Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 09:52 PM EDT

PDB ID	:	8E2P
Title	:	Crystal structure of TadA*8.20 in a complex with ssDNA
Authors	:	Feliciano, P.R.; Lee, S.J.; Ciaramella, G.
Deposited on	:	2022-08-15
Resolution	:	2.72 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

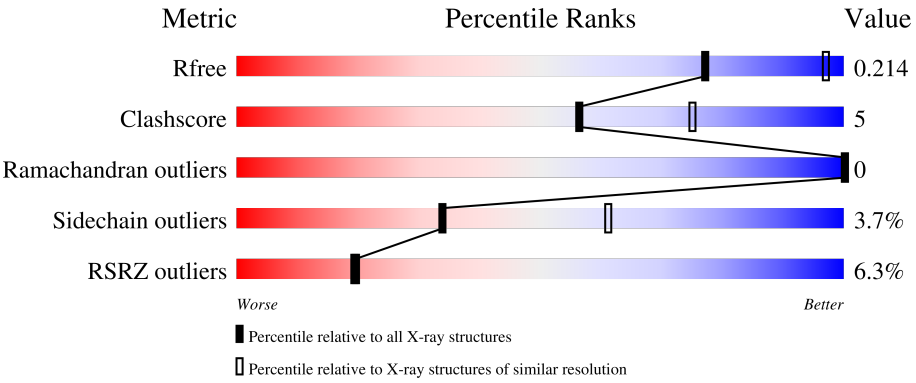
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	167	7% 75% 15% • 10%
1	B	167	4% 81% 11% • 8%
1	C	167	5% 80% 11% 10%
1	D	167	8% 71% 18% • 10%
2	E	13	8% 69% 23% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	13	54% 23% 23%
2	G	13	54% 23% 23%
2	H	13	8% 62% 23% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5577 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 tRNA-specific adenosine deaminase 8.20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1138	719	213	194	12			
1	B	154	Total	C	N	O	S	0	0	0
			1191	753	223	203	12			
1	C	151	Total	C	N	O	S	0	0	0
			1152	727	212	201	12			
1	D	151	Total	C	N	O	S	0	0	0
			1161	731	218	201	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	TRP	conflict	UNP W8T8U5
A	36	LEU	HIS	conflict	UNP W8T8U5
A	48	ALA	PRO	conflict	UNP W8T8U5
A	51	LEU	ARG	conflict	UNP W8T8U5
A	76	TYR	ILE	conflict	UNP W8T8U5
A	82	SER	VAL	conflict	UNP W8T8U5
A	84	PHE	LEU	conflict	UNP W8T8U5
A	106	VAL	ALA	conflict	UNP W8T8U5
A	108	ASN	ASP	conflict	UNP W8T8U5
A	146	CYS	SER	conflict	UNP W8T8U5
A	147	ARG	ASP	conflict	UNP W8T8U5
A	152	PRO	ARG	conflict	UNP W8T8U5
A	154	ARG	GLN	conflict	UNP W8T8U5
A	155	VAL	GLU	conflict	UNP W8T8U5
A	156	PHE	ILE	conflict	UNP W8T8U5
A	157	ASN	LYS	conflict	UNP W8T8U5
B	23	ARG	TRP	conflict	UNP W8T8U5
B	36	LEU	HIS	conflict	UNP W8T8U5
B	48	ALA	PRO	conflict	UNP W8T8U5
B	51	LEU	ARG	conflict	UNP W8T8U5
B	76	TYR	ILE	conflict	UNP W8T8U5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	SER	VAL	conflict	UNP W8T8U5
B	84	PHE	LEU	conflict	UNP W8T8U5
B	106	VAL	ALA	conflict	UNP W8T8U5
B	108	ASN	ASP	conflict	UNP W8T8U5
B	146	CYS	SER	conflict	UNP W8T8U5
B	147	ARG	ASP	conflict	UNP W8T8U5
B	152	PRO	ARG	conflict	UNP W8T8U5
B	154	ARG	GLN	conflict	UNP W8T8U5
B	155	VAL	GLU	conflict	UNP W8T8U5
B	156	PHE	ILE	conflict	UNP W8T8U5
B	157	ASN	LYS	conflict	UNP W8T8U5
C	23	ARG	TRP	conflict	UNP W8T8U5
C	36	LEU	HIS	conflict	UNP W8T8U5
C	48	ALA	PRO	conflict	UNP W8T8U5
C	51	LEU	ARG	conflict	UNP W8T8U5
C	76	TYR	ILE	conflict	UNP W8T8U5
C	82	SER	VAL	conflict	UNP W8T8U5
C	84	PHE	LEU	conflict	UNP W8T8U5
C	106	VAL	ALA	conflict	UNP W8T8U5
C	108	ASN	ASP	conflict	UNP W8T8U5
C	146	CYS	SER	conflict	UNP W8T8U5
C	147	ARG	ASP	conflict	UNP W8T8U5
C	152	PRO	ARG	conflict	UNP W8T8U5
C	154	ARG	GLN	conflict	UNP W8T8U5
C	155	VAL	GLU	conflict	UNP W8T8U5
C	156	PHE	ILE	conflict	UNP W8T8U5
C	157	ASN	LYS	conflict	UNP W8T8U5
D	23	ARG	TRP	conflict	UNP W8T8U5
D	36	LEU	HIS	conflict	UNP W8T8U5
D	48	ALA	PRO	conflict	UNP W8T8U5
D	51	LEU	ARG	conflict	UNP W8T8U5
D	76	TYR	ILE	conflict	UNP W8T8U5
D	82	SER	VAL	conflict	UNP W8T8U5
D	84	PHE	LEU	conflict	UNP W8T8U5
D	106	VAL	ALA	conflict	UNP W8T8U5
D	108	ASN	ASP	conflict	UNP W8T8U5
D	146	CYS	SER	conflict	UNP W8T8U5
D	147	ARG	ASP	conflict	UNP W8T8U5
D	152	PRO	ARG	conflict	UNP W8T8U5
D	154	ARG	GLN	conflict	UNP W8T8U5
D	155	VAL	GLU	conflict	UNP W8T8U5
D	156	PHE	ILE	conflict	UNP W8T8U5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	157	ASN	LYS	conflict	UNP W8T8U5

