



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 07:42 pm BST

PDB ID : 6DKD  
Title : Yeast Ddi2 Cyanamide Hydratase  
Authors : Moore, S.A.; Xiao, W.; Li, J.  
Deposited on : 2018-05-29  
Resolution : 3.00 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.

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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 : 2.11  
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) : 2.11

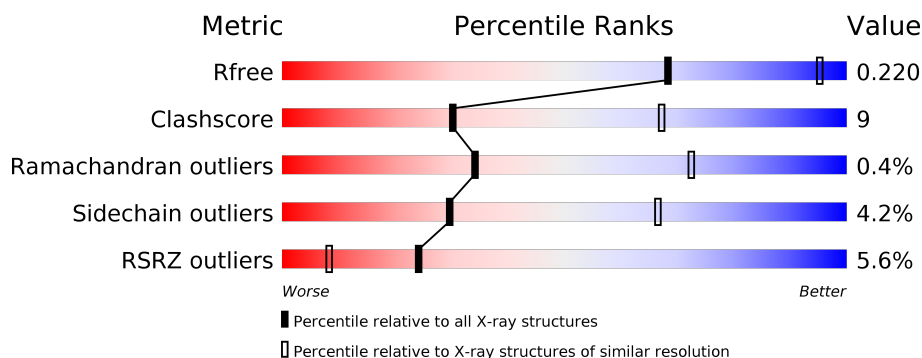
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	<div> <div>78%</div> <div>17%</div> <div>...</div> </div>
1	B	234	<div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	C	234	<div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	D	234	<div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	E	234	<div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	F	234	<div> <div>82%</div> <div>15%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	234	
1	H	234	
1	I	234	

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
3	SO4	B	305	-	-	-	X
3	SO4	D	302	-	-	-	X
3	SO4	D	305	-	-	-	X
3	SO4	E	305	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32110 atoms, of which 15747 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
1	A	229	Total	C	H	N	O	S	0	0	0
			3512	1129	1738	301	338	6			
1	B	230	Total	C	H	N	O	S	0	0	0
			3542	1137	1753	305	341	6			
1	C	230	Total	C	H	N	O	S	0	0	0
			3576	1145	1773	309	343	6			
1	D	229	Total	C	H	N	O	S	0	0	0
			3567	1142	1769	308	342	6			
1	E	229	Total	C	H	N	O	S	0	0	0
			3567	1142	1769	308	342	6			
1	F	230	Total	C	H	N	O	S	0	0	0
			3555	1139	1761	308	341	6			
1	G	229	Total	C	H	N	O	S	0	0	0
			3533	1134	1749	304	340	6			
1	H	225	Total	C	H	N	O	S	0	0	0
			3408	1096	1683	297	327	5			
1	I	226	Total	C	H	N	O	S	0	0	0
			3529	1129	1752	305	337	6			

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	137	ASN	HIS	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	137	ASN	HIS	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	137	ASN	HIS	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	137	ASN	HIS	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	137	ASN	HIS	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	137	ASN	HIS	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	137	ASN	HIS	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	137	ASN	HIS	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	137	ASN	HIS	engineered mutation	UNP A7A1Y4

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

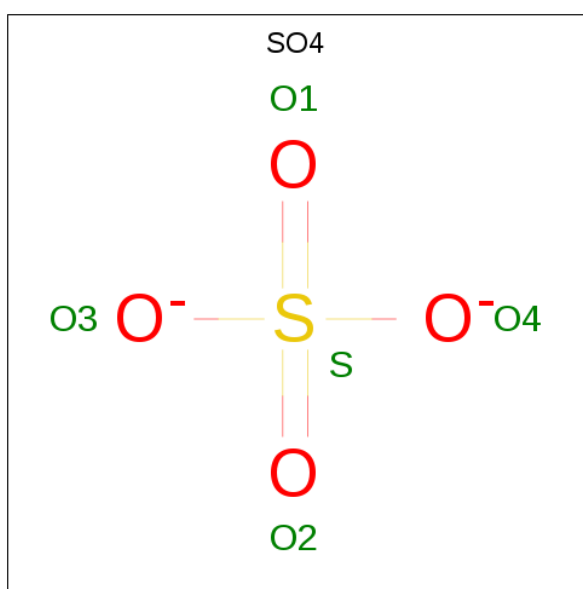
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 4 is water.

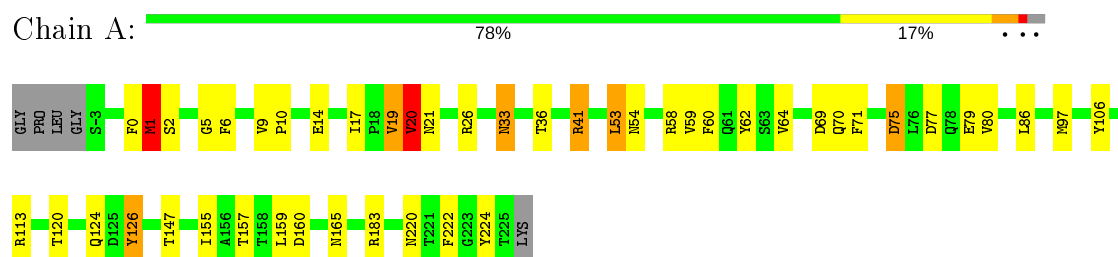


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	19	Total 19	O 19	0	0
4	C	36	Total 36	O 36	0	0
4	D	37	Total 37	O 37	0	0
4	E	42	Total 42	O 42	0	0
4	F	18	Total 18	O 18	0	0
4	G	12	Total 12	O 12	0	0

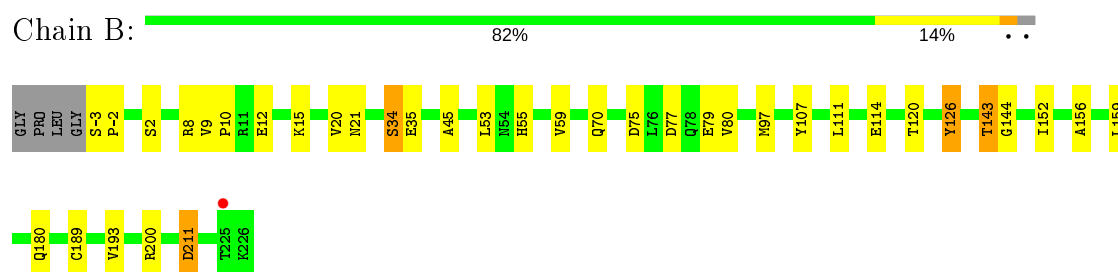
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

