Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 08:18 PM EDT

PDB ID	:	8E2S
Title	:	Crystal structure of TadAC-1.19
Authors	:	Feliciano, P.R.; Lee, S.J.; Ciaramella, G.
Deposited on	:	2022-08-15
Resolution	:	2.95 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:

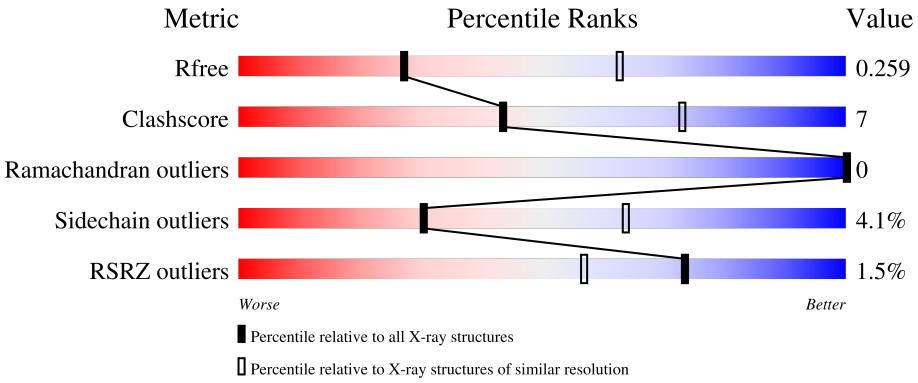
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	2% 77% 14% 8%
1	B	167	70% 20% 10%
1	C	167	66% 22% 10%
1	D	167	71% 16% 13%
1	E	167	79% 13% 7%

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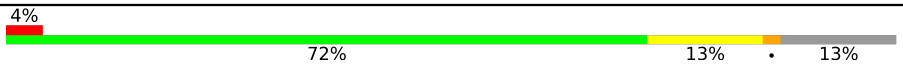
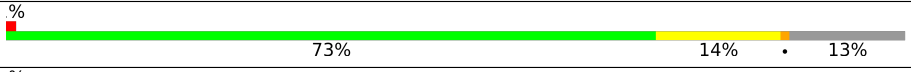
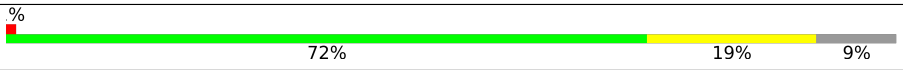
Mol	Chain	Length	Quality of chain
1	F	167	
1	G	167	
1	H	167	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9113 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 1.19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1153	723	216	203	11			
1	B	151	Total	C	N	O	S	0	1	0
			1158	724	216	206	12			
1	C	150	Total	C	N	O	S	0	3	0
			1166	731	224	199	12			
1	D	146	Total	C	N	O	S	0	1	0
			1116	704	205	196	11			
1	E	155	Total	C	N	O	S	0	0	0
			1131	711	208	201	11			
1	F	146	Total	C	N	O	S	0	0	0
			1107	695	206	195	11			
1	G	146	Total	C	N	O	S	0	0	0
			1083	677	200	195	11			
1	H	152	Total	C	N	O	S	0	1	0
			1142	718	211	202	11			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	TRP	conflict	UNP W8T8U5
A	27	GLY	GLU	conflict	UNP W8T8U5
A	36	LEU	HIS	conflict	UNP W8T8U5
A	48	ALA	PRO	conflict	UNP W8T8U5
A	49	ASN	ILE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	27	GLY	GLU	conflict	UNP W8T8U5
B	36	LEU	HIS	conflict	UNP W8T8U5
B	48	ALA	PRO	conflict	UNP W8T8U5
B	49	ASN	ILE	conflict	UNP W8T8U5
B	51	LEU	ARG	conflict	UNP W8T8U5
B	76	TYR	ILE	conflict	UNP W8T8U5
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	27	GLY	GLU	conflict	UNP W8T8U5
C	36	LEU	HIS	conflict	UNP W8T8U5
C	48	ALA	PRO	conflict	UNP W8T8U5
C	49	ASN	ILE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	27	GLY	GLU	conflict	UNP W8T8U5
D	36	LEU	HIS	conflict	UNP W8T8U5
D	48	ALA	PRO	conflict	UNP W8T8U5
D	49	ASN	ILE	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
D	157	ASN	LYS	conflict	UNP W8T8U5
E	23	ARG	TRP	conflict	UNP W8T8U5
E	27	GLY	GLU	conflict	UNP W8T8U5
E	36	LEU	HIS	conflict	UNP W8T8U5
E	48	ALA	PRO	conflict	UNP W8T8U5
E	49	ASN	ILE	conflict	UNP W8T8U5
E	51	LEU	ARG	conflict	UNP W8T8U5
E	76	TYR	ILE	conflict	UNP W8T8U5
E	82	SER	VAL	conflict	UNP W8T8U5
E	84	PHE	LEU	conflict	UNP W8T8U5
E	106	VAL	ALA	conflict	UNP W8T8U5
E	108	ASN	ASP	conflict	UNP W8T8U5
E	146	CYS	SER	conflict	UNP W8T8U5
E	147	ARG	ASP	conflict	UNP W8T8U5
E	152	PRO	ARG	conflict	UNP W8T8U5
E	154	ARG	GLN	conflict	UNP W8T8U5
E	155	VAL	GLU	conflict	UNP W8T8U5
E	156	PHE	ILE	conflict	UNP W8T8U5
E	157	ASN	LYS	conflict	UNP W8T8U5
F	23	ARG	TRP	conflict	UNP W8T8U5
F	27	GLY	GLU	conflict	UNP W8T8U5
F	36	LEU	HIS	conflict	UNP W8T8U5
F	48	ALA	PRO	conflict	UNP W8T8U5
F	49	ASN	ILE	conflict	UNP W8T8U5
F	51	LEU	ARG	conflict	UNP W8T8U5
F	76	TYR	ILE	conflict	UNP W8T8U5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	82	SER	VAL	conflict	UNP W8T8U5
F	84	PHE	LEU	conflict	UNP W8T8U5
F	106	VAL	ALA	conflict	UNP W8T8U5
F	108	ASN	ASP	conflict	UNP W8T8U5
F	146	CYS	SER	conflict	UNP W8T8U5
F	147	ARG	ASP	conflict	UNP W8T8U5
F	152	PRO	ARG	conflict	UNP W8T8U5
F	154	ARG	GLN	conflict	UNP W8T8U5
F	155	VAL	GLU	conflict	UNP W8T8U5
F	156	PHE	ILE	conflict	UNP W8T8U5
F	157	ASN	LYS	conflict	UNP W8T8U5
G	23	ARG	TRP	conflict	UNP W8T8U5
G	27	GLY	GLU	conflict	UNP W8T8U5
G	36	LEU	HIS	conflict	UNP W8T8U5
G	48	ALA	PRO	conflict	UNP W8T8U5
G	49	ASN	ILE	conflict	UNP W8T8U5
G	51	LEU	ARG	conflict	UNP W8T8U5
G	76	TYR	ILE	conflict	UNP W8T8U5
G	82	SER	VAL	conflict	UNP W8T8U5
G	84	PHE	LEU	conflict	UNP W8T8U5
G	106	VAL	ALA	conflict	UNP W8T8U5
G	108	ASN	ASP	conflict	UNP W8T8U5
G	146	CYS	SER	conflict	UNP W8T8U5
G	147	ARG	ASP	conflict	UNP W8T8U5
G	152	PRO	ARG	conflict	UNP W8T8U5
G	154	ARG	GLN	conflict	UNP W8T8U5
G	155	VAL	GLU	conflict	UNP W8T8U5
G	156	PHE	ILE	conflict	UNP W8T8U5
G	157	ASN	LYS	conflict	UNP W8T8U5
H	23	ARG	TRP	conflict	UNP W8T8U5
H	27	GLY	GLU	conflict	UNP W8T8U5
H	36	LEU	HIS	conflict	UNP W8T8U5
H	48	ALA	PRO	conflict	UNP W8T8U5
H	49	ASN	ILE	conflict	UNP W8T8U5
H	51	LEU	ARG	conflict	UNP W8T8U5
H	76	TYR	ILE	conflict	UNP W8T8U5
H	82	SER	VAL	conflict	UNP W8T8U5
H	84	PHE	LEU	conflict	UNP W8T8U5
H	106	VAL	ALA	conflict	UNP W8T8U5
H	108	ASN	ASP	conflict	UNP W8T8U5
H	146	CYS	SER	conflict	UNP W8T8U5
H	147	ARG	ASP	conflict	UNP W8T8U5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	152	PRO	ARG	conflict	UNP W8T8U5
H	154	ARG	GLN	conflict	UNP W8T8U5
H	155	VAL	GLU	conflict	UNP W8T8U5
H	156	PHE	ILE	conflict	UNP W8T8U5
H	157	ASN	LYS	conflict	UNP W8T8U5

