



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:01 AM UTC

PDB ID : 9P8Z / pdb_00009p8z
Title : Crystal Structure of GTP cyclohydrolase 1 (FolE) from Mycobacterium tuberculosis
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-06-23
Resolution : 2.74 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

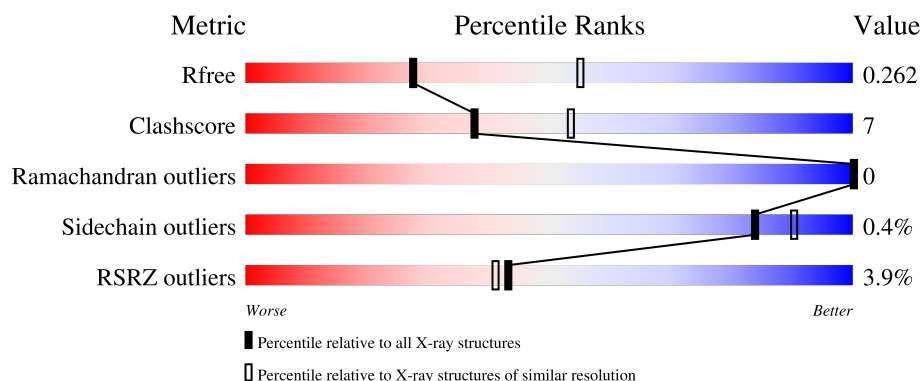
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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 $\leq 5\%$. 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	223	
1	B	223	
1	C	223	
1	D	223	
1	E	223	

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Mol	Chain	Length	Quality of chain
1	F	223	3% 68% 16% 16%
1	G	223	2% 73% 10% 16%
1	H	223	% 70% 15% 15%
1	I	223	4% 68% 17% 15%
1	J	223	2% 72% 13% 15%
1	K	223	3% 70% 14% 16%
1	L	223	5% 66% 17% 17%
1	M	223	2% 72% 12% 17%
1	N	223	2% 77% 9% 15%
1	O	223	4% 70% 13% 17%
1	P	223	2% 70% 14% 16%
1	Q	223	2% 78% 6% 16%
1	R	223	9% 70% 13% 17%
1	S	223	5% 68% 16% 16%
1	T	223	% 74% 11% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29166 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 GTP cyclohydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1450	907	260	275	8			
1	B	189	Total	C	N	O	S	0	0	0
			1469	919	266	276	8			
1	C	189	Total	C	N	O	S	0	0	0
			1461	916	261	276	8			
1	D	189	Total	C	N	O	S	0	0	0
			1467	919	264	276	8			
1	E	189	Total	C	N	O	S	0	0	0
			1469	919	266	276	8			
1	F	188	Total	C	N	O	S	0	0	0
			1451	908	261	274	8			
1	G	187	Total	C	N	O	S	0	0	0
			1442	905	258	271	8			
1	H	190	Total	C	N	O	S	0	0	0
			1476	925	267	276	8			
1	I	189	Total	C	N	O	S	0	0	0
			1468	919	266	275	8			
1	J	189	Total	C	N	O	S	0	0	0
			1469	919	266	276	8			
1	K	188	Total	C	N	O	S	0	0	0
			1452	910	259	275	8			
1	L	186	Total	C	N	O	S	0	0	0
			1441	904	257	272	8			
1	M	186	Total	C	N	O	S	0	0	0
			1441	904	257	272	8			
1	N	190	Total	C	N	O	S	0	0	0
			1477	925	267	277	8			
1	O	184	Total	C	N	O	S	0	0	0
			1413	885	254	266	8			
1	P	188	Total	C	N	O	S	0	0	0
			1456	913	260	275	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	188	Total	C	N	O	S	0	0	0
			1462	916	263	275	8			
1	R	185	Total	C	N	O	S	0	0	0
			1430	895	262	265	8			
1	S	187	Total	C	N	O	S	0	0	0
			1442	904	257	273	8			
1	T	189	Total	C	N	O	S	0	0	0
			1465	917	265	275	8			