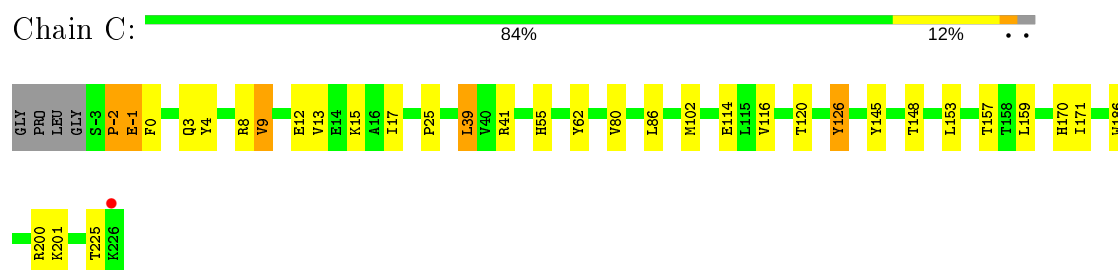
- Molecule 1: DNA damage-inducible protein



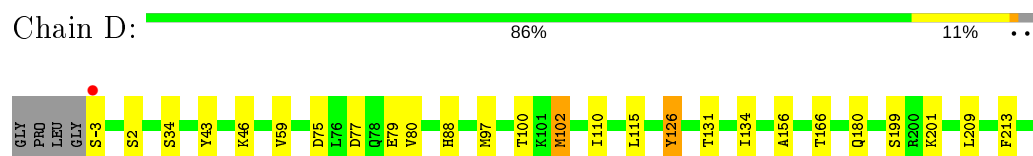
- Molecule 1: DNA damage-inducible protein



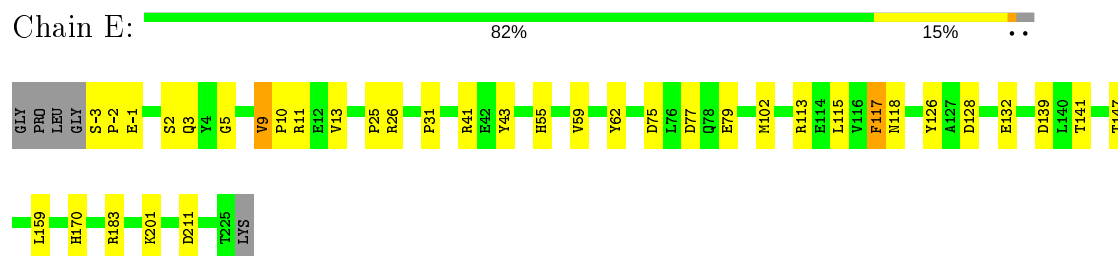
- Molecule 1: DNA damage-inducible protein



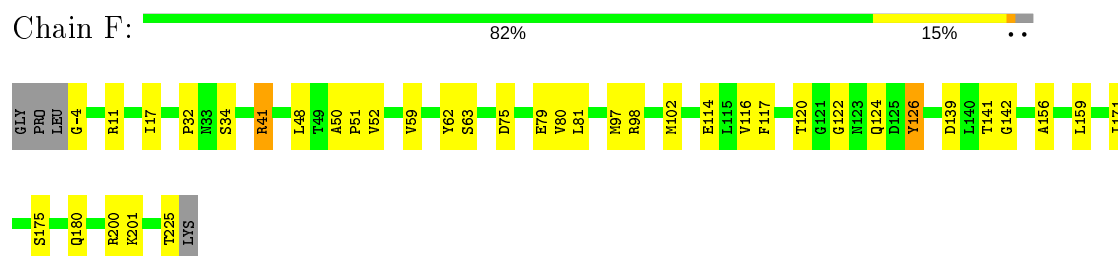
- Molecule 1: DNA damage-inducible protein



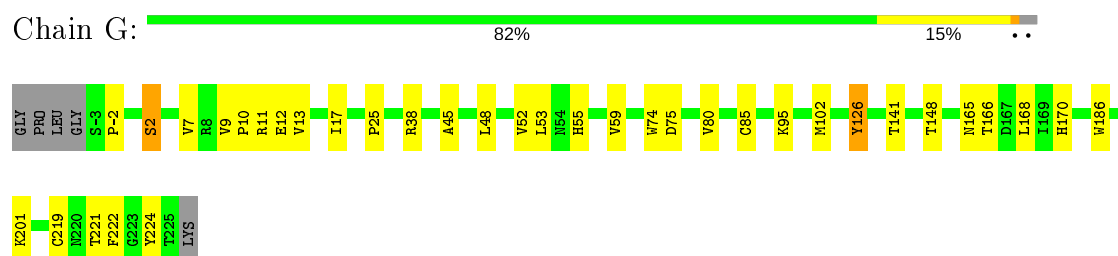
- Molecule 1: DNA damage-inducible protein



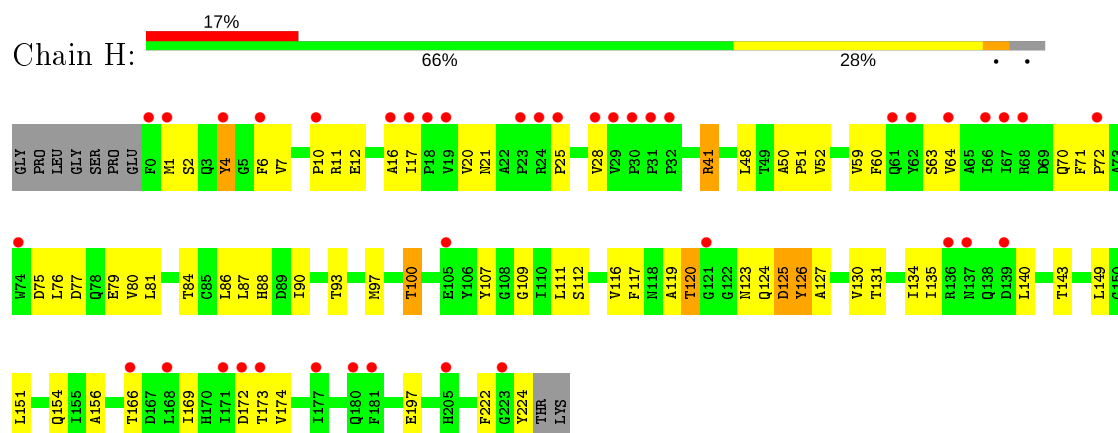
- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein