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*CP*TP*CP*GP*GP*CP*TP*(D8A)P *CP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			268	125	51	79	13			
2	F	10	Total	C	N	O	P	0	0	0
			207	96	41	60	10			
2	G	10	Total	C	N	O	P	0	0	0
			207	96	41	60	10			
2	H	11	Total	C	N	O	P	0	0	0
			227	106	43	67	11			

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	9	Total	O	0	0
			9	9		
4	C	5	Total	O	0	0
			5	5		
4	D	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

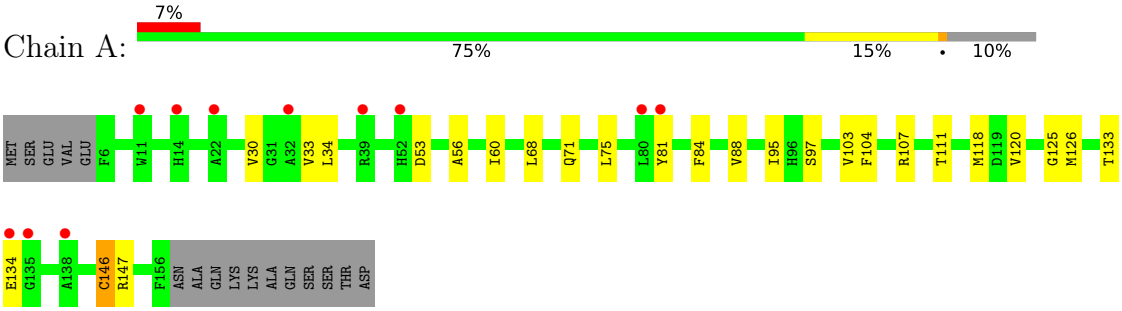
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	3	Total O 3 3	0	0

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.

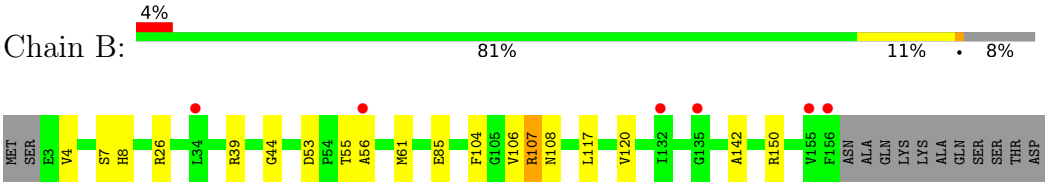
• Molecule 1: tRNA-specific adenosine deaminase 8.20

Chain A:



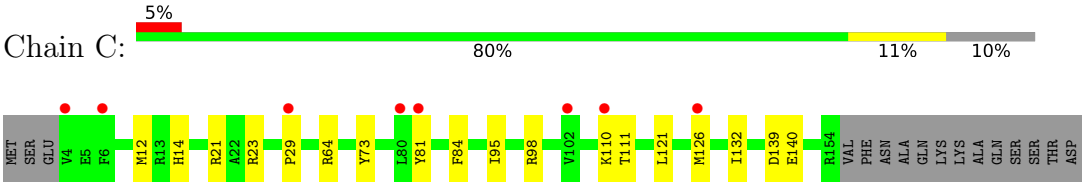
• Molecule 1: tRNA-specific adenosine deaminase 8.20

Chain B:



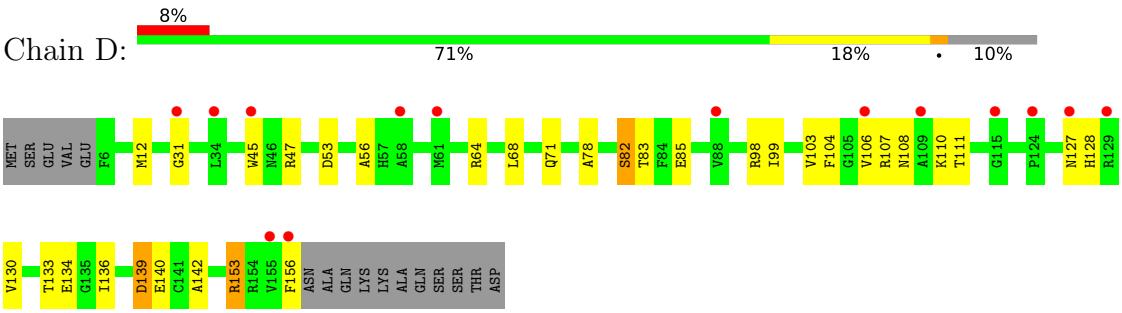
• Molecule 1: tRNA-specific adenosine deaminase 8.20

