



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2023 – 03:34 PM EDT

PDB ID : 6DKA  
Title : Yeast Ddi2 Cyanamide Hydratase  
Authors : Moore, S.A.; Xiao, W.; Li, J.  
Deposited on : 2018-05-29  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

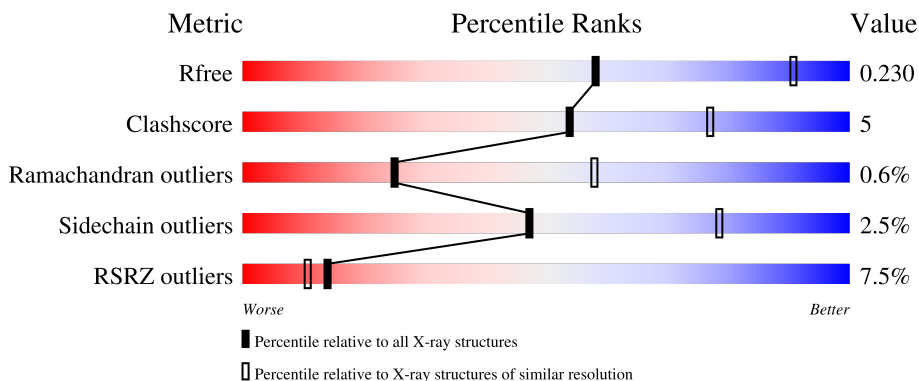
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	234	88% 9% ..
1	B	234	87% 11% ..
1	C	234	92% 5% ..
1	D	234	88% 9% .
1	E	234	90% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	234	<p>90% 8% ..</p>
1	G	234	<p>88% 9% .</p>
1	H	234	<p>20% 73% 23% ..</p>
1	I	234	<p>36% 73% 23% ..</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	305	-	-	X	-
4	SO4	F	301	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 32496 atoms, of which 15894 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 DNA damage-inducible protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	230	3555	1143	1759	306	341	6	0	1	0
1	B	230	3554	1143	1758	306	341	6	0	1	0
1	C	230	3594	1153	1780	310	345	6	0	1	0
1	D	229	3572	1145	1772	309	340	6	0	0	0
1	E	230	3578	1149	1770	310	343	6	0	0	0
1	F	232	3604	1159	1783	312	344	6	0	1	0
1	G	229	3554	1140	1762	308	338	6	0	0	0
1	H	227	3512	1128	1741	303	335	5	0	0	0
1	I	226	3534	1132	1755	306	335	6	0	0	0

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A7A1Y4
A	-6	PRO	-	expression tag	UNP A7A1Y4
A	-5	LEU	-	expression tag	UNP A7A1Y4
A	-4	GLY	-	expression tag	UNP A7A1Y4
A	-3	SER	-	expression tag	UNP A7A1Y4
A	-2	PRO	-	expression tag	UNP A7A1Y4
A	-1	GLU	-	expression tag	UNP A7A1Y4
A	0	PHE	-	expression tag	UNP A7A1Y4
A	157	VAL	THR	engineered mutation	UNP A7A1Y4
B	-7	GLY	-	expression tag	UNP A7A1Y4
B	-6	PRO	-	expression tag	UNP A7A1Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP A7A1Y4
B	-4	GLY	-	expression tag	UNP A7A1Y4
B	-3	SER	-	expression tag	UNP A7A1Y4
B	-2	PRO	-	expression tag	UNP A7A1Y4
B	-1	GLU	-	expression tag	UNP A7A1Y4
B	0	PHE	-	expression tag	UNP A7A1Y4
B	157	VAL	THR	engineered mutation	UNP A7A1Y4
C	-7	GLY	-	expression tag	UNP A7A1Y4
C	-6	PRO	-	expression tag	UNP A7A1Y4
C	-5	LEU	-	expression tag	UNP A7A1Y4
C	-4	GLY	-	expression tag	UNP A7A1Y4
C	-3	SER	-	expression tag	UNP A7A1Y4
C	-2	PRO	-	expression tag	UNP A7A1Y4
C	-1	GLU	-	expression tag	UNP A7A1Y4
C	0	PHE	-	expression tag	UNP A7A1Y4
C	157	VAL	THR	engineered mutation	UNP A7A1Y4
D	-7	GLY	-	expression tag	UNP A7A1Y4
D	-6	PRO	-	expression tag	UNP A7A1Y4
D	-5	LEU	-	expression tag	UNP A7A1Y4
D	-4	GLY	-	expression tag	UNP A7A1Y4
D	-3	SER	-	expression tag	UNP A7A1Y4
D	-2	PRO	-	expression tag	UNP A7A1Y4
D	-1	GLU	-	expression tag	UNP A7A1Y4
D	0	PHE	-	expression tag	UNP A7A1Y4
D	157	VAL	THR	engineered mutation	UNP A7A1Y4
E	-7	GLY	-	expression tag	UNP A7A1Y4
E	-6	PRO	-	expression tag	UNP A7A1Y4
E	-5	LEU	-	expression tag	UNP A7A1Y4
E	-4	GLY	-	expression tag	UNP A7A1Y4
E	-3	SER	-	expression tag	UNP A7A1Y4
E	-2	PRO	-	expression tag	UNP A7A1Y4
E	-1	GLU	-	expression tag	UNP A7A1Y4
E	0	PHE	-	expression tag	UNP A7A1Y4
E	157	VAL	THR	engineered mutation	UNP A7A1Y4
F	-7	GLY	-	expression tag	UNP A7A1Y4
F	-6	PRO	-	expression tag	UNP A7A1Y4
F	-5	LEU	-	expression tag	UNP A7A1Y4
F	-4	GLY	-	expression tag	UNP A7A1Y4
F	-3	SER	-	expression tag	UNP A7A1Y4
F	-2	PRO	-	expression tag	UNP A7A1Y4
F	-1	GLU	-	expression tag	UNP A7A1Y4
F	0	PHE	-	expression tag	UNP A7A1Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	157	VAL	THR	engineered mutation	UNP A7A1Y4
G	-7	GLY	-	expression tag	UNP A7A1Y4
G	-6	PRO	-	expression tag	UNP A7A1Y4
G	-5	LEU	-	expression tag	UNP A7A1Y4
G	-4	GLY	-	expression tag	UNP A7A1Y4
G	-3	SER	-	expression tag	UNP A7A1Y4
G	-2	PRO	-	expression tag	UNP A7A1Y4
G	-1	GLU	-	expression tag	UNP A7A1Y4
G	0	PHE	-	expression tag	UNP A7A1Y4
G	157	VAL	THR	engineered mutation	UNP A7A1Y4
H	-7	GLY	-	expression tag	UNP A7A1Y4
H	-6	PRO	-	expression tag	UNP A7A1Y4
H	-5	LEU	-	expression tag	UNP A7A1Y4
H	-4	GLY	-	expression tag	UNP A7A1Y4
H	-3	SER	-	expression tag	UNP A7A1Y4
H	-2	PRO	-	expression tag	UNP A7A1Y4
H	-1	GLU	-	expression tag	UNP A7A1Y4
H	0	PHE	-	expression tag	UNP A7A1Y4
H	157	VAL	THR	engineered mutation	UNP A7A1Y4
I	-7	GLY	-	expression tag	UNP A7A1Y4
I	-6	PRO	-	expression tag	UNP A7A1Y4
I	-5	LEU	-	expression tag	UNP A7A1Y4
I	-4	GLY	-	expression tag	UNP A7A1Y4
I	-3	SER	-	expression tag	UNP A7A1Y4
I	-2	PRO	-	expression tag	UNP A7A1Y4
I	-1	GLU	-	expression tag	UNP A7A1Y4
I	0	PHE	-	expression tag	UNP A7A1Y4
I	157	VAL	THR	engineered mutation	UNP A7A1Y4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

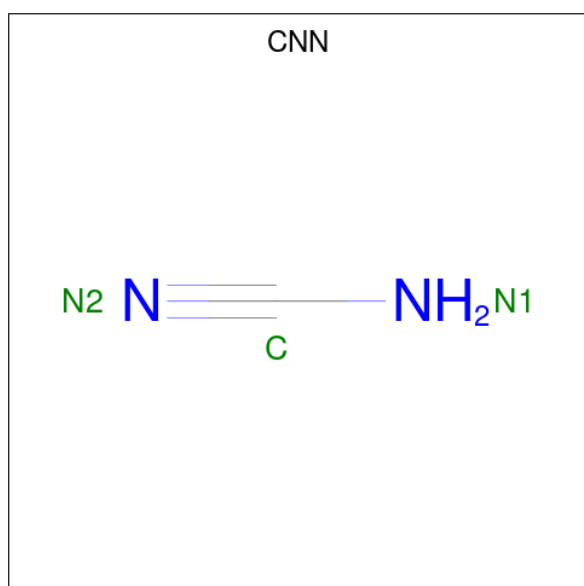
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0

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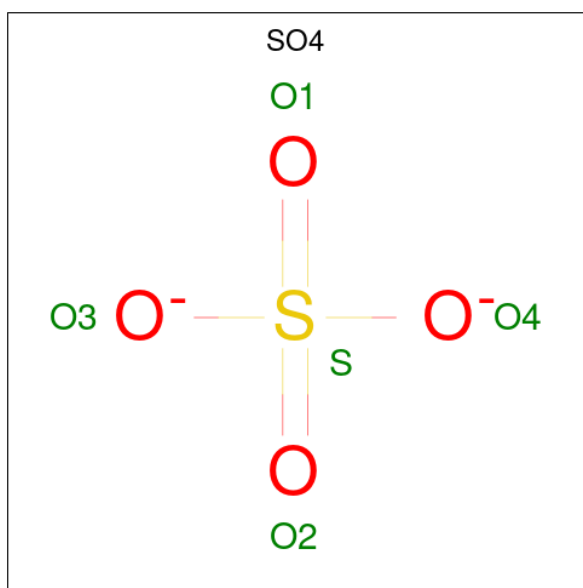
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	Zn 1	0	0
2	G	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0

- Molecule 3 is CYANAMIDE (three-letter code: CNN) (formula:  $\text{CH}_2\text{N}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 5	C 1	H 2	N 2	0	0
3	B	1	Total 5	C 1	H 2	N 2	0	0
3	C	1	Total 5	C 1	H 2	N 2	0	0
3	D	1	Total 5	C 1	H 2	N 2	0	0
3	E	1	Total 5	C 1	H 2	N 2	0	0
3	F	1	Total 5	C 1	H 2	N 2	0	0
3	G	1	Total 5	C 1	H 2	N 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	35	Total	O	0	0
			35	35		
5	C	58	Total	O	0	0
			58	58		
5	D	35	Total	O	0	0
			35	35		
5	E	48	Total	O	0	0
			48	48		
5	F	30	Total	O	0	0
			30	30		