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P9WN57
A	-19	ALA	-	expression tag	UNP P9WN57
A	-18	HIS	-	expression tag	UNP P9WN57
A	-17	HIS	-	expression tag	UNP P9WN57
A	-16	HIS	-	expression tag	UNP P9WN57
A	-15	HIS	-	expression tag	UNP P9WN57
A	-14	HIS	-	expression tag	UNP P9WN57
A	-13	HIS	-	expression tag	UNP P9WN57
A	-12	MET	-	expression tag	UNP P9WN57
A	-11	GLY	-	expression tag	UNP P9WN57
A	-10	THR	-	expression tag	UNP P9WN57
A	-9	LEU	-	expression tag	UNP P9WN57
A	-8	GLU	-	expression tag	UNP P9WN57
A	-7	ALA	-	expression tag	UNP P9WN57
A	-6	GLN	-	expression tag	UNP P9WN57
A	-5	THR	-	expression tag	UNP P9WN57
A	-4	GLN	-	expression tag	UNP P9WN57
A	-3	GLY	-	expression tag	UNP P9WN57
A	-2	PRO	-	expression tag	UNP P9WN57
A	-1	GLY	-	expression tag	UNP P9WN57
A	0	SER	-	expression tag	UNP P9WN57
B	-20	MET	-	expression tag	UNP P9WN57
B	-19	ALA	-	expression tag	UNP P9WN57
B	-18	HIS	-	expression tag	UNP P9WN57
B	-17	HIS	-	expression tag	UNP P9WN57
B	-16	HIS	-	expression tag	UNP P9WN57
B	-15	HIS	-	expression tag	UNP P9WN57
B	-14	HIS	-	expression tag	UNP P9WN57
B	-13	HIS	-	expression tag	UNP P9WN57
B	-12	MET	-	expression tag	UNP P9WN57
B	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	THR	-	expression tag	UNP P9WN57
B	-9	LEU	-	expression tag	UNP P9WN57
B	-8	GLU	-	expression tag	UNP P9WN57
B	-7	ALA	-	expression tag	UNP P9WN57
B	-6	GLN	-	expression tag	UNP P9WN57
B	-5	THR	-	expression tag	UNP P9WN57
B	-4	GLN	-	expression tag	UNP P9WN57
B	-3	GLY	-	expression tag	UNP P9WN57
B	-2	PRO	-	expression tag	UNP P9WN57
B	-1	GLY	-	expression tag	UNP P9WN57
B	0	SER	-	expression tag	UNP P9WN57
C	-20	MET	-	expression tag	UNP P9WN57
C	-19	ALA	-	expression tag	UNP P9WN57
C	-18	HIS	-	expression tag	UNP P9WN57
C	-17	HIS	-	expression tag	UNP P9WN57
C	-16	HIS	-	expression tag	UNP P9WN57
C	-15	HIS	-	expression tag	UNP P9WN57
C	-14	HIS	-	expression tag	UNP P9WN57
C	-13	HIS	-	expression tag	UNP P9WN57
C	-12	MET	-	expression tag	UNP P9WN57
C	-11	GLY	-	expression tag	UNP P9WN57
C	-10	THR	-	expression tag	UNP P9WN57
C	-9	LEU	-	expression tag	UNP P9WN57
C	-8	GLU	-	expression tag	UNP P9WN57
C	-7	ALA	-	expression tag	UNP P9WN57
C	-6	GLN	-	expression tag	UNP P9WN57
C	-5	THR	-	expression tag	UNP P9WN57
C	-4	GLN	-	expression tag	UNP P9WN57
C	-3	GLY	-	expression tag	UNP P9WN57
C	-2	PRO	-	expression tag	UNP P9WN57
C	-1	GLY	-	expression tag	UNP P9WN57
C	0	SER	-	expression tag	UNP P9WN57
D	-20	MET	-	expression tag	UNP P9WN57
D	-19	ALA	-	expression tag	UNP P9WN57
D	-18	HIS	-	expression tag	UNP P9WN57
D	-17	HIS	-	expression tag	UNP P9WN57
D	-16	HIS	-	expression tag	UNP P9WN57
D	-15	HIS	-	expression tag	UNP P9WN57
D	-14	HIS	-	expression tag	UNP P9WN57
D	-13	HIS	-	expression tag	UNP P9WN57
D	-12	MET	-	expression tag	UNP P9WN57
D	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	THR	-	expression tag	UNP P9WN57
D	-9	LEU	-	expression tag	UNP P9WN57
D	-8	GLU	-	expression tag	UNP P9WN57
D	-7	ALA	-	expression tag	UNP P9WN57
D	-6	GLN	-	expression tag	UNP P9WN57
D	-5	THR	-	expression tag	UNP P9WN57
D	-4	GLN	-	expression tag	UNP P9WN57
D	-3	GLY	-	expression tag	UNP P9WN57
D	-2	PRO	-	expression tag	UNP P9WN57
D	-1	GLY	-	expression tag	UNP P9WN57
D	0	SER	-	expression tag	UNP P9WN57
E	-20	MET	-	expression tag	UNP P9WN57
E	-19	ALA	-	expression tag	UNP P9WN57
E	-18	HIS	-	expression tag	UNP P9WN57
E	-17	HIS	-	expression tag	UNP P9WN57
E	-16	HIS	-	expression tag	UNP P9WN57
E	-15	HIS	-	expression tag	UNP P9WN57
E	-14	HIS	-	expression tag	UNP P9WN57
E	-13	HIS	-	expression tag	UNP P9WN57
E	-12	MET	-	expression tag	UNP P9WN57
E	-11	GLY	-	expression tag	UNP P9WN57
E	-10	THR	-	expression tag	UNP P9WN57
E	-9	LEU	-	expression tag	UNP P9WN57
E	-8	GLU	-	expression tag	UNP P9WN57
E	-7	ALA	-	expression tag	UNP P9WN57
E	-6	GLN	-	expression tag	UNP P9WN57
E	-5	THR	-	expression tag	UNP P9WN57
E	-4	GLN	-	expression tag	UNP P9WN57
E	-3	GLY	-	expression tag	UNP P9WN57
E	-2	PRO	-	expression tag	UNP P9WN57
E	-1	GLY	-	expression tag	UNP P9WN57
E	0	SER	-	expression tag	UNP P9WN57
F	-20	MET	-	expression tag	UNP P9WN57
F	-19	ALA	-	expression tag	UNP P9WN57
F	-18	HIS	-	expression tag	UNP P9WN57
F	-17	HIS	-	expression tag	UNP P9WN57
F	-16	HIS	-	expression tag	UNP P9WN57
F	-15	HIS	-	expression tag	UNP P9WN57
F	-14	HIS	-	expression tag	UNP P9WN57
F	-13	HIS	-	expression tag	UNP P9WN57
F	-12	MET	-	expression tag	UNP P9WN57
F	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	THR	-	expression tag	UNP P9WN57
F	-9	LEU	-	expression tag	UNP P9WN57
F	-8	GLU	-	expression tag	UNP P9WN57
F	-7	ALA	-	expression tag	UNP P9WN57
F	-6	GLN	-	expression tag	UNP P9WN57
F	-5	THR	-	expression tag	UNP P9WN57
F	-4	GLN	-	expression tag	UNP P9WN57
F	-3	GLY	-	expression tag	UNP P9WN57
F	-2	PRO	-	expression tag	UNP P9WN57
F	-1	GLY	-	expression tag	UNP P9WN57
F	0	SER	-	expression tag	UNP P9WN57
G	-20	MET	-	expression tag	UNP P9WN57
G	-19	ALA	-	expression tag	UNP P9WN57
G	-18	HIS	-	expression tag	UNP P9WN57
G	-17	HIS	-	expression tag	UNP P9WN57
G	-16	HIS	-	expression tag	UNP P9WN57
G	-15	HIS	-	expression tag	UNP P9WN57
G	-14	HIS	-	expression tag	UNP P9WN57
G	-13	HIS	-	expression tag	UNP P9WN57
G	-12	MET	-	expression tag	UNP P9WN57
G	-11	GLY	-	expression tag	UNP P9WN57