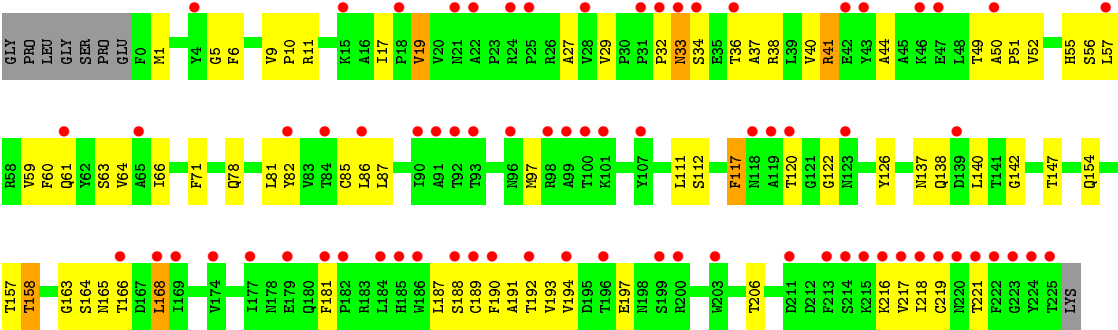


- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.64Å 264.64Å 119.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.77 – 3.00 39.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.77-3.00) 96.5 (39.77-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.194 , 0.221 0.195 , 0.220	Depositor DCC
$R_{free}$ test set	2310 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: ZN, SO4

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	0.34	0/1815	0.58	0/2483
1	B	0.33	0/1830	0.58	0/2502
1	C	0.35	0/1844	0.60	0/2518
1	D	0.34	0/1839	0.58	0/2511
1	E	0.36	0/1839	0.61	1/2511 (0.0%)
1	F	0.34	0/1835	0.57	0/2507
1	G	0.31	0/1825	0.55	0/2495
1	H	0.35	0/1764	0.64	0/2416
1	I	0.31	0/1817	0.58	0/2480
All	All	0.34	0/16408	0.59	1/22423 (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	C	0	1
1	D	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	-3	SER	C-N-CD	-7.47	104.17	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	-2	PRO	Peptide
1	D	-3	SER	Peptide
1	F	-4	GLY	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1774	1738	1726	43	0
1	B	1789	1753	1743	24	0
1	C	1803	1773	1769	19	0
1	D	1798	1769	1767	16	0
1	E	1798	1769	1767	23	0
1	F	1794	1761	1755	21	0
1	G	1784	1749	1741	17	0
1	H	1725	1683	1664	73	0
1	I	1777	1752	1752	66	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	10	0	0	0	0
3	B	20	0	0	0	0
3	C	25	0	0	0	0
3	D	35	0	0	0	0
3	E	20	0	0	2	0
3	F	15	0	0	1	0
3	G	10	0	0	0	0
4	A	13	0	0	1	0
4	B	19	0	0	0	0
4	C	36	0	0	3	0
4	D	37	0	0	1	0
4	E	42	0	0	3	0
4	F	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	12	0	0	0	0
All	All	16363	15747	15684	295	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 9.

The worst 5 of 295 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:E:118:ASN:ND2	4:E:401:HOH:O	1.91	1.02
1:I:190:PHE:CD1	1:I:217:VAL:HG21	2.01	0.96
1:I:32:PRO:HB2	1:I:37:ALA:HB1	1.50	0.94
1:H:76:LEU:HD11	1:H:80:VAL:HG11	1.52	0.92
1:H:4:TYR:HA	1:H:80:VAL:HG21	1.54	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/234 (97%)	216 (95%)	8 (4%)	3 (1%)	12	45
1	B	228/234 (97%)	222 (97%)	5 (2%)	1 (0%)	34	72
1	C	228/234 (97%)	221 (97%)	6 (3%)	1 (0%)	34	72
1	D	227/234 (97%)	220 (97%)	7 (3%)	0	100	100
1	E	227/234 (97%)	220 (97%)	6 (3%)	1 (0%)	34	72
1	F	228/234 (97%)	223 (98%)	5 (2%)	0	100	100
1	G	227/234 (97%)	219 (96%)	7 (3%)	1 (0%)	34	72
1	H	223/234 (95%)	208 (93%)	14 (6%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	224/234 (96%)	214 (96%)	9 (4%)	1 (0%)	34 72
All	All	2039/2106 (97%)	1963 (96%)	67 (3%)	9 (0%)	34 72

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	C	-1	GLU
1	E	-2	PRO
1	H	119	ALA
1	A	20	VAL

### 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	192/202 (95%)	182 (95%)	10 (5%)	23 59
1	B	194/202 (96%)	186 (96%)	8 (4%)	30 67
1	C	197/202 (98%)	189 (96%)	8 (4%)	30 67
1	D	197/202 (98%)	191 (97%)	6 (3%)	41 75
1	E	197/202 (98%)	189 (96%)	8 (4%)	30 67
1	F	195/202 (96%)	187 (96%)	8 (4%)	30 67
1	G	194/202 (96%)	187 (96%)	7 (4%)	35 70
1	H	183/202 (91%)	174 (95%)	9 (5%)	25 61
1	I	195/202 (96%)	186 (95%)	9 (5%)	27 64
All	All	1744/1818 (96%)	1671 (96%)	73 (4%)	30 66

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	13	VAL
1	F	41	ARG

*Continued on next page...*

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Mol	Chain	Res	Type
1	I	97	MET
1	E	139	ASP
1	F	114	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	GLN
1	I	137	ASN
1	I	205	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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	$\# Z  > 2$
3	SO4	D	303	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	F	302	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	F	304	-	4,4,4	0.13	0	6,6,6	0.16	0
3	SO4	E	302	-	4,4,4	0.12	0	6,6,6	0.25	0
3	SO4	E	305	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	A	303	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	E	303	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	E	304	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	D	302	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.12	0
3	SO4	C	302	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	G	303	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	G	301	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	D	307	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	F	303	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	D	306	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	C	304	-	4,4,4	0.13	0	6,6,6	0.19	0
3	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.13	0
3	SO4	D	305	-	4,4,4	0.15	0	6,6,6	0.12	0
3	SO4	C	305	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	D	308	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	C	306	-	4,4,4	0.15	0	6,6,6	0.05	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	SO4	1	0
3	E	305	SO4	1	0
3	E	303	SO4	1	0

