WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 10:29 PM JST

PDB ID	:	6JZV
Title	:	Crystal structure of SufU from Bacillus subtilis
Authors	:	Fujishiro, T.; Takahashi, Y.
Deposited on	:	2019-05-04
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

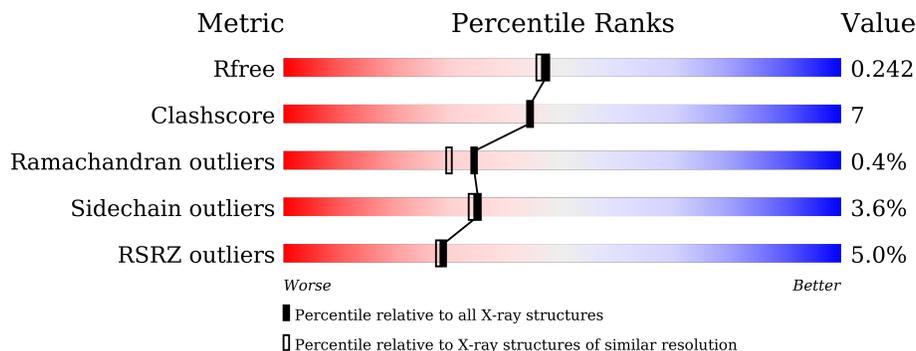|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.242
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		3.6%
RSRZ outliers		5.0%

Worse   Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	155	6% / 77% / 13% · 9%
1	B	155	3% / 79% / 10% · 9%
1	C	155	5% / 81% / 8% · 10%
1	D	155	4% / 68% / 15% · 12%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4318 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-dependent sulfurtransferase SufU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1081	668	183	218	12			
1	B	141	Total	C	N	O	S	0	0	0
			1080	670	183	215	12			
1	C	139	Total	C	N	O	S	0	0	0
			1066	661	180	213	12			
1	D	136	Total	C	N	O	S	0	0	0
			1034	642	177	203	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	LEU	-	expression tag	UNP O32163
A	149	GLU	-	expression tag	UNP O32163
A	150	HIS	-	expression tag	UNP O32163
A	151	HIS	-	expression tag	UNP O32163
A	152	HIS	-	expression tag	UNP O32163
A	153	HIS	-	expression tag	UNP O32163
A	154	HIS	-	expression tag	UNP O32163
A	155	HIS	-	expression tag	UNP O32163
B	148	LEU	-	expression tag	UNP O32163
B	149	GLU	-	expression tag	UNP O32163
B	150	HIS	-	expression tag	UNP O32163
B	151	HIS	-	expression tag	UNP O32163
B	152	HIS	-	expression tag	UNP O32163
B	153	HIS	-	expression tag	UNP O32163
B	154	HIS	-	expression tag	UNP O32163
B	155	HIS	-	expression tag	UNP O32163
C	148	LEU	-	expression tag	UNP O32163
C	149	GLU	-	expression tag	UNP O32163
C	150	HIS	-	expression tag	UNP O32163
C	151	HIS	-	expression tag	UNP O32163
C	152	HIS	-	expression tag	UNP O32163

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Chain	Residue	Modelled	Actual	Comment	Reference
C	153	HIS	-	expression tag	UNP O32163
C	154	HIS	-	expression tag	UNP O32163
C	155	HIS	-	expression tag	UNP O32163
D	148	LEU	-	expression tag	UNP O32163
D	149	GLU	-	expression tag	UNP O32163
D	150	HIS	-	expression tag	UNP O32163
D	151	HIS	-	expression tag	UNP O32163
D	152	HIS	-	expression tag	UNP O32163
D	153	HIS	-	expression tag	UNP O32163
D	154	HIS	-	expression tag	UNP O32163
D	155	HIS	-	expression tag	UNP O32163

- 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	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	11	Total 11	O 11	0	0
3	C	18	Total 18	O 18	0	0
3	D	10	Total 10	O 10	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.
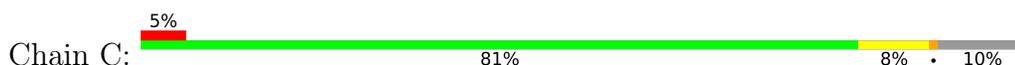
• Molecule 1: Zinc-dependent sulfurtransferase SufU