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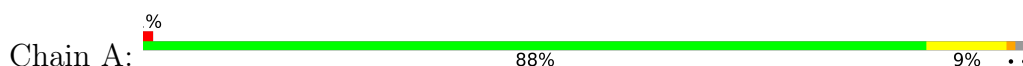
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	G	19	Total O 19 19	0	0
5	H	2	Total O 2 2	0	0

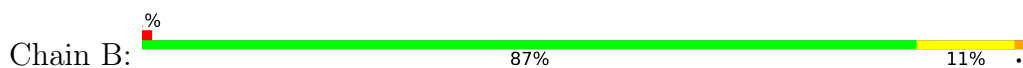
### 3 Residue-property plots [i](#)

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: DNA damage-inducible protein



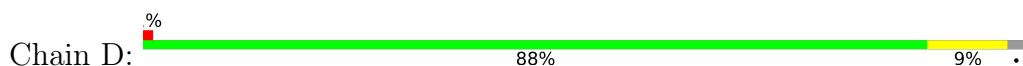
- Molecule 1: DNA damage-inducible protein



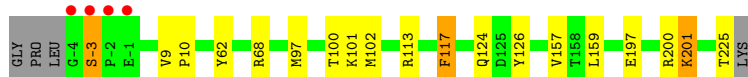
- Molecule 1: DNA damage-inducible protein



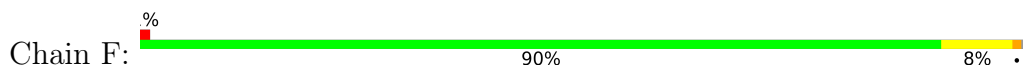
- Molecule 1: DNA damage-inducible protein



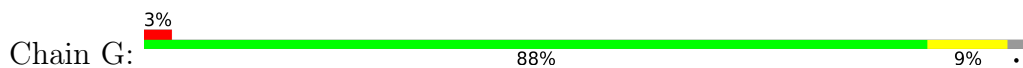
- Molecule 1: DNA damage-inducible protein



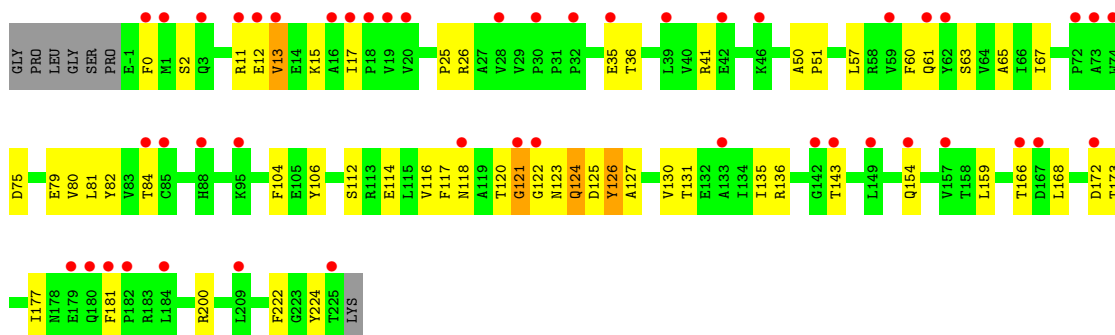
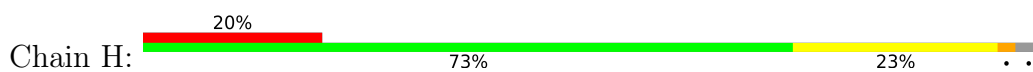
- Molecule 1: DNA damage-inducible protein



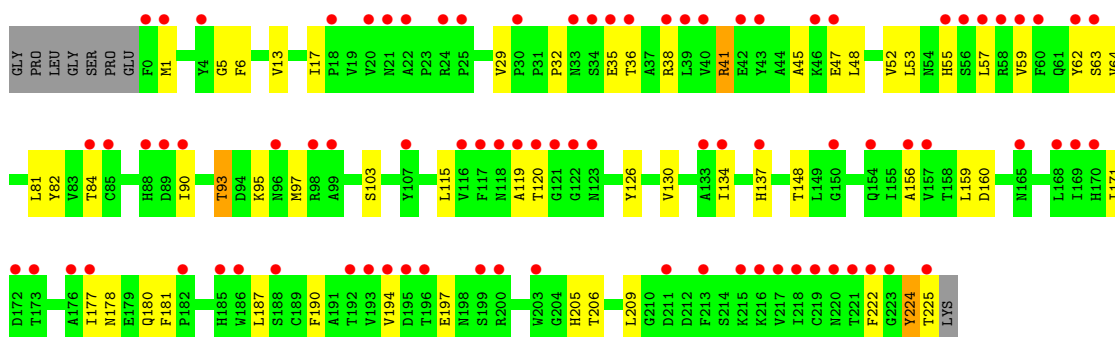
- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	263.43Å 263.43Å 119.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 2.90 29.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.97-2.90) 96.7 (29.97-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.198 , 0.230 0.198 , 0.230	Depositor DCC
$R_{free}$ test set	2569 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtrriage
Anisotropy	0.507	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CNN, 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	0/1841	0.54	0/2517
1	B	0.30	0/1841	0.54	0/2517
1	C	0.31	0/1859	0.55	0/2538
1	D	0.30	0/1842	0.54	0/2515
1	E	0.31	0/1850	0.55	0/2525
1	F	0.28	0/1867	0.51	0/2549
1	G	0.28	0/1834	0.51	0/2506
1	H	0.31	0/1812	0.58	1/2476 (0.0%)
1	I	0.38	1/1820 (0.1%)	0.58	1/2484 (0.0%)
All	All	0.31	1/16566 (0.0%)	0.54	2/22627 (0.0%)

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	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	93	THR	CB-CG2	-9.57	1.20	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	117	PHE	N-CA-CB	-5.34	100.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	41	ARG	NE-CZ-NH1	-5.32	117.64	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	SER	Peptide
1	E	-3	SER	Peptide

## 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	1796	1759	1750	12	1
1	B	1796	1758	1750	15	0
1	C	1814	1780	1780	10	0
1	D	1800	1772	1770	14	0
1	E	1808	1770	1777	11	0
1	F	1821	1783	1794	17	0
1	G	1792	1762	1755	13	0
1	H	1771	1741	1733	39	1
1	I	1779	1755	1755	46	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	3	2	2	0	0
3	B	3	2	2	0	0
3	C	3	2	2	1	0
3	D	3	2	2	0	0
3	E	3	2	2	1	0
3	F	3	2	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	3	2	2	0	0
4	A	15	0	0	2	0
4	B	20	0	0	1	0
4	C	25	0	0	2	0
4	D	25	0	0	1	0
4	E	15	0	0	0	0
4	F	15	0	0	4	0
4	G	10	0	0	1	0
4	H	5	0	0	1	0
5	A	38	0	0	0	0
5	B	35	0	0	0	0
5	C	58	0	0	1	0
5	D	35	0	0	0	0
5	E	48	0	0	0	0
5	F	30	0	0	0	0
5	G	19	0	0	0	0
5	H	2	0	0	0	0
All	All	16602	15894	15878	171	1

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 5.

The worst 5 of 171 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:I:48:LEU:HD23	1:I:93:THR:CG2	1.86	1.04
1:B:2:SER:OG	1:B:75:ASP:OD2	1.80	0.99
1:A:2:SER:OG	1:A:75:ASP:OD2	1.84	0.96
1:E:200:ARG:NH2	4:G:303:SO4:O3	2.01	0.94
1:F:200:ARG:NH2	4:F:301:SO4:O4	2.06	0.89

All (1) 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)
1:A:82:TYR:OH	1:H:121:GLY:O[3_566]	1.97	0.23



## 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	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	34	66
1	B	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	34	66
1	C	229/234 (98%)	223 (97%)	5 (2%)	1 (0%)	34	66
1	D	227/234 (97%)	220 (97%)	6 (3%)	1 (0%)	34	66
1	E	228/234 (97%)	222 (97%)	5 (2%)	1 (0%)	34	66
1	F	231/234 (99%)	224 (97%)	4 (2%)	3 (1%)	12	37
1	G	227/234 (97%)	221 (97%)	5 (2%)	1 (0%)	34	66
1	H	225/234 (96%)	214 (95%)	8 (4%)	3 (1%)	12	37
1	I	224/234 (96%)	217 (97%)	5 (2%)	2 (1%)	17	48
All	All	2049/2106 (97%)	1985 (97%)	50 (2%)	14 (1%)	25	54

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	121	GLY
1	H	124	GLN
1	A	13	VAL
1	B	13	VAL
1	D	-1	GLU

### 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	195/202 (96%)	189 (97%)	6 (3%)	40	74
1	B	195/202 (96%)	189 (97%)	6 (3%)	40	74
1	C	199/202 (98%)	193 (97%)	6 (3%)	41	75
1	D	197/202 (98%)	192 (98%)	5 (2%)	47	78
1	E	198/202 (98%)	191 (96%)	7 (4%)	36	70
1	F	200/202 (99%)	198 (99%)	2 (1%)	76	92
1	G	195/202 (96%)	193 (99%)	2 (1%)	76	92
1	H	192/202 (95%)	188 (98%)	4 (2%)	53	81
1	I	195/202 (96%)	189 (97%)	6 (3%)	40	74
All	All	1766/1818 (97%)	1722 (98%)	44 (2%)	47	78

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	201	LYS
1	H	35	GLU
1	E	225	THR
1	G	39	LEU
1	H	126	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	D	78	GLN
1	E	124	GLN
1	I	54	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 42 ligands modelled in this entry, 9 are monoatomic - leaving 33 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	F	305	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	E	305	-	4,4,4	0.12	0	6,6,6	0.19	0
4	SO4	D	306	-	4,4,4	0.16	0	6,6,6	0.14	0
4	SO4	G	303	-	4,4,4	0.10	0	6,6,6	0.43	0
4	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.11	0
3	CNN	C	302	2	1,2,2	1.72	0	0,1,1	-	-
4	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	D	304	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	D	305	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	F	304	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	B	306	-	4,4,4	0.13	0	6,6,6	0.11	0
3	CNN	B	303	2	1,2,2	1.67	0	0,1,1	-	-
4	SO4	E	304	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	F	301	-	4,4,4	0.14	0	6,6,6	0.18	0
3	CNN	E	302	2	1,2,2	1.77	0	0,1,1	-	-
4	SO4	D	301	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	D	307	-	4,4,4	0.13	0	6,6,6	0.11	0
4	SO4	C	304	-	4,4,4	0.13	0	6,6,6	0.15	0
4	SO4	A	304	-	4,4,4	0.15	0	6,6,6	0.14	0
4	SO4	G	304	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	C	307	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	C	306	-	4,4,4	0.12	0	6,6,6	0.14	0
3	CNN	A	302	2	1,2,2	1.54	0	0,1,1	-	-
3	CNN	G	302	2	1,2,2	1.56	0	0,1,1	-	-
4	SO4	A	305	-	4,4,4	0.15	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	B	305	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	H	302	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	E	303	-	4,4,4	0.13	0	6,6,6	0.09	0
3	CNN	F	303	2	1,2,2	1.67	0	0,1,1	-	-
3	CNN	D	303	2	1,2,2	1.58	0	0,1,1	-	-
4	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