## 5.7 Other polymers [i](#)

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 [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	229/234 (97%)	-0.29	0 100 100	54, 73, 103, 132	0
1	B	230/234 (98%)	-0.34	1 (0%) 92 79	48, 68, 92, 126	0
1	C	230/234 (98%)	-0.50	1 (0%) 92 79	38, 54, 78, 140	0
1	D	229/234 (97%)	-0.43	1 (0%) 92 79	39, 54, 75, 116	0
1	E	229/234 (97%)	-0.46	0 100 100	39, 51, 76, 122	0
1	F	230/234 (98%)	-0.39	0 100 100	44, 59, 87, 118	0
1	G	229/234 (97%)	-0.30	0 100 100	49, 77, 105, 141	0
1	H	225/234 (96%)	0.85	40 (17%) 1 0	89, 144, 194, 243	0
1	I	226/234 (96%)	1.41	73 (32%) 0 0	97, 182, 230, 280	0
All	All	2057/2106 (97%)	-0.05	116 (5%) 24 8	38, 68, 191, 280	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	225	THR	6.8
1	I	218	ILE	6.6
1	I	99	ALA	5.7
1	H	139	ASP	5.7
1	I	220	ASN	5.2

### 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](#)

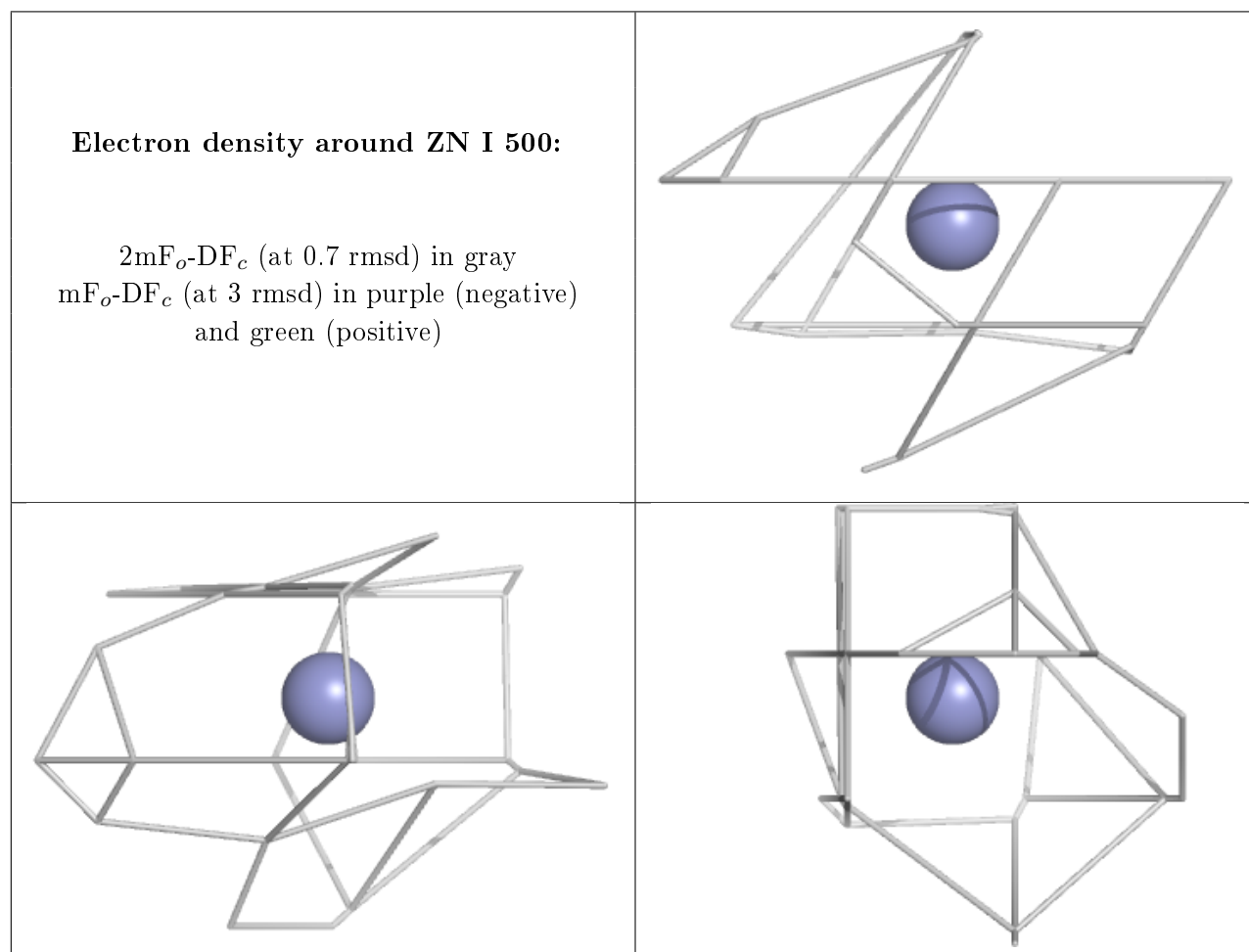
There are no carbohydrates in this entry.