- 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
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	13	Total O 13 13	0	0
3	C	4	Total O 4 4	0	0
3	D	6	Total O 6 6	0	0
3	E	2	Total O 2 2	0	0
3	F	5	Total O 5 5	0	0

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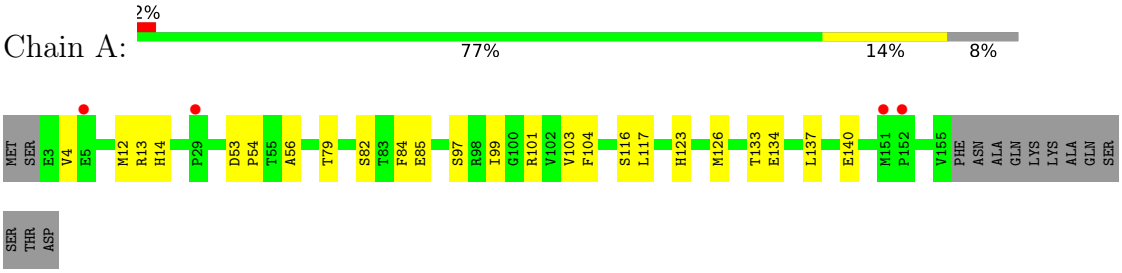
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	9	Total O 9 9	0	0
3	H	5	Total O 5 5	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

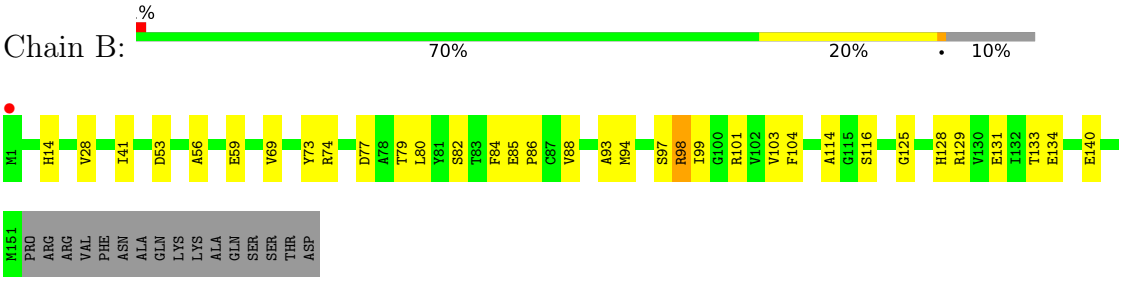
• Molecule 1: tRNA-specific adenosine deaminase 1.19

Chain A:



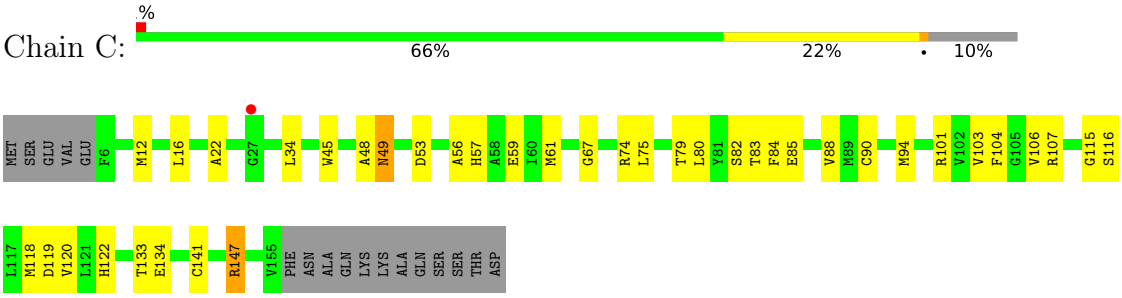
• Molecule 1: tRNA-specific adenosine deaminase 1.19

Chain B:



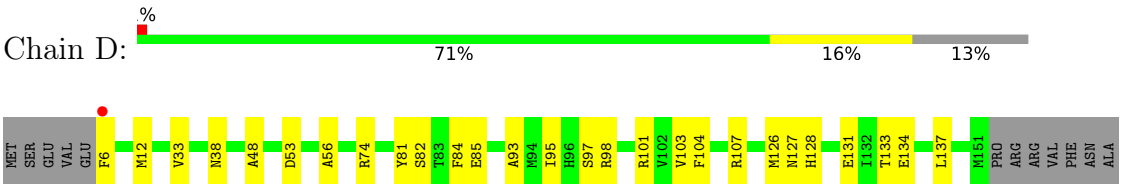
• Molecule 1: tRNA-specific adenosine deaminase 1.19

Chain C:



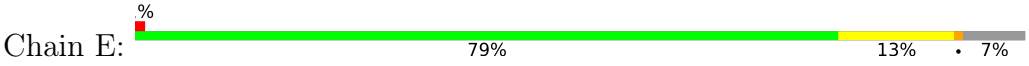
• Molecule 1: tRNA-specific adenosine deaminase 1.19

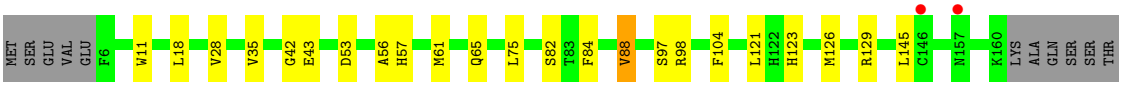
Chain D:



• Molecule 1: tRNA-specific adenosine deaminase 1.19

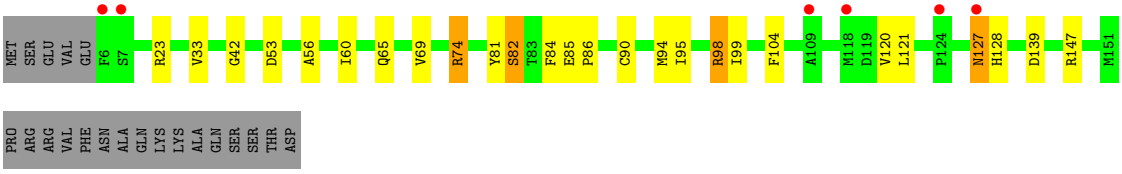
Chain E:





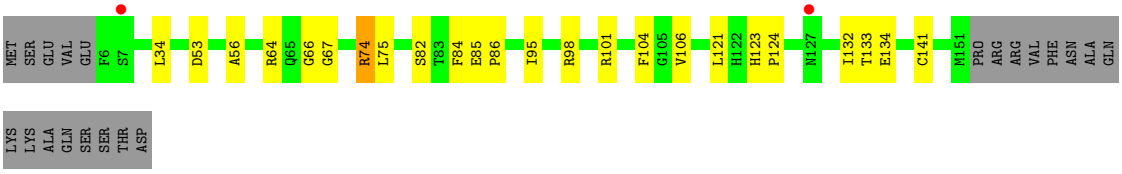
• Molecule 1: tRNA-specific adenosine deaminase 1.19

Chain F:



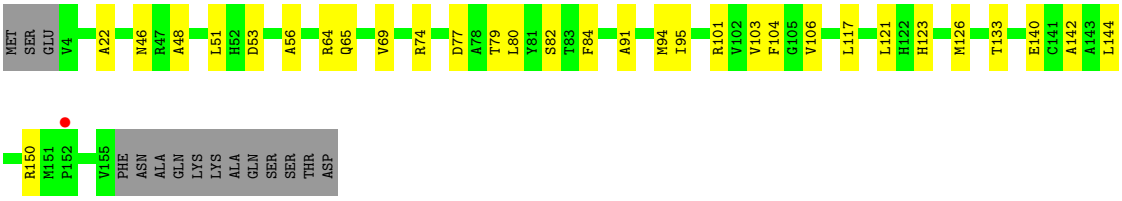
• Molecule 1: tRNA-specific adenosine deaminase 1.19

Chain G:



• Molecule 1: tRNA-specific adenosine deaminase 1.19

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.49Å 63.40Å 95.17Å 87.89° 82.82° 77.14°	Depositor
Resolution (Å)	51.49 – 2.95 51.49 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.0 (51.49-2.95) 97.0 (51.49-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.261 0.219 , 0.259	Depositor DCC
R_{free} test set	1363 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	1.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9113	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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

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	0.23	0/1177	0.49	0/1597
1	B	0.27	0/1182	0.52	0/1600
1	C	0.24	0/1191	0.51	0/1613
1	D	0.24	0/1140	0.50	0/1544
1	E	0.25	0/1155	0.50	0/1573
1	F	0.26	0/1131	0.50	0/1534
1	G	0.26	0/1105	0.50	0/1502
1	H	0.27	0/1166	0.54	0/1584
All	All	0.25	0/9247	0.51	0/12547