G	-10	THR	-	expression tag	UNP P9WN57
G	-9	LEU	-	expression tag	UNP P9WN57
G	-8	GLU	-	expression tag	UNP P9WN57
G	-7	ALA	-	expression tag	UNP P9WN57
G	-6	GLN	-	expression tag	UNP P9WN57
G	-5	THR	-	expression tag	UNP P9WN57
G	-4	GLN	-	expression tag	UNP P9WN57
G	-3	GLY	-	expression tag	UNP P9WN57
G	-2	PRO	-	expression tag	UNP P9WN57
G	-1	GLY	-	expression tag	UNP P9WN57
G	0	SER	-	expression tag	UNP P9WN57
H	-20	MET	-	expression tag	UNP P9WN57
H	-19	ALA	-	expression tag	UNP P9WN57
H	-18	HIS	-	expression tag	UNP P9WN57
H	-17	HIS	-	expression tag	UNP P9WN57
H	-16	HIS	-	expression tag	UNP P9WN57
H	-15	HIS	-	expression tag	UNP P9WN57
H	-14	HIS	-	expression tag	UNP P9WN57
H	-13	HIS	-	expression tag	UNP P9WN57
H	-12	MET	-	expression tag	UNP P9WN57
H	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	THR	-	expression tag	UNP P9WN57
H	-9	LEU	-	expression tag	UNP P9WN57
H	-8	GLU	-	expression tag	UNP P9WN57
H	-7	ALA	-	expression tag	UNP P9WN57
H	-6	GLN	-	expression tag	UNP P9WN57
H	-5	THR	-	expression tag	UNP P9WN57
H	-4	GLN	-	expression tag	UNP P9WN57
H	-3	GLY	-	expression tag	UNP P9WN57
H	-2	PRO	-	expression tag	UNP P9WN57
H	-1	GLY	-	expression tag	UNP P9WN57
H	0	SER	-	expression tag	UNP P9WN57
I	-20	MET	-	expression tag	UNP P9WN57
I	-19	ALA	-	expression tag	UNP P9WN57
I	-18	HIS	-	expression tag	UNP P9WN57
I	-17	HIS	-	expression tag	UNP P9WN57
I	-16	HIS	-	expression tag	UNP P9WN57
I	-15	HIS	-	expression tag	UNP P9WN57
I	-14	HIS	-	expression tag	UNP P9WN57
I	-13	HIS	-	expression tag	UNP P9WN57
I	-12	MET	-	expression tag	UNP P9WN57
I	-11	GLY	-	expression tag	UNP P9WN57
I	-10	THR	-	expression tag	UNP P9WN57
I	-9	LEU	-	expression tag	UNP P9WN57
I	-8	GLU	-	expression tag	UNP P9WN57
I	-7	ALA	-	expression tag	UNP P9WN57
I	-6	GLN	-	expression tag	UNP P9WN57
I	-5	THR	-	expression tag	UNP P9WN57
I	-4	GLN	-	expression tag	UNP P9WN57
I	-3	GLY	-	expression tag	UNP P9WN57
I	-2	PRO	-	expression tag	UNP P9WN57
I	-1	GLY	-	expression tag	UNP P9WN57
I	0	SER	-	expression tag	UNP P9WN57
J	-20	MET	-	expression tag	UNP P9WN57
J	-19	ALA	-	expression tag	UNP P9WN57
J	-18	HIS	-	expression tag	UNP P9WN57
J	-17	HIS	-	expression tag	UNP P9WN57
J	-16	HIS	-	expression tag	UNP P9WN57
J	-15	HIS	-	expression tag	UNP P9WN57
J	-14	HIS	-	expression tag	UNP P9WN57
J	-13	HIS	-	expression tag	UNP P9WN57
J	-12	MET	-	expression tag	UNP P9WN57
J	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-10	THR	-	expression tag	UNP P9WN57
J	-9	LEU	-	expression tag	UNP P9WN57
J	-8	GLU	-	expression tag	UNP P9WN57
J	-7	ALA	-	expression tag	UNP P9WN57
J	-6	GLN	-	expression tag	UNP P9WN57
J	-5	THR	-	expression tag	UNP P9WN57
J	-4	GLN	-	expression tag	UNP P9WN57
J	-3	GLY	-	expression tag	UNP P9WN57
J	-2	PRO	-	expression tag	UNP P9WN57
J	-1	GLY	-	expression tag	UNP P9WN57
J	0	SER	-	expression tag	UNP P9WN57
K	-20	MET	-	expression tag	UNP P9WN57
K	-19	ALA	-	expression tag	UNP P9WN57
K	-18	HIS	-	expression tag	UNP P9WN57
K	-17	HIS	-	expression tag	UNP P9WN57
K	-16	HIS	-	expression tag	UNP P9WN57
K	-15	HIS	-	expression tag	UNP P9WN57
K	-14	HIS	-	expression tag	UNP P9WN57
K	-13	HIS	-	expression tag	UNP P9WN57
K	-12	MET	-	expression tag	UNP P9WN57
K	-11	GLY	-	expression tag	UNP P9WN57
K	-10	THR	-	expression tag	UNP P9WN57
K	-9	LEU	-	expression tag	UNP P9WN57
K	-8	GLU	-	expression tag	UNP P9WN57
K	-7	ALA	-	expression tag	UNP P9WN57
K	-6	GLN	-	expression tag	UNP P9WN57
K	-5	THR	-	expression tag	UNP P9WN57
K	-4	GLN	-	expression tag	UNP P9WN57
K	-3	GLY	-	expression tag	UNP P9WN57
K	-2	PRO	-	expression tag	UNP P9WN57
K	-1	GLY	-	expression tag	UNP P9WN57
K	0	SER	-	expression tag	UNP P9WN57
L	-20	MET	-	expression tag	UNP P9WN57
L	-19	ALA	-	expression tag	UNP P9WN57
L	-18	HIS	-	expression tag	UNP P9WN57
L	-17	HIS	-	expression tag	UNP P9WN57
L	-16	HIS	-	expression tag	UNP P9WN57
L	-15	HIS	-	expression tag	UNP P9WN57
L	-14	HIS	-	expression tag	UNP P9WN57
L	-13	HIS	-	expression tag	UNP P9WN57
L	-12	MET	-	expression tag	UNP P9WN57
L	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-10	THR	-	expression tag	UNP P9WN57
L	-9	LEU	-	expression tag	UNP P9WN57
L	-8	GLU	-	expression tag	UNP P9WN57
L	-7	ALA	-	expression tag	UNP P9WN57
L	-6	GLN	-	expression tag	UNP P9WN57
L	-5	THR	-	expression tag	UNP P9WN57
L	-4	GLN	-	expression tag	UNP P9WN57
L	-3	GLY	-	expression tag	UNP P9WN57
L	-2	PRO	-	expression tag	UNP P9WN57
L	-1	GLY	-	expression tag	UNP P9WN57
L	0	SER	-	expression tag	UNP P9WN57
M	-20	MET	-	expression tag	UNP P9WN57
M	-19	ALA	-	expression tag	UNP P9WN57
M	-18	HIS	-	expression tag	UNP P9WN57
M	-17	HIS	-	expression tag	UNP P9WN57
M	-16	HIS	-	expression tag	UNP P9WN57
M	-15	HIS	-	expression tag	UNP P9WN57
M	-14	HIS	-	expression tag	UNP P9WN57
M	-13	HIS	-	expression tag	UNP P9WN57
M	-12	MET	-	expression tag	UNP P9WN57
M	-11	GLY	-	expression tag	UNP P9WN57
M	-10	THR	-	expression tag	UNP P9WN57
M	-9	LEU	-	expression tag	UNP P9WN57
M	-8	GLU	-	expression tag	UNP P9WN57
M	-7	ALA	-	expression tag	UNP P9WN57
M	-6	GLN	-	expression tag	UNP P9WN57
M	-5	THR	-	expression tag	UNP P9WN57
M	-4	GLN	-	expression tag	UNP P9WN57
M	-3	GLY	-	expression tag	UNP P9WN57
M	-2	PRO	-	expression tag	UNP P9WN57
M	-1	GLY	-	expression tag	UNP P9WN57
M	0	SER	-	expression tag	UNP P9WN57