Chain C:



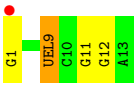
• Molecule 1: tRNA-specific adenosine deaminase 8.20

Chain D:



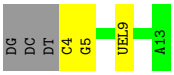
• Molecule 2: DNA (5'-D(P*GP*CP*TP*CP*GP*GP*CP*TP*(D8A)P*CP*GP*GP*A)-3')

Chain E:



• Molecule 2: DNA (5'-D(P*GP*CP*TP*CP*GP*GP*CP*TP*(D8A)P*CP*GP*GP*A)-3')

Chain F:

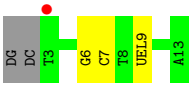


• Molecule 2: DNA (5'-D(P*GP*CP*TP*CP*GP*GP*CP*TP*(D8A)P*CP*GP*GP*A)-3')

Chain G:

• Molecule 2: DNA (5'-D(P*GP*CP*TP*CP*GP*GP*CP*TP*(D8A)P*CP*GP*GP*A)-3')

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.67Å 84.67Å 214.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.34 – 2.72 43.34 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.34-2.72) 100.0 (43.34-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	415.51 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.190 , 0.218 0.189 , 0.214	Depositor DCC
R_{free} test set	1155 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.337 for -h,-k,l	Xtriage
Reported twinning fraction	0.400 for -h,-k,l	Depositor
Outliers	0 of 24773 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5577	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.24	0/1163	0.49	0/1577
1	B	0.23	0/1217	0.49	0/1646
1	C	0.23	0/1177	0.47	0/1595
1	D	0.23	0/1186	0.50	0/1606
2	E	0.50	0/275	0.88	0/420
2	F	0.47	0/207	0.78	0/315
2	G	0.60	0/207	0.85	0/315
2	H	0.51	0/229	0.88	0/349
All	All	0.30	0/5661	0.57	0/7823

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1138	0	1101	14	0
1	B	1191	0	1173	13	0
1	C	1152	0	1122	9	0
1	D	1161	0	1137	19	0
2	E	268	0	135	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	207	0	101	2	0
2	G	207	0	101	1	0
2	H	227	0	113	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	9	0	0	0	0
4	C	5	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	3	0	0	0	0
All	All	5577	0	4983	53	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 5.

All (53) 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:D:139:ASP:HA	1:D:153:ARG:HH21	1.39	0.85
1:A:88:VAL:HG11	1:B:120:VAL:HG11	1.74	0.70
1:C:23:ARG:HB2	1:C:29:PRO:HB3	1.77	0.67
1:D:45:TRP:HE1	1:D:47:ARG:HD3	1.61	0.65
1:C:95:ILE:HD13	1:C:126:MET:HG2	1.77	0.64
1:B:150:ARG:NH1	2:F:5:DG:N7	2.47	0.63
2:G:6:DG:H2"	2:G:7:DC:H5"	1.79	0.63
1:A:103:VAL:HG22	1:A:133:THR:HB	1.84	0.60
1:B:150:ARG:NH2	2:F:4:DC:OP2	2.35	0.59
1:D:78:ALA:HB3	1:D:99:ILE:HG22	1.87	0.56
1:B:106:VAL:HG11	1:B:142:ALA:HB2	1.88	0.55
1:A:33:VAL:HG12	1:A:81:TYR:HB2	1.89	0.54
1:D:103:VAL:HG22	1:D:133:THR:HB	1.89	0.54
1:D:68:LEU:O	1:D:71:GLN:NE2	2.40	0.53
1:D:110:LYS:HG2	1:D:111:THR:HG23	1.91	0.53
1:C:64:ARG:HH12	1:D:64:ARG:CZ	2.22	0.52
1:C:110:LYS:HD3	1:C:111:THR:HG23	1.92	0.52
1:A:125:GLY:HA3	1:B:117:LEU:HD11	1.91	0.52
1:A:146:CYS:SG	1:A:147:ARG:N	2.83	0.51
1:D:85:GLU:OE1	1:D:108:ASN:N	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASP:HB3	1:D:56:ALA:HB2	1.94	0.50
1:D:12:MET:HG2	1:D:136:ILE:HG22	1.93	0.49
2:E:11:DG:H5"	2:E:12:DG:H3'	1.93	0.49
1:D:45:TRP:NE1	1:D:47:ARG:HD3	2.28	0.47
1:A:53:ASP:HB3	1:A:56:ALA:HB2	1.96	0.47
1:A:104:PHE:HE2	1:A:107:ARG:HG2	1.78	0.47
1:A:118:MET:HE1	1:B:120:VAL:HG22	1.96	0.47
1:C:95:ILE:O	1:C:98:ARG:HD3	2.15	0.47
1:A:68:LEU:O	1:A:71:GLN:NE2	2.46	0.47
1:D:31:GLY:H	1:D:83:THR:HG1	1.63	0.47
1:B:53:ASP:HB3	1:B:56:ALA:HB2	1.98	0.46
1:C:140:GLU:N	1:C:140:GLU:OE2	2.49	0.46
1:A:34:LEU:HD21	1:A:75:LEU:HD13	1.97	0.45
1:D:106:VAL:HG11	1:D:142:ALA:HB2	1.98	0.45
1:D:98:ARG:HG3	1:D:128:HIS:CG	2.51	0.45
1:B:7:SER:OG	1:B:8:HIS:N	2.50	0.45
1:D:140:GLU:N	1:D:140:GLU:OE1	2.51	0.44
1:C:12:MET:HE2	1:C:81:TYR:HD1	1.83	0.43
1:A:30:VAL:HG11	2:E:9:UEL:N1	2.33	0.43
1:B:4:VAL:HG21	1:C:14:HIS:CG	2.54	0.43
1:D:128:HIS:CD2	1:D:130:VAL:HG22	2.54	0.43
1:A:60:ILE:HG23	1:B:55:THR:HG21	2.00	0.43
1:A:111:THR:OG1	2:E:9:UEL:OP2	2.36	0.43
1:B:104:PHE:CE2	1:B:107:ARG:HG2	2.55	0.42
1:D:107:ARG:NH1	1:D:134:GLU:OE2	2.53	0.42
2:H:6:DG:O3'	2:H:7:DC:H4'	2.20	0.41
1:D:98:ARG:HA	1:D:128:HIS:CD2	2.55	0.41
1:B:85:GLU:OE1	1:B:108:ASN:N	2.48	0.41
1:B:44:GLY:HA2	1:B:61:MET:SD	2.61	0.41
1:A:95:ILE:HG21	1:A:126:MET:HG2	2.03	0.41
1:D:82:SER:O	1:D:104:PHE:HA	2.21	0.41
1:C:121:LEU:HD12	1:C:132:ILE:HD11	2.02	0.41
2:E:1:DG:H8	2:E:1:DG:H5'	1.86	0.40