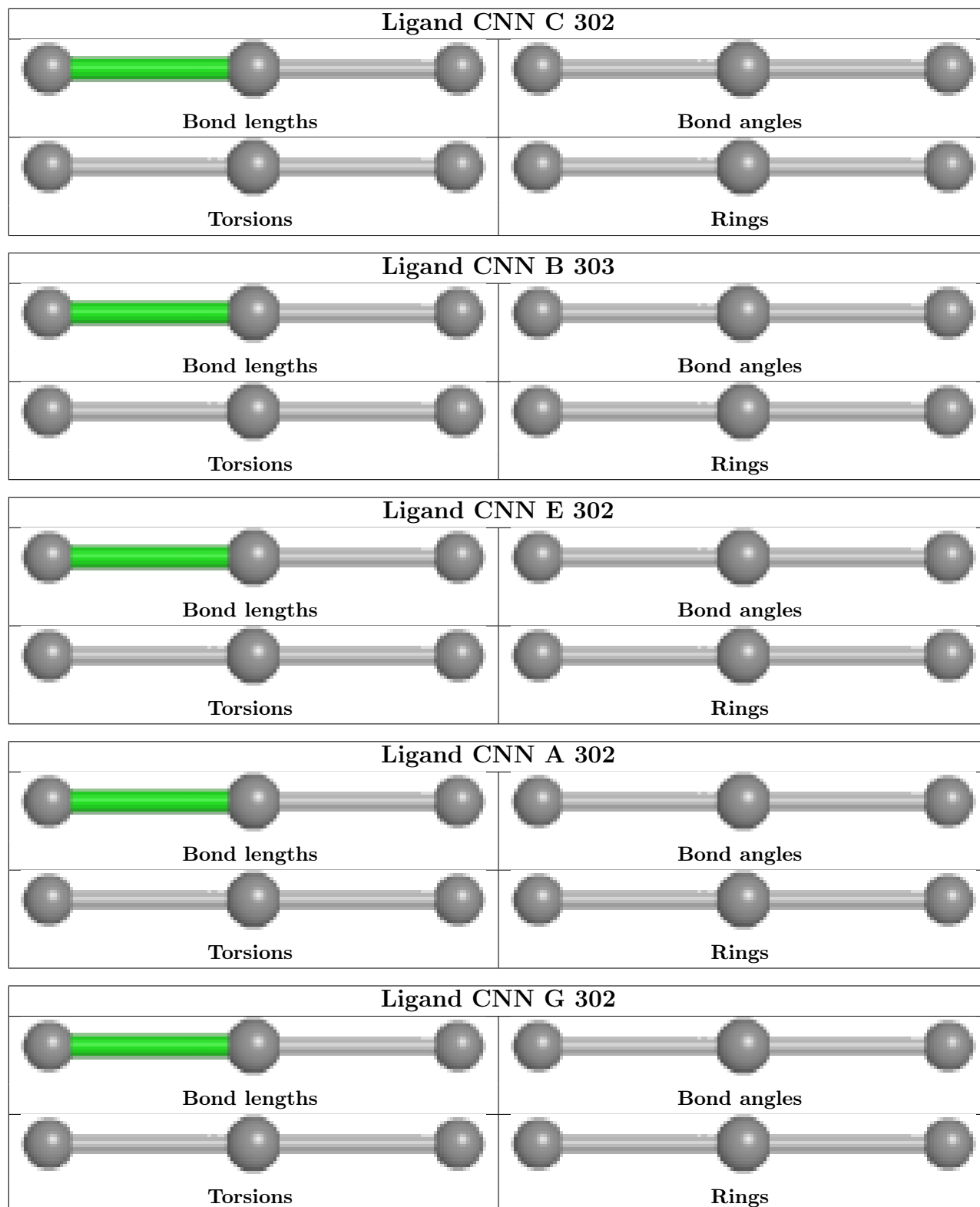
There are no torsion outliers.

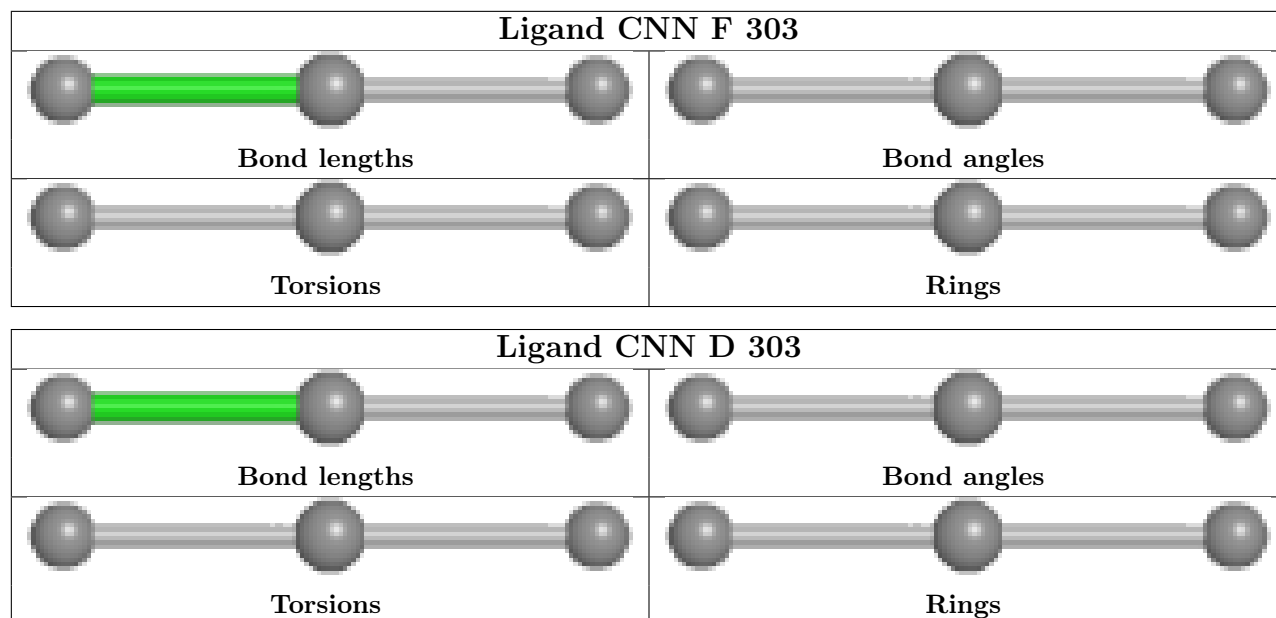
There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	305	SO4	1	0
4	G	303	SO4	1	0
3	C	302	CNN	1	0
4	B	301	SO4	1	0
4	C	305	SO4	2	0
4	F	301	SO4	3	0
3	E	302	CNN	1	0
4	D	301	SO4	1	0
4	A	304	SO4	1	0
4	A	305	SO4	1	0
4	H	302	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	230/234 (98%)	-0.17	3 (1%) 77 77	37, 54, 77, 121	0
1	B	230/234 (98%)	-0.19	2 (0%) 84 84	35, 51, 73, 117	0
1	C	230/234 (98%)	-0.15	2 (0%) 84 84	33, 43, 67, 142	0
1	D	229/234 (97%)	-0.19	2 (0%) 84 84	33, 48, 70, 126	0
1	E	230/234 (98%)	-0.22	4 (1%) 70 69	30, 44, 70, 189	0
1	F	232/234 (99%)	-0.15	3 (1%) 77 77	41, 54, 79, 127	0
1	G	229/234 (97%)	0.01	6 (2%) 56 52	42, 66, 92, 115	0
1	H	227/234 (97%)	0.98	47 (20%) 1 0	67, 115, 153, 190	0
1	I	226/234 (96%)	1.70	85 (37%) 0 0	77, 142, 178, 230	0
All	All	2063/2106 (97%)	0.18	154 (7%) 14 11	30, 55, 147, 230	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	225	THR	8.1
1	I	85	CYS	6.7
1	I	88	HIS	5.9
1	H	180	GLN	5.9
1	I	120	THR	5.9

### 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZN	I	500	1/1	0.71	0.18	113,113,113,113	1
4	SO4	A	304	5/5	0.86	0.35	101,101,102,102	5
4	SO4	B	305	5/5	0.87	0.35	102,102,102,103	5
4	SO4	F	305	5/5	0.87	0.32	106,107,107,107	0
4	SO4	C	306	5/5	0.88	0.25	79,79,80,81	5
4	SO4	D	305	5/5	0.89	0.30	99,101,101,102	0
4	SO4	E	304	5/5	0.89	0.26	100,100,100,101	5
3	CNN	B	303	3/3	0.89	0.43	83,85,104,104	5
4	SO4	B	304	5/5	0.90	0.25	95,95,95,96	0
4	SO4	D	306	5/5	0.90	0.42	51,52,52,52	5
2	ZN	H	301	1/1	0.90	0.25	117,117,117,117	1
2	ZN	G	301	1/1	0.90	0.18	102,102,102,102	1
4	SO4	H	302	5/5	0.90	0.25	85,86,86,86	5
4	SO4	F	301	5/5	0.91	0.33	37,38,38,40	5
4	SO4	B	301	5/5	0.91	0.23	46,47,48,48	5
4	SO4	B	306	5/5	0.91	0.21	79,79,79,79	5
4	SO4	A	305	5/5	0.92	0.37	40,42,44,48	5
4	SO4	D	307	5/5	0.92	0.25	78,79,80,80	5
4	SO4	C	305	5/5	0.92	0.22	43,44,44,44	5
4	SO4	D	301	5/5	0.93	0.20	87,91,94,95	5
4	SO4	G	303	5/5	0.93	0.20	41,41,42,44	5
3	CNN	D	303	3/3	0.93	0.40	74,79,99,99	5
3	CNN	G	302	3/3	0.94	0.43	106,111,137,137	5
4	SO4	D	304	5/5	0.94	0.18	83,84,84,84	0
4	SO4	F	304	5/5	0.94	0.18	85,85,85,85	0
4	SO4	C	303	5/5	0.94	0.25	89,89,89,89	5
2	ZN	D	302	1/1	0.94	0.14	71,71,71,71	1
4	SO4	G	304	5/5	0.94	0.25	48,48,48,48	5
3	CNN	A	302	3/3	0.94	0.31	69,71,87,87	5
3	CNN	C	302	3/3	0.95	0.21	63,67,82,82	5
2	ZN	E	301	1/1	0.95	0.08	67,67,67,67	1
2	ZN	B	302	1/1	0.95	0.09	82,82,82,82	1
4	SO4	C	307	5/5	0.95	0.36	75,76,76,76	5
3	CNN	E	302	3/3	0.96	0.29	68,72,90,90	5
4	SO4	A	303	5/5	0.96	0.18	73,73,73,74	0
3	CNN	F	303	3/3	0.96	0.26	70,73,90,90	5
4	SO4	E	303	5/5	0.97	0.17	80,81,81,81	5