## 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, 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.

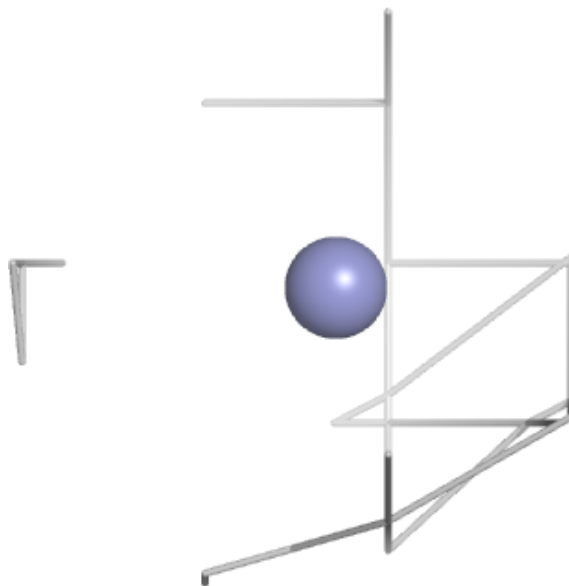
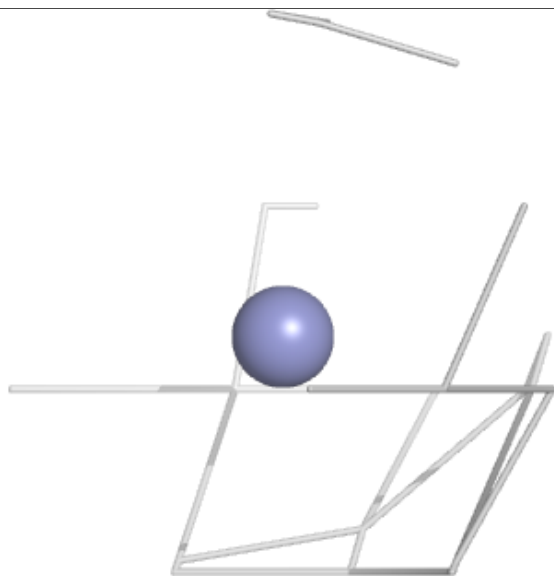
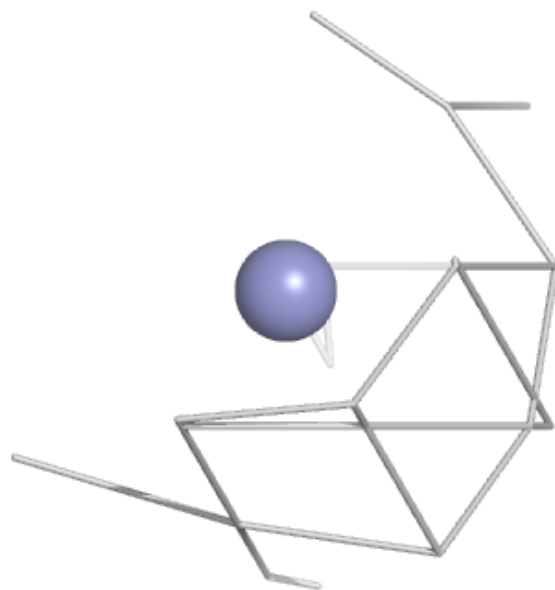
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	I	500	1/1	-0.02	0.28	132,132,132,132	1
3	SO4	D	305	5/5	0.00	0.52	200,205,213,214	0
3	SO4	D	302	5/5	0.52	0.46	189,195,198,203	0
3	SO4	B	305	5/5	0.63	0.55	164,165,171,212	0
3	SO4	D	307	5/5	0.74	0.34	149,149,157,165	0
3	SO4	B	304	5/5	0.77	0.36	134,139,154,156	0
3	SO4	E	305	5/5	0.78	0.56	92,94,103,107	5
3	SO4	B	302	5/5	0.80	0.18	157,158,170,174	0
2	ZN	H	500	1/1	0.83	0.13	135,135,135,135	1
3	SO4	F	302	5/5	0.85	0.23	114,122,127,132	0
3	SO4	C	303	5/5	0.85	0.30	126,132,137,154	0
3	SO4	D	308	5/5	0.86	0.36	105,107,110,111	5
3	SO4	C	306	5/5	0.86	0.43	114,118,122,123	5
3	SO4	A	302	5/5	0.87	0.22	106,114,118,119	0
2	ZN	B	301	1/1	0.89	0.17	85,85,85,85	1
2	ZN	F	301	1/1	0.89	0.21	86,86,86,86	1
2	ZN	D	301	1/1	0.90	0.10	73,73,73,73	1
2	ZN	G	302	1/1	0.90	0.06	99,99,99,99	1
3	SO4	B	303	5/5	0.90	0.21	124,136,144,151	0
3	SO4	D	306	5/5	0.90	0.23	109,115,120,120	0
3	SO4	E	304	5/5	0.90	0.25	100,104,106,113	0
3	SO4	A	303	5/5	0.91	0.17	114,115,118,126	0
3	SO4	C	302	5/5	0.92	0.21	106,109,114,116	0
3	SO4	G	301	5/5	0.92	0.20	102,107,113,114	0
3	SO4	F	304	5/5	0.92	0.18	105,108,109,109	0
3	SO4	E	303	5/5	0.93	0.22	110,116,119,121	0
3	SO4	F	303	5/5	0.93	0.26	134,147,160,160	0
3	SO4	D	304	5/5	0.93	0.18	105,106,108,108	0
2	ZN	C	301	1/1	0.93	0.12	79,79,79,79	1
3	SO4	G	303	5/5	0.93	0.24	115,115,119,121	0
3	SO4	C	305	5/5	0.94	0.17	100,107,108,119	0
3	SO4	C	304	5/5	0.94	0.20	101,103,104,107	0
2	ZN	E	301	1/1	0.95	0.08	71,71,71,71	1
3	SO4	D	303	5/5	0.95	0.19	94,101,105,111	0
2	ZN	A	301	1/1	0.96	0.17	85,85,85,85	1
3	SO4	E	302	5/5	0.98	0.16	56,58,68,72	0

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



**Electron density around ZN H 500:**

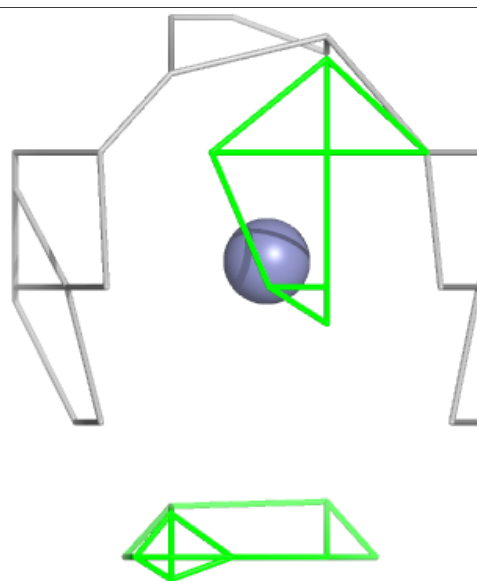
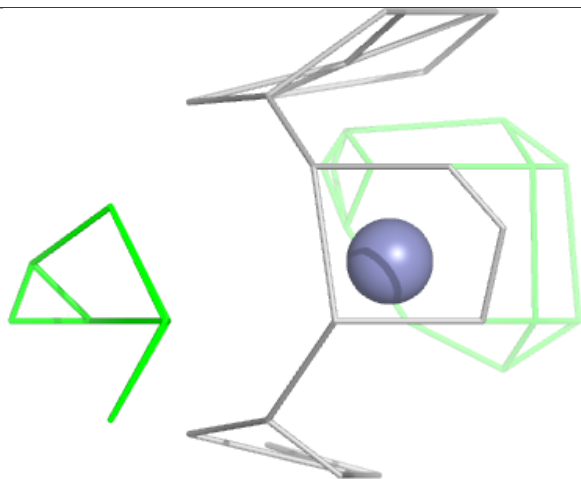
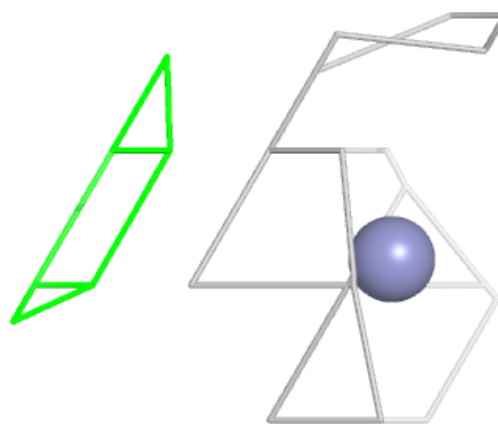
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