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	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
1	B	152/167 (91%)	148 (97%)	4 (3%)	0	100	100
1	C	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
1	D	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
All	All	599/668 (90%)	583 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	110/135 (82%)	105 (96%)	5 (4%)	27	53
1	B	119/135 (88%)	116 (98%)	3 (2%)	47	75
1	C	115/135 (85%)	111 (96%)	4 (4%)	36	63
1	D	116/135 (86%)	111 (96%)	5 (4%)	29	55
All	All	460/540 (85%)	443 (96%)	17 (4%)	34	61

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

Mol	Chain	Res	Type
1	A	84	PHE
1	A	97	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	VAL
1	A	134	GLU
1	A	146	CYS
1	B	26	ARG
1	B	39	ARG
1	B	107	ARG
1	C	21	ARG
1	C	73	TYR
1	C	84	PHE
1	C	139	ASP
1	D	82	SER
1	D	127	ASN
1	D	139	ASP
1	D	153	ARG
1	D	156	PHE

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

Mol	Chain	Res	Type
1	A	65	GLN
1	C	38	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	UEL	H	9	3,2	16,23,24	4.91	10 (62%)	14,33,36	1.57	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	UEL	F	9	3,2	16,23,24	4.89	10 (62%)	14,33,36	1.51	3 (21%)
2	UEL	G	9	3,2	16,23,24	4.90	10 (62%)	14,33,36	1.48	3 (21%)
2	UEL	E	9	3,2	16,23,24	4.91	10 (62%)	14,33,36	1.56	3 (21%)

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
2	UEL	H	9	3,2	-	1/3/31/32	0/3/3/3
2	UEL	F	9	3,2	-	1/3/31/32	0/3/3/3
2	UEL	G	9	3,2	-	1/3/31/32	0/3/3/3
2	UEL	E	9	3,2	-	1/3/31/32	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	9	UEL	N7-N8	-11.06	1.14	1.34
2	E	9	UEL	N7-N8	-11.06	1.14	1.34
2	G	9	UEL	N7-N8	-11.05	1.14	1.34
2	F	9	UEL	N7-N8	-11.00	1.14	1.34
2	G	9	UEL	N8-N9	-9.55	1.17	1.34
2	H	9	UEL	N8-N9	-9.53	1.17	1.34
2	F	9	UEL	N8-N9	-9.52	1.17	1.34
2	E	9	UEL	N8-N9	-9.49	1.17	1.34
2	E	9	UEL	C2-N1	8.40	1.49	1.34
2	H	9	UEL	C2-N1	8.35	1.49	1.34
2	F	9	UEL	C2-N1	8.33	1.49	1.34
2	G	9	UEL	C2-N1	8.30	1.48	1.34
2	F	9	UEL	C4-N3	-6.36	1.18	1.37
2	H	9	UEL	C4-N3	-6.34	1.18	1.37
2	G	9	UEL	C4-N3	-6.34	1.18	1.37
2	E	9	UEL	C4-N3	-6.32	1.18	1.37
2	H	9	UEL	C5-C4	3.61	1.55	1.41
2	G	9	UEL	C5-C4	3.61	1.55	1.41
2	F	9	UEL	C5-C4	3.60	1.55	1.41
2	E	9	UEL	C5-C4	3.56	1.55	1.41
2	H	9	UEL	O4'-C1'	3.40	1.50	1.42
2	E	9	UEL	O4'-C1'	3.37	1.49	1.42
2	G	9	UEL	O4'-C1'	3.32	1.49	1.42
2	F	9	UEL	O4'-C1'	3.30	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	9	UEL	C5-N7	3.15	1.38	1.34
2	F	9	UEL	O6-C6	-3.13	1.28	1.40
2	G	9	UEL	C5-N7	3.12	1.38	1.34
2	H	9	UEL	O6-C6	-3.12	1.28	1.40
2	E	9	UEL	O6-C6	-3.12	1.28	1.40
2	G	9	UEL	O6-C6	-3.11	1.28	1.40
2	E	9	UEL	C5-N7	3.08	1.38	1.34
2	F	9	UEL	C5-N7	3.07	1.38	1.34
2	E	9	UEL	C2'-C3'	-2.70	1.45	1.52
2	H	9	UEL	C2'-C3'	-2.51	1.46	1.52
2	F	9	UEL	C2'-C3'	-2.51	1.46	1.52
2	G	9	UEL	C2'-C3'	-2.46	1.46	1.52
2	G	9	UEL	C2-N3	-2.12	1.26	1.29
2	F	9	UEL	C2-N3	-2.08	1.26	1.29
2	H	9	UEL	C2-N3	-2.06	1.26	1.29
2	E	9	UEL	C2-N3	-2.05	1.26	1.29

