



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:08 pm BST

PDB ID : 6AIT
Title : Crystal structure of E. coli BepA
Authors : Umar, M.S.M.; Tanaka, Y.; Kamikubo, H.; Tsukazaki, T.
Deposited on : 2018-08-24
Resolution : 2.60 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

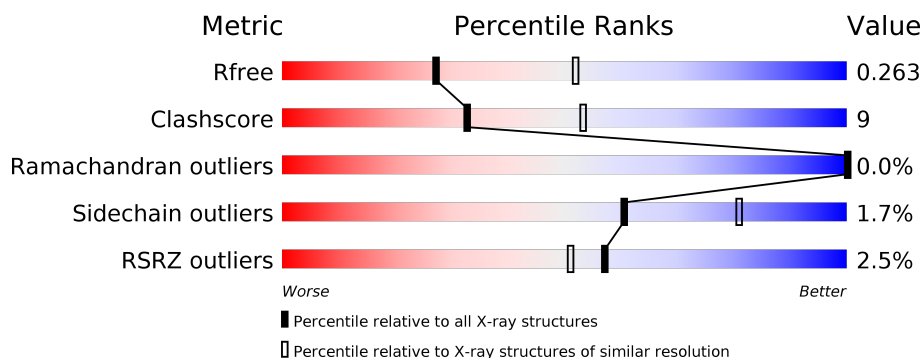
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 ≥ 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	439	<div> <div>0%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	439	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	C	439	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>5%</div> </div> </div>
1	D	439	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	E	439	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>7%</div> </div> </div>
1	F	439	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>• 8%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19732 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 Beta-barrel assembly-enhancing protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3297	2046	608	631	12			
1	B	418	Total	C	N	O	S	0	0	0
			3288	2041	606	629	12			
1	C	415	Total	C	N	O	S	0	0	0
			3272	2032	603	625	12			
1	D	416	Total	C	N	O	S	0	0	0
			3279	2035	604	628	12			
1	E	410	Total	C	N	O	S	0	0	0
			3235	2009	596	619	11			
1	F	406	Total	C	N	O	S	0	0	0
			3197	1982	588	615	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	see sequence details	UNP P66948
B	44	GLY	-	see sequence details	UNP P66948
C	44	GLY	-	see sequence details	UNP P66948
D	44	GLY	-	see sequence details	UNP P66948
E	44	GLY	-	see sequence details	UNP P66948
F	44	GLY	-	see sequence details	UNP P66948

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

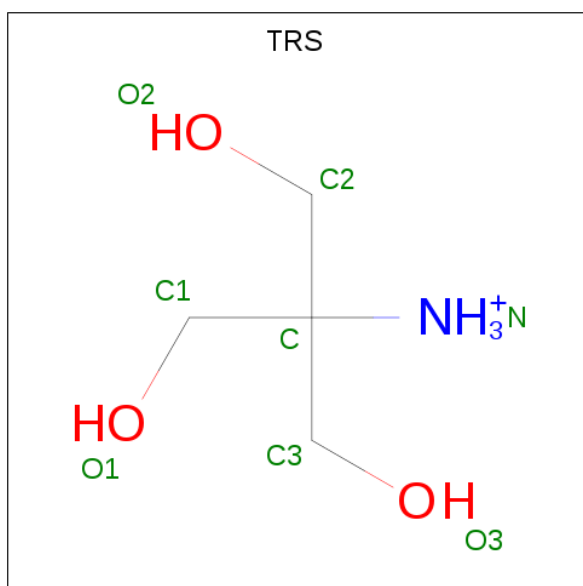
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	E	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total 35	O 35	0	0
4	B	15	Total 15	O 15	0	0
4	C	14	Total 14	O 14	0	0
4	D	17	Total 17	O 17	0	0
4	E	16	Total 16	O 16	0	0
4	F	13	Total 13	O 13	0	0

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 ($\text{RSRZ} > 2$). 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.