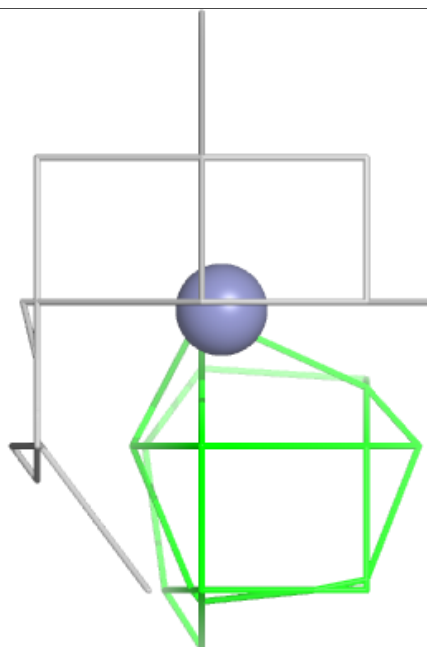
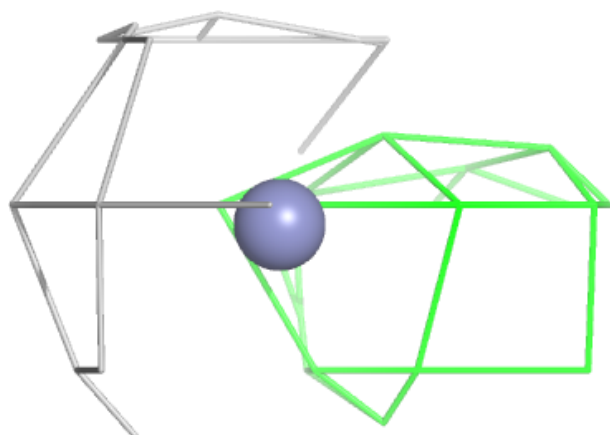
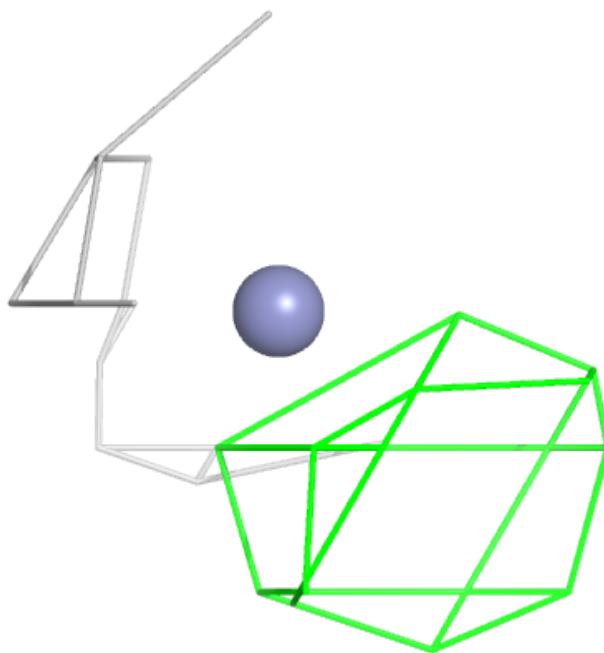
**Electron density around ZN B 301:**

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



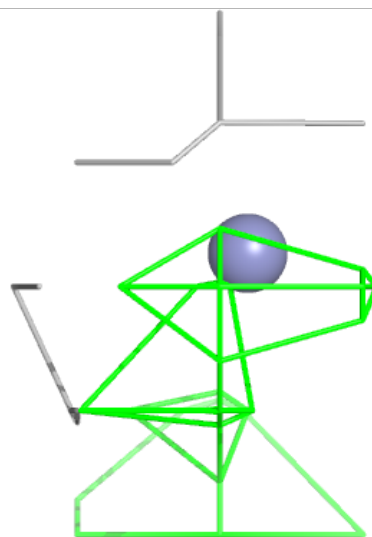
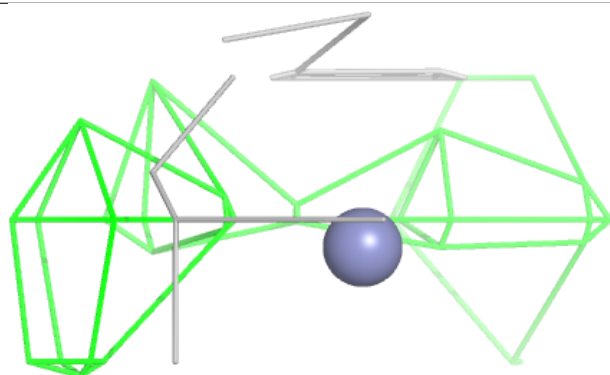
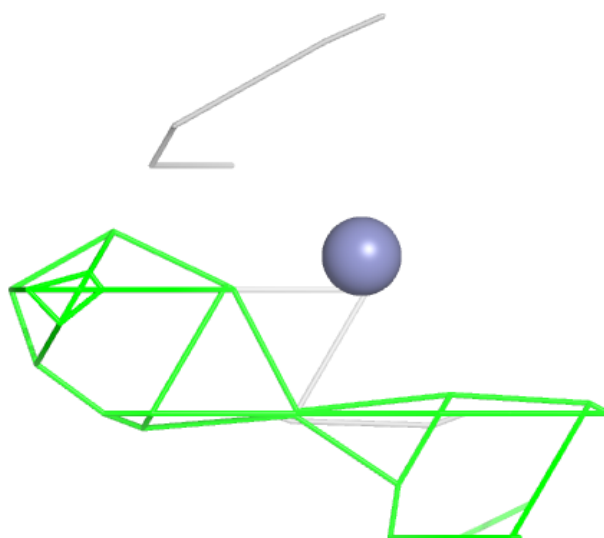
**Electron density around ZN F 301:**