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	9	UEL	C2'-C1'-N9	-3.66	109.36	113.67
2	H	9	UEL	C2'-C1'-N9	-3.61	109.41	113.67
2	F	9	UEL	C2'-C1'-N9	-3.27	109.81	113.67
2	G	9	UEL	C2'-C1'-N9	-3.13	109.98	113.67
2	E	9	UEL	C4-N3-C2	2.66	126.33	115.55
2	F	9	UEL	C4-N3-C2	2.59	126.03	115.55
2	H	9	UEL	C4-N3-C2	2.58	126.02	115.55
2	G	9	UEL	C4-N3-C2	2.56	125.94	115.55
2	E	9	UEL	C4'-O4'-C1'	-2.39	103.67	109.45
2	H	9	UEL	C2'-C3'-C4'	2.20	107.35	102.76
2	F	9	UEL	C2'-C3'-C4'	2.15	107.25	102.76
2	G	9	UEL	C2'-C3'-C4'	2.13	107.21	102.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	9	UEL	O4'-C4'-C5'-O5'
2	H	9	UEL	O4'-C4'-C5'-O5'
2	F	9	UEL	O4'-C4'-C5'-O5'
2	G	9	UEL	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	9	UEL	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	151/167 (90%)	0.86	11 (7%) 15 13	49, 61, 79, 108	0
1	B	154/167 (92%)	0.71	6 (3%) 39 39	50, 58, 76, 90	0
1	C	151/167 (90%)	0.82	8 (5%) 26 25	56, 66, 93, 123	0
1	D	151/167 (90%)	0.87	14 (9%) 8 7	60, 69, 90, 145	0
2	E	12/13 (92%)	0.32	1 (8%) 11 10	52, 58, 108, 120	0
2	F	9/13 (69%)	0.20	0 100 100	55, 61, 67, 76	0
2	G	9/13 (69%)	0.44	0 100 100	60, 70, 71, 81	0
2	H	10/13 (76%)	0.50	1 (10%) 7 5	56, 63, 83, 104	0
All	All	647/720 (89%)	0.79	41 (6%) 20 19	49, 64, 85, 145	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	GLY	4.9
1	D	156	PHE	4.4
1	B	132	ILE	4.2
1	A	14	HIS	4.1
1	C	6	PHE	3.5
1	A	80	LEU	3.5
1	D	88	VAL	3.4
1	A	22	ALA	3.3
1	D	127	ASN	3.1
1	C	81	TYR	3.0
1	A	138	ALA	2.9
1	D	155	VAL	2.8
1	A	81	TYR	2.8
1	D	61	MET	2.7
2	E	1	DG	2.7
1	B	56	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	2.6
1	A	134	GLU	2.5
1	A	39	ARG	2.5
1	C	80	LEU	2.5
1	C	126	MET	2.4
1	C	110	LYS	2.3
1	B	34	LEU	2.3
1	B	155	VAL	2.3
1	D	58	ALA	2.2
1	D	109	ALA	2.2
1	D	129	ARG	2.2
1	A	32	ALA	2.1
1	A	52	HIS	2.1
1	A	11	TRP	2.1
1	D	45	TRP	2.1
1	D	34	LEU	2.1
2	H	3	DT	2.1
1	B	156	PHE	2.1
1	C	29	PRO	2.1
1	D	124	PRO	2.1
1	D	115	GLY	2.1
1	C	4	VAL	2.0
1	D	106	VAL	2.0
1	D	31	GLY	2.0
1	C	102	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	UEL	G	9	21/22	0.86	0.19	51,55,64,65	0
2	UEL	E	9	21/22	0.89	0.21	51,54,57,57	0
2	UEL	F	9	21/22	0.92	0.16	49,52,57,62	0
2	UEL	H	9	21/22	0.93	0.17	61,64,69,75	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