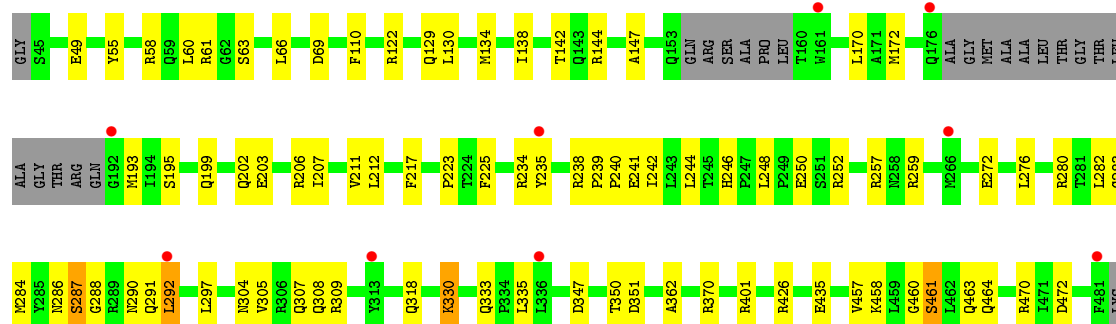
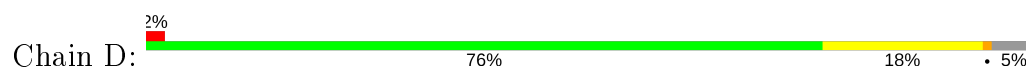
- Chain A:**
-
- %
- 82%
- 12%
- 5%
- GLY S45 L60 D69 G80 M81 R82 L83 V84 S85 H86 F94 E103 F110 N113 Y123 N126 E127 S128 Q129 V141 L146 M150 Q154 ARG SER ALA PRO LEU T160 W161 I168 L169 L170 A171 M172 Q176 ALA GLY MET ALA ALA LEU THR CTV
- THR LEU ALA GLY THR ARG GLN G192 M193 I194 T197 M200 R206 F217 F225 K228 R238 R259 S270 R280 M284 Y285 D298 K302 R306 L317 R329 T350 Q356 L366 R370 F404 K407 K458 L459 G460 S464
- L462 Q463 Q464 A465 B466 R475 Q476 L477 R480 F481 K492

- Chain B:
-
- 77% 2% 18% 5%

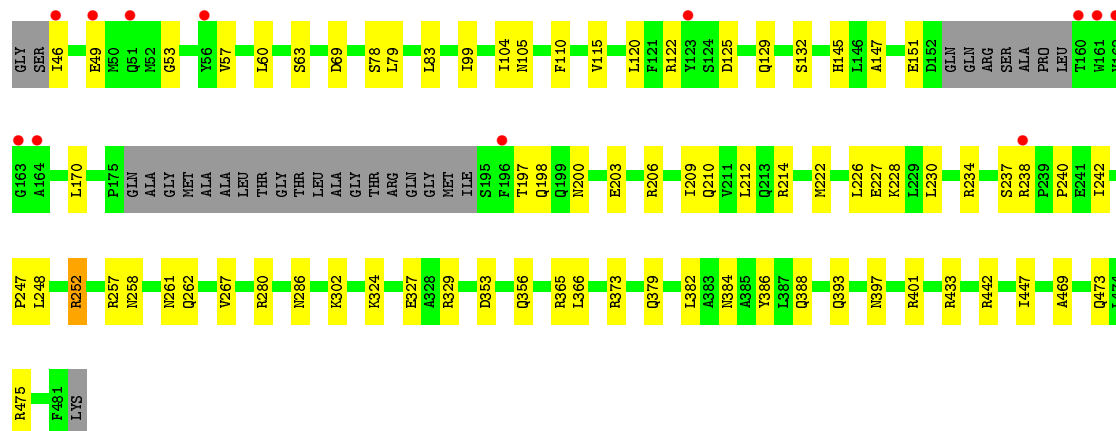
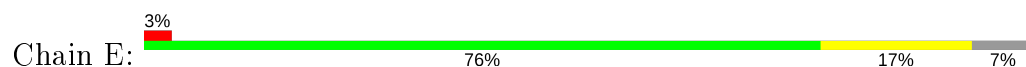
- Chain C:
-
- 78% 16% 3% 5%
- G44 S45 Q48 Q51 L60 D69 M105 G112 R122 V141 T142 Q143 R148 T153 G1N A164 L170 P175 G1N A1A G1Y M1E A1A A1A L1U T1R G1Y T1R L1U A1A G1Y T1R A1R G1N G1Y M1I S195 Q1O
- Q202 E203 R206 L207 V211 L212 Q213 P219 Q220 L230 D231 Q232 Y235 T242 R259 A256 M261 Q262 M263 R264 Y267 R280 N290 L297 R302 G303 N304 V305 R306 Q307 Q308 R309 A310 A311 R315 Q318 E321 A322 N323 R324 Y325 R329 C326