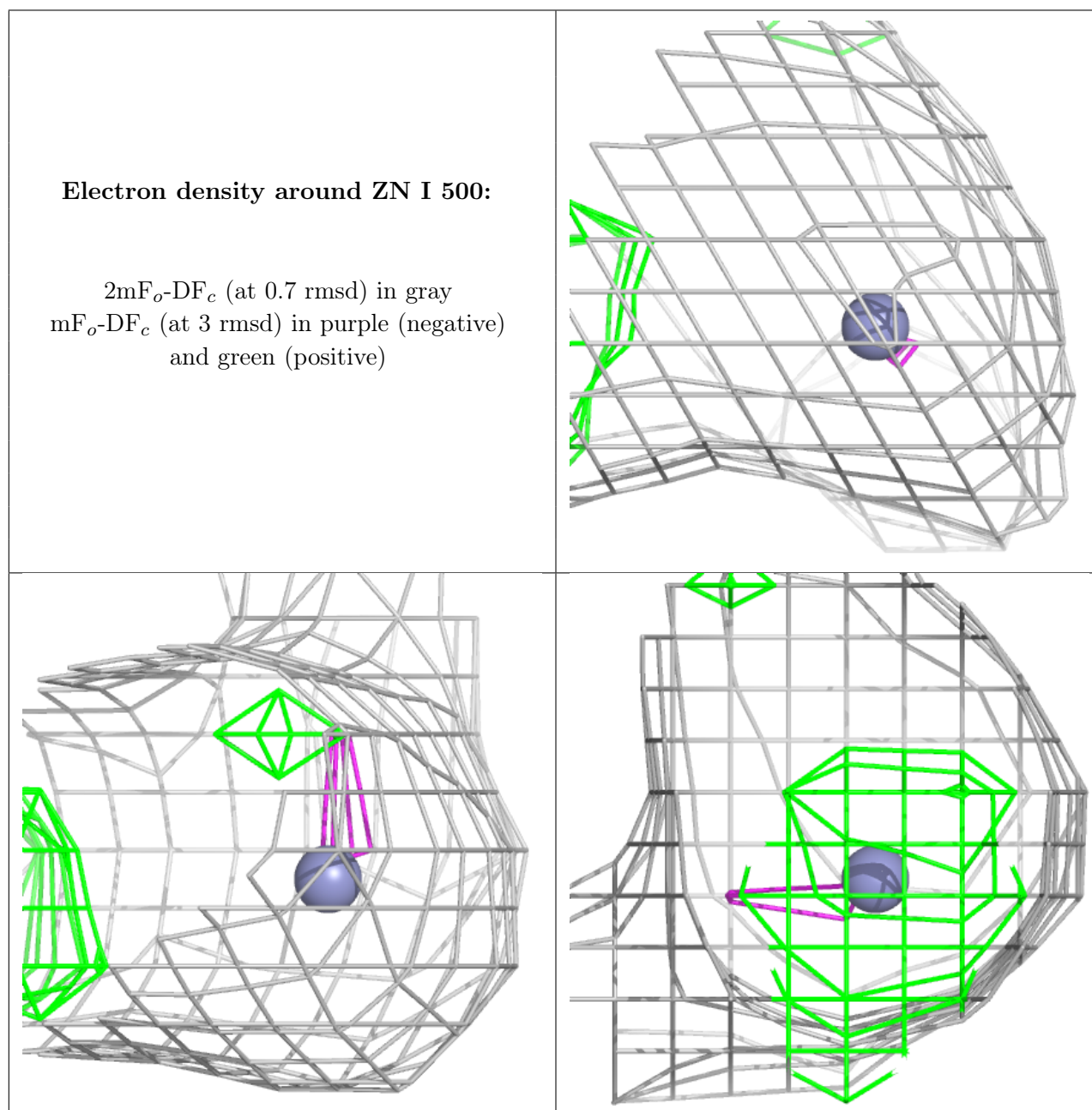
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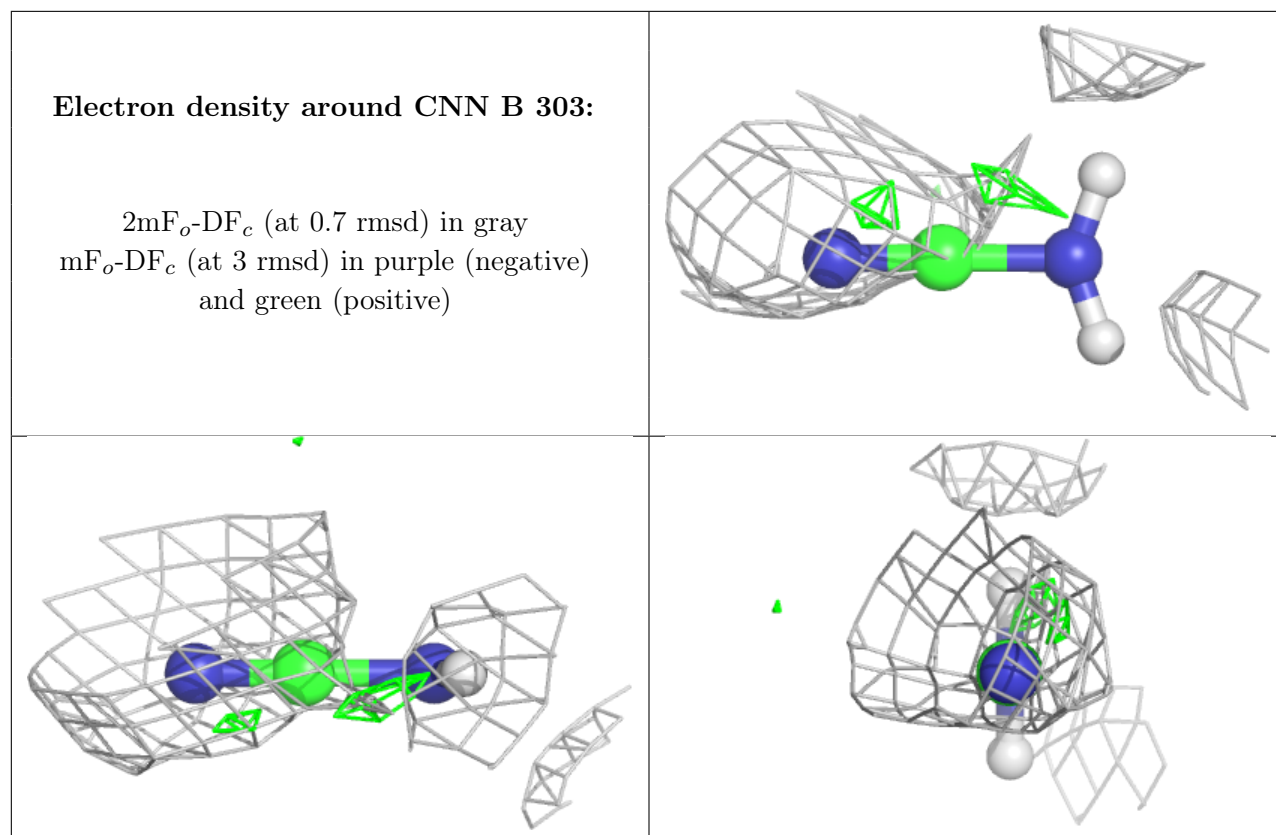


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	C	304	5/5	0.97	0.17	76,77,77,78	0
4	SO4	E	305	5/5	0.97	0.12	61,61,62,62	0
2	ZN	C	301	1/1	0.98	0.10	62,62,62,62	1
2	ZN	F	302	1/1	0.98	0.12	69,69,69,69	1
2	ZN	A	301	1/1	0.99	0.08	68,68,68,68	1

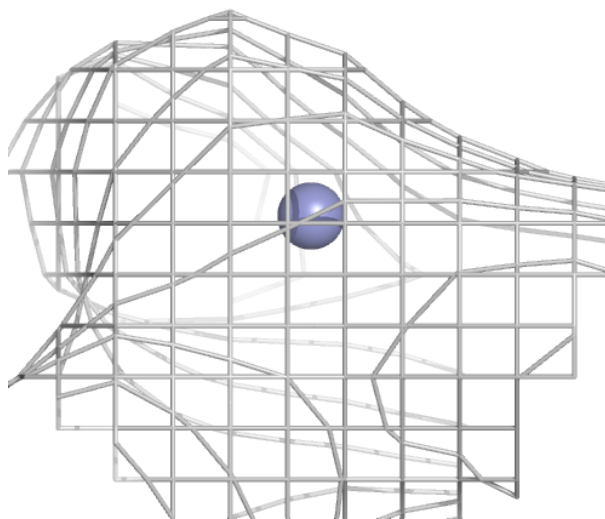
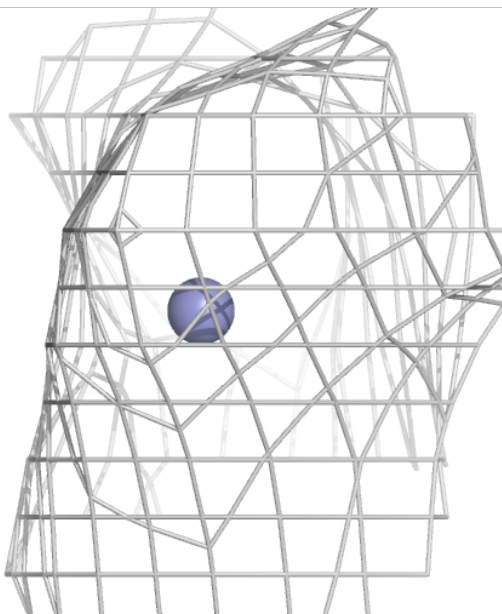
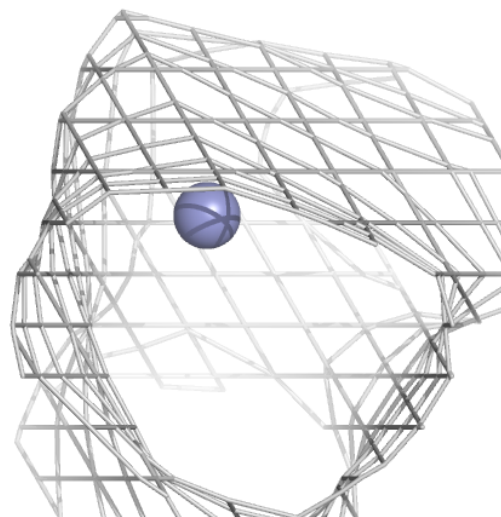
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