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	1153	0	1111	13	0
1	B	1158	0	1115	17	0
1	C	1166	0	1127	22	0
1	D	1116	0	1075	15	0
1	E	1131	0	1059	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1107	0	1063	15	0
1	G	1083	0	1027	14	0
1	H	1142	0	1092	17	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
3	A	5	0	0	0	0
3	B	13	0	0	0	0
3	C	4	0	0	0	0
3	D	6	0	0	0	0
3	E	2	0	0	0	0
3	F	5	0	0	0	0
3	G	9	0	0	0	0
3	H	5	0	0	0	0
All	All	9113	0	8669	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (118) 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:F:74:ARG:HD3	1:F:98:ARG:HG3	1.75	0.69
1:E:88:VAL:HG21	1:F:120:VAL:HG21	1.77	0.66
1:B:74:ARG:HD3	1:B:98:ARG:HG3	1.76	0.66
1:G:95:ILE:HD11	1:G:121:LEU:HA	1.78	0.65
1:F:95:ILE:HD11	1:F:121:LEU:HA	1.80	0.63
1:D:98:ARG:NH2	1:D:128:HIS:HB2	2.16	0.61
1:A:53:ASP:HB3	1:A:56:ALA:HB2	1.82	0.60
1:F:98:ARG:NH1	1:F:128:HIS:HB2	2.17	0.60
1:G:123:HIS:HE1	1:H:117:LEU:HD11	1.64	0.59
1:C:53:ASP:HB3	1:C:56:ALA:HB2	1.84	0.59
1:C:57:HIS:O	1:C:61:MET:HG2	2.02	0.59
1:G:74:ARG:HD3	1:G:98:ARG:HG3	1.83	0.59
1:D:12:MET:HB3	1:D:137:LEU:HD12	1.85	0.58
1:E:53:ASP:HB3	1:E:56:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:THR:HG23	1:C:101:ARG:HB3	1.87	0.57
1:C:118:MET:HG3	1:C:120:VAL:HG13	1.85	0.57
1:F:23:ARG:O	1:F:147:ARG:NH2	2.37	0.57
1:A:101:ARG:NH1	1:A:133:THR:OG1	2.38	0.57
1:B:129:ARG:NH1	1:B:131:GLU:OE2	2.39	0.56
1:B:79:THR:HG23	1:B:101:ARG:HB3	1.87	0.55
1:B:53:ASP:HB3	1:B:56:ALA:HB2	1.88	0.54
1:H:95:ILE:HD11	1:H:121:LEU:HA	1.89	0.54
1:B:41:ILE:HB	1:B:69:VAL:HG21	1.90	0.54
1:F:82:SER:O	1:F:104:PHE:HA	2.08	0.54
1:H:53:ASP:HB3	1:H:56:ALA:HB2	1.91	0.53
1:B:85:GLU:HG3	1:B:114:ALA:HB3	1.90	0.53
1:E:18:LEU:HD21	1:E:43:GLU:HB3	1.89	0.53
1:H:79:THR:HG23	1:H:101:ARG:HB3	1.91	0.52
1:D:33:VAL:HG12	1:D:81:TYR:HB2	1.90	0.52
1:G:82:SER:O	1:G:104:PHE:HA	2.10	0.51
1:H:82:SER:O	1:H:104:PHE:HA	2.10	0.51
1:C:106:VAL:HG23	1:C:141:CYS:HB2	1.92	0.51
1:H:106:VAL:HG11	1:H:142:ALA:HB2	1.92	0.51
1:E:42:GLY:HA2	1:E:65:GLN:HG2	1.92	0.51
1:G:101:ARG:NH1	1:G:133:THR:OG1	2.43	0.51
1:G:67:GLY:HA2	1:G:75:LEU:HD21	1.91	0.51
1:D:53:ASP:HB3	1:D:56:ALA:HB2	1.93	0.51
1:G:53:ASP:HB3	1:G:56:ALA:HB2	1.93	0.51
1:A:82:SER:O	1:A:104:PHE:HA	2.10	0.50
1:B:82:SER:O	1:B:104:PHE:HA	2.11	0.50
1:F:85:GLU:HG2	1:F:86:PRO:HD2	1.93	0.50
1:A:12:MET:HB3	1:A:137:LEU:HD22	1.94	0.50
1:H:65:GLN:O	1:H:69:VAL:HG23	2.12	0.50
1:C:59:GLU:HB3	1:C:80:LEU:HD21	1.93	0.50
1:C:82:SER:O	1:C:104:PHE:HA	2.11	0.50
1:E:75:LEU:HD12	1:E:97:SER:HB2	1.94	0.50
1:A:117:LEU:HD11	1:B:125:GLY:HA3	1.93	0.49
1:C:85:GLU:OE1	1:C:116:SER:OG	2.22	0.49
1:F:53:ASP:HB3	1:F:56:ALA:HB2	1.93	0.49
1:D:103:VAL:HG13	1:D:133:THR:HB	1.94	0.48
1:A:79:THR:HG23	1:A:101:ARG:HB3	1.95	0.48
1:B:59:GLU:HB3	1:B:80:LEU:HD21	1.94	0.48
1:E:57:HIS:O	1:E:61:MET:HG2	2.13	0.48
1:D:98:ARG:HH21	1:D:128:HIS:HB2	1.76	0.48
1:D:82:SER:O	1:D:104:PHE:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:LEU:HD23	1:G:66:GLY:HA3	1.96	0.48
1:C:104:PHE:O	1:C:134:GLU:HA	2.15	0.47
1:F:98:ARG:HH12	1:F:127:ASN:HB2	1.80	0.47
1:C:67:GLY:HA2	1:C:75:LEU:HD21	1.96	0.47
1:D:107:ARG:HD3	1:D:134:GLU:OE1	2.15	0.47
1:E:82:SER:O	1:E:104:PHE:HA	2.14	0.47
1:F:65:GLN:O	1:F:69:VAL:HG23	2.14	0.47
1:D:95:ILE:HD13	1:D:126:MET:SD	2.55	0.46
1:D:74:ARG:CZ	1:D:98:ARG:HD2	2.46	0.46
1:E:123:HIS:HB3	1:E:126:MET:HG2	1.97	0.46
1:H:123:HIS:HB3	1:H:126:MET:HG2	1.98	0.46
1:G:34:LEU:HD21	1:G:75:LEU:HD13	1.98	0.46
1:C:147:ARG:HE	1:C:147:ARG:HB2	1.69	0.45
1:F:98:ARG:HH22	1:F:127:ASN:HB2	1.80	0.45
1:H:91:ALA:HA	1:H:94:MET:HG3	1.99	0.45
1:C:34:LEU:HD21	1:C:75:LEU:HD13	1.98	0.45
1:A:13:ARG:NH1	1:A:140:GLU:OE1	2.47	0.45
1:A:54:PRO:HA	1:B:73:TYR:HD2	1.82	0.45
1:H:48:ALA:HA	1:H:56:ALA:HB3	1.98	0.45
1:A:104:PHE:O	1:A:134:GLU:HA	2.18	0.44
1:C:16:LEU:HD22	1:C:83:THR:HG22	2.00	0.44
1:C:119:ASP:OD2	1:C:122:HIS:HB2	2.18	0.44
1:G:106:VAL:HG22	1:G:141:CYS:HB3	1.99	0.44
1:B:94:MET:HB3	1:B:99:ILE:HD11	1.98	0.44
1:G:85:GLU:HG2	1:G:86:PRO:HD2	2.00	0.44
1:C:49:ASN:O	1:C:49:ASN:ND2	2.49	0.44
1:H:103:VAL:HG22	1:H:133:THR:HB	1.99	0.44
1:C:22:ALA:HB2	1:C:45:TRP:HB2	2.01	0.43
1:C:74:ARG:NH1	1:H:77:ASP:OD1	2.51	0.43
1:C:103:VAL:HG22	1:C:133:THR:HB	2.00	0.43
1:F:94:MET:HB3	1:F:99:ILE:HD11	2.00	0.43
1:C:85:GLU:HB2	1:C:107:ARG:HA	2.01	0.43
1:D:6:PHE:HD2	1:D:38:ASN:HB3	1.83	0.43
1:F:42:GLY:HA2	1:F:65:GLN:OE1	2.18	0.43
1:G:121:LEU:HD12	1:G:132:ILE:HD11	2.00	0.43
1:G:64:ARG:HH12	1:H:64:ARG:CD	2.32	0.43
1:A:123:HIS:HB3	1:A:126:MET:HG2	2.01	0.42
1:B:93:ALA:O	1:B:97:SER:OG	2.31	0.42
1:E:28:VAL:HG13	1:E:145:LEU:HA	2.02	0.42
1:B:103:VAL:HA	1:B:133:THR:O	2.19	0.42
1:A:97:SER:HB2	1:A:99:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:LEU:HD23	1:H:144:LEU:HA	1.87	0.42
1:D:85:GLU:HB2	1:D:107:ARG:HA	2.02	0.42
1:A:103:VAL:HG22	1:A:133:THR:HB	2.02	0.41
1:A:85:GLU:OE1	1:A:116:SER:OG	2.28	0.41
1:D:48:ALA:HA	1:D:56:ALA:HB3	2.03	0.41
1:B:86:PRO:HB3	1:B:94:MET:HE1	2.02	0.41
1:C:90:CYS:O	1:C:94:MET:HG3	2.20	0.41
1:E:121:LEU:O	1:E:129:ARG:HA	2.20	0.41
1:H:51:LEU:HD23	1:H:51:LEU:O	2.21	0.41
1:F:90:CYS:O	1:F:94:MET:HG3	2.21	0.41
1:B:98:ARG:HA	1:B:128:HIS:CD2	2.56	0.41
1:H:22:ALA:HB1	1:H:46:ASN:HB2	2.03	0.41
1:C:48:ALA:HA	1:C:56:ALA:HB3	2.02	0.41
1:D:101:ARG:HG3	1:D:131:GLU:HB2	2.03	0.41
1:D:93:ALA:O	1:D:97:SER:OG	2.29	0.41
1:G:123:HIS:HA	1:G:124:PRO:HD3	1.90	0.41
1:H:103:VAL:HA	1:H:133:THR:O	2.21	0.40
1:B:104:PHE:CZ	1:B:134:GLU:HB3	2.56	0.40
1:B:104:PHE:O	1:B:134:GLU:HA	2.22	0.40
1:E:11:TRP:CD2	1:E:35:VAL:HG21	2.56	0.40
1:C:115:GLY:N	1:C:118:MET:O	2.52	0.40
1:F:33:VAL:HG13	1:F:81:TYR:HB2	2.03	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	151/167 (90%)	146 (97%)	5 (3%)	0	100	100
1	B	150/167 (90%)	145 (97%)	5 (3%)	0	100	100
1	C	151/167 (90%)	146 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	145/167 (87%)	139 (96%)	6 (4%)	0	100	100
1	E	153/167 (92%)	143 (94%)	10 (6%)	0	100	100
1	F	144/167 (86%)	139 (96%)	5 (4%)	0	100	100
1	G	144/167 (86%)	138 (96%)	6 (4%)	0	100	100
1	H	151/167 (90%)	144 (95%)	7 (5%)	0	100	100
All	All	1189/1336 (89%)	1140 (96%)	49 (4%)	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	113/134 (84%)	110 (97%)	3 (3%)	44	74
1	B	115/134 (86%)	106 (92%)	9 (8%)	12	38
1	C	114/134 (85%)	109 (96%)	5 (4%)	28	62
1	D	109/134 (81%)	107 (98%)	2 (2%)	59	82
1	E	106/134 (79%)	103 (97%)	3 (3%)	43	74
1	F	109/134 (81%)	102 (94%)	7 (6%)	17	47
1	G	105/134 (78%)	102 (97%)	3 (3%)	42	73
1	H	111/134 (83%)	105 (95%)	6 (5%)	22	54
All	All	882/1072 (82%)	844 (96%)	38 (4%)	30	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	14	HIS
1	A	84	PHE
1	B	14	HIS
1	B	28	VAL

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Mol	Chain	Res	Type
1	B	77	ASP
1	B	84	PHE
1	B	88	VAL
1	B	98	ARG
1	B	116	SER
1	B	140[A]	GLU
1	B	140[B]	GLU
1	C	12	MET
1	C	49	ASN
1	C	84	PHE
1	C	88	VAL
1	C	147	ARG
1	D	84	PHE
1	D	127	ASN
1	E	84	PHE
1	E	88	VAL
1	E	98	ARG
1	F	60	ILE
1	F	74	ARG
1	F	82	SER
1	F	84	PHE
1	F	98	ARG
1	F	127	ASN
1	F	139	ASP
1	G	74	ARG
1	G	84	PHE
1	G	134	GLU
1	H	74	ARG
1	H	80[A]	LEU
1	H	80[B]	LEU
1	H	84	PHE
1	H	140	GLU
1	H	150	ARG