N	-20	MET	-	expression tag	UNP P9WN57
N	-19	ALA	-	expression tag	UNP P9WN57
N	-18	HIS	-	expression tag	UNP P9WN57
N	-17	HIS	-	expression tag	UNP P9WN57
N	-16	HIS	-	expression tag	UNP P9WN57
N	-15	HIS	-	expression tag	UNP P9WN57
N	-14	HIS	-	expression tag	UNP P9WN57
N	-13	HIS	-	expression tag	UNP P9WN57
N	-12	MET	-	expression tag	UNP P9WN57
N	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-10	THR	-	expression tag	UNP P9WN57
N	-9	LEU	-	expression tag	UNP P9WN57
N	-8	GLU	-	expression tag	UNP P9WN57
N	-7	ALA	-	expression tag	UNP P9WN57
N	-6	GLN	-	expression tag	UNP P9WN57
N	-5	THR	-	expression tag	UNP P9WN57
N	-4	GLN	-	expression tag	UNP P9WN57
N	-3	GLY	-	expression tag	UNP P9WN57
N	-2	PRO	-	expression tag	UNP P9WN57
N	-1	GLY	-	expression tag	UNP P9WN57
N	0	SER	-	expression tag	UNP P9WN57
O	-20	MET	-	expression tag	UNP P9WN57
O	-19	ALA	-	expression tag	UNP P9WN57
O	-18	HIS	-	expression tag	UNP P9WN57
O	-17	HIS	-	expression tag	UNP P9WN57
O	-16	HIS	-	expression tag	UNP P9WN57
O	-15	HIS	-	expression tag	UNP P9WN57
O	-14	HIS	-	expression tag	UNP P9WN57
O	-13	HIS	-	expression tag	UNP P9WN57
O	-12	MET	-	expression tag	UNP P9WN57
O	-11	GLY	-	expression tag	UNP P9WN57
O	-10	THR	-	expression tag	UNP P9WN57
O	-9	LEU	-	expression tag	UNP P9WN57
O	-8	GLU	-	expression tag	UNP P9WN57
O	-7	ALA	-	expression tag	UNP P9WN57
O	-6	GLN	-	expression tag	UNP P9WN57
O	-5	THR	-	expression tag	UNP P9WN57
O	-4	GLN	-	expression tag	UNP P9WN57
O	-3	GLY	-	expression tag	UNP P9WN57
O	-2	PRO	-	expression tag	UNP P9WN57
O	-1	GLY	-	expression tag	UNP P9WN57
O	0	SER	-	expression tag	UNP P9WN57
P	-20	MET	-	expression tag	UNP P9WN57
P	-19	ALA	-	expression tag	UNP P9WN57
P	-18	HIS	-	expression tag	UNP P9WN57
P	-17	HIS	-	expression tag	UNP P9WN57
P	-16	HIS	-	expression tag	UNP P9WN57
P	-15	HIS	-	expression tag	UNP P9WN57
P	-14	HIS	-	expression tag	UNP P9WN57
P	-13	HIS	-	expression tag	UNP P9WN57
P	-12	MET	-	expression tag	UNP P9WN57
P	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-10	THR	-	expression tag	UNP P9WN57
P	-9	LEU	-	expression tag	UNP P9WN57
P	-8	GLU	-	expression tag	UNP P9WN57
P	-7	ALA	-	expression tag	UNP P9WN57
P	-6	GLN	-	expression tag	UNP P9WN57
P	-5	THR	-	expression tag	UNP P9WN57
P	-4	GLN	-	expression tag	UNP P9WN57
P	-3	GLY	-	expression tag	UNP P9WN57
P	-2	PRO	-	expression tag	UNP P9WN57
P	-1	GLY	-	expression tag	UNP P9WN57
P	0	SER	-	expression tag	UNP P9WN57
Q	-20	MET	-	expression tag	UNP P9WN57
Q	-19	ALA	-	expression tag	UNP P9WN57
Q	-18	HIS	-	expression tag	UNP P9WN57
Q	-17	HIS	-	expression tag	UNP P9WN57
Q	-16	HIS	-	expression tag	UNP P9WN57
Q	-15	HIS	-	expression tag	UNP P9WN57
Q	-14	HIS	-	expression tag	UNP P9WN57
Q	-13	HIS	-	expression tag	UNP P9WN57
Q	-12	MET	-	expression tag	UNP P9WN57
Q	-11	GLY	-	expression tag	UNP P9WN57
Q	-10	THR	-	expression tag	UNP P9WN57
Q	-9	LEU	-	expression tag	UNP P9WN57
Q	-8	GLU	-	expression tag	UNP P9WN57
Q	-7	ALA	-	expression tag	UNP P9WN57
Q	-6	GLN	-	expression tag	UNP P9WN57
Q	-5	THR	-	expression tag	UNP P9WN57
Q	-4	GLN	-	expression tag	UNP P9WN57
Q	-3	GLY	-	expression tag	UNP P9WN57
Q	-2	PRO	-	expression tag	UNP P9WN57
Q	-1	GLY	-	expression tag	UNP P9WN57
Q	0	SER	-	expression tag	UNP P9WN57
R	-20	MET	-	expression tag	UNP P9WN57
R	-19	ALA	-	expression tag	UNP P9WN57
R	-18	HIS	-	expression tag	UNP P9WN57
R	-17	HIS	-	expression tag	UNP P9WN57
R	-16	HIS	-	expression tag	UNP P9WN57
R	-15	HIS	-	expression tag	UNP P9WN57
R	-14	HIS	-	expression tag	UNP P9WN57
R	-13	HIS	-	expression tag	UNP P9WN57
R	-12	MET	-	expression tag	UNP P9WN57
R	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-10	THR	-	expression tag	UNP P9WN57
R	-9	LEU	-	expression tag	UNP P9WN57
R	-8	GLU	-	expression tag	UNP P9WN57
R	-7	ALA	-	expression tag	UNP P9WN57
R	-6	GLN	-	expression tag	UNP P9WN57
R	-5	THR	-	expression tag	UNP P9WN57
R	-4	GLN	-	expression tag	UNP P9WN57
R	-3	GLY	-	expression tag	UNP P9WN57
R	-2	PRO	-	expression tag	UNP P9WN57
R	-1	GLY	-	expression tag	UNP P9WN57
R	0	SER	-	expression tag	UNP P9WN57
S	-20	MET	-	expression tag	UNP P9WN57
S	-19	ALA	-	expression tag	UNP P9WN57
S	-18	HIS	-	expression tag	UNP P9WN57
S	-17	HIS	-	expression tag	UNP P9WN57
S	-16	HIS	-	expression tag	UNP P9WN57
S	-15	HIS	-	expression tag	UNP P9WN57
S	-14	HIS	-	expression tag	UNP P9WN57
S	-13	HIS	-	expression tag	UNP P9WN57
S	-12	MET	-	expression tag	UNP P9WN57
S	-11	GLY	-	expression tag	UNP P9WN57
S	-10	THR	-	expression tag	UNP P9WN57
S	-9	LEU	-	expression tag	UNP P9WN57
S	-8	GLU	-	expression tag	UNP P9WN57
S	-7	ALA	-	expression tag	UNP P9WN57
S	-6	GLN	-	expression tag	UNP P9WN57
S	-5	THR	-	expression tag	UNP P9WN57
S	-4	GLN	-	expression tag	UNP P9WN57
S	-3	GLY	-	expression tag	UNP P9WN57
S	-2	PRO	-	expression tag	UNP P9WN57
S	-1	GLY	-	expression tag	UNP P9WN57
S	0	SER	-	expression tag	UNP P9WN57
T	-20	MET	-	expression tag	UNP P9WN57
T	-19	ALA	-	expression tag	UNP P9WN57
T	-18	HIS	-	expression tag	UNP P9WN57
T	-17	HIS	-	expression tag	UNP P9WN57
T	-16	HIS	-	expression tag	UNP P9WN57
T	-15	HIS	-	expression tag	UNP P9WN57
T	-14	HIS	-	expression tag	UNP P9WN57
T	-13	HIS	-	expression tag	UNP P9WN57
T	-12	MET	-	expression tag	UNP P9WN57
T	-11	GLY	-	expression tag	UNP P9WN57