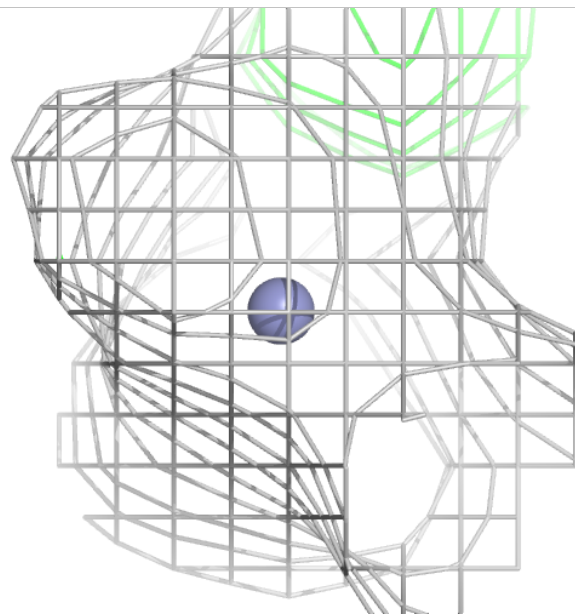
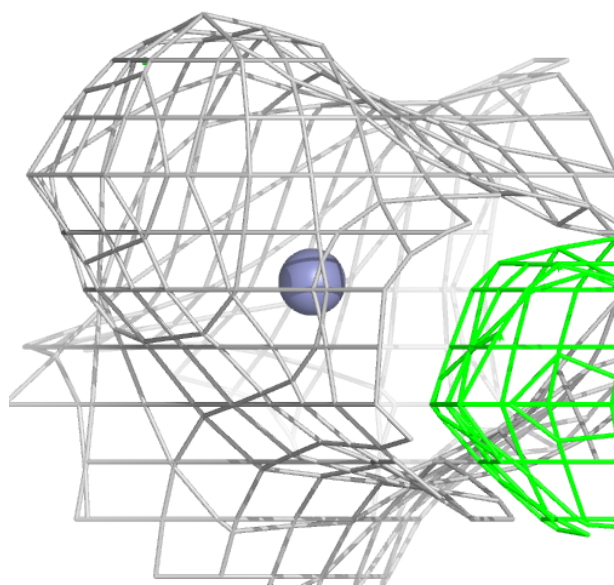
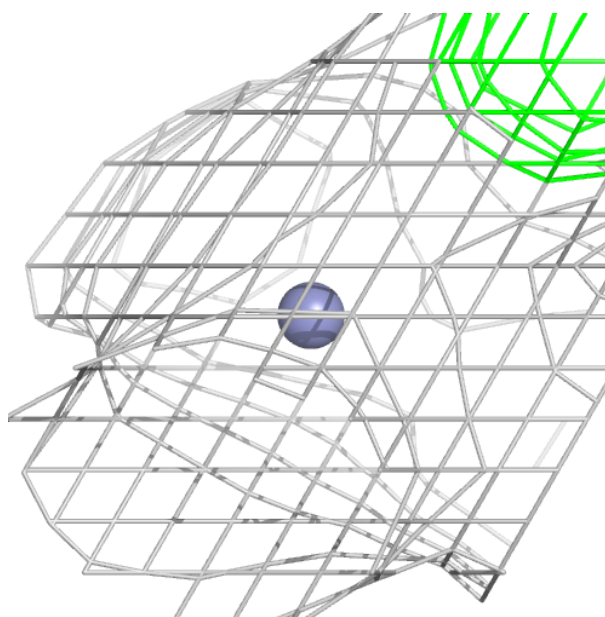
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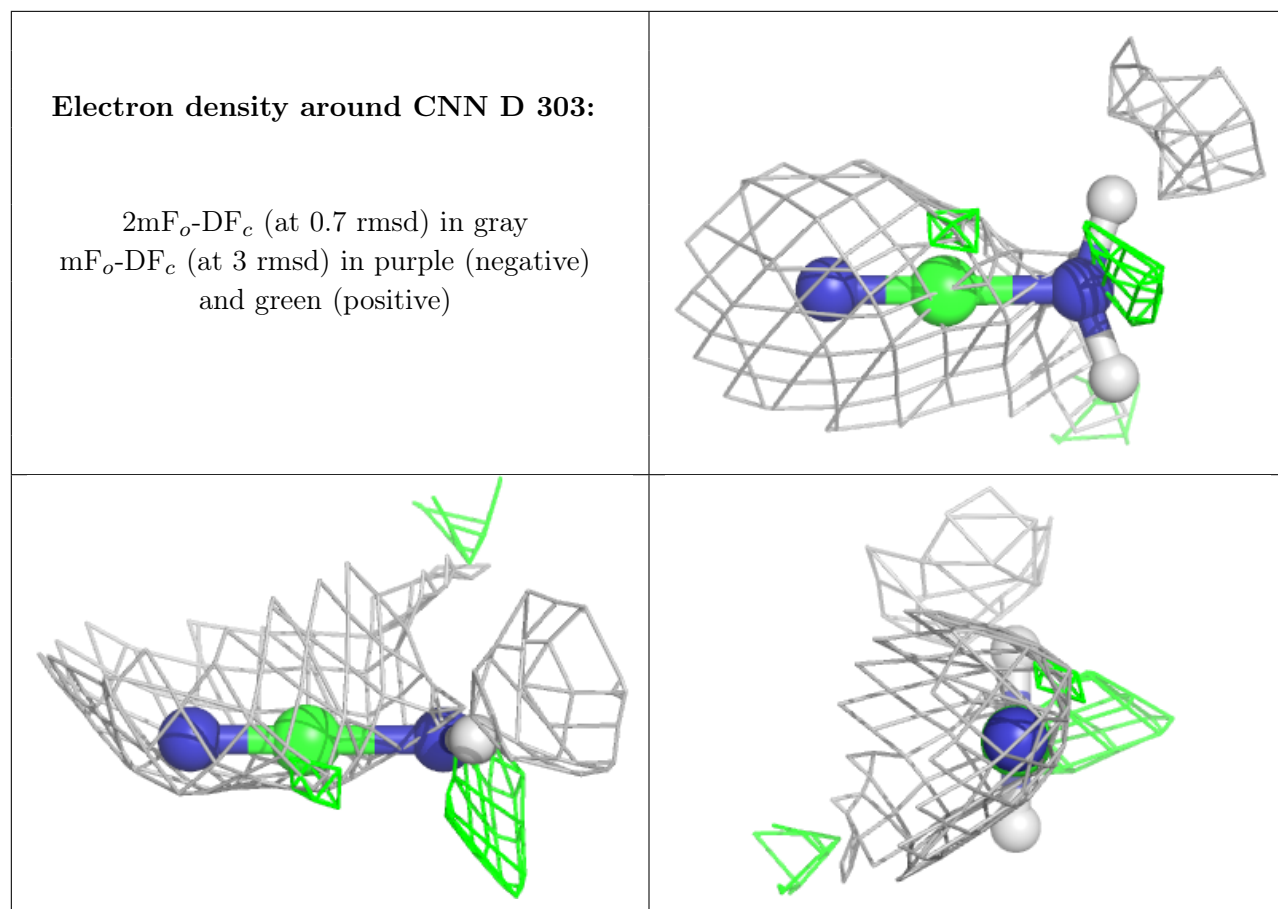
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN G 301:**

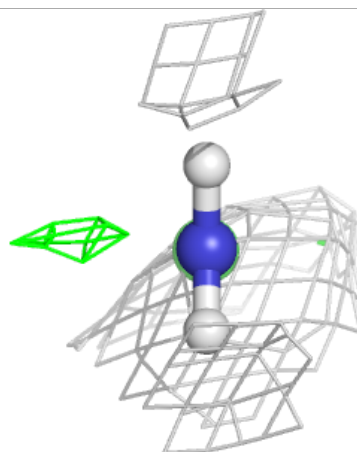
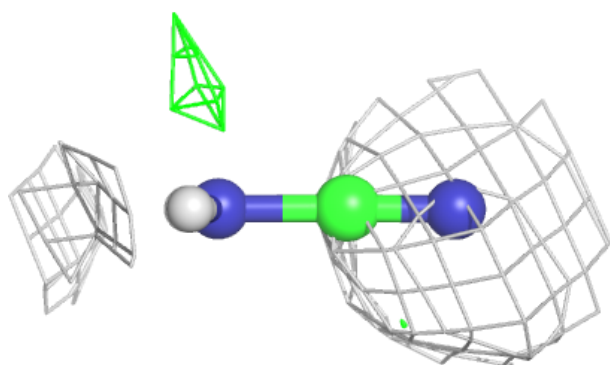
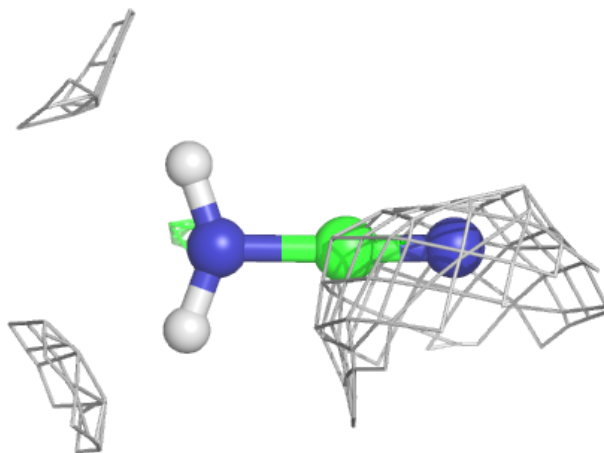
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and green (positive)