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

Mol	Chain	Res	Type
1	B	127	ASN
1	D	38	ASN
1	G	123	HIS
1	H	52	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	153/167 (91%)	-0.15	4 (2%)	56	39	18, 28, 47, 64	0
1	B	151/167 (90%)	-0.16	1 (0%)	87	76	18, 29, 45, 56	0
1	C	150/167 (89%)	0.00	1 (0%)	87	76	21, 32, 46, 59	0
1	D	146/167 (87%)	-0.14	1 (0%)	87	76	18, 28, 42, 51	0
1	E	155/167 (92%)	0.02	2 (1%)	77	61	22, 32, 51, 63	0
1	F	146/167 (87%)	0.16	6 (4%)	37	24	24, 37, 50, 60	0
1	G	146/167 (87%)	-0.07	2 (1%)	75	59	23, 32, 48, 81	0
1	H	152/167 (91%)	-0.10	1 (0%)	87	76	20, 30, 47, 79	0
All	All	1199/1336 (89%)	-0.05	18 (1%)	73	57	18, 31, 49, 81	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	157	ASN	4.0
1	A	151	MET	3.7
1	H	152	PRO	3.2
1	F	6	PHE	3.2
1	C	27	GLY	3.0
1	A	152	PRO	2.7
1	B	1	MET	2.5
1	D	6	PHE	2.4
1	A	29	PRO	2.4
1	F	7	SER	2.4
1	G	127	ASN	2.4
1	F	124	PRO	2.2
1	A	5	GLU	2.2
1	E	146	CYS	2.1
1	G	7	SER	2.1
1	F	109	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	127	ASN	2.0
1	F	118	MET	2.0

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)

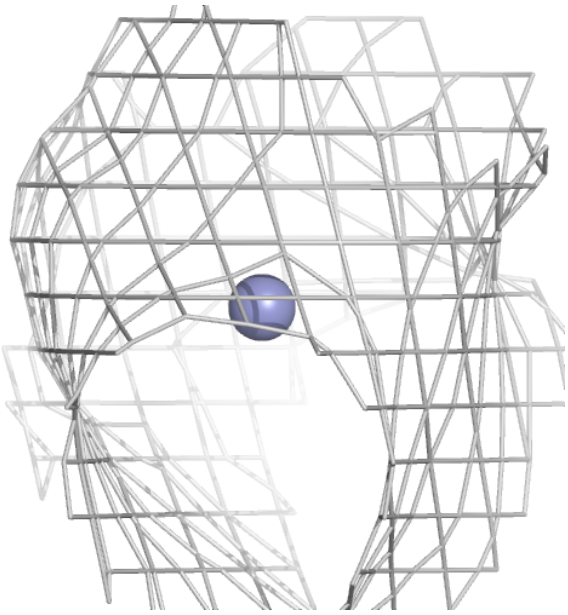
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

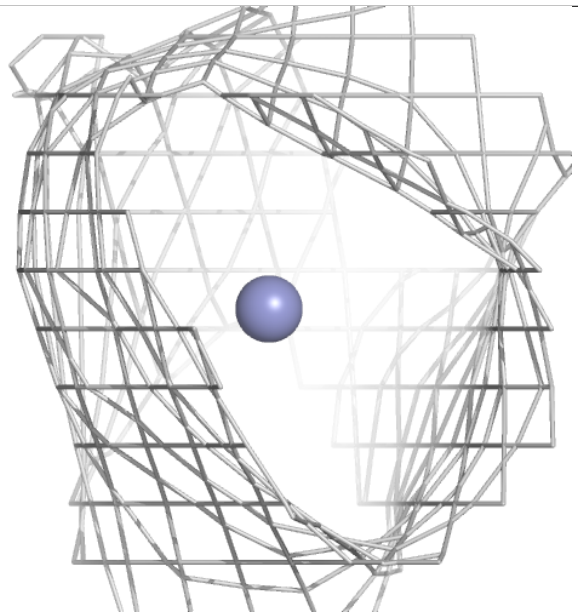
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	201	1/1	0.98	0.10	26,26,26,26	0
2	ZN	C	201	1/1	0.98	0.12	31,31,31,31	0
2	ZN	A	201	1/1	0.99	0.06	31,31,31,31	0
2	ZN	D	201	1/1	0.99	0.09	26,26,26,26	0
2	ZN	E	201	1/1	0.99	0.09	26,26,26,26	0
2	ZN	F	201	1/1	0.99	0.08	33,33,33,33	0
2	ZN	G	201	1/1	0.99	0.08	22,22,22,22	0
2	ZN	H	201	1/1	0.99	0.06	21,21,21,21	0

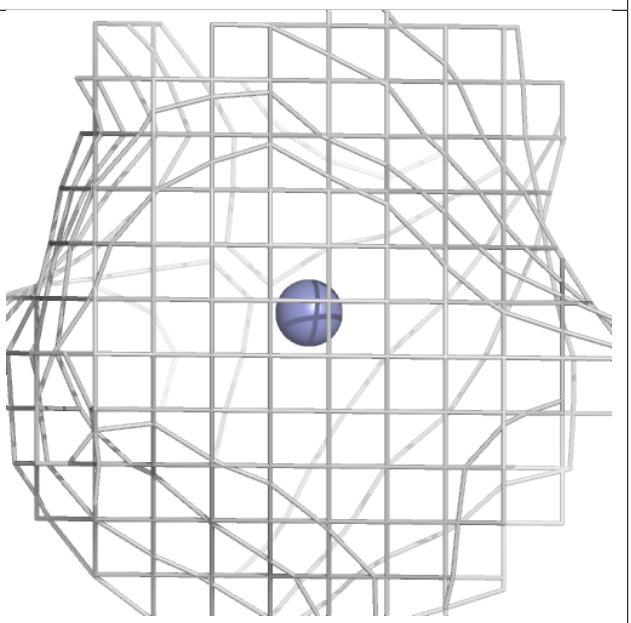
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