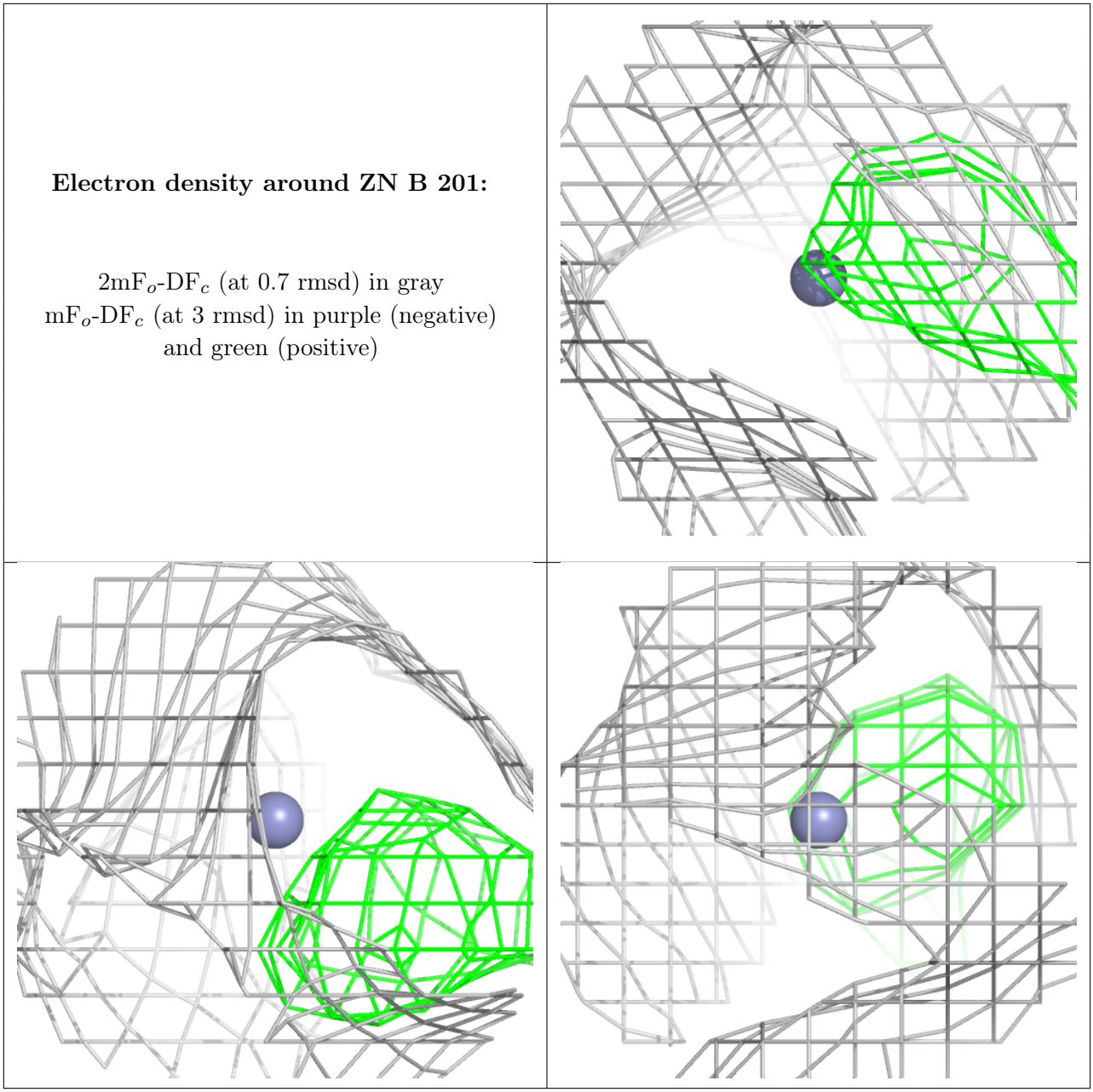
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	ZN	B	201	1/1	0.71	0.19	61,61,61,61	0
3	ZN	A	201	1/1	0.91	0.12	52,52,52,52	0
3	ZN	C	201	1/1	0.91	0.12	58,58,58,58	0
3	ZN	D	201	1/1	0.91	0.21	61,61,61,61	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.

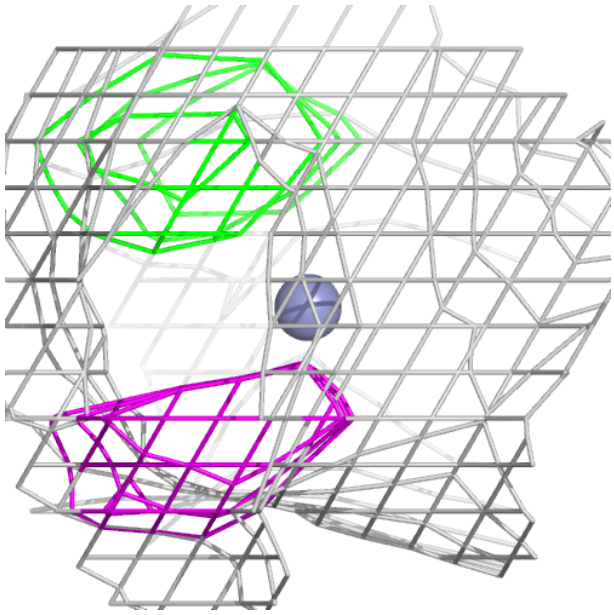
Electron density around ZN B 201:

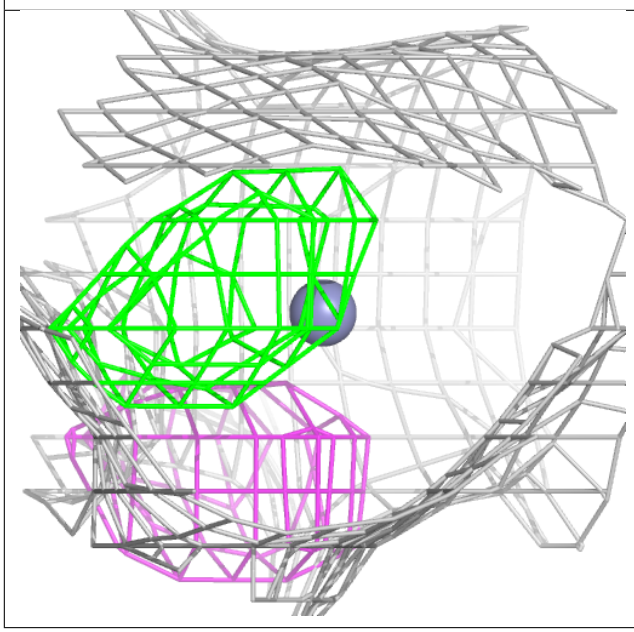
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

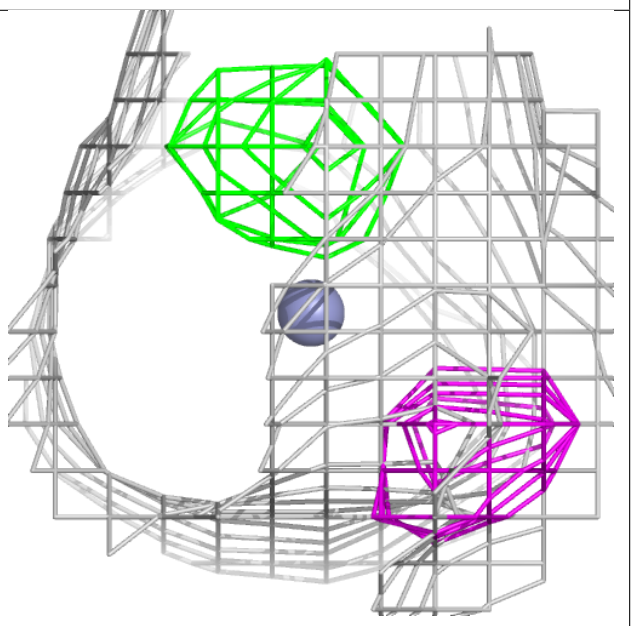


Electron density around ZN A 201:

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

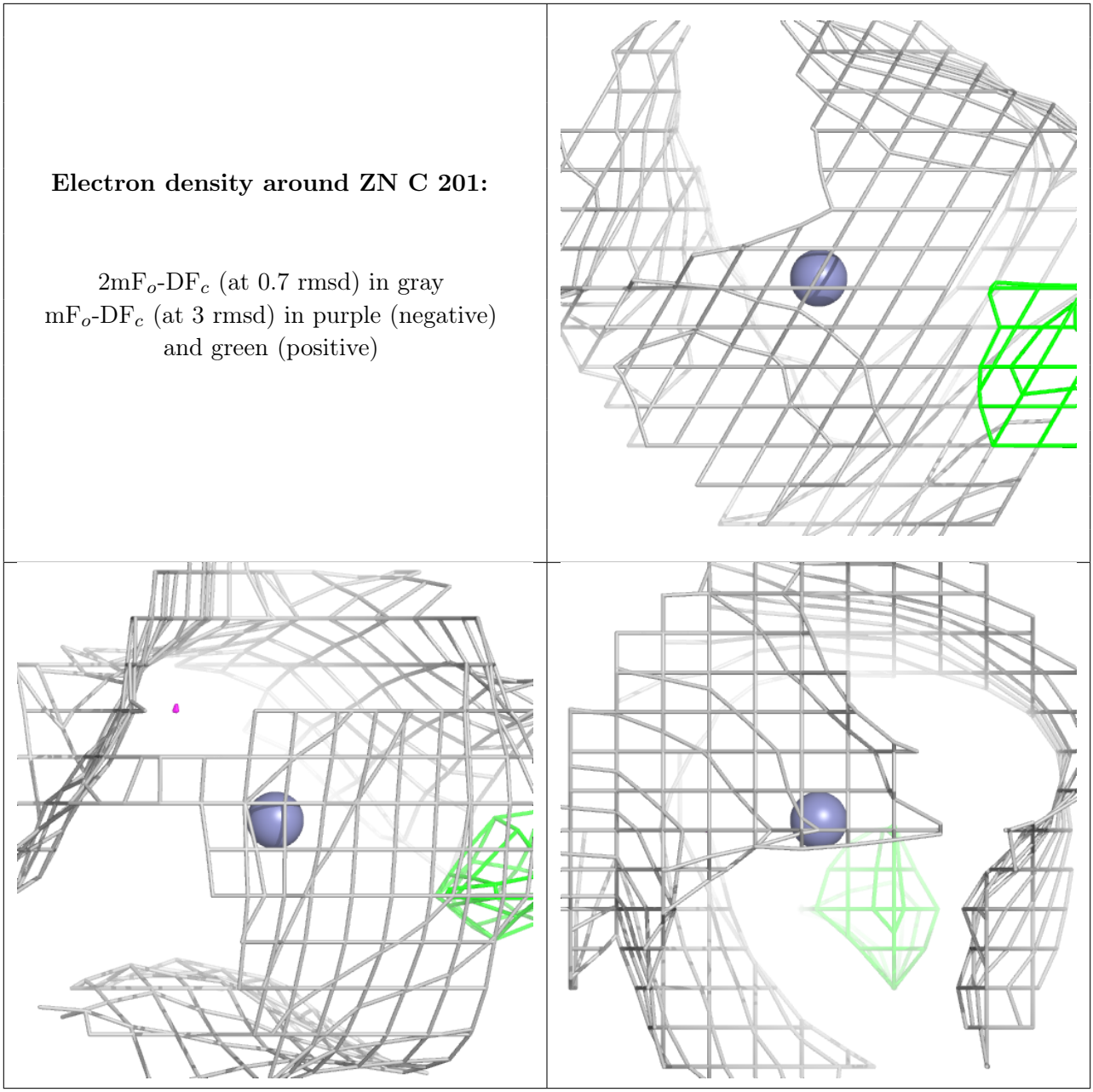






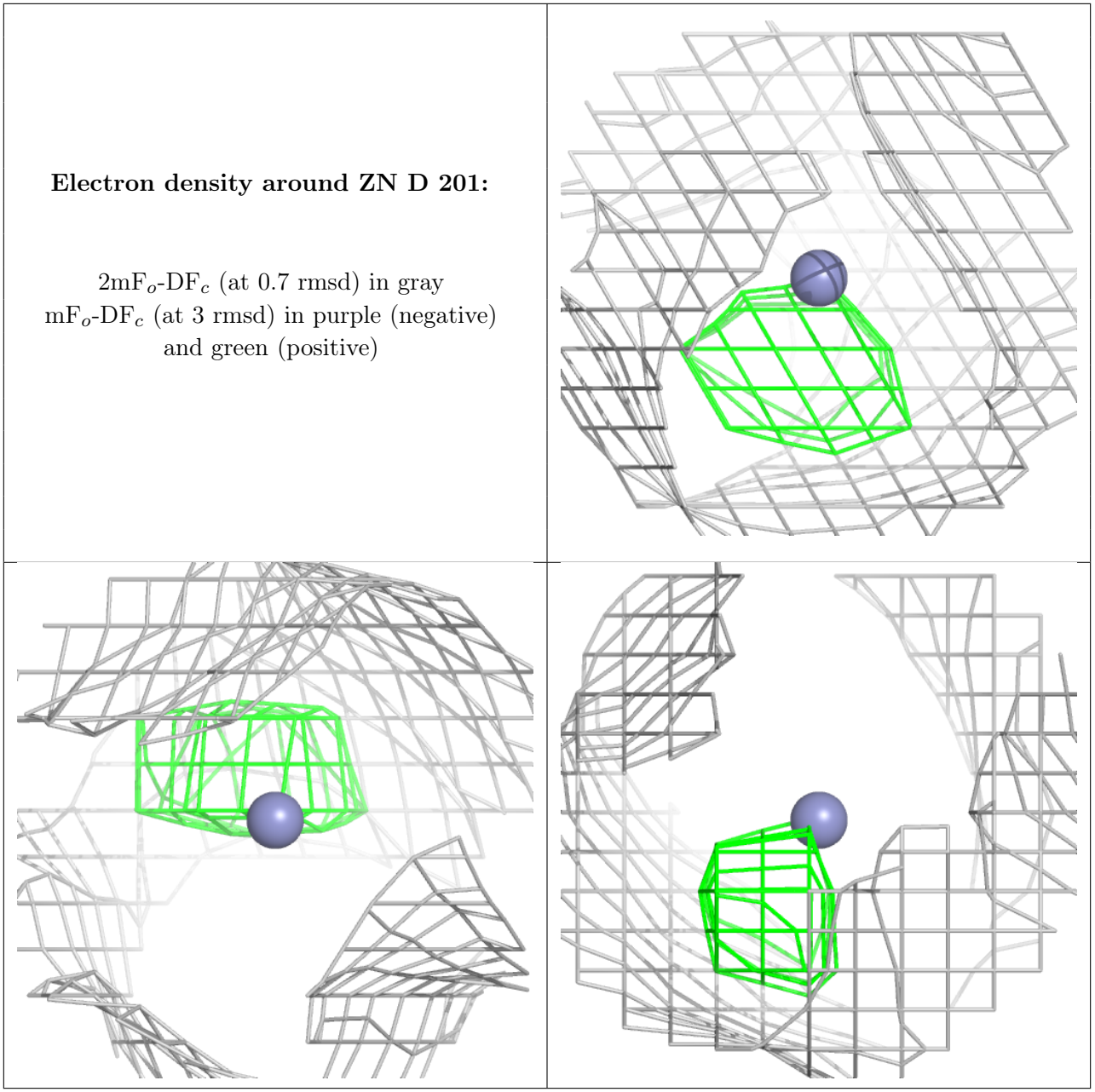
Electron density around ZN C 201:

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



Electron density around ZN D 201:

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



6.5 Other polymers

There are no such residues in this entry.