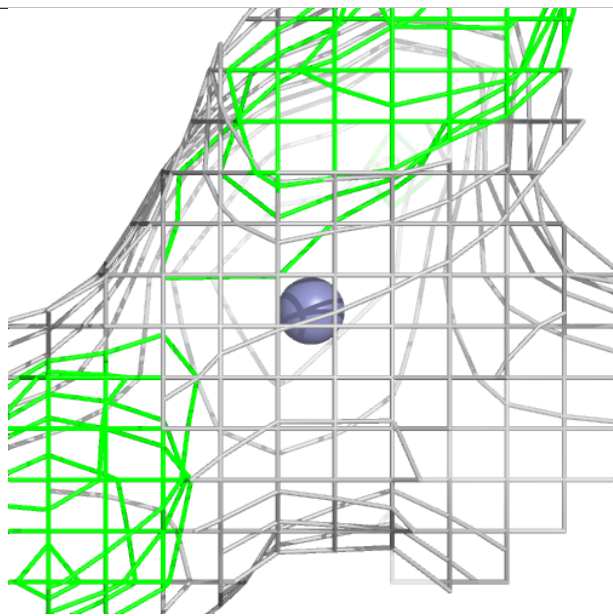
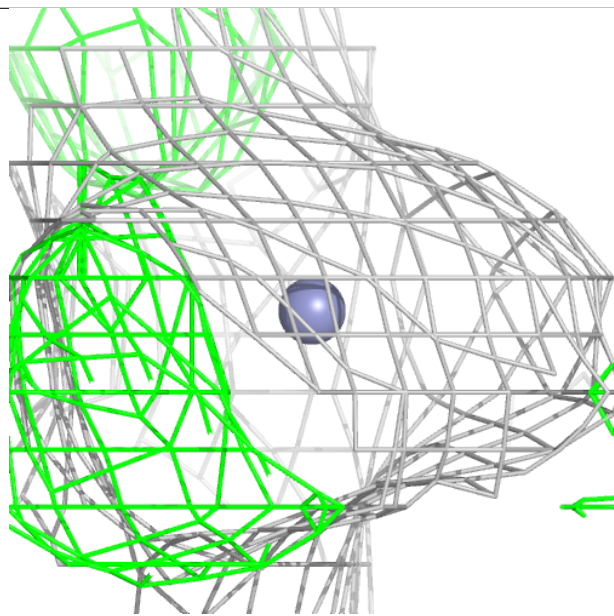
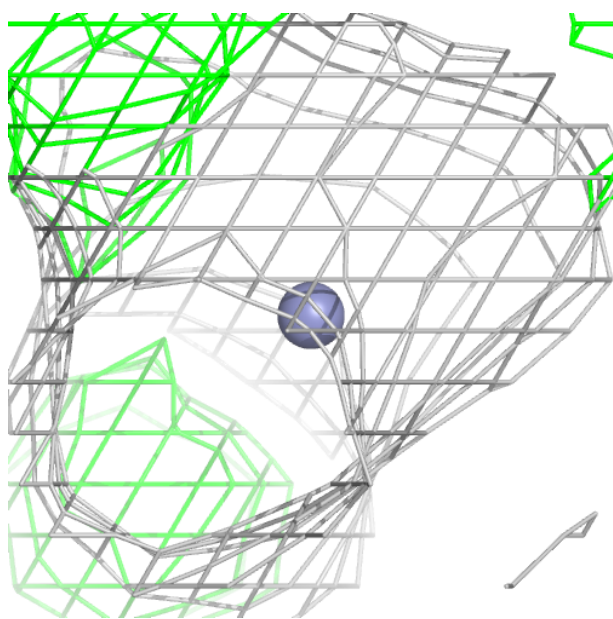
**Electron density around CNN G 302:**

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and green (positive)



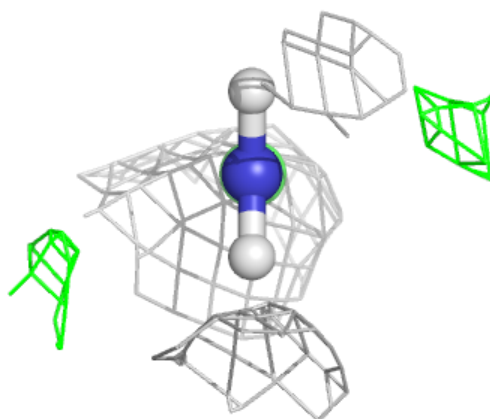
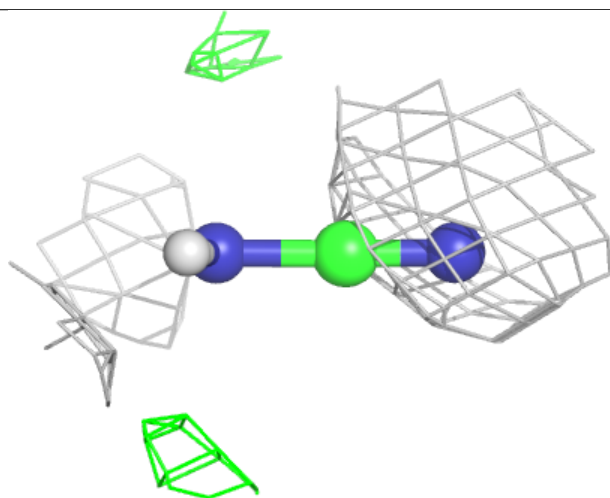
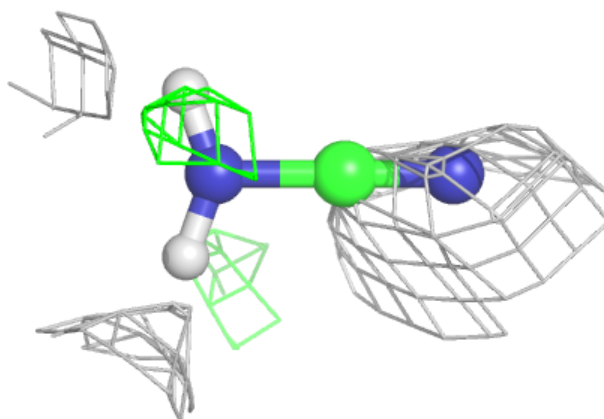
**Electron density around ZN D 302:**

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



**Electron density around CNN A 302:**

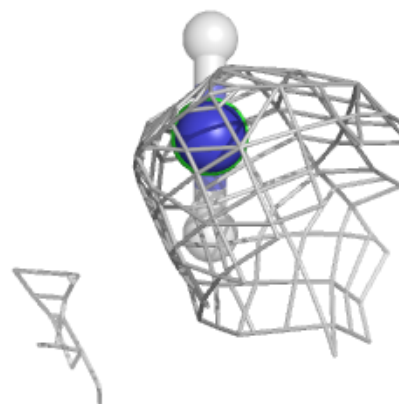
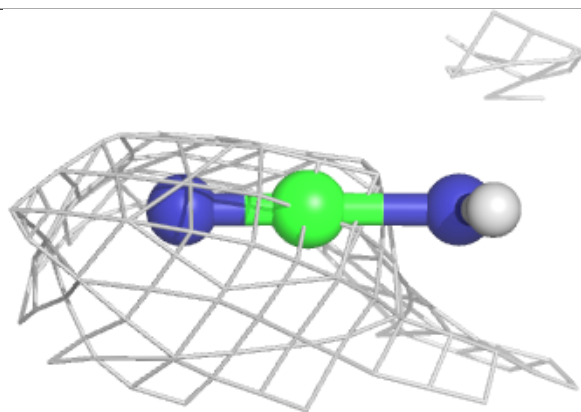
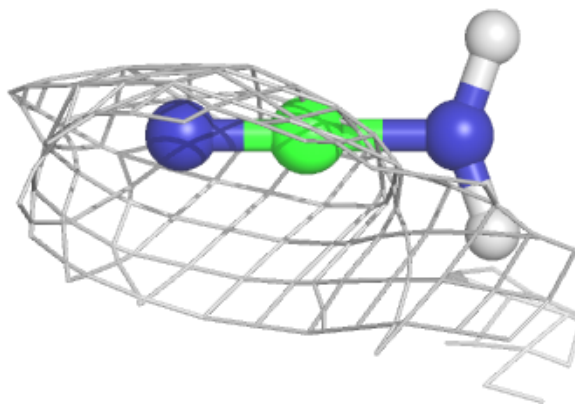
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





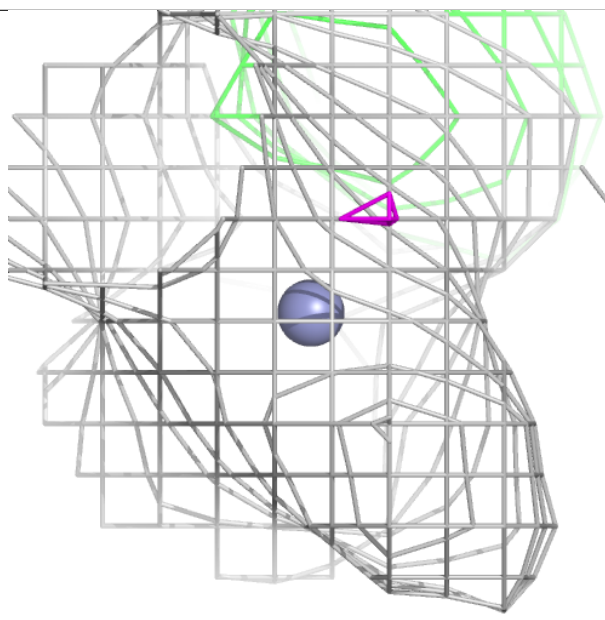
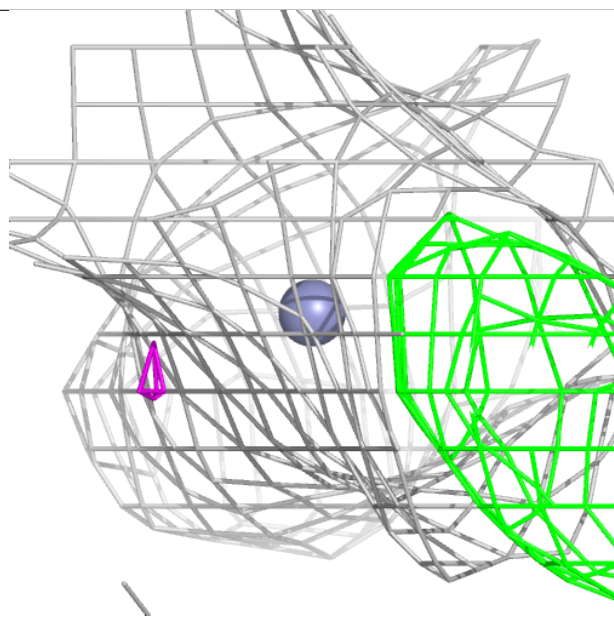
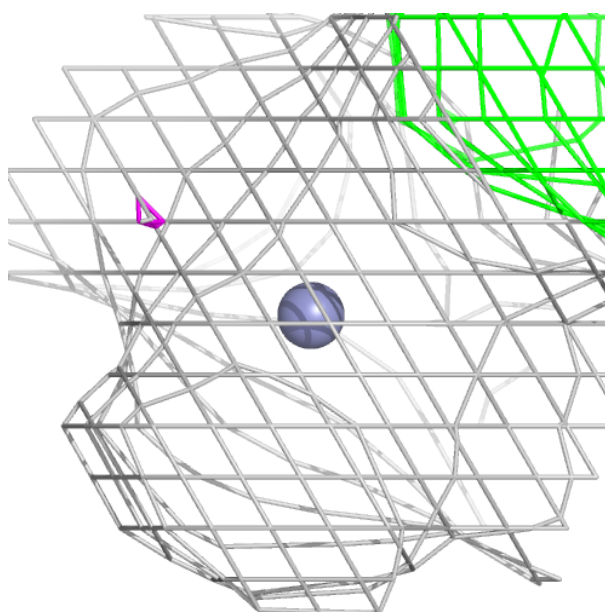
**Electron density around CNN C 302:**