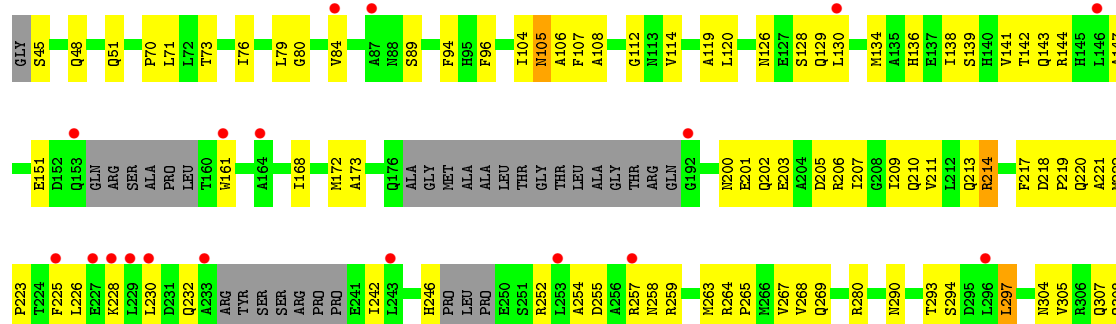
- Molecule 1: Beta-barrel assembly-enhancing protease



- Molecule 1: Beta-barrel assembly-enhancing protease



- Molecule 1: Beta-barrel assembly-enhancing protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 104.67Å 104.97Å 113.61° 105.84° 104.03°	Depositor
Resolution (Å)	48.59 – 2.60 48.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.59-2.60) 98.2 (48.59-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.206 , 0.263 0.206 , 0.263	Depositor DCC
R_{free} test set	2016 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,l,-h-k-l 0.000 for h,-h-k-l,k 0.000 for -h,-l,-k 0.000 for -h,-k,h+k+l 0.000 for -h,h+k+l,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19732	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TRS

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	0.27	0/3351	0.42	0/4530
1	B	0.27	0/3342	0.43	0/4518
1	C	0.29	0/3326	0.44	0/4496
1	D	0.26	0/3333	0.44	1/4507 (0.0%)
1	E	0.28	0/3289	0.45	0/4449
1	F	0.28	0/3244	0.47	1/4380 (0.0%)
All	All	0.27	0/19885	0.44	2/26880 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	LEU	CA-CB-CG	5.73	128.48	115.30
1	F	297	LEU	CB-CG-CD1	5.40	120.18	111.00

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	3297	0	3234	37	0
1	B	3288	0	3226	51	0
1	C	3272	0	3211	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3279	0	3213	59	0
1	E	3235	0	3169	55	0
1	F	3197	0	3127	81	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
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
3	D	8	0	12	1	0
3	E	8	0	12	0	0
3	F	8	0	12	2	0
4	A	35	0	0	2	0
4	B	15	0	0	0	0
4	C	14	0	0	0	0
4	D	17	0	0	1	0
4	E	16	0	0	1	0
4	F	13	0	0	0	0
All	All	19732	0	19252	337	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 337 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:C:475:ARG:O	1:C:479:GLU:OE2	1.80	0.97
1:B:253:LEU:HD21	1:B:257:ARG:HD2	1.52	0.90
1:C:373:ARG:NE	1:C:373:ARG:O	2.06	0.89
1:D:283:GLY:HA2	1:D:292:LEU:HD22	1.57	0.87
1:D:282:LEU:HB3	1:D:292:LEU:HB3	1.59	0.84

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	412/439 (94%)	403 (98%)	9 (2%)	0	100	100
1	B	412/439 (94%)	403 (98%)	9 (2%)	0	100	100
1	C	409/439 (93%)	402 (98%)	7 (2%)	0	100	100
1	D	410/439 (93%)	402 (98%)	7 (2%)	1 (0%)	47	71
1	E	404/439 (92%)	396 (98%)	8 (2%)	0	100	100
1	F	396/439 (90%)	385 (97%)	11 (3%)	0	100	100
All	All	2443/2634 (93%)	2391 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	287	SER

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	344/356 (97%)	340 (99%)	4 (1%)	71	87
1	B	342/356 (96%)	335 (98%)	7 (2%)	55	78
1	C	341/356 (96%)	336 (98%)	5 (2%)	65	83
1	D	342/356 (96%)	337 (98%)	5 (2%)	65	83
1	E	337/356 (95%)	330 (98%)	7 (2%)	53	77
1	F	332/356 (93%)	326 (98%)	6 (2%)	59	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2038/2136 (95%)	2004 (98%)	34 (2%)	60 81