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-10	THR	-	expression tag	UNP P9WN57
T	-9	LEU	-	expression tag	UNP P9WN57
T	-8	GLU	-	expression tag	UNP P9WN57
T	-7	ALA	-	expression tag	UNP P9WN57
T	-6	GLN	-	expression tag	UNP P9WN57
T	-5	THR	-	expression tag	UNP P9WN57
T	-4	GLN	-	expression tag	UNP P9WN57
T	-3	GLY	-	expression tag	UNP P9WN57
T	-2	PRO	-	expression tag	UNP P9WN57
T	-1	GLY	-	expression tag	UNP P9WN57
T	0	SER	-	expression tag	UNP P9WN57

- Molecule 2 is ZINC ION (CCD ID: 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
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0
2	M	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	1	Total 1	Zn 1	0	0
2	O	1	Total 1	Zn 1	0	0
2	P	1	Total 1	Zn 1	0	0
2	Q	1	Total 1	Zn 1	0	0
2	R	1	Total 1	Zn 1	0	0
2	S	1	Total 1	Zn 1	0	0
2	T	1	Total 1	Zn 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Cl 1	0	0
3	G	1	Total 1	Cl 1	0	0
3	J	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	O 1	0	0
4	C	3	Total 3	O 3	0	0
4	D	2	Total 2	O 2	0	0
4	E	5	Total 5	O 5	0	0
4	F	2	Total 2	O 2	0	0
4	G	3	Total 3	O 3	0	0
4	H	6	Total 6	O 6	0	0