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



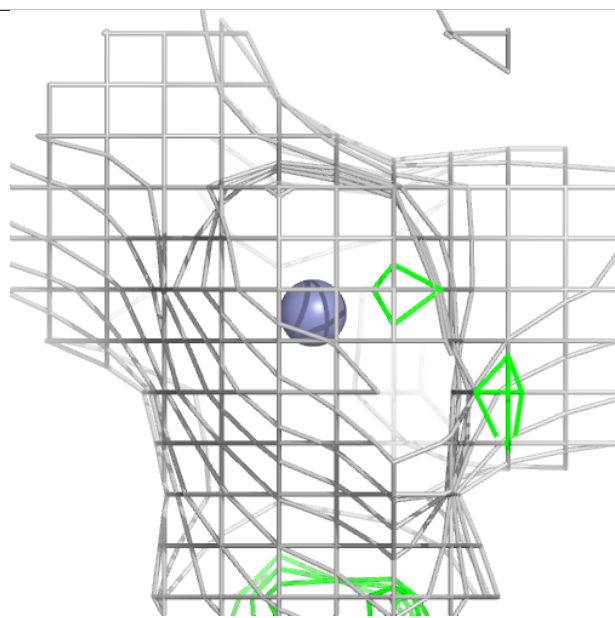
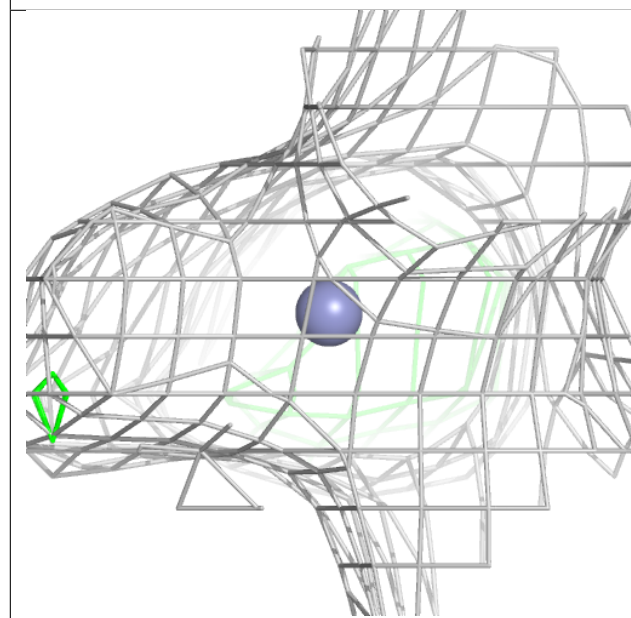
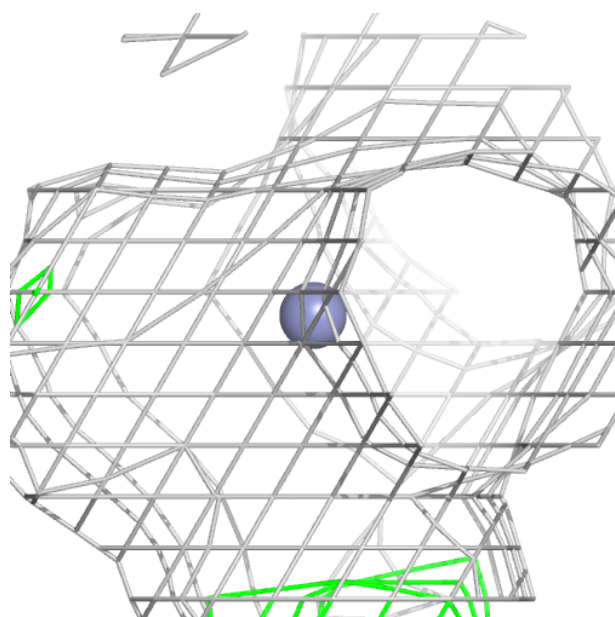
**Electron density around ZN E 301:**

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



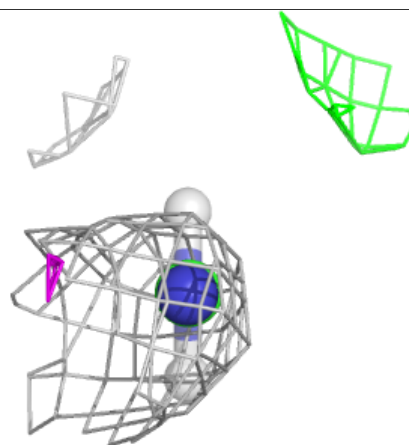
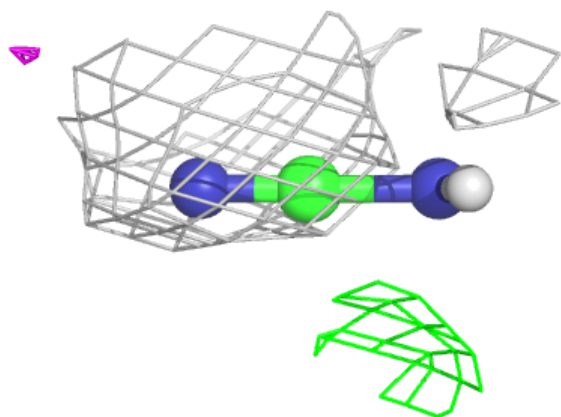
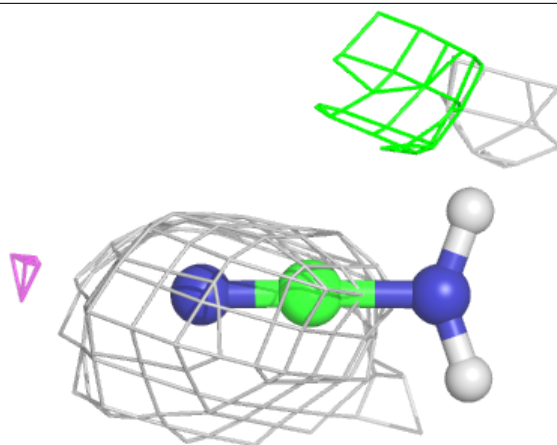
**Electron density around ZN B 302:**

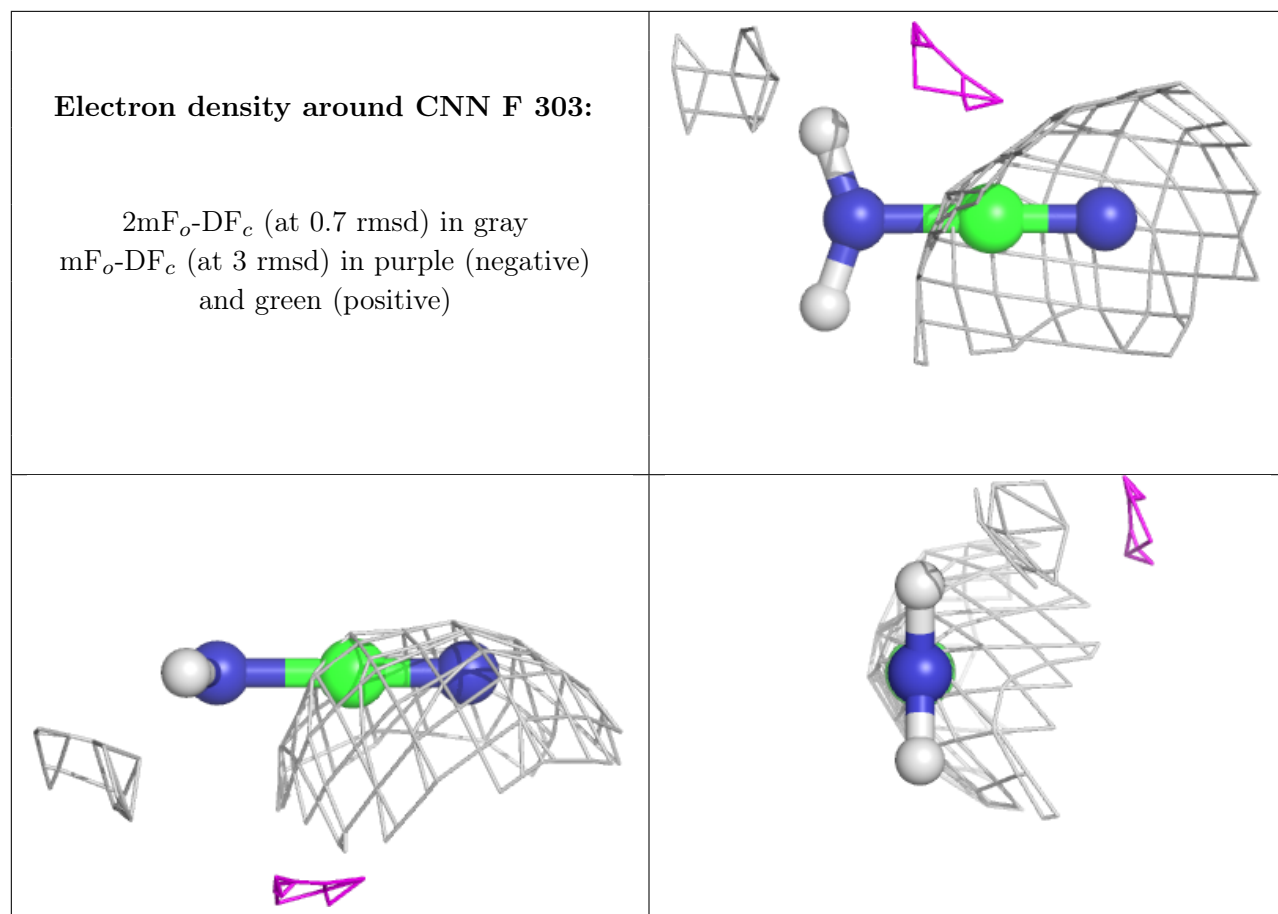
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CNN E 302:**

