of which 6762 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	H	N	O	S	0	1	0
			2269	716	1126	199	221	7			
1	B	155	Total	C	H	N	O	S	0	0	0
			2243	708	1115	197	216	7			
1	C	156	Total	C	H	N	O	S	0	0	0
			2263	714	1126	199	217	7			
1	D	159	Total	C	H	N	O	S	0	1	0
			2325	733	1156	203	226	7			
1	E	156	Total	C	H	N	O	S	0	1	0
			2275	718	1130	199	220	8			
1	F	152	Total	C	H	N	O	S	0	1	0
			2231	706	1109	195	213	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	LEU	-	expression tag	UNP A0A0D6GQL3
A	159	GLU	-	expression tag	UNP A0A0D6GQL3
A	160	HIS	-	expression tag	UNP A0A0D6GQL3
A	161	HIS	-	expression tag	UNP A0A0D6GQL3
A	162	HIS	-	expression tag	UNP A0A0D6GQL3
A	163	HIS	-	expression tag	UNP A0A0D6GQL3
A	164	HIS	-	expression tag	UNP A0A0D6GQL3
A	165	HIS	-	expression tag	UNP A0A0D6GQL3
B	158	LEU	-	expression tag	UNP A0A0D6GQL3
B	159	GLU	-	expression tag	UNP A0A0D6GQL3
B	160	HIS	-	expression tag	UNP A0A0D6GQL3
B	161	HIS	-	expression tag	UNP A0A0D6GQL3
B	162	HIS	-	expression tag	UNP A0A0D6GQL3
B	163	HIS	-	expression tag	UNP A0A0D6GQL3
B	164	HIS	-	expression tag	UNP A0A0D6GQL3
B	165	HIS	-	expression tag	UNP A0A0D6GQL3
C	158	LEU	-	expression tag	UNP A0A0D6GQL3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	159	GLU	-	expression tag	UNP A0A0D6GQL3
C	160	HIS	-	expression tag	UNP A0A0D6GQL3
C	161	HIS	-	expression tag	UNP A0A0D6GQL3
C	162	HIS	-	expression tag	UNP A0A0D6GQL3
C	163	HIS	-	expression tag	UNP A0A0D6GQL3
C	164	HIS	-	expression tag	UNP A0A0D6GQL3
C	165	HIS	-	expression tag	UNP A0A0D6GQL3
D	158	LEU	-	expression tag	UNP A0A0D6GQL3
D	159	GLU	-	expression tag	UNP A0A0D6GQL3
D	160	HIS	-	expression tag	UNP A0A0D6GQL3
D	161	HIS	-	expression tag	UNP A0A0D6GQL3
D	162	HIS	-	expression tag	UNP A0A0D6GQL3
D	163	HIS	-	expression tag	UNP A0A0D6GQL3
D	164	HIS	-	expression tag	UNP A0A0D6GQL3
D	165	HIS	-	expression tag	UNP A0A0D6GQL3
E	158	LEU	-	expression tag	UNP A0A0D6GQL3
E	159	GLU	-	expression tag	UNP A0A0D6GQL3
E	160	HIS	-	expression tag	UNP A0A0D6GQL3
E	161	HIS	-	expression tag	UNP A0A0D6GQL3
E	162	HIS	-	expression tag	UNP A0A0D6GQL3
E	163	HIS	-	expression tag	UNP A0A0D6GQL3
E	164	HIS	-	expression tag	UNP A0A0D6GQL3
E	165	HIS	-	expression tag	UNP A0A0D6GQL3
F	158	LEU	-	expression tag	UNP A0A0D6GQL3
F	159	GLU	-	expression tag	UNP A0A0D6GQL3
F	160	HIS	-	expression tag	UNP A0A0D6GQL3
F	161	HIS	-	expression tag	UNP A0A0D6GQL3
F	162	HIS	-	expression tag	UNP A0A0D6GQL3
F	163	HIS	-	expression tag	UNP A0A0D6GQL3
F	164	HIS	-	expression tag	UNP A0A0D6GQL3
F	165	HIS	-	expression tag	UNP A0A0D6GQL3

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0

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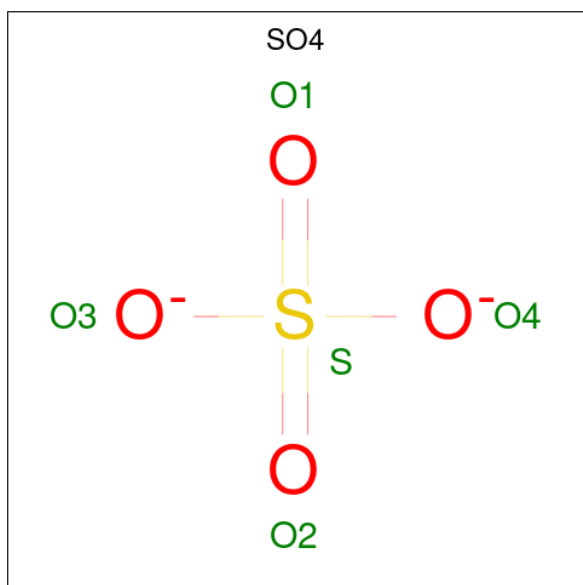
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

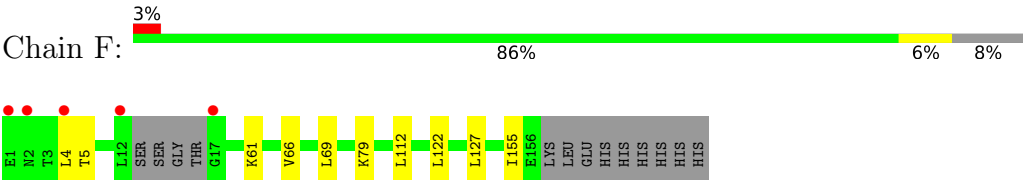
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	135	Total O 135 135	0	0
5	B	149	Total O 149 149	0	0
5	C	163	Total O 163 163	0	0
5	D	147	Total O 147 147	0	0
5	E	131	Total O 131 131	0	0
5	F	124	Total O 124 124	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.84Å 69.47Å 95.29Å 90.00° 116.89° 90.00°	Depositor
Resolution (Å)	35.88 – 1.70 84.99 – 1.53	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.88-1.70) 75.9 (84.99-1.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.178 , 0.219 0.185 , 0.217	Depositor DCC
R_{free} test set	2000 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14487	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 4.75% 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, SO4, CU

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	0.42	0/1171	0.66	0/1588
1	B	0.40	0/1156	0.65	0/1568
1	C	0.40	0/1165	0.66	0/1579
1	D	0.41	0/1197	0.66	0/1622
1	E	0.42	0/1173	0.64	0/1590
1	F	0.39	0/1149	0.63	0/1556
All	All	0.41	0/7011	0.65	0/9503

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1143	1126	1124	6	0
1	B	1128	1115	1114	7	0
1	C	1137	1126	1124	11	0
1	D	1169	1156	1154	5	0
1	E	1145	1130	1128	8	0
1	F	1122	1109	1107	8	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	135	0	0	3	0
5	B	149	0	0	0	0
5	C	163	0	0	2	0
5	D	147	0	0	0	0
5	E	131	0	0	2	0
5	F	124	0	0	0	0
All	All	7725	6762	6751	38	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 3.