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	361	GLU
1	D	426	ARG
1	F	214	ARG
1	D	284	MET
1	B	148	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	261	ASN
1	D	74	GLN
1	F	290	ASN
1	C	290	ASN
1	C	356	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	TRS	F	502	-	7,7,7	0.33	0	9,9,9	0.65	0
3	TRS	D	502	-	7,7,7	0.32	0	9,9,9	0.46	0
3	TRS	B	502	-	7,7,7	0.33	0	9,9,9	0.37	0
3	TRS	C	502	-	7,7,7	0.34	0	9,9,9	0.43	0
3	TRS	E	502	-	7,7,7	0.30	0	9,9,9	0.23	0
3	TRS	A	502	-	7,7,7	0.30	0	9,9,9	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	F	502	-	-	1/9/9/9	-
3	TRS	D	502	-	-	2/9/9/9	-
3	TRS	B	502	-	-	3/9/9/9	-
3	TRS	C	502	-	-	1/9/9/9	-
3	TRS	E	502	-	-	0/9/9/9	-
3	TRS	A	502	-	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	TRS	N-C-C1-O1
3	B	502	TRS	C1-C-C2-O2
3	B	502	TRS	C3-C-C2-O2
3	B	502	TRS	N-C-C2-O2
3	C	502	TRS	N-C-C1-O1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	502	TRS	2	0
3	D	502	TRS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/439 (95%)	-0.14	4 (0%) 82 80	43, 63, 110, 175	0
1	B	418/439 (95%)	-0.05	8 (1%) 66 62	41, 76, 119, 165	0
1	C	415/439 (94%)	0.08	11 (2%) 54 48	39, 75, 129, 173	0
1	D	416/439 (94%)	-0.05	9 (2%) 62 56	40, 80, 122, 154	0
1	E	410/439 (93%)	0.04	12 (2%) 51 45	43, 74, 135, 190	0
1	F	406/439 (92%)	0.16	18 (4%) 34 27	43, 84, 147, 187	0
All	All	2483/2634 (94%)	0.01	62 (2%) 57 51	39, 75, 131, 190	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	GLY	7.7
1	E	164	ALA	7.5
1	E	160	THR	6.5
1	B	192	GLY	6.4
1	B	177	ALA	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

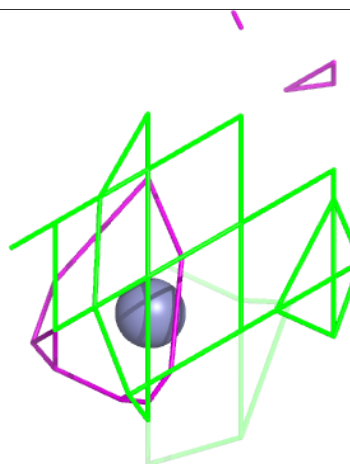
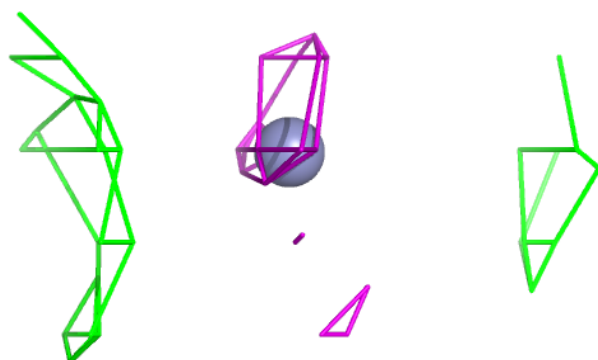
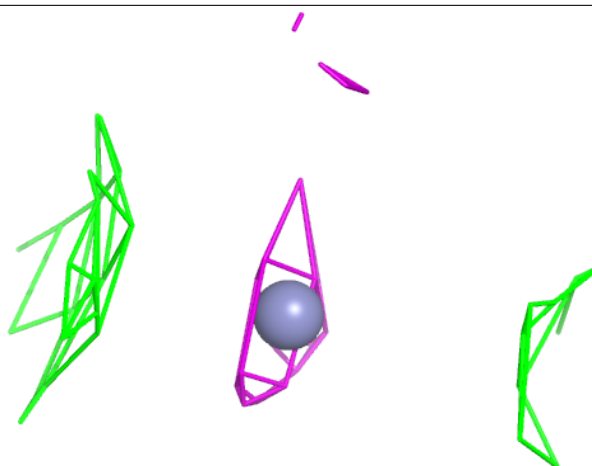
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