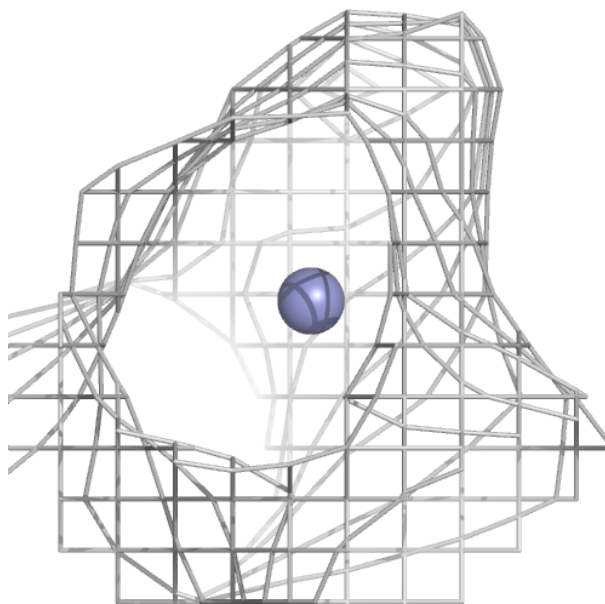
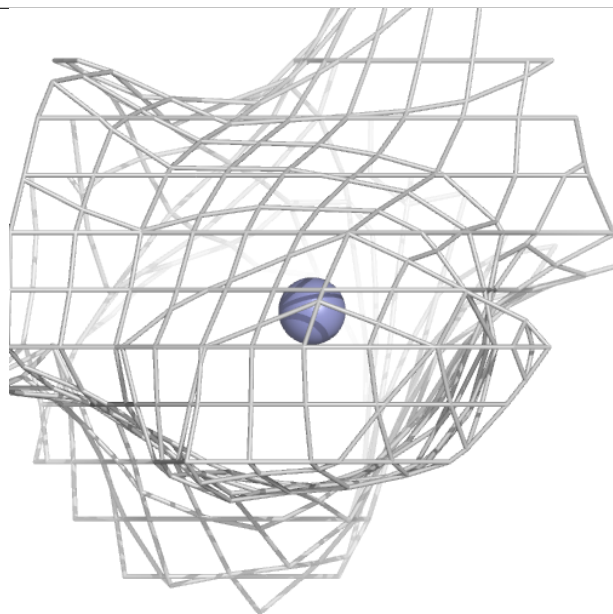
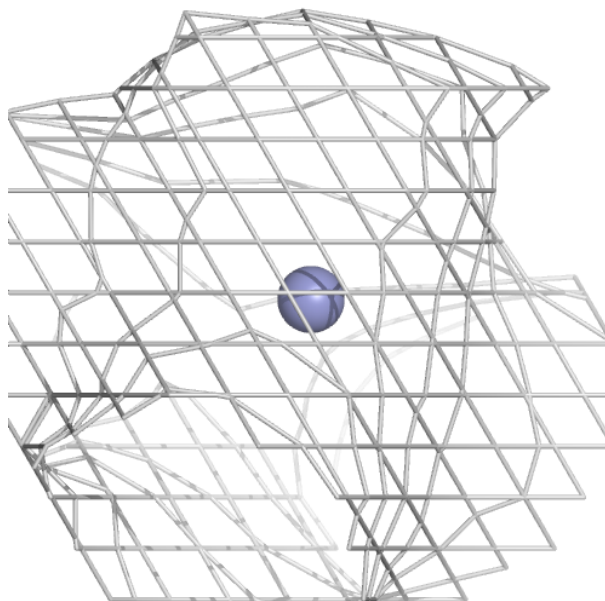
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





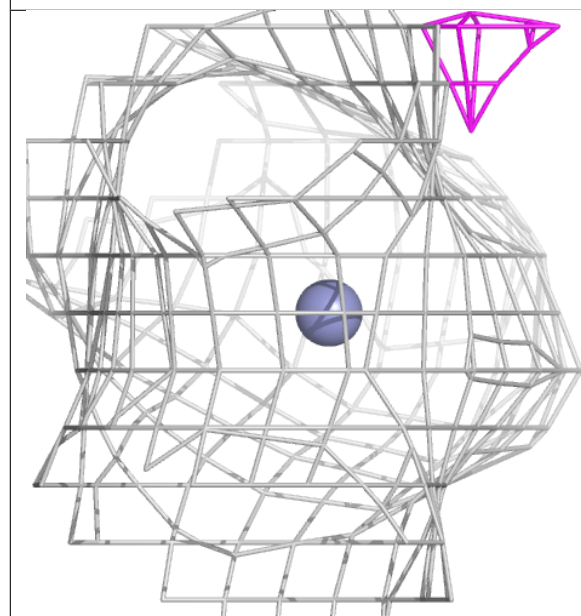
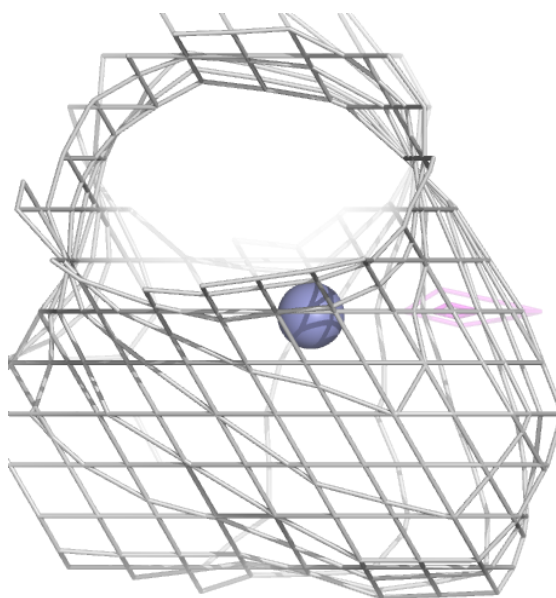
**Electron density around ZN C 301:**

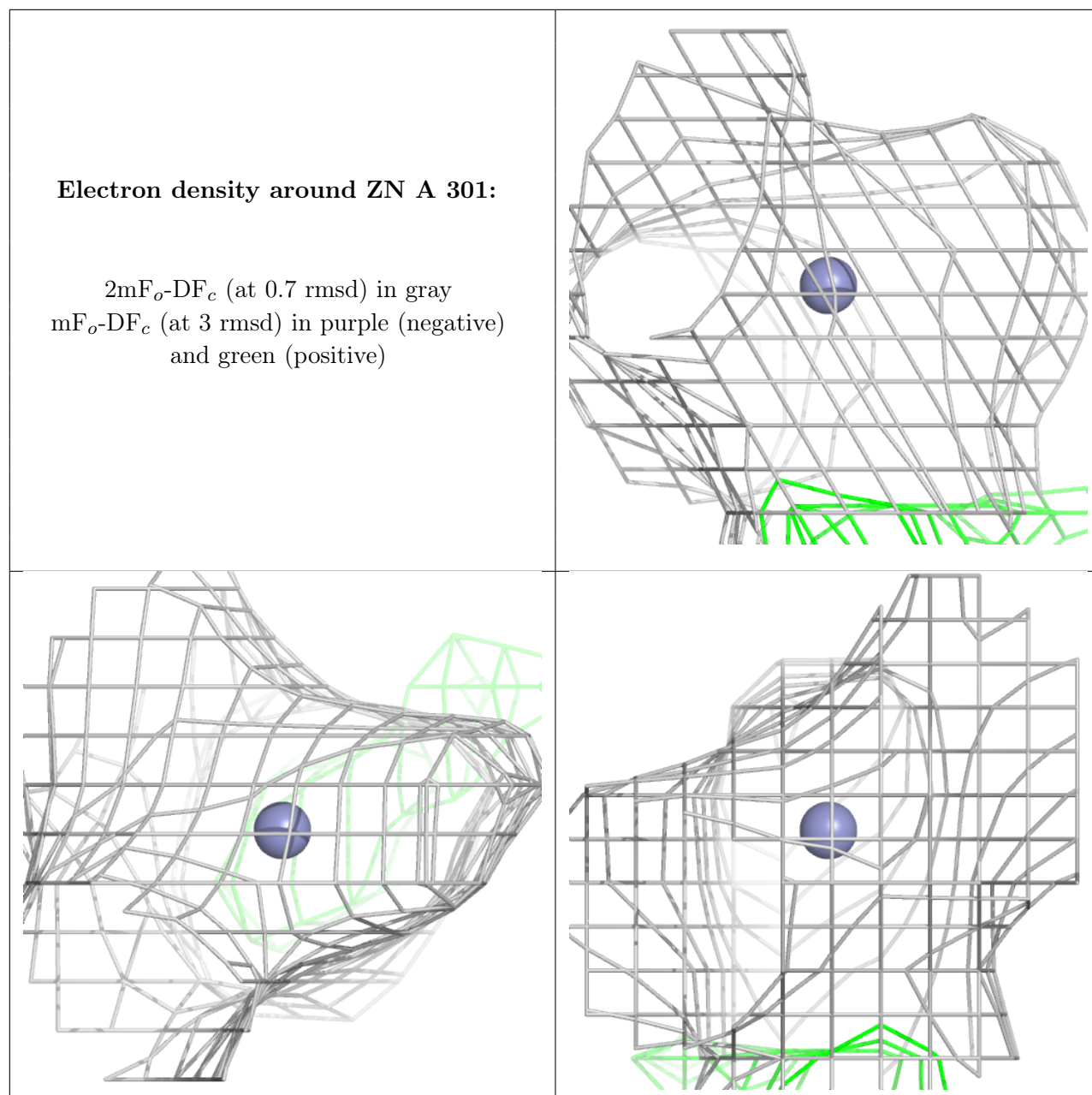
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN F 302:**

$2mF_o-DF_c$  (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.