All (38) 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:B:42:THR:HG21	1:C:117:LYS:HB3	1.83	0.61
5:A:424:HOH:O	1:C:57:MET:HE1	2.04	0.58
1:D:42:THR:HG21	1:D:131:LYS:HE2	1.87	0.57
1:A:4:LEU:HD21	1:A:123:LYS:HE2	1.87	0.56
5:A:424:HOH:O	1:C:57:MET:CE	2.54	0.56
1:D:41:LEU:HD23	1:D:150:PHE:CE2	2.42	0.54
1:F:127:LEU:HG	1:F:155:ILE:HD11	1.91	0.52
1:F:122:LEU:HB3	1:F:155:ILE:HD13	1.92	0.52
1:B:127:LEU:HG	1:B:155:ILE:HD11	1.92	0.50
1:F:61:LYS:HG3	1:F:66:VAL:HG21	1.94	0.50
1:C:7:LYS:HD3	1:C:22:GLU:HB3	1.91	0.50
1:A:122:LEU:HB3	1:A:155:ILE:HD13	1.94	0.49
1:B:70:MET:HE1	1:E:117:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASN:N	5:C:304:HOH:O	2.45	0.49
1:E:4:LEU:HD12	1:E:119:LEU:HD22	1.95	0.48
1:D:45:ILE:CD1	1:D:100:VAL:HG22	2.43	0.48
1:A:57:MET:CE	1:A:57:MET:HA	2.44	0.48
1:E:83:HIS:CE1	1:E:95:ASP:CG	2.88	0.47
1:B:60:MET:SD	1:B:65:GLU:HG2	2.55	0.47
1:E:122:LEU:HB3	1:E:155:ILE:HD13	1.96	0.46
1:F:4:LEU:HD23	1:F:5:THR:N	2.29	0.46
1:B:12:LEU:HD23	1:C:120:SER:HB2	1.97	0.46
1:D:42:THR:CG2	1:D:131:LYS:HE2	2.46	0.46
1:C:57:MET:HE3	1:C:57:MET:HB3	1.72	0.45
1:C:2:ASN:ND2	5:C:306:HOH:O	2.49	0.45
1:B:100:VAL:HG11	1:D:45:ILE:HD11	1.97	0.45
1:C:122:LEU:HB3	1:C:155:ILE:HD13	1.99	0.45
1:A:156:GLU:HG2	5:A:411:HOH:O	2.16	0.44
1:C:114:PRO:HG3	1:F:112:LEU:HD22	2.00	0.44
1:E:4:LEU:HG	1:E:119:LEU:HD13	1.99	0.43
1:F:61:LYS:HE2	1:F:69:LEU:HD21	2.00	0.43
1:E:91:GLY:HA3	5:E:371:HOH:O	2.19	0.42
1:E:111:LEU:HA	5:E:330:HOH:O	2.19	0.42
1:A:20:ILE:HB	1:A:39:ASN:O	2.20	0.42
1:A:4:LEU:HD21	1:A:123:LYS:CE	2.48	0.41
1:B:70:MET:HE3	1:E:117:LYS:HB3	2.03	0.41
1:C:114:PRO:HG3	1:F:112:LEU:CD2	2.51	0.40
1:F:79:LYS:O	1:F:79:LYS:CG	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/165 (94%)	152 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
1	C	154/165 (93%)	151 (98%)	3 (2%)	0	100	100
1	D	158/165 (96%)	155 (98%)	3 (2%)	0	100	100
1	E	155/165 (94%)	154 (99%)	1 (1%)	0	100	100
1	F	149/165 (90%)	146 (98%)	3 (2%)	0	100	100
All	All	924/990 (93%)	910 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/131 (94%)	122 (99%)	1 (1%)	81	74
1	B	121/131 (92%)	121 (100%)	0	100	100
1	C	122/131 (93%)	121 (99%)	1 (1%)	81	74
1	D	126/131 (96%)	126 (100%)	0	100	100
1	E	123/131 (94%)	122 (99%)	1 (1%)	81	74
1	F	120/131 (92%)	120 (100%)	0	100	100
All	All	735/786 (94%)	732 (100%)	3 (0%)	91	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	C	79	LYS
1	E	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2	ASN
1	F	53	ASN

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 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	203	-	4,4,4	0.14	0	6,6,6	0.26	0
4	SO4	C	204	-	4,4,4	0.14	0	6,6,6	0.19	0
4	SO4	C	203	-	4,4,4	0.22	0	6,6,6	0.27	0
4	SO4	D	203	-	4,4,4	0.11	0	6,6,6	0.13	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/165 (94%)	-0.39	1 (0%) 89 91	13, 20, 36, 73	0
1	B	155/165 (93%)	-0.38	1 (0%) 89 91	13, 19, 35, 67	0
1	C	156/165 (94%)	-0.37	0 100 100	13, 19, 40, 57	0
1	D	159/165 (96%)	-0.42	1 (0%) 89 91	13, 19, 37, 57	0
1	E	156/165 (94%)	-0.20	2 (1%) 77 81	15, 23, 45, 70	0
1	F	152/165 (92%)	-0.14	5 (3%) 46 51	15, 24, 46, 63	0
All	All	934/990 (94%)	-0.32	10 (1%) 80 83	13, 21, 41, 73	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	17	GLY	6.8
1	E	1	GLU	4.6
1	F	1	GLU	4.4
1	A	1	GLU	3.8
1	B	1	GLU	3.7
1	F	2	ASN	3.4
1	F	12	LEU	3.2
1	F	4	LEU	2.7
1	E	2	ASN	2.5
1	D	158	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