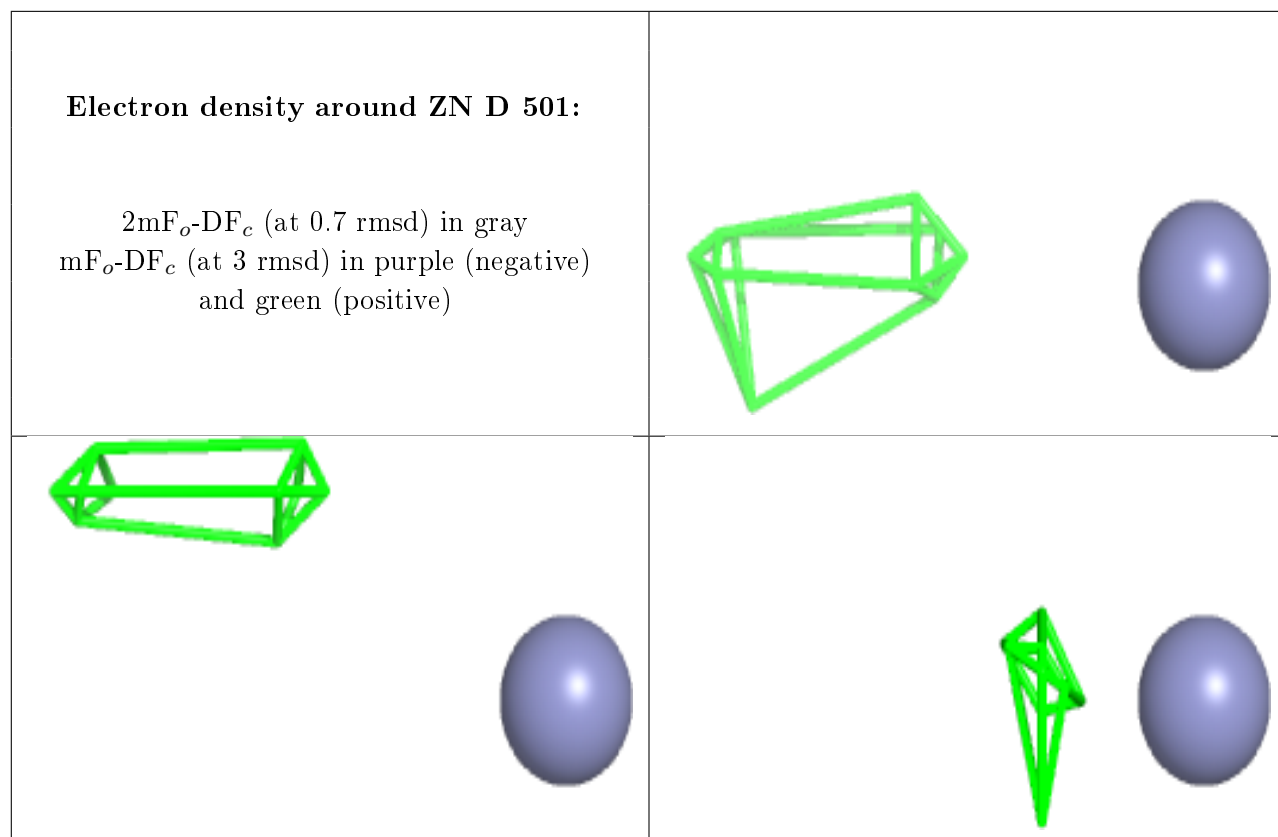
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	F	501	1/1	0.85	0.04	104,104,104,104	0
3	TRS	E	502	8/8	0.85	0.19	75,91,97,102	0
3	TRS	C	502	8/8	0.88	0.27	91,98,100,101	0
3	TRS	F	502	8/8	0.88	0.23	68,76,86,88	0
3	TRS	D	502	8/8	0.89	0.19	84,88,90,95	0
3	TRS	A	502	8/8	0.90	0.16	69,81,84,87	0
3	TRS	B	502	8/8	0.91	0.17	85,89,91,93	0
2	ZN	D	501	1/1	0.98	0.18	77,77,77,77	0
2	ZN	E	501	1/1	0.99	0.10	76,76,76,76	0
2	ZN	B	501	1/1	0.99	0.14	67,67,67,67	0
2	ZN	A	501	1/1	0.99	0.21	76,76,76,76	0
2	ZN	C	501	1/1	0.99	0.13	56,56,56,56	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 F 501:

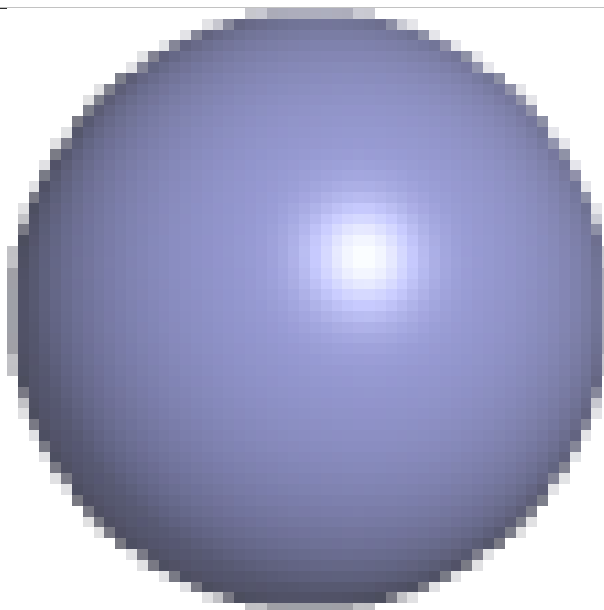
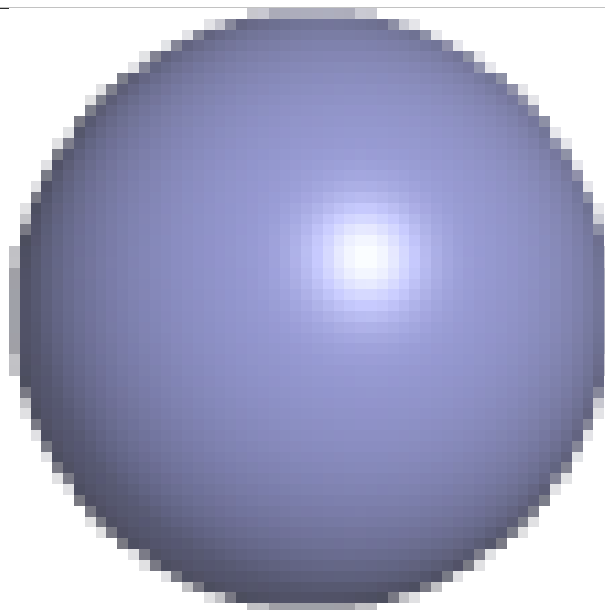
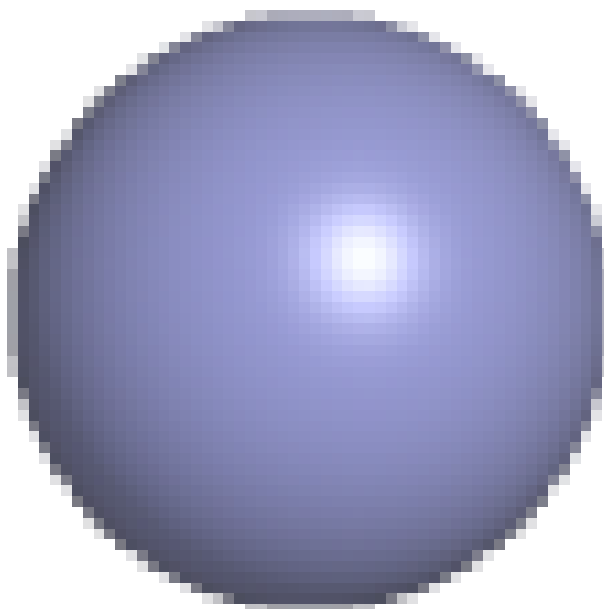
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





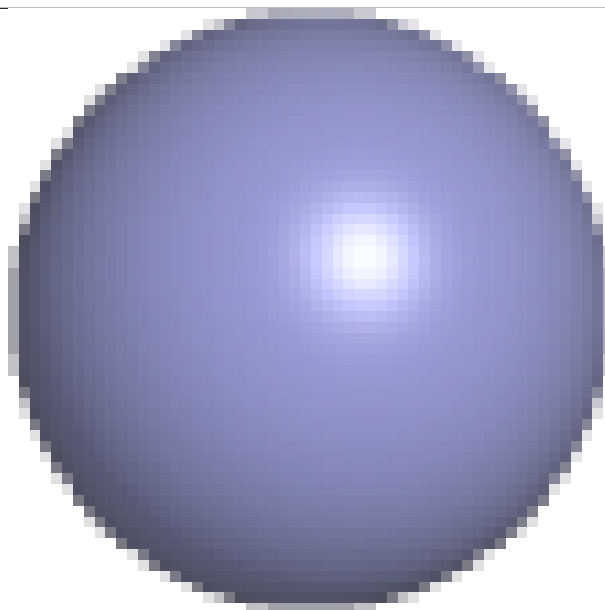
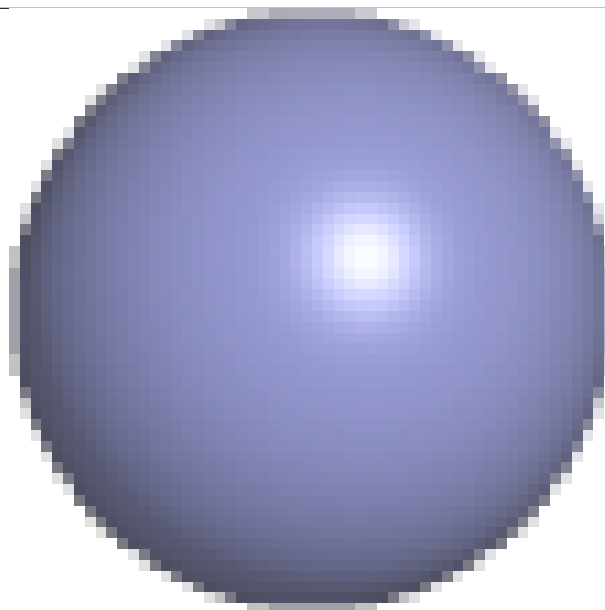
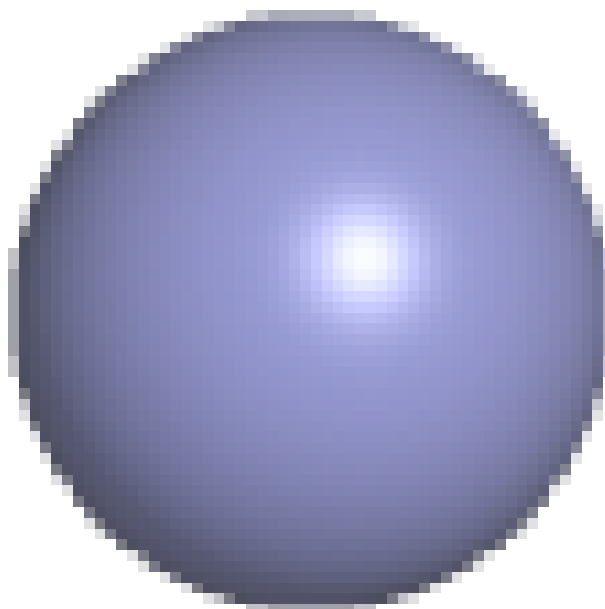
Electron density around ZN E 501:

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



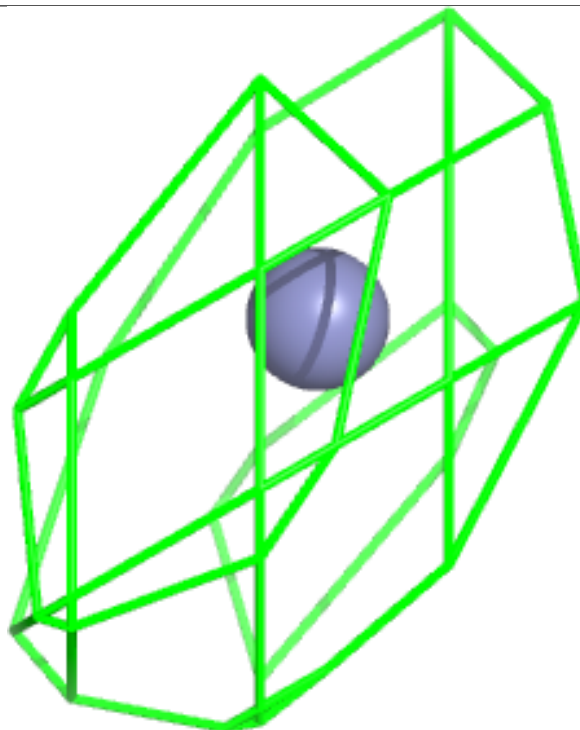
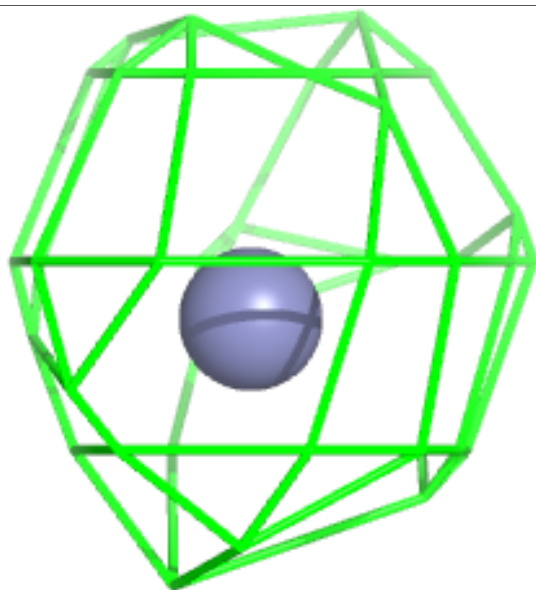
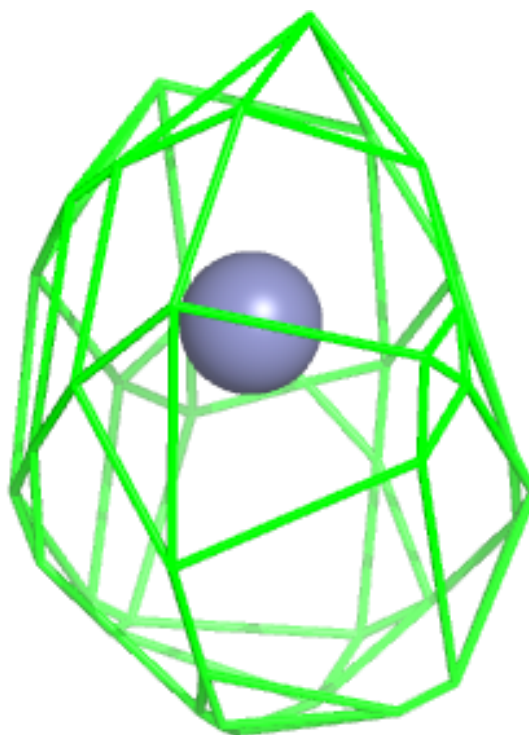
Electron density around ZN B 501:

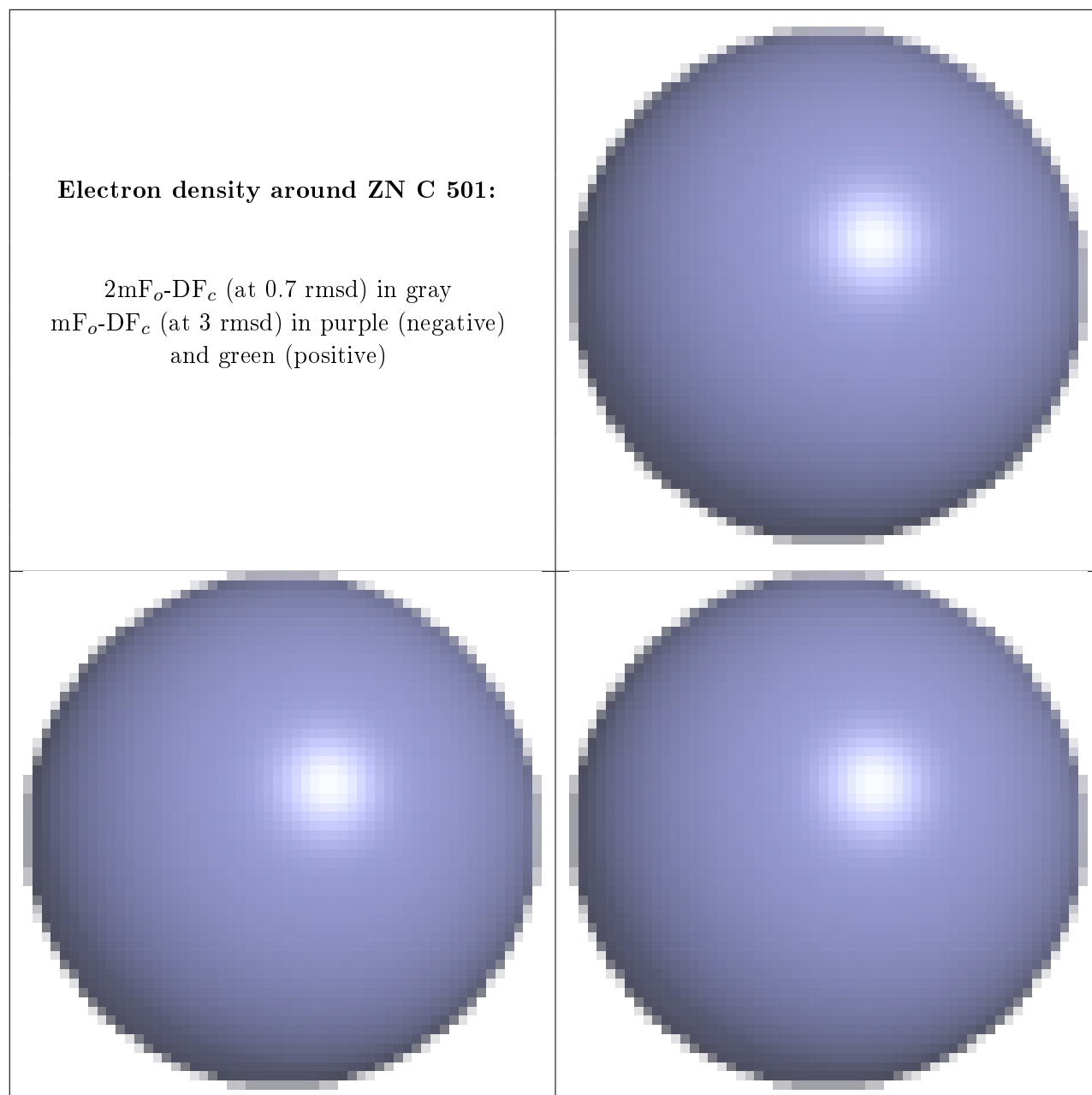
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 501:

$2mF_o-DF_c$ (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.