Chain A:

• Molecule 1: Zinc-dependent sulfurtransferase SufU

Chain B:

• Molecule 1: Zinc-dependent sulfurtransferase SufU

Chain C:

• Molecule 1: Zinc-dependent sulfurtransferase SufU

Chain D:
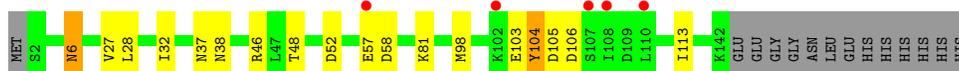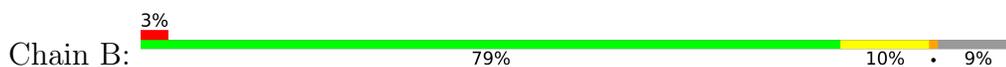
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	35.32Å 54.45Å 70.38Å 68.99° 75.86° 72.54°	Depositor
Resolution (Å)	49.41 – 2.00 49.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.41-2.00) 92.9 (49.41-2.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.211 , 0.242 0.211 , 0.242	Depositor DCC
R_{free} test set	1558 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 46.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.167 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4318	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.30	0/1092	0.54	0/1463
1	B	0.30	0/1092	0.55	0/1463
1	C	0.29	0/1078	0.53	0/1445
1	D	0.30	0/1044	0.54	0/1397
All	All	0.30	0/4306	0.54	0/5768

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	1081	0	1078	16	0
1	B	1080	0	1080	12	0
1	C	1066	0	1062	8	0
1	D	1034	0	1043	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	0	0	0
3	C	18	0	0	1	0
3	D	10	0	0	0	0
All	All	4318	0	4263	56	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 (56) 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:122:PHE:HD2	1:A:125:ARG:HG2	1.36	0.89
1:D:38:ASN:HD21	1:D:127:LYS:HG2	1.47	0.79
1:A:122:PHE:CD2	1:A:125:ARG:HG2	2.23	0.72
1:D:34:VAL:HG13	1:D:138:LYS:HD2	1.71	0.72
1:A:38:ASN:ND2	3:A:301:HOH:O	2.23	0.71
1:D:44:ARG:HB3	1:D:44:ARG:HH11	1.59	0.68
1:D:120:SER:HA	1:D:126:ILE:HD11	1.75	0.67
1:D:52:ASP:HB2	1:D:57:GLU:HG3	1.76	0.66
1:D:38:ASN:HD22	1:D:131:LEU:HD13	1.61	0.65
1:C:104:TYR:H	1:C:104:TYR:HD1	1.44	0.65
1:D:38:ASN:ND2	1:D:127:LYS:HG2	2.11	0.64
1:D:119:VAL:HG12	1:D:126:ILE:HD13	1.81	0.63
1:C:52:ASP:HB2	1:C:57:GLU:HG3	1.80	0.62
1:B:98:MET:HE1	1:B:113:ILE:HG22	1.83	0.58
1:A:98:MET:HE1	1:A:114:GLU:HA	1.85	0.58
1:B:27:VAL:HG12	1:D:44:ARG:HH22	1.68	0.58
1:A:32:ILE:HD11	1:A:143:GLU:HG3	1.85	0.57
1:B:52:ASP:HB2	1:B:57:GLU:HG3	1.86	0.57
1:A:27:VAL:HG13	1:A:48:THR:HG21	1.87	0.56
1:A:32:ILE:O	1:A:48:THR:HA	2.07	0.54
1:B:46:ARG:NH1	1:D:37:ASN:OD1	2.39	0.54
1:A:122:PHE:CE2	1:A:124:ALA:HB3	2.42	0.54
1:B:28:LEU:O	1:D:44:ARG:NH2	2.35	0.54
1:C:98:MET:HE3	1:C:114:GLU:HA	1.90	0.54
1:D:58:ASP:OD1	1:D:81:LYS:HE3	2.08	0.53
1:D:27:VAL:HG13	1:D:48:THR:HG21	1.92	0.51
1:B:27:VAL:HB	1:D:44:ARG:NH1	2.26	0.51
1:B:28:LEU:C	1:D:44:ARG:HH21	2.15	0.49
1:D:107:SER:O	1:D:108:ILE:HD13	2.13	0.49
1:A:89:LEU:HD21	1:A:140:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG12	1:D:29:ASN:OD1	2.13	0.49
1:D:44:ARG:HB3	1:D:44:ARG:NH1	2.27	0.48
1:D:33:VAL:HG22	1:D:48:THR:HG22	1.95	0.48
1:A:103:GLU:HG2	1:A:105:ASP:HB2	1.96	0.47
1:D:51:LEU:HD13	1:D:85:ILE:HD11	1.96	0.47
1:D:55:ILE:HG13	1:D:55:ILE:O	2.14	0.47
1:D:108:ILE:HD12	1:D:108:ILE:HA	1.79	0.47
1:C:98:MET:CE	1:C:114:GLU:HA	2.44	0.47
1:D:36:MET:HE3	1:D:36:MET:HB2	1.69	0.46
1:A:34:VAL:HG21	1:A:139:GLY:HA2	1.98	0.46
1:B:6:ASN:HD22	1:B:6:ASN:N	2.14	0.45
1:C:32:ILE:O	1:C:48:THR:HA	2.17	0.44
1:D:55:ILE:HD11	1:D:57:GLU:OE1	2.18	0.44
1:A:34:VAL:HG13	1:A:138:LYS:HD3	2.01	0.43
1:C:2:SER:HB2	1:C:5:ALA:HB3	2.02	0.42
1:A:110:LEU:HB3	1:A:113:ILE:HB	2.01	0.42
1:D:32:ILE:O	1:D:48:THR:HA	2.19	0.42
1:B:98:MET:HB2	1:B:104:TYR:CG	2.55	0.42
1:B:37:ASN:OD1	1:B:38:ASN:N	2.53	0.41
1:B:58:ASP:OD1	1:B:81:LYS:NZ	2.39	0.41
1:C:25:LYS:NZ	3:C:302:HOH:O	2.50	0.41
1:C:89:LEU:HD21	1:C:140:VAL:HG23	2.03	0.41
1:A:7:LEU:O	1:A:7:LEU:HD22	2.21	0.41
1:A:33:VAL:HG12	1:D:29:ASN:CG	2.40	0.41
1:D:36:MET:HE3	1:D:135:ALA:HA	2.03	0.41
1:B:32:ILE:O	1:B:48:THR:HA	2.21	0.41