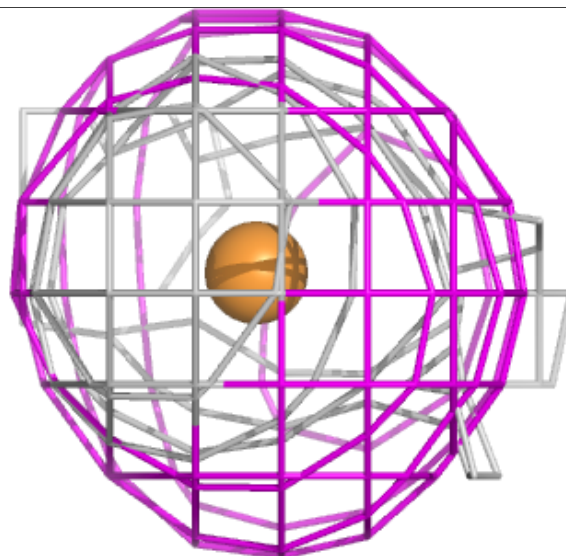
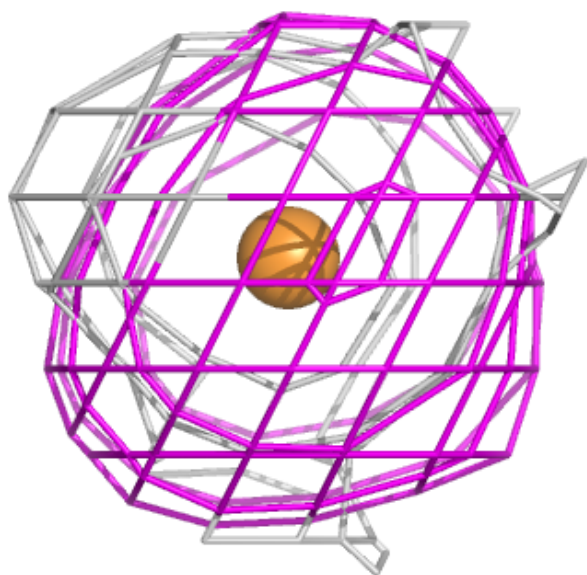
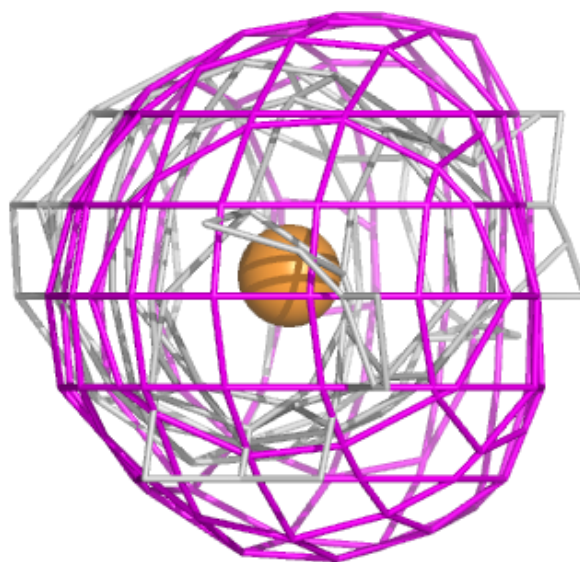
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	D	203	5/5	0.86	0.23	36,40,46,58	0
2	CU	C	202	1/1	0.89	0.43	39,39,39,39	0
2	CU	B	202	1/1	0.91	0.54	39,39,39,39	0
4	SO4	C	203	5/5	0.94	0.13	27,31,32,34	0
4	SO4	B	203	5/5	0.94	0.22	28,29,43,48	0
4	SO4	C	204	5/5	0.96	0.18	32,38,46,57	0
2	CU	E	201	1/1	0.96	0.54	46,46,46,46	0
2	CU	F	202	1/1	0.97	0.55	44,44,44,44	0
3	ZN	E	202	1/1	0.97	0.04	20,20,20,20	0
2	CU	D	202	1/1	0.98	0.49	42,42,42,42	0
2	CU	A	201	1/1	0.98	0.55	35,35,35,35	0
3	ZN	F	201	1/1	0.99	0.04	13,13,13,13	0
3	ZN	B	201	1/1	0.99	0.04	10,10,10,10	0
3	ZN	C	201	1/1	0.99	0.04	10,10,10,10	0
3	ZN	D	201	1/1	0.99	0.04	11,11,11,11	0
3	ZN	A	202	1/1	0.99	0.03	11,11,11,11	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.

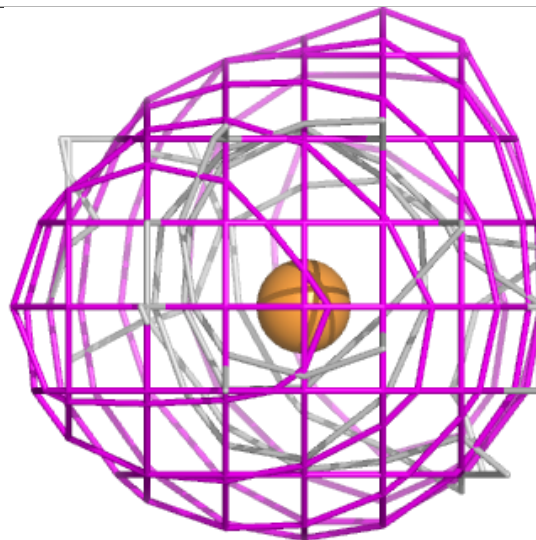
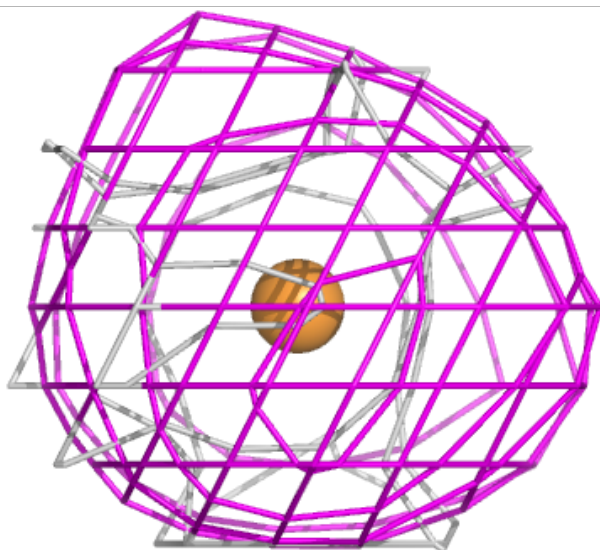
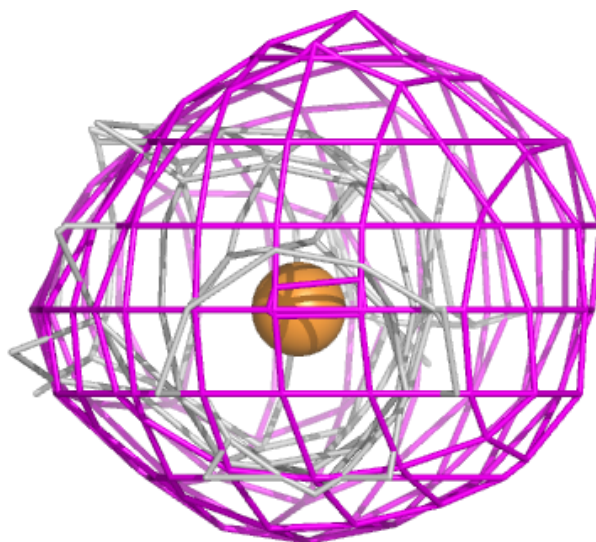
Electron density around CU C 202:

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



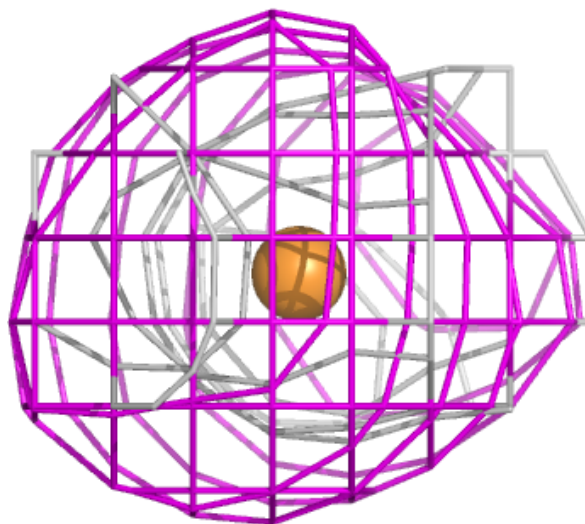
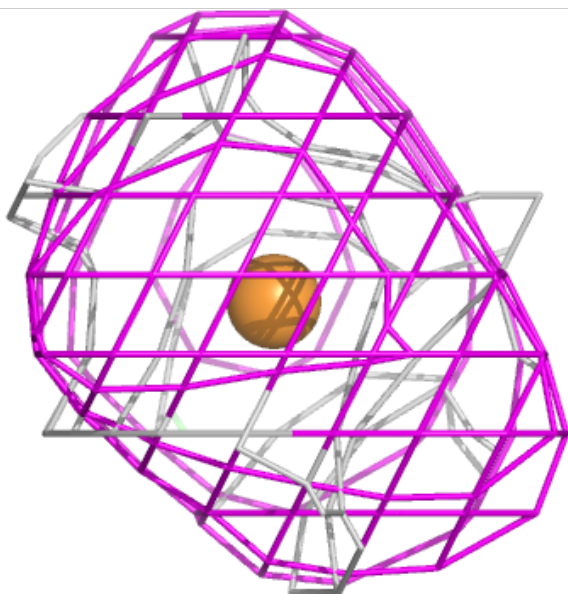
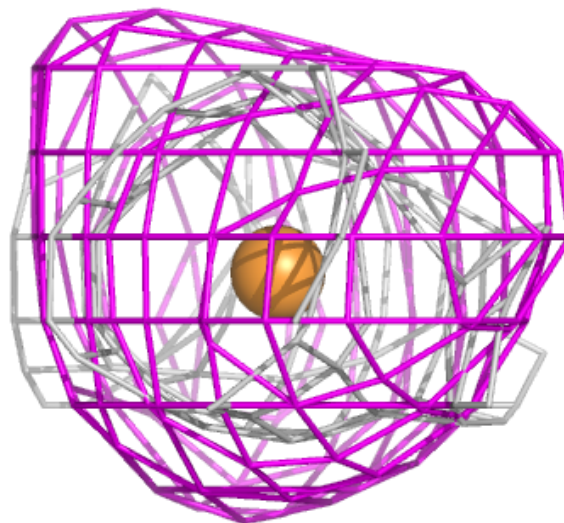
Electron density around CU B 202:

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



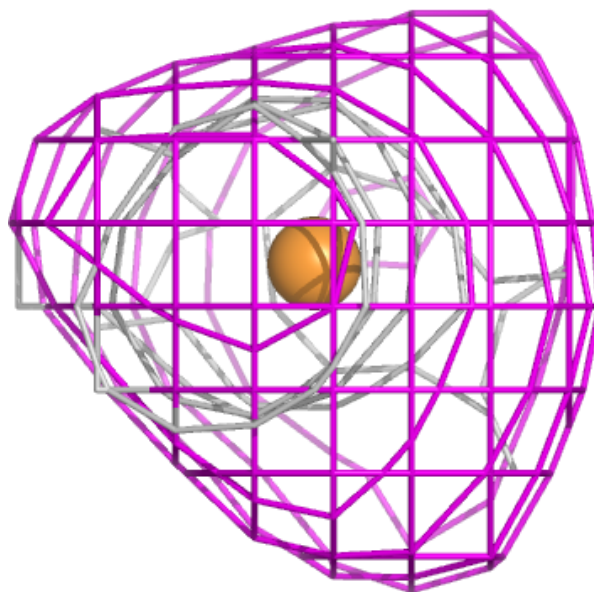
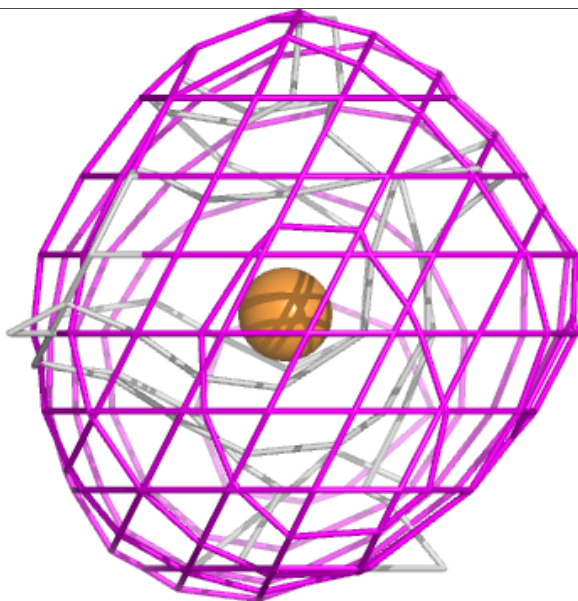
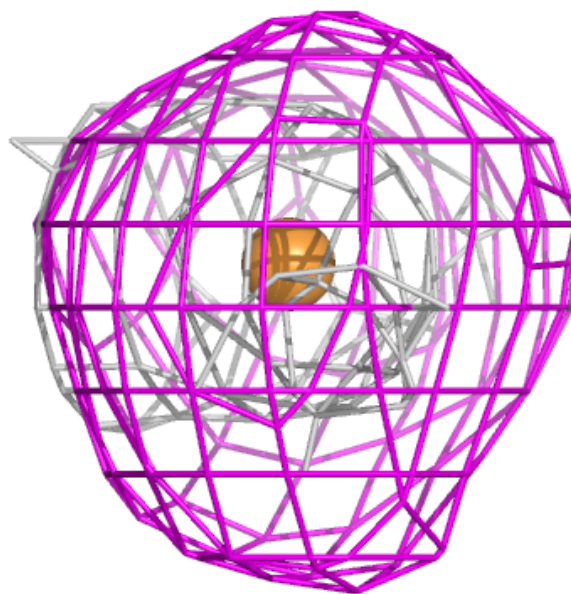
Electron density around CU E 201:

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



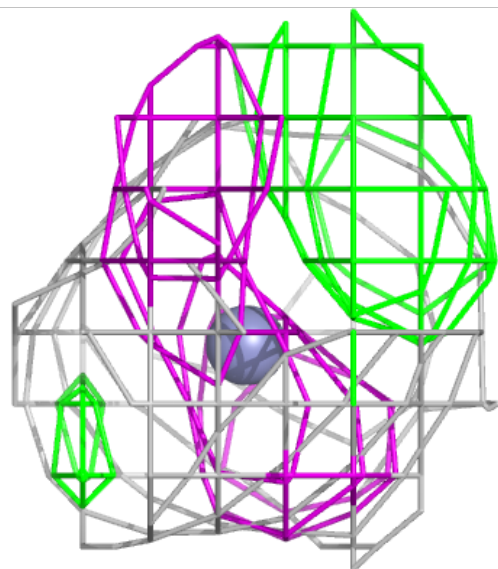
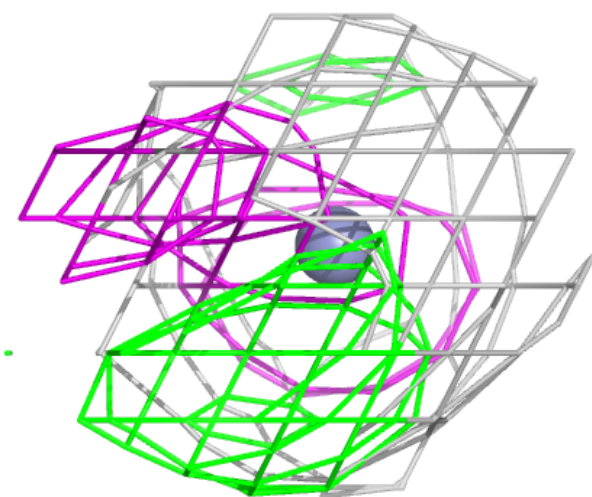
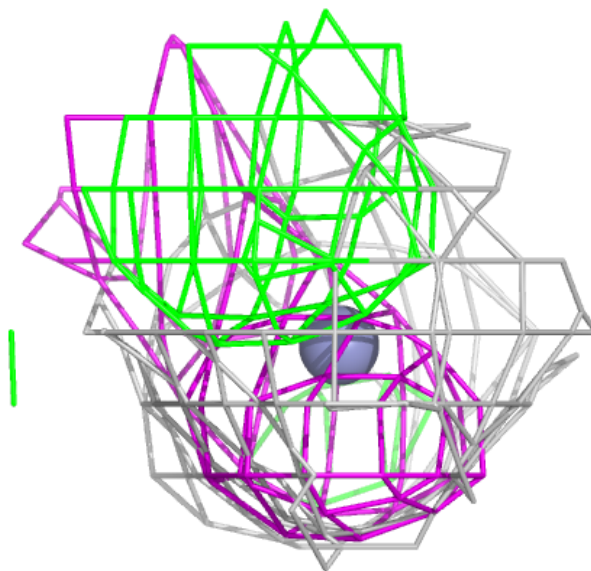
Electron density around CU F 202:

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



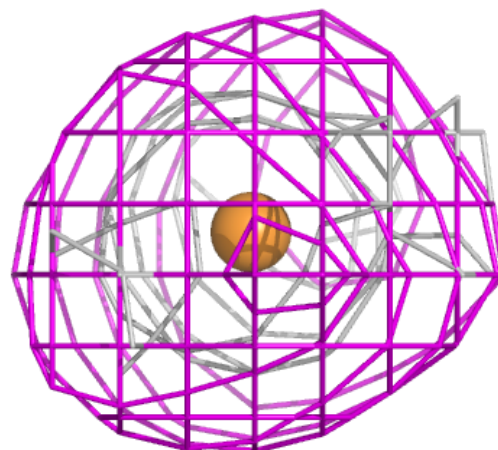
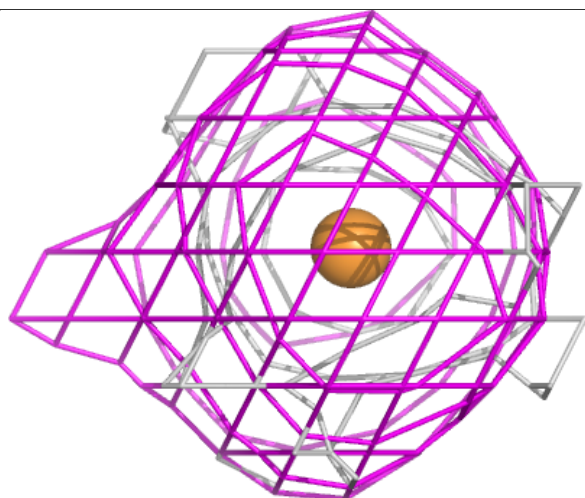
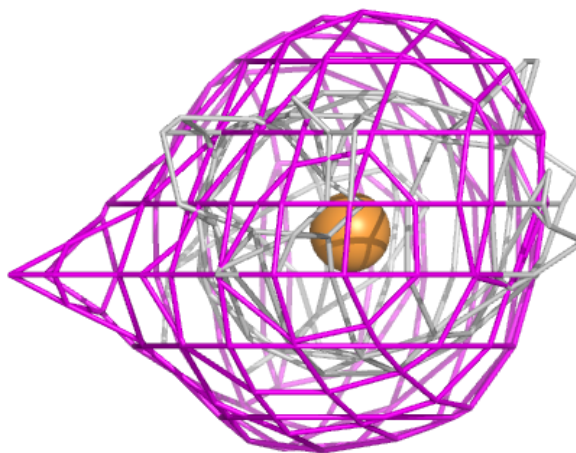
Electron density around ZN E 202:

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



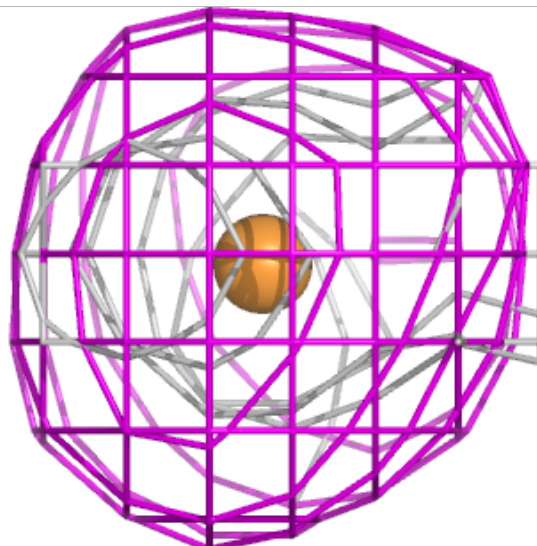
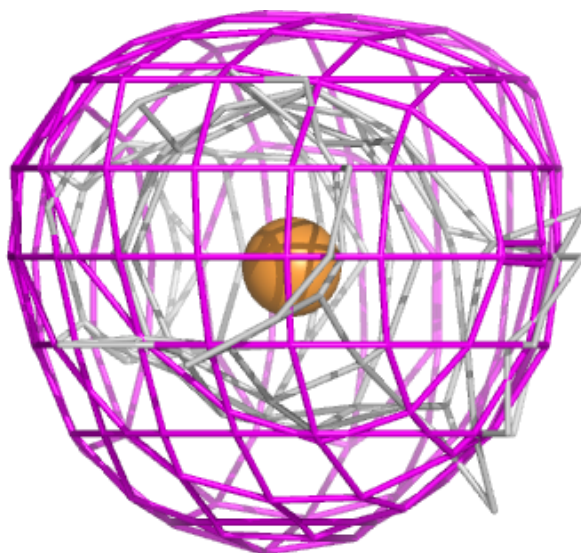
Electron density around CU D 202:

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



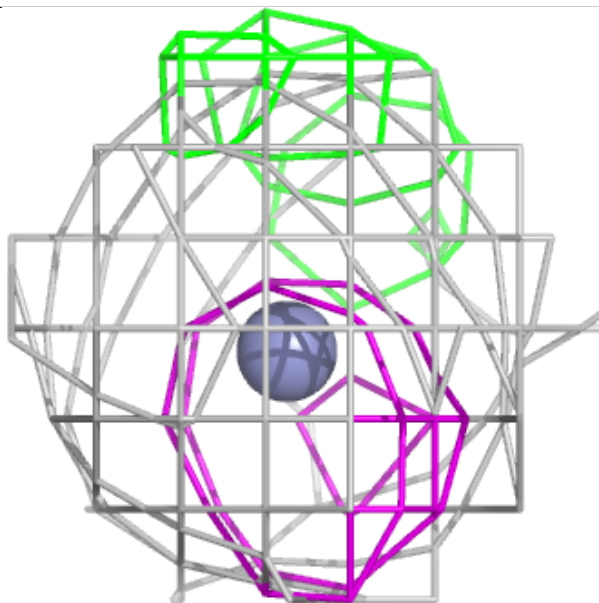
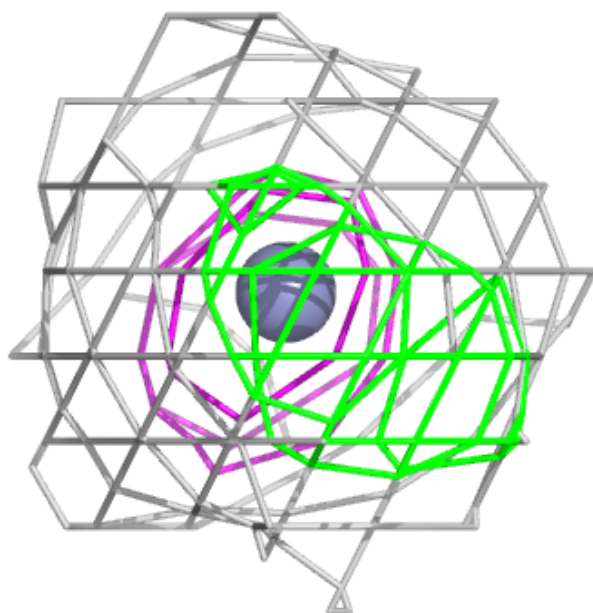
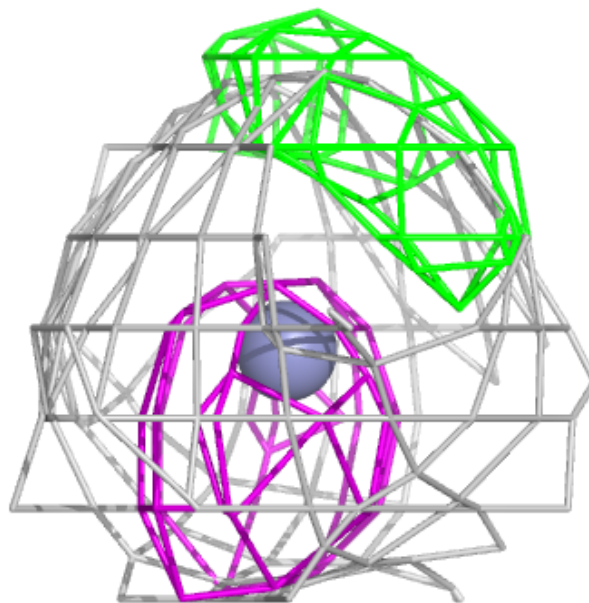
Electron density around CU A 201:

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



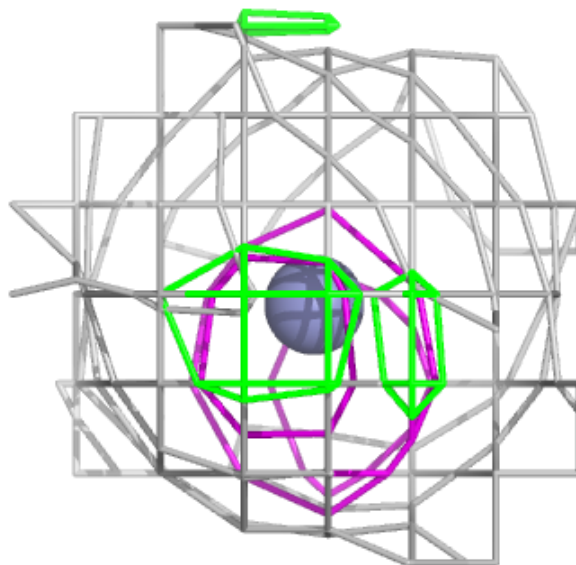
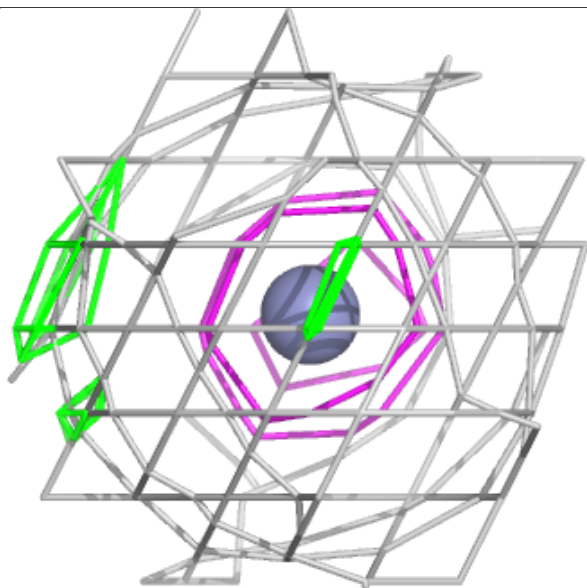
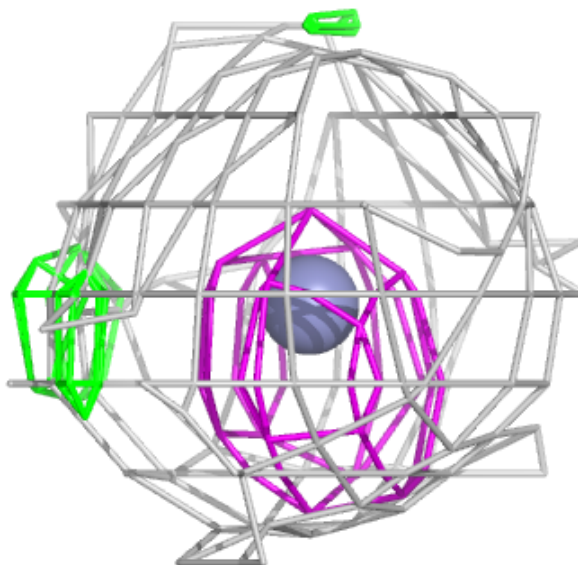
Electron density around ZN F 201:

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



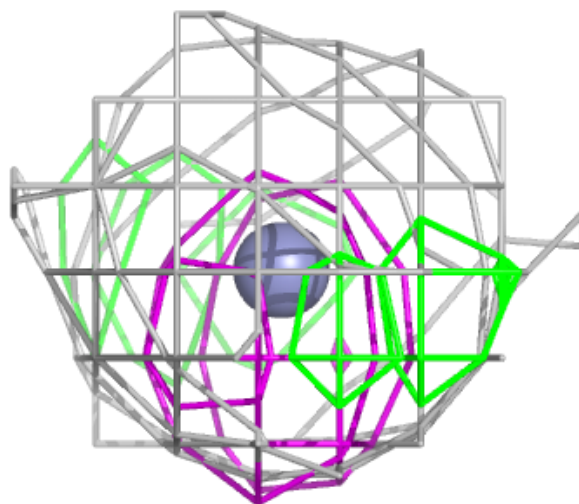
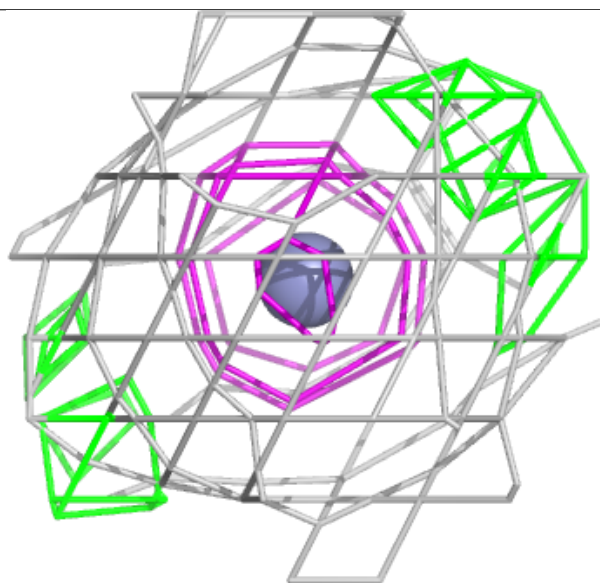
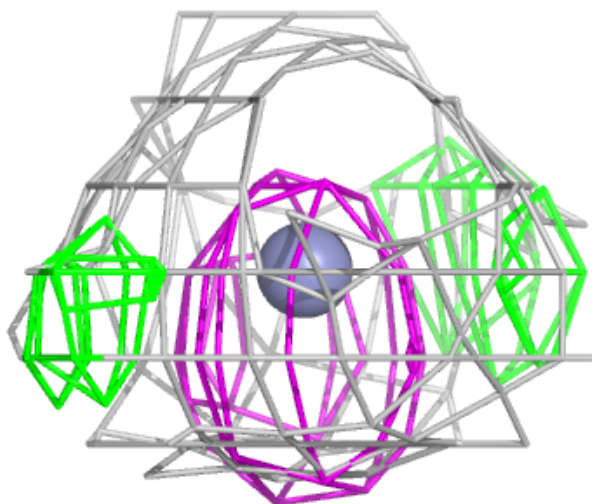
Electron density around ZN B 201:

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



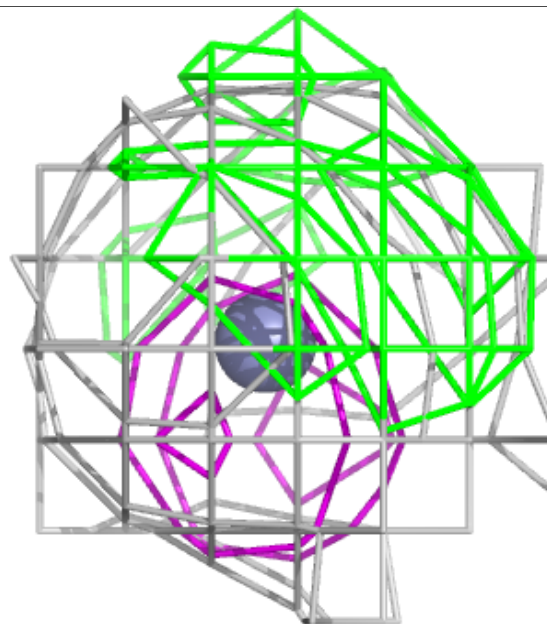
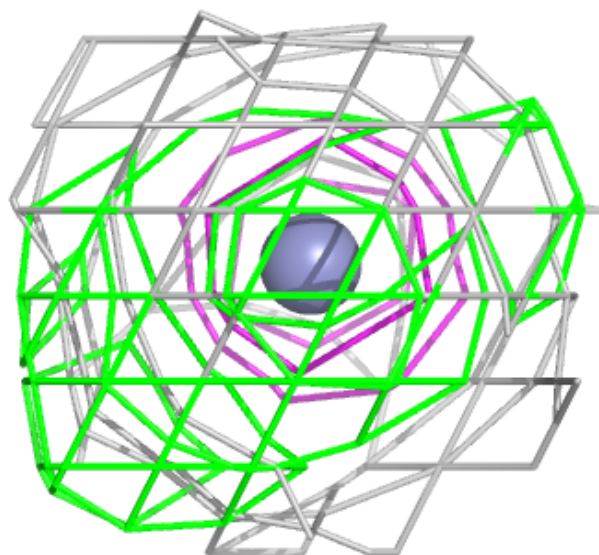
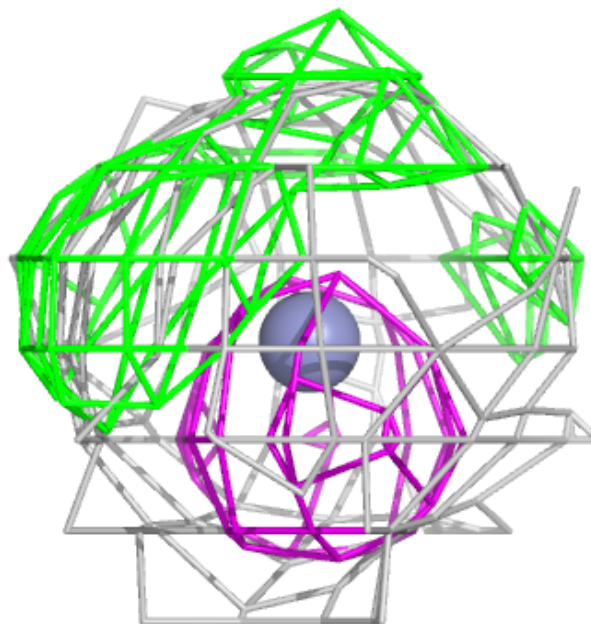
Electron density around ZN C 201:

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



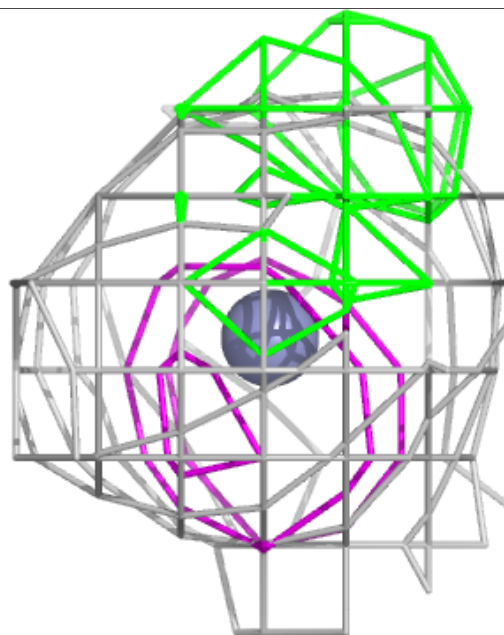
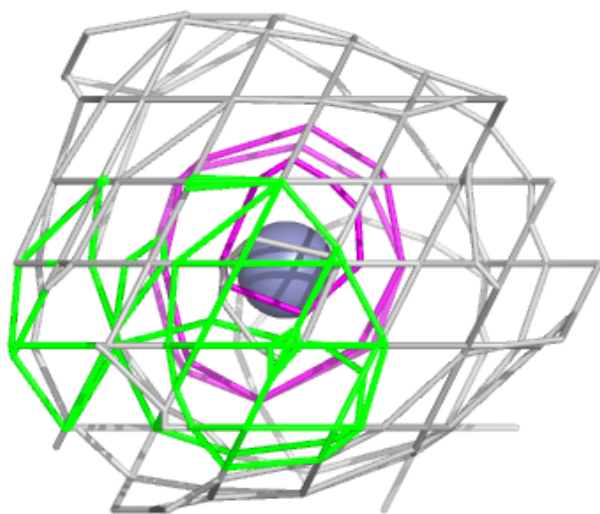
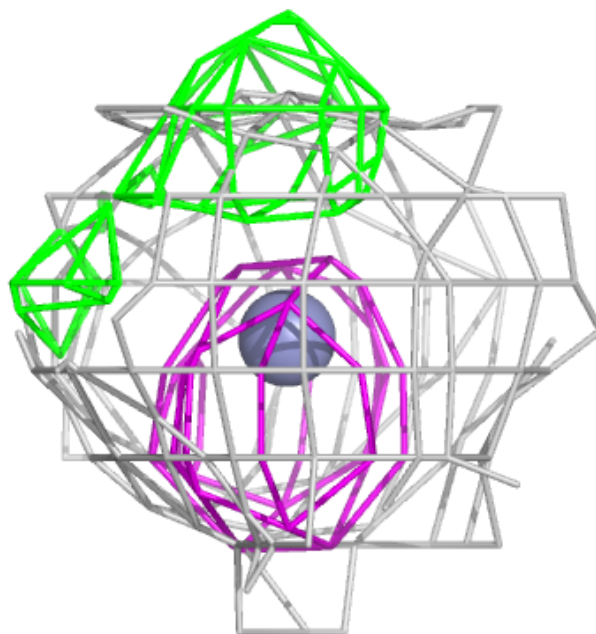
Electron density around ZN D 201:

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



Electron density around ZN A 202:

$2mF_o-DF_c$ (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.