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



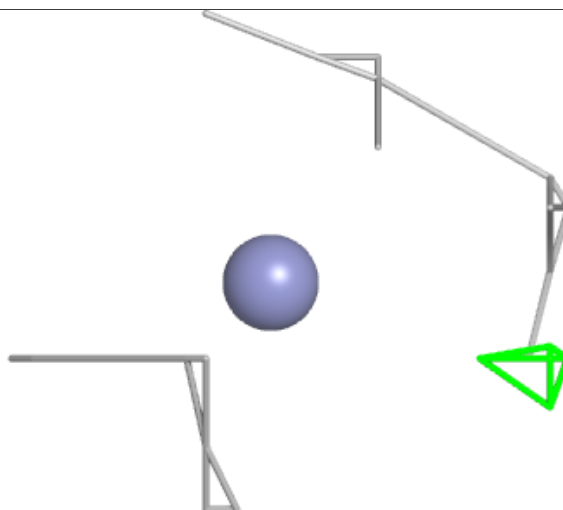
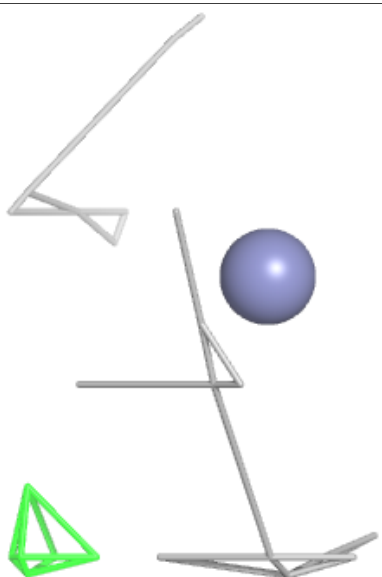
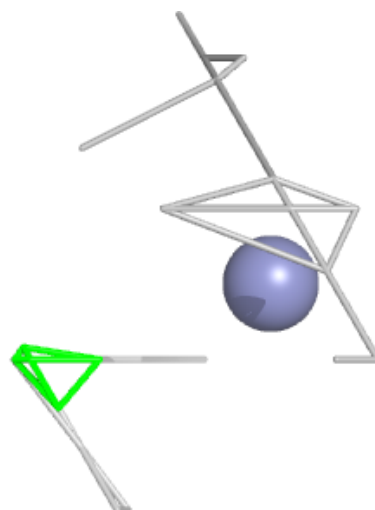
**Electron density around ZN D 301:**

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



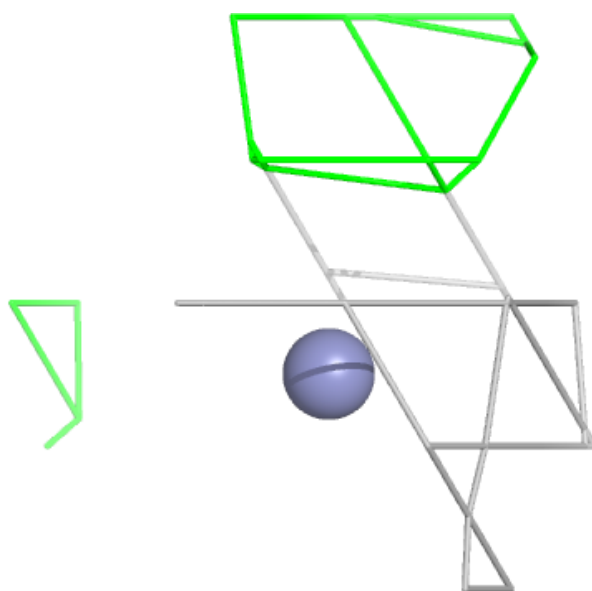
**Electron density around ZN G 302:**

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

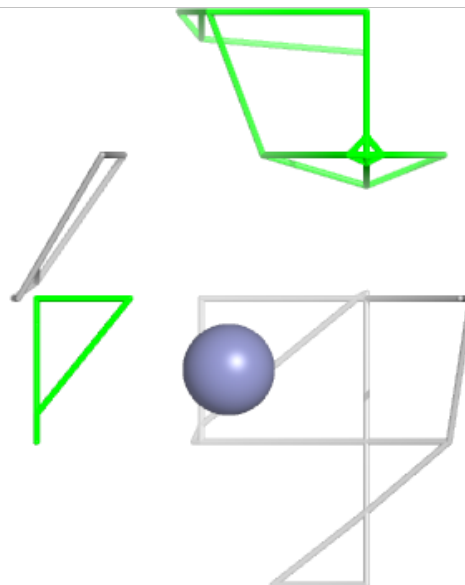
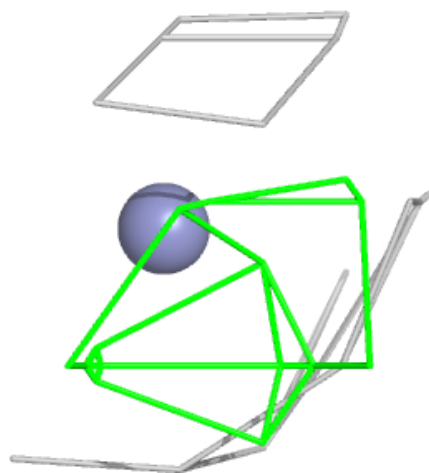