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	139/155 (90%)	135 (97%)	4 (3%)	0	100	100
1	B	139/155 (90%)	133 (96%)	4 (3%)	2 (1%)	11	5
1	C	137/155 (88%)	135 (98%)	2 (2%)	0	100	100
1	D	132/155 (85%)	130 (98%)	2 (2%)	0	100	100
All	All	547/620 (88%)	533 (97%)	12 (2%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	TYR
1	B	105	ASP

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	120/132 (91%)	119 (99%)	1 (1%)	81	86
1	B	120/132 (91%)	117 (98%)	3 (2%)	47	49
1	C	119/132 (90%)	116 (98%)	3 (2%)	47	49
1	D	115/132 (87%)	105 (91%)	10 (9%)	10	6
All	All	474/528 (90%)	457 (96%)	17 (4%)	35	34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	B	6	ASN
1	B	103	GLU
1	B	106	ASP
1	C	45	ILE
1	C	102	LYS
1	C	104	TYR
1	D	7	LEU
1	D	36	MET

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Mol	Chain	Res	Type
1	D	38	ASN
1	D	40	THR
1	D	44	ARG
1	D	55	ILE
1	D	81	LYS
1	D	93	LYS
1	D	100	GLN
1	D	108	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	B	6	ASN
1	B	29	ASN
1	D	38	ASN
1	D	117	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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 ⓘ