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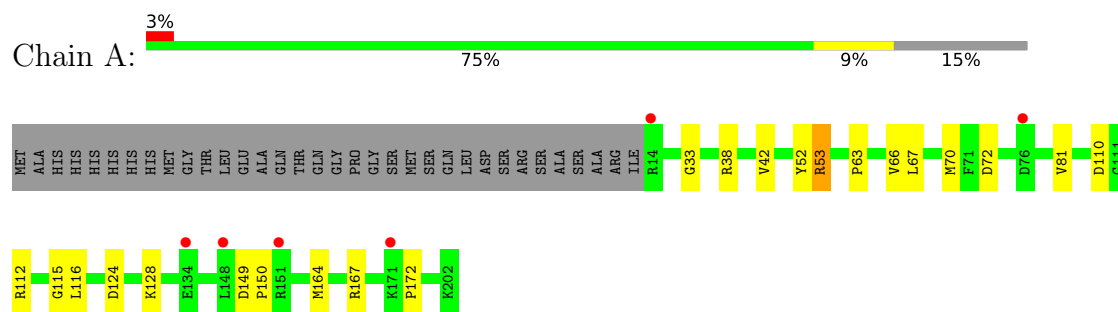
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total 1	O 1	0	0
4	M	3	Total 3	O 3	0	0
4	N	5	Total 5	O 5	0	0
4	O	4	Total 4	O 4	0	0
4	P	1	Total 1	O 1	0	0
4	R	4	Total 4	O 4	0	0
4	S	2	Total 2	O 2	0	0

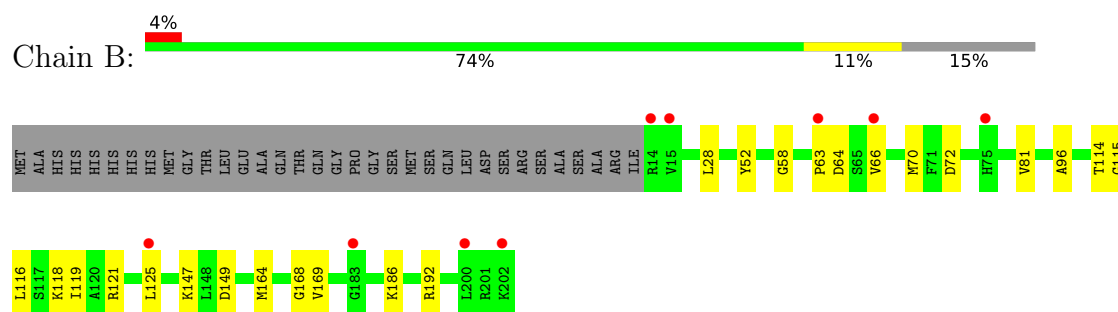
3 Residue-property plots [i](#)

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

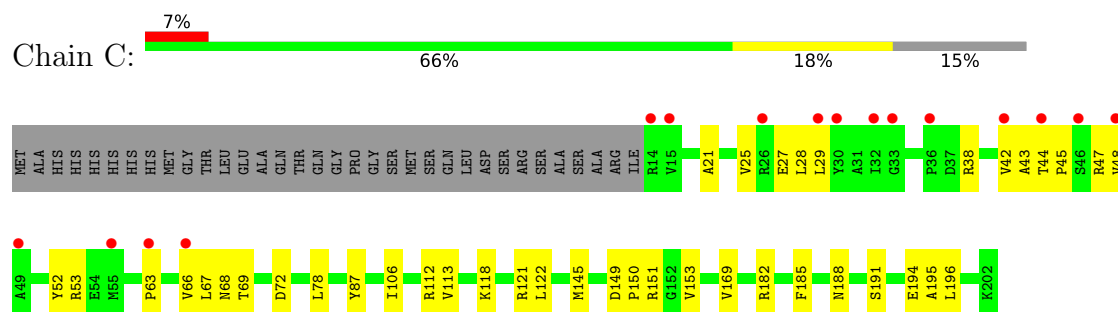
• Molecule 1: GTP cyclohydrolase 1



• Molecule 1: GTP cyclohydrolase 1

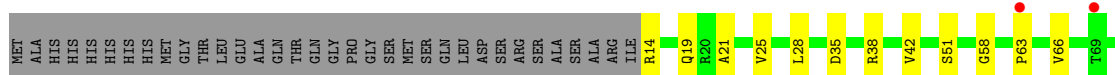


• Molecule 1: GTP cyclohydrolase 1

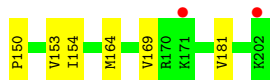
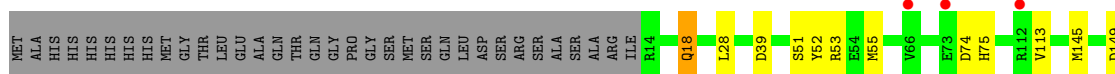
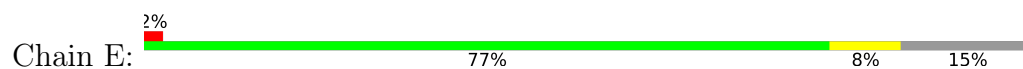