**Electron density around ZN C 301:**

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

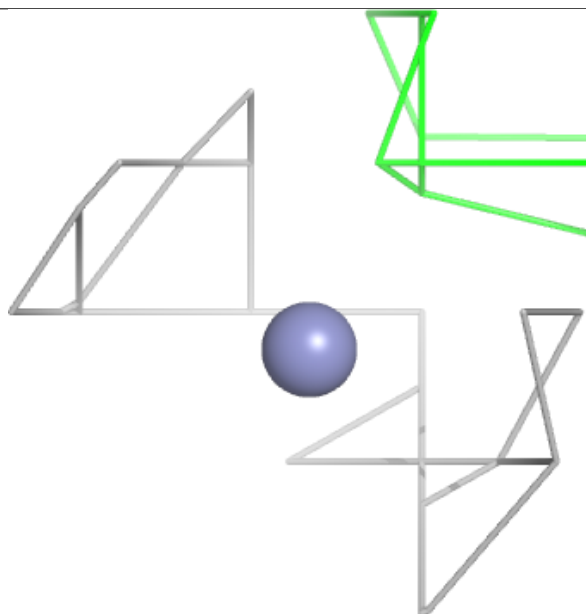
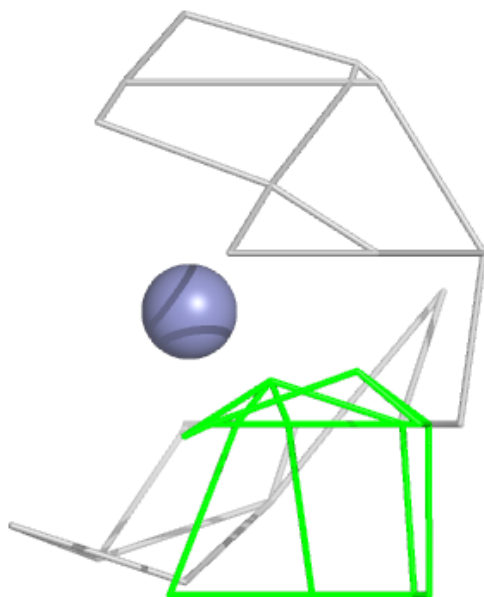
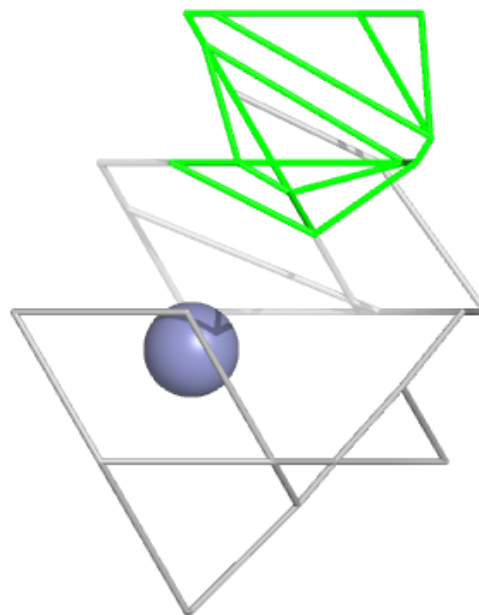


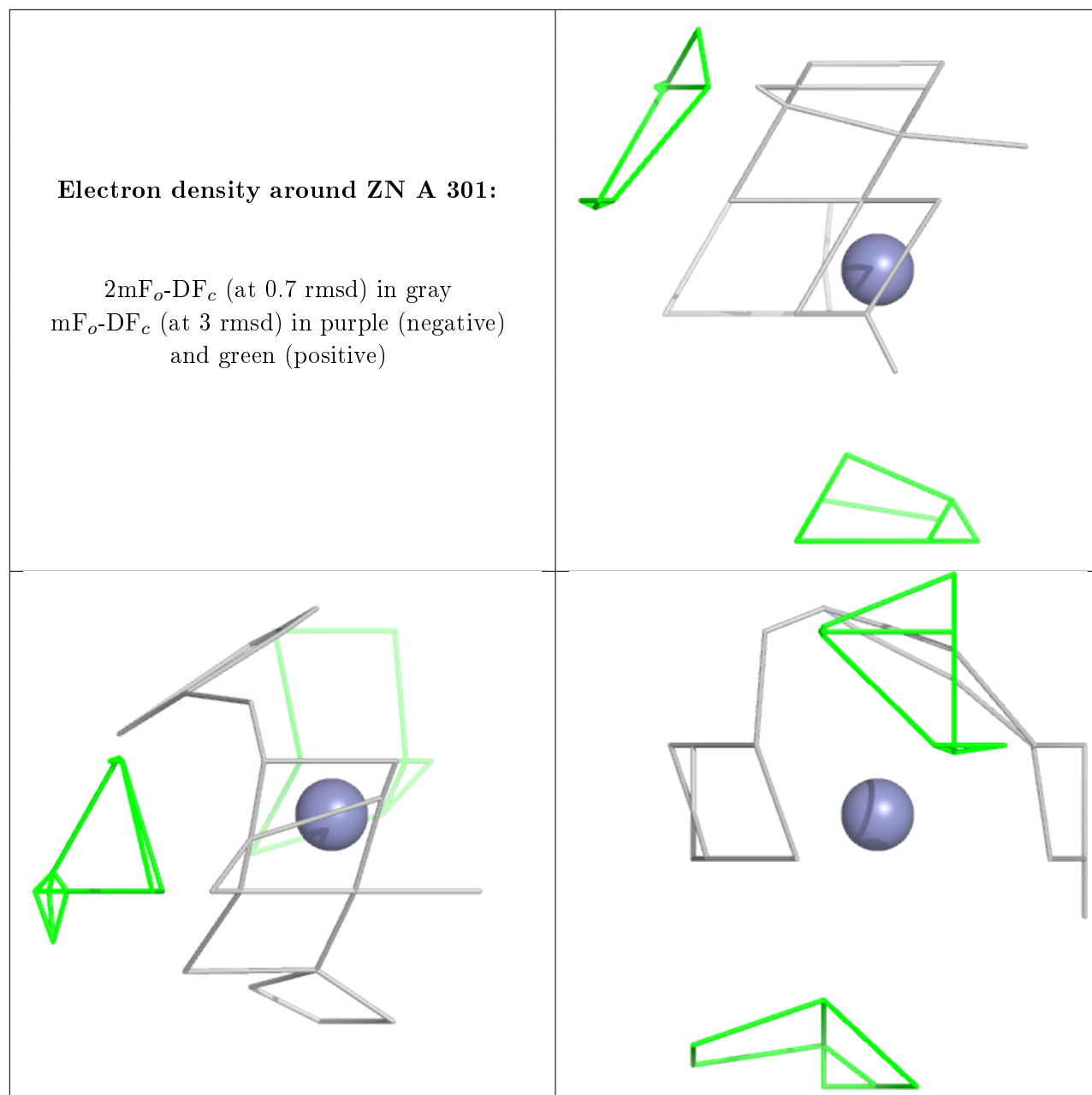
7



**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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.