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(Å²)	Q<0.9
1	A	141/155 (90%)	0.40	9 (6%)	19	18	19, 39, 84, 118	0
1	B	141/155 (90%)	0.25	5 (3%)	44	43	18, 39, 80, 102	0
1	C	139/155 (89%)	0.27	8 (5%)	23	22	21, 38, 83, 115	0
1	D	136/155 (87%)	0.27	6 (4%)	34	33	20, 40, 71, 96	0
All	All	557/620 (89%)	0.30	28 (5%)	28	28	18, 39, 81, 118	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ILE	6.1
1	C	108	ILE	5.6
1	B	107	SER	5.1
1	C	107	SER	4.6
1	A	104	TYR	4.5
1	C	104	TYR	4.2
1	D	108	ILE	4.0
1	C	30	ASP	3.9
1	A	144	GLU	3.7
1	A	107	SER	3.4
1	B	102	LYS	3.2
1	A	122	PHE	3.1
1	C	121	LYS	2.9
1	C	2	SER	2.8
1	D	40	THR	2.7
1	A	121	LYS	2.6
1	B	57	GLU	2.6
1	D	107	SER	2.6
1	C	122	PHE	2.3
1	B	110	LEU	2.2
1	A	123	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	108	ILE	2.2
1	D	44	ARG	2.2
1	D	110	LEU	2.1
1	A	106	ASP	2.1
1	D	100	GLN	2.1
1	C	105	ASP	2.1
1	A	100	GLN	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(Å^2)	Q<0.9
2	ZN	C	201	1/1	0.92	0.07	33,33,33,33	0
2	ZN	A	201	1/1	0.94	0.06	34,34,34,34	0
2	ZN	B	201	1/1	0.97	0.05	33,33,33,33	0
2	ZN	D	201	1/1	0.97	0.06	31,31,31,31	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.
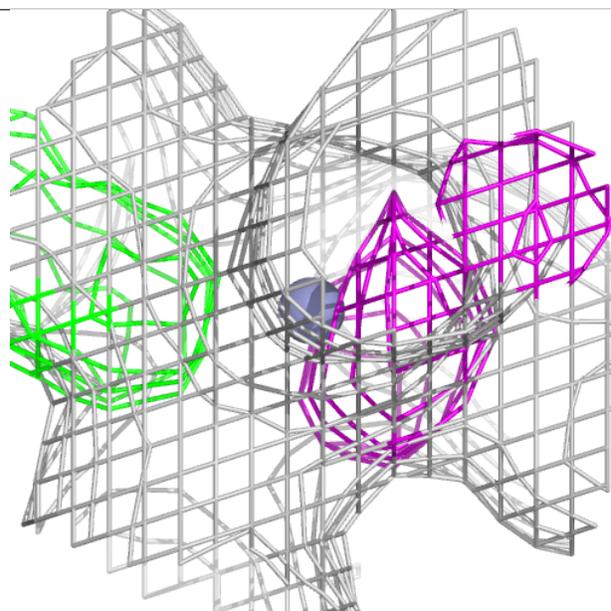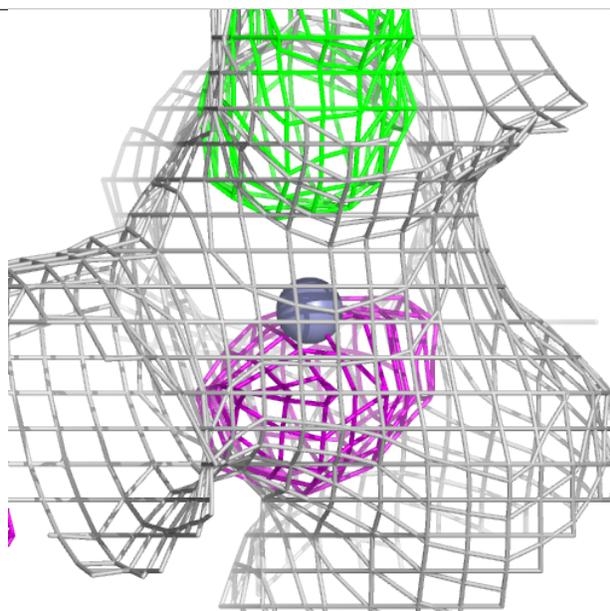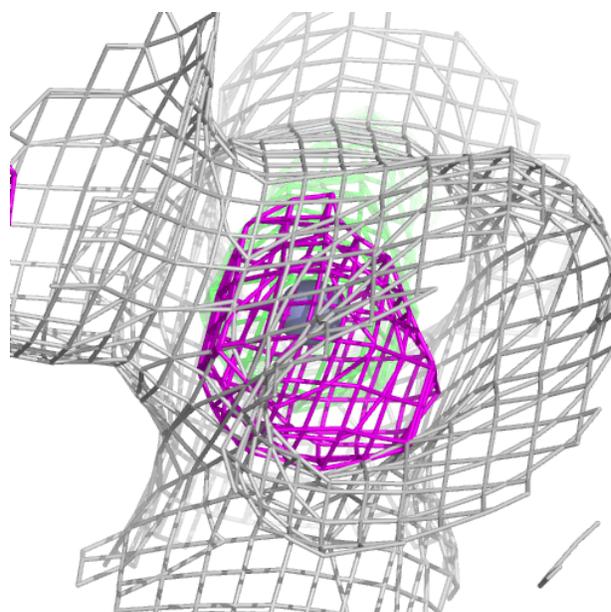
WORLDWIDE
wwPDB
PROTEIN DATA BANK