• Molecule 1: GTP cyclohydrolase 1

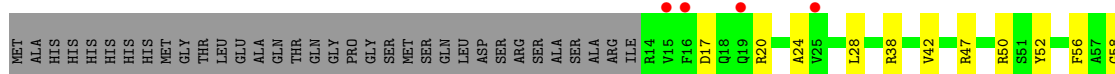




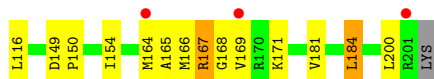
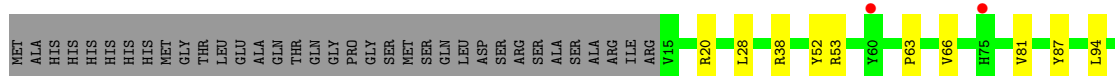
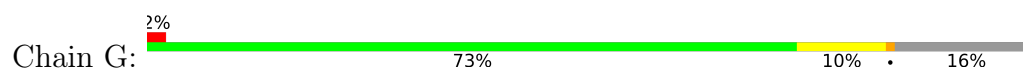
• Molecule 1: GTP cyclohydrolase 1



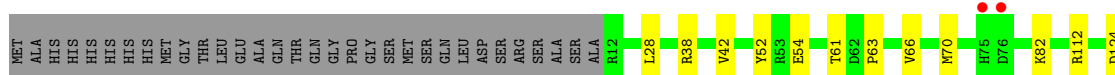
• Molecule 1: GTP cyclohydrolase 1



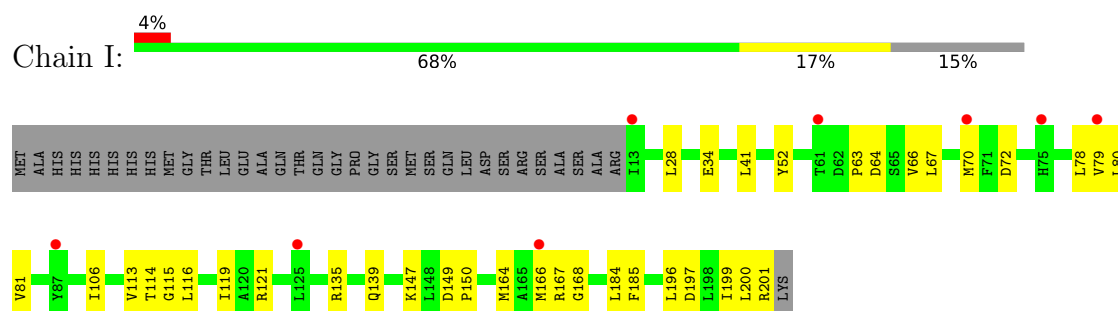
• Molecule 1: GTP cyclohydrolase 1



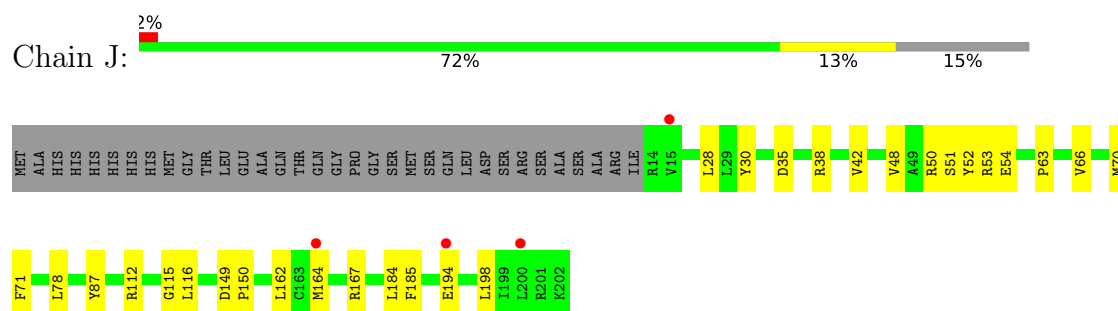
• Molecule 1: GTP cyclohydrolase 1



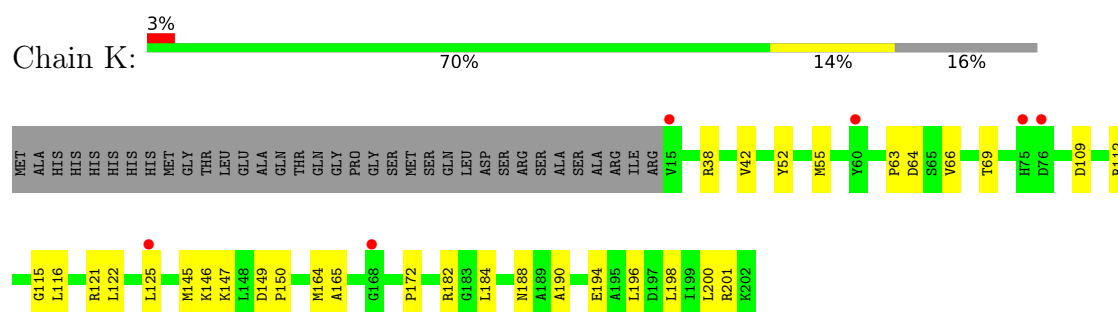
- Molecule 1: GTP cyclohydrolase 1



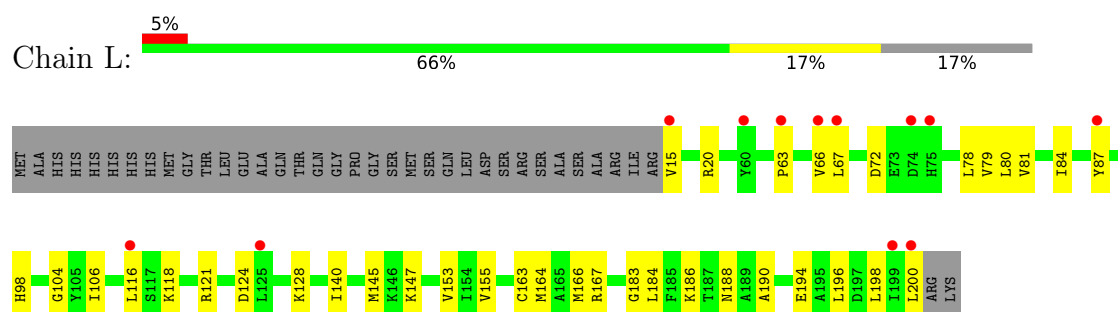
- Molecule 1: GTP cyclohydrolase 1



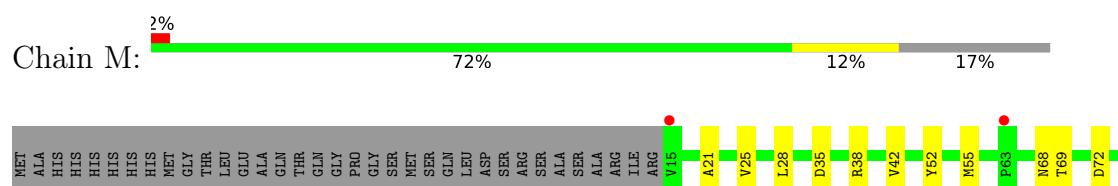
- Molecule 1: GTP cyclohydrolase 1

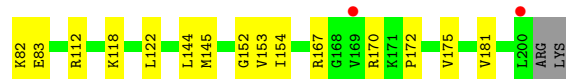


- Molecule 1: GTP cyclohydrolase 1

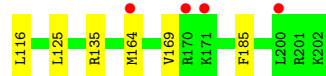
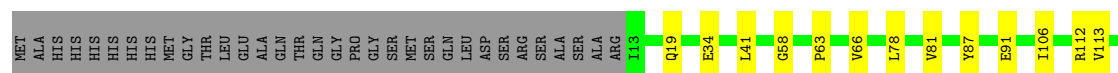
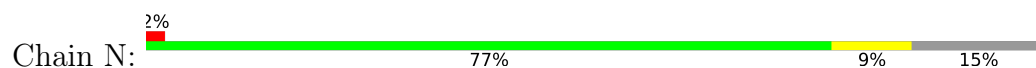


- Molecule 1: GTP cyclohydrolase 1

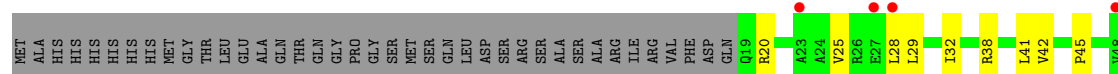




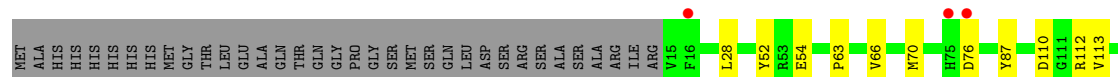
- Molecule 1: GTP cyclohydrolase 1



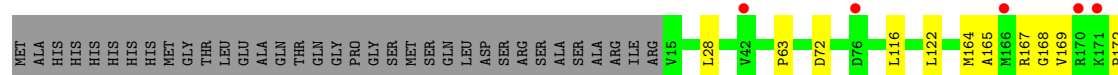
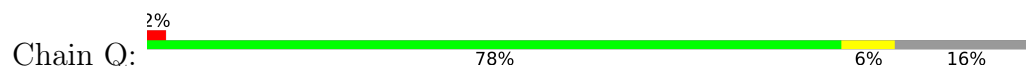
- Molecule 1: GTP cyclohydrolase 1



- Molecule 1: GTP cyclohydrolase 1

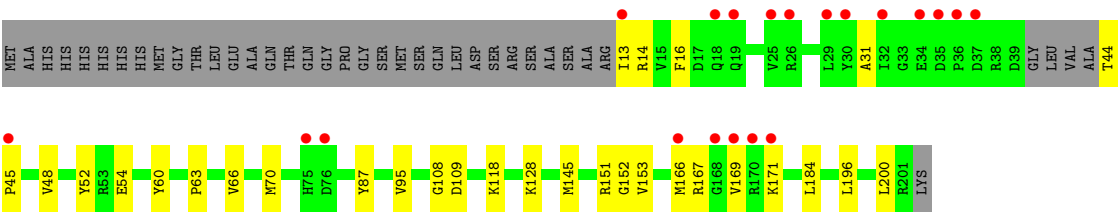


- Molecule 1: GTP cyclohydrolase 1

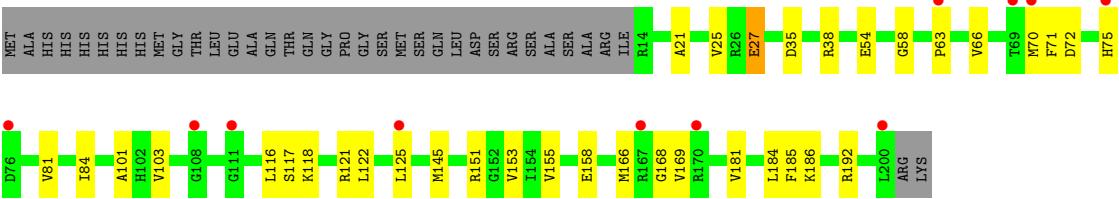


- Molecule 1: GTP cyclohydrolase 1

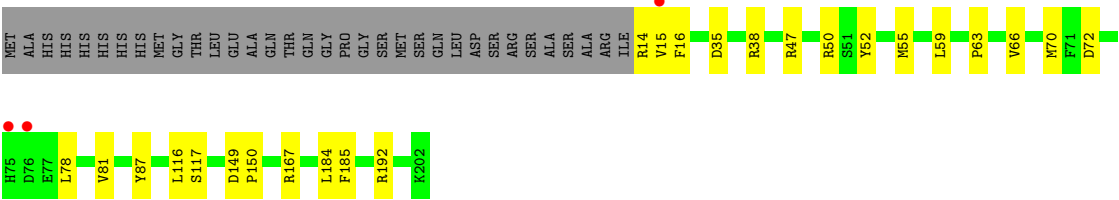
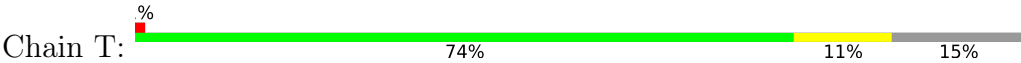




● Molecule 1: GTP cyclohydrolase 1



● Molecule 1: GTP cyclohydrolase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.55Å 109.12Å 122.55Å 89.11° 88.12° 77.95°	Depositor
Resolution (Å)	48.76 – 2.74 48.76 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.76-2.74) 96.3 (48.76-2.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.73Å)	Xtriage
Refinement program	PHENIX (2.0_5723: ???)	Depositor
R, R_{free}	0.210 , 0.259 0.215 , 0.262	Depositor DCC
R_{free} test set	5683 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29166	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7214e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.22	0/1473	0.45	0/1994
1	B	0.20	0/1493	0.43	0/2019
1	C	0.20	0/1485	0.44	0/2009
1	D	0.20	0/1491	0.43	0/2016
1	E	0.18	0/1493	0.42	0/2019
1	F	0.20	0/1475	0.42	0/1998
1	G	0.21	0/1466	0.47	0/1986
1	H	0.18	0/1500	0.43	0/2030
1	I	0.20	0/1492	0.44	0/2019
1	J	0.19	0/1493	0.42	0/2019
1	K	0.21	0/1476	0.45	0/1998
1	L	0.22	0/1465	0.46	0/1984
1	M	0.21	0/1465	0.44	0/1984
1	N	0.25	0/1501	0.47	0/2030
1	O	0.19	0/1436	0.43	0/1944
1	P	0.19	0/1480	0.42	0/2002
1	Q	0.19	0/1486	0.40	0/2009
1	R	0.20	0/1453	0.45	0/1965
1	S	0.20	0/1466	0.46	0/1987
1	T	0.19	0/1489	0.41	0/2014
All	All	0.20	0/29578	0.44	0/40026