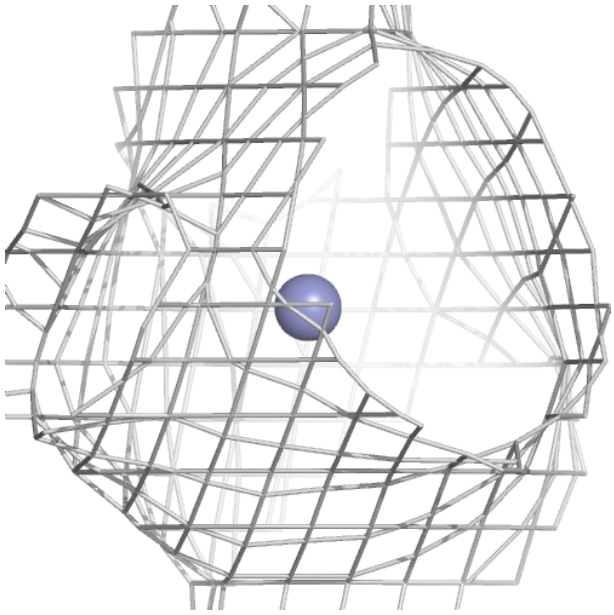


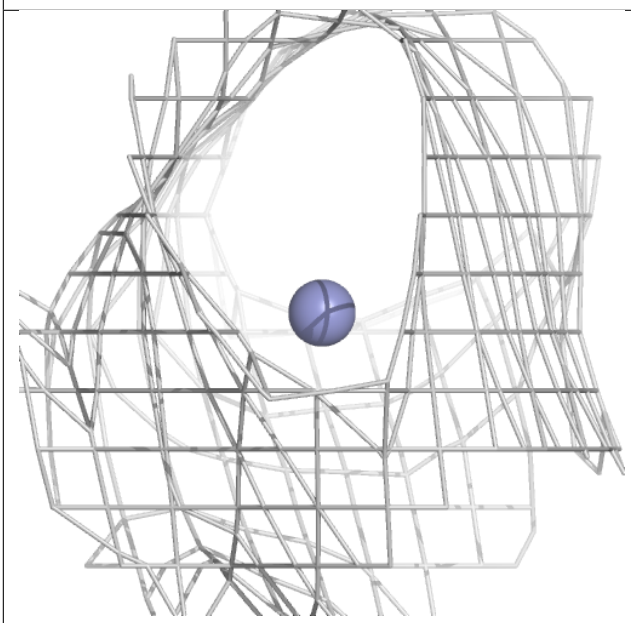


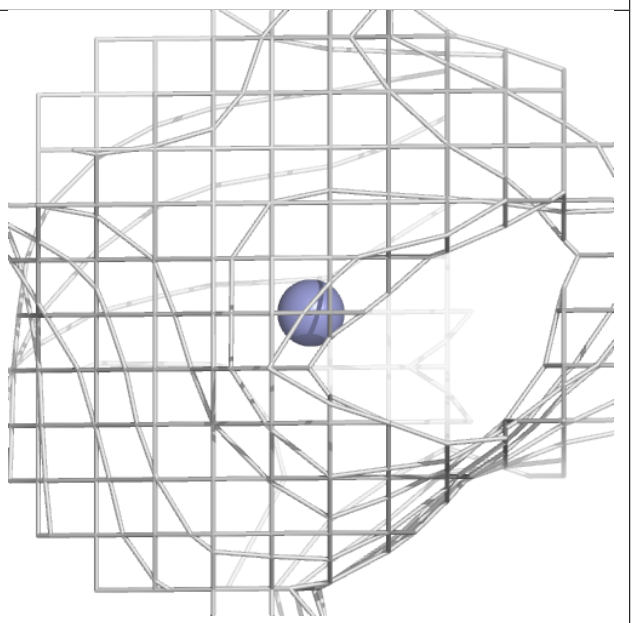


Electron density around ZN C 201:

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

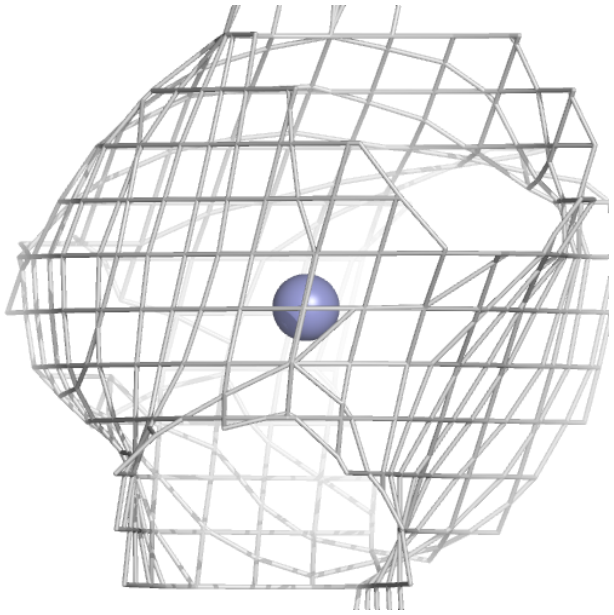


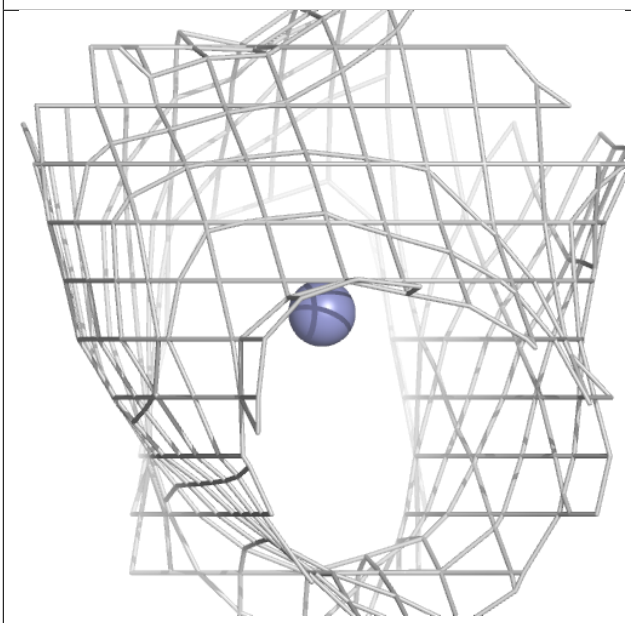


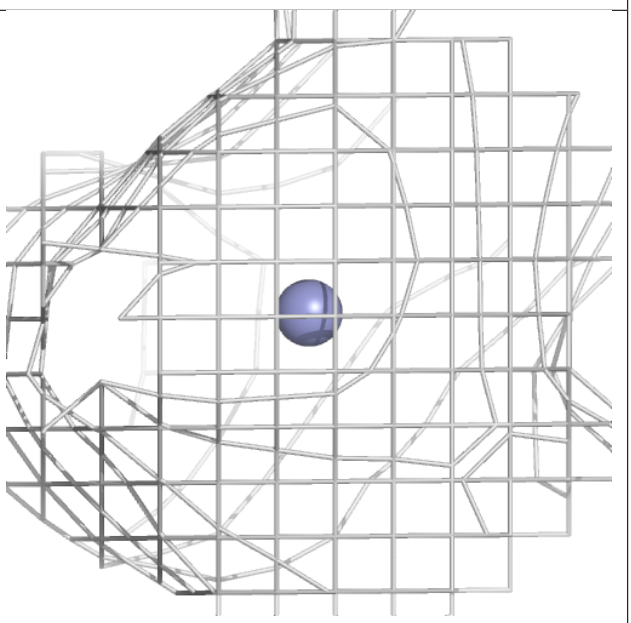


Electron density around ZN A 201:

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

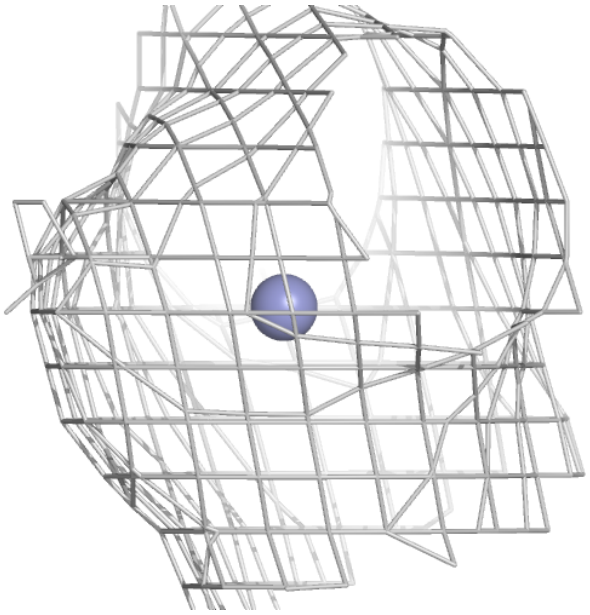


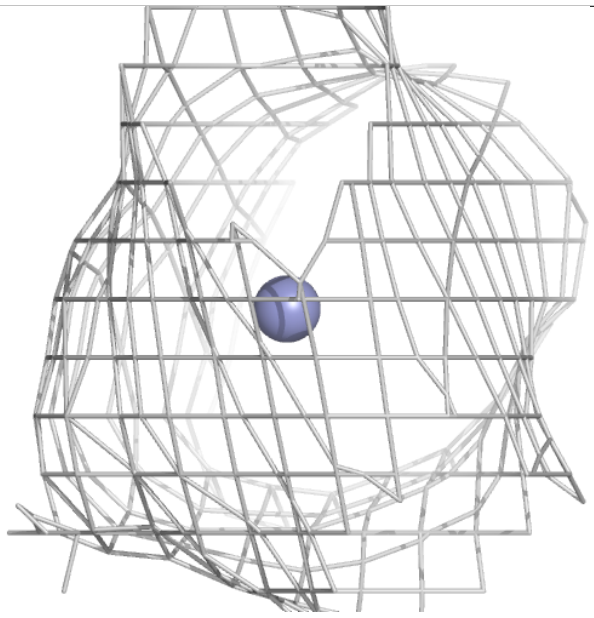


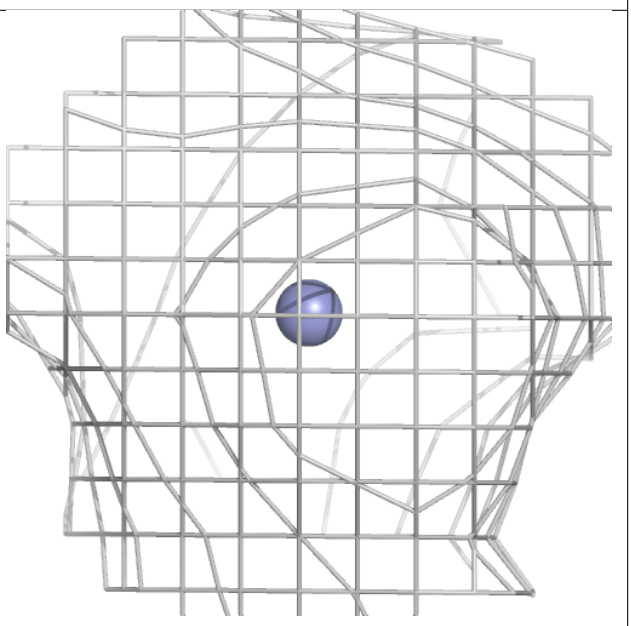


Electron density around ZN D 201:

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

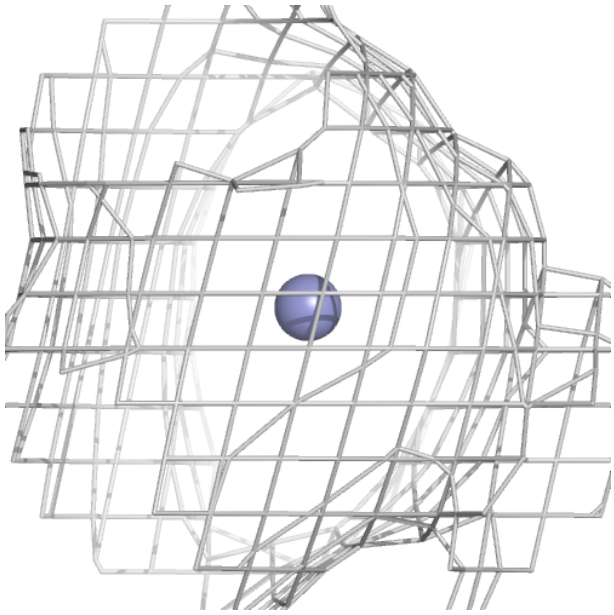


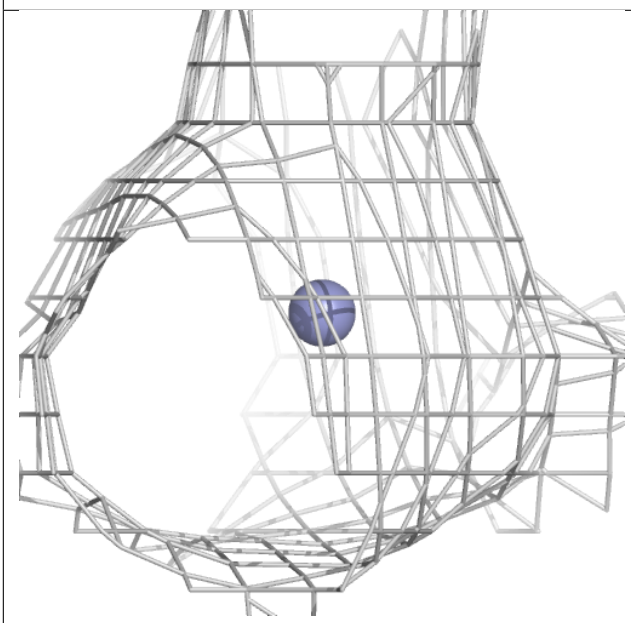




Electron density around ZN E 201:

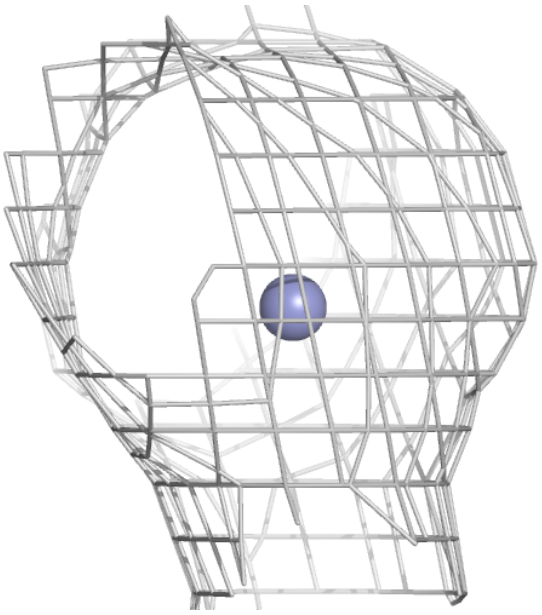
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

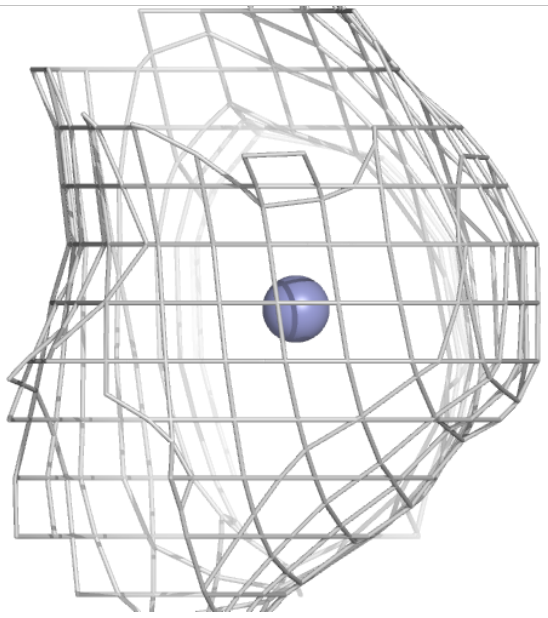


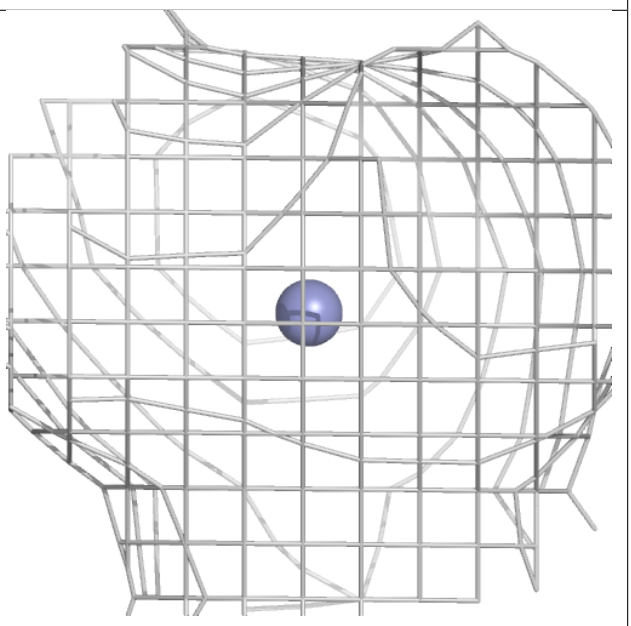


Electron density around ZN F 201:

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

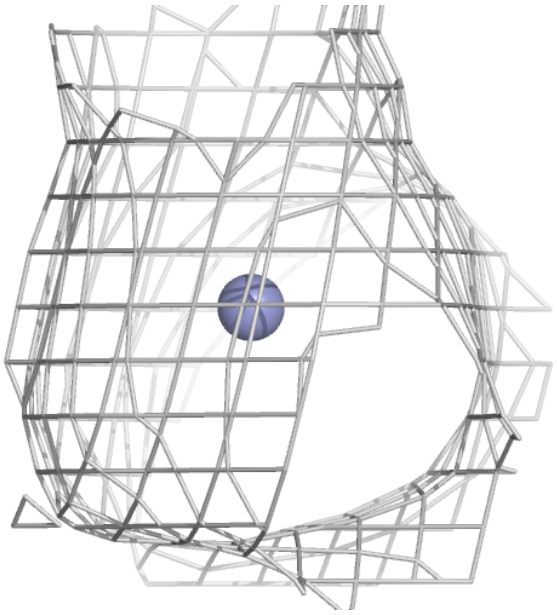


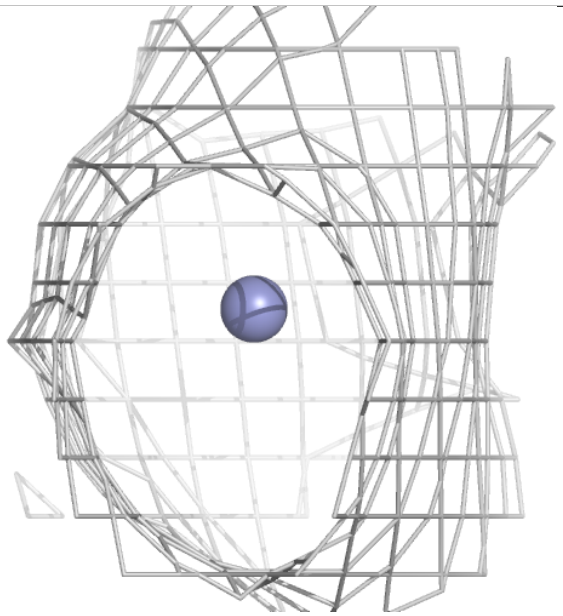


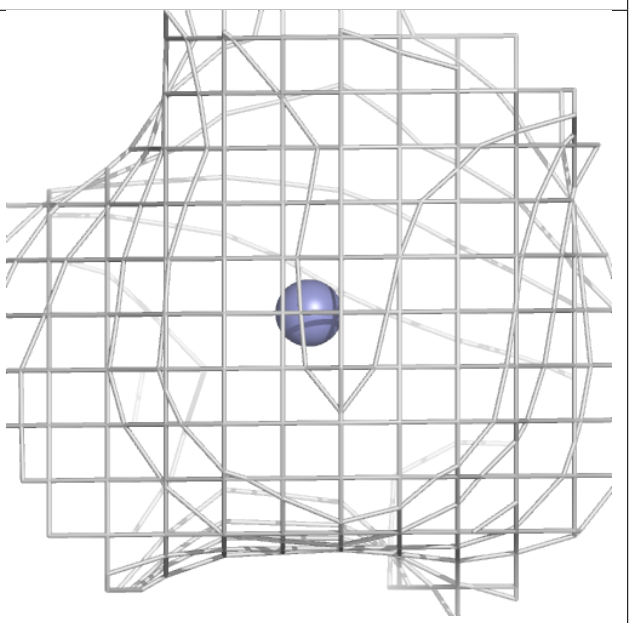


Electron density around ZN G 201:

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

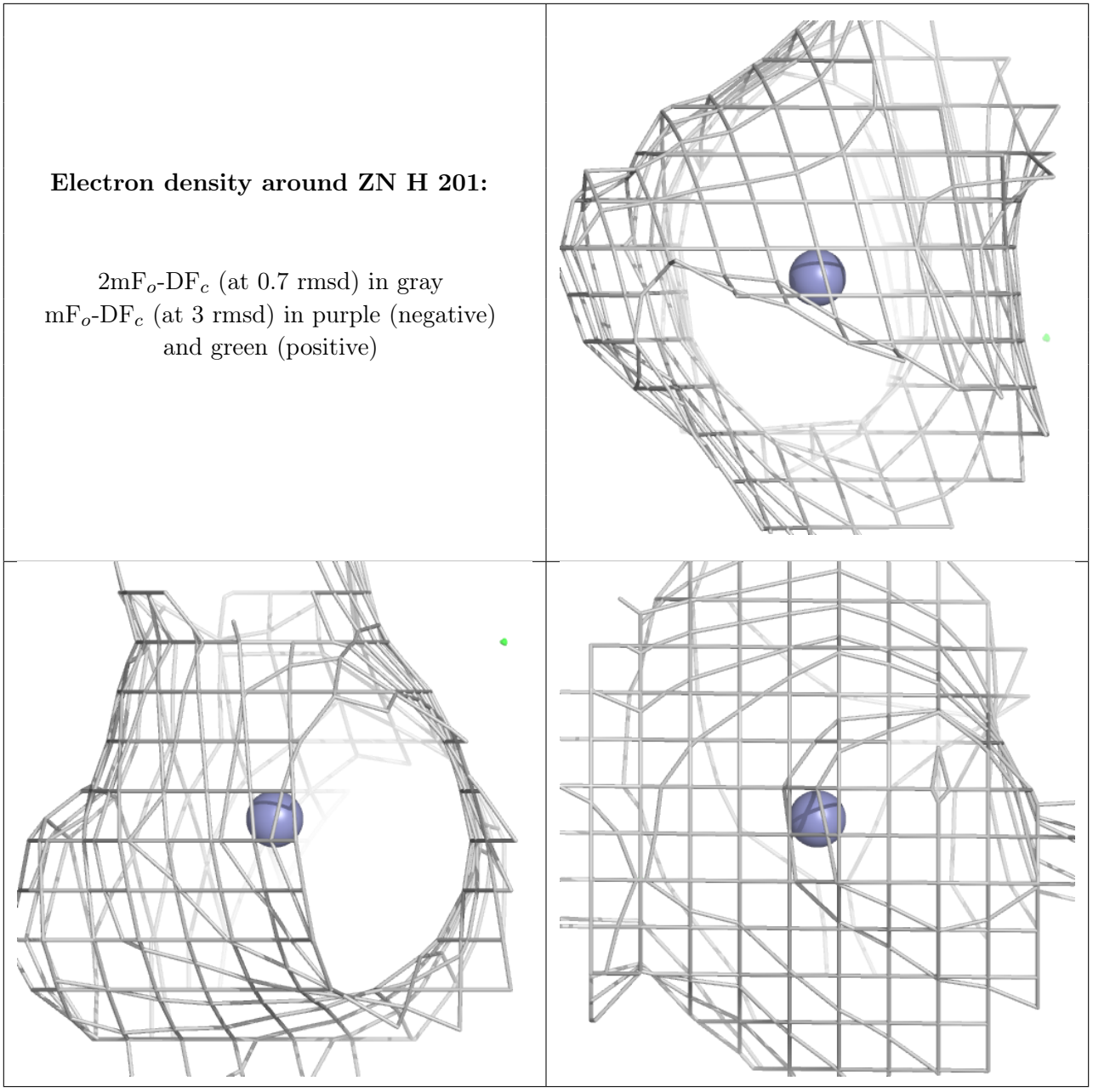






Electron density around ZN H 201:

$2mF_o$-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.