Electron density around ZN C 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
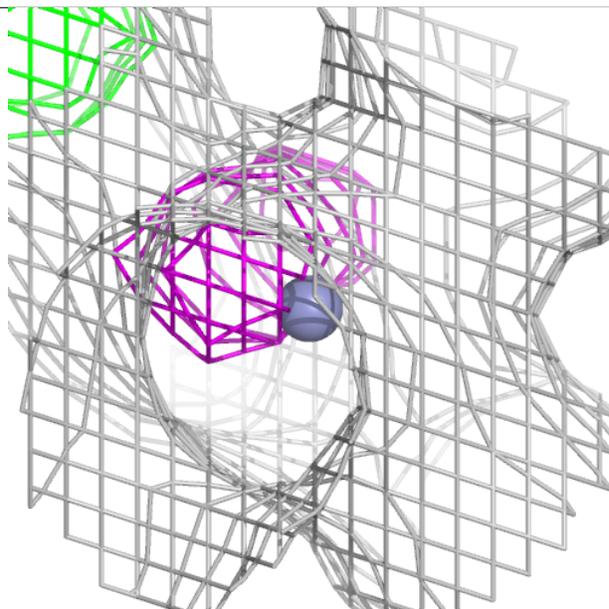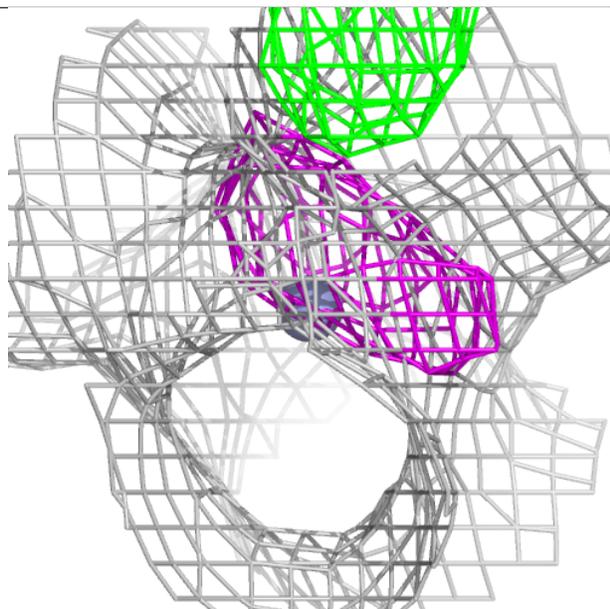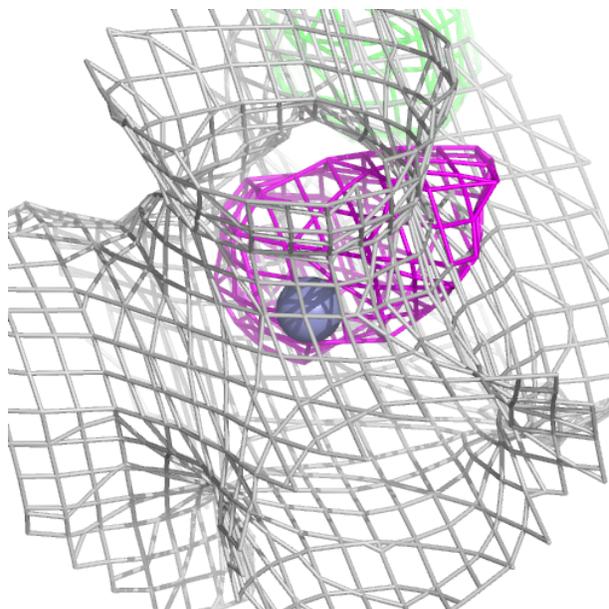mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
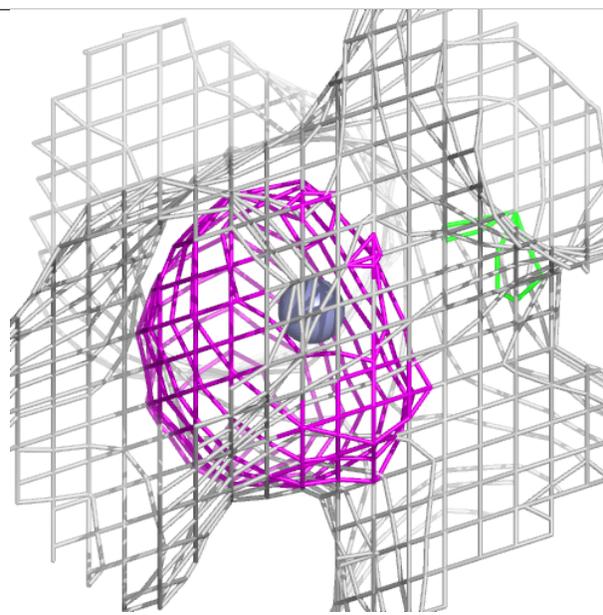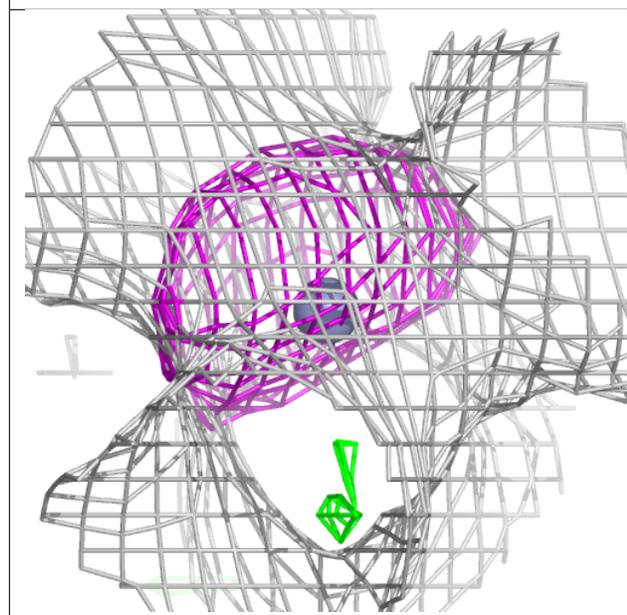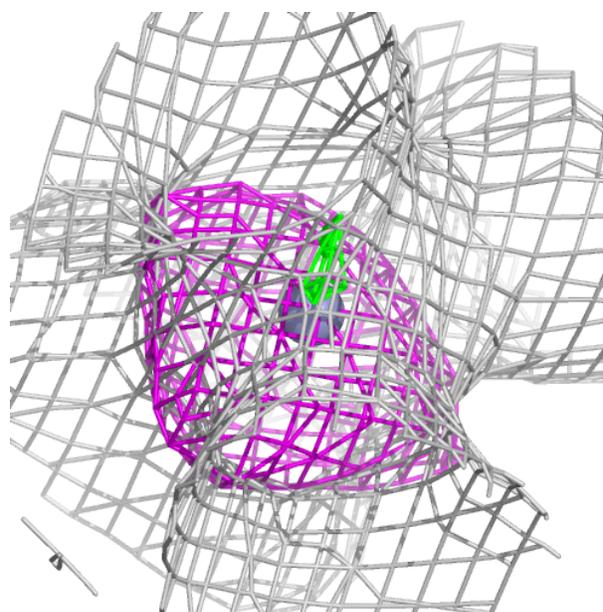
Electron density around ZN A 201:

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

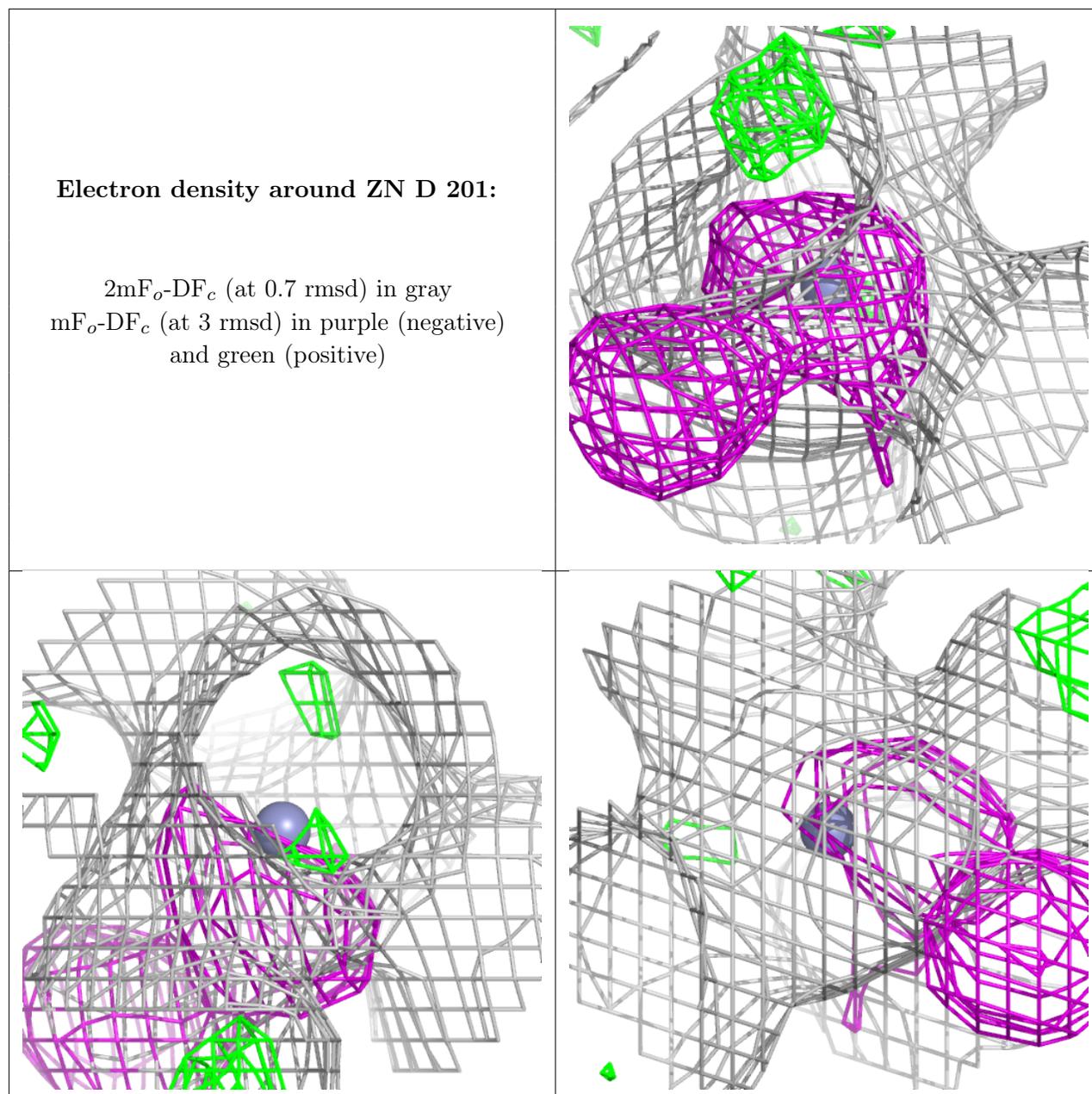Electron density around ZN B 201:

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

Electron density around ZN D 201:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.