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	ARG	Sidechain
1	G	167	ARG	Sidechain
1	G	53	ARG	Sidechain

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	1450	0	1446	18	0
1	B	1469	0	1475	31	0
1	C	1461	0	1464	38	0
1	D	1467	0	1475	30	0
1	E	1469	0	1475	11	0
1	F	1451	0	1444	30	0
1	G	1442	0	1445	21	0
1	H	1476	0	1486	23	0
1	I	1468	0	1475	34	0
1	J	1469	0	1475	29	0
1	K	1452	0	1451	29	0
1	L	1441	0	1447	34	0
1	M	1441	0	1447	21	0
1	N	1477	0	1486	17	0
1	O	1413	0	1417	29	0
1	P	1456	0	1462	22	0
1	Q	1462	0	1473	14	0
1	R	1430	0	1427	28	0
1	S	1442	0	1438	28	0
1	T	1465	0	1469	21	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	1	0
3	J	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	5	0	0	0	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
4	H	6	0	0	0	0
4	I	1	0	0	0	0
4	M	3	0	0	0	0
4	N	5	0	0	0	0
4	O	4	0	0	0	0
4	P	1	0	0	0	0
4	R	4	0	0	0	0
4	S	2	0	0	0	0
All	All	29166	0	29177	405	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 (405) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:LEU:HD11	1:I:199:ILE:HD11	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:MET:HE2	1:H:153:VAL:HG23	1.61	0.81
1:B:118:LYS:HE3	1:B:118:LYS:HA	1.64	0.79
1:C:52:TYR:CE2	1:F:28:LEU:HD21	2.19	0.78
1:C:44:THR:HG22	1:C:45:PRO:HD3	1.66	0.78
1:M:52:TYR:CE2	1:P:28:LEU:HD21	2.20	0.76
1:O:28:LEU:HD21	1:R:52:TYR:HE2	1.49	0.76
1:R:171:LYS:H	1:R:171:LYS:HD3	1.51	0.75
1:G:28:LEU:HD21	1:J:52:TYR:CE2	2.22	0.74
1:F:116:LEU:HD21	1:H:171:LYS:HD3	1.68	0.74
1:O:28:LEU:HD21	1:R:52:TYR:CE2	2.23	0.73
1:E:52:TYR:CE2	1:H:28:LEU:HD21	2.24	0.73
1:B:81:VAL:HG13	1:B:116:LEU:HD12	1.72	0.72
1:L:81:VAL:HG22	1:L:116:LEU:HD22	1.72	0.71
1:F:196:LEU:O	1:F:200:LEU:HD22	1.91	0.71
1:R:171:LYS:H	1:R:171:LYS:CD	2.03	0.70
1:M:28:LEU:HD21	1:P:52:TYR:HE2	1.57	0.70
1:P:195:ALA:O	1:P:199:ILE:HD13	1.92	0.70
1:K:146:LYS:HE3	1:K:147:LYS:CE	2.22	0.69
1:C:69:THR:HG23	1:C:112:ARG:NH1	2.06	0.69
1:C:67:LEU:HD21	1:C:122:LEU:HD12	1.75	0.69
1:M:38:ARG:O	1:M:42:VAL:HG23	1.93	0.69
1:I:80:LEU:HD11	1:I:199:ILE:CD1	2.23	0.67
1:M:68:ASN:OD1	1:M:118:LYS:HG3	1.94	0.67
1:I:81:VAL:HG13	1:I:116:LEU:HD12	1.75	0.67
1:C:27:GLU:HG3	1:F:20:ARG:HG2	1.77	0.66
1:G:154:ILE:HD13	1:G:181:VAL:HG12	1.78	0.66
1:O:29:LEU:HD12	1:O:41:LEU:HD13	1.76	0.66
1:T:81:VAL:HG22	1:T:116:LEU:HD23	1.78	0.66
1:L:66:VAL:HG11	1:L:121:ARG:HD3	1.79	0.65
1:K:172:PRO:HB3	1:N:87:TYR:OH	1.96	0.65
1:G:165:ALA:HB1	1:J:87:TYR:CZ	2.32	0.65
1:P:54:GLU:O	1:P:128:LYS:HD3	1.97	0.64
1:M:145:MET:SD	1:M:153:VAL:HG23	2.37	0.64
1:O:20:ARG:HB3	1:R:31:ALA:HB2	1.79	0.64
1:G:28:LEU:HD21	1:J:52:TYR:HE2	1.64	0.63
1:Q:28:LEU:HD21	1:T:52:TYR:HE2	1.62	0.63
1:S:145:MET:SD	1:S:153:VAL:HG23	2.39	0.63
1:J:194:GLU:O	1:J:198:LEU:HD12	1.99	0.62
1:L:194:GLU:O	1:L:198:LEU:HD12	2.00	0.62
1:B:81:VAL:HG22	1:B:116:LEU:HD11	1.81	0.62
1:M:69:THR:HG22	1:M:112:ARG:NH2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:PRO:O	1:L:66:VAL:HG22	2.01	0.61
1:N:34:GLU:HG2	1:N:41:LEU:HD11	1.83	0.61
1:M:172:PRO:HB3	1:P:87:TYR:OH	2.01	0.61
1:G:168:GLY:O	1:I:115:GLY:HA2	2.01	0.60
1:L:196:LEU:O	1:L:200:LEU:HD23	2.00	0.60
1:H:70:MET:HE1	1:J:167:ARG:HB3	1.82	0.60
1:B:149:ASP:OD1	1:B:149:ASP:O	2.18	0.60
1:C:121:ARG:HG3	1:C:121:ARG:HH11	1.67	0.60
1:T:63:PRO:O	1:T:66:VAL:HG22	2.02	0.60
1:K:38:ARG:O	1:K:42:VAL:HG23	2.00	0.60
1:L:81:VAL:CG2	1:L:116:LEU:HD22	2.32	0.59
1:O:29:LEU:HD13	1:O:32:ILE:HD11	1.84	0.59
1:E:51:SER:O	1:E:55:MET:HG3	2.03	0.59
1:K:69:THR:HG22	1:K:112:ARG:NH2	2.18	0.59
1:L:163:CYS:O	1:L:166:MET:HE2	2.03	0.59
1:C:106:ILE:HG21	1:C:151:ARG:HE	1.66	0.59
1:A:72:ASP:HA	1:I:164:MET:HE3	1.85	0.59
1:F:164:MET:HB3	1:F:170:ARG:HG3	1.85	0.58
1:O:162:LEU:HD22	1:R:87:TYR:HE2	1.68	0.58
1:T:185:PHE:O	1:T:192:ARG:HG3	2.03	0.58
1:I:66:VAL:HG11	1:I:121:ARG:HG2	1.85	0.58
1:O:53:ARG:HH11	1:O:53:ARG:HB2	1.69	0.58
1:D:194:GLU:O	1:D:198:LEU:HD12	2.03	0.58
1:R:171:LYS:HD3	1:R:171:LYS:N	2.19	0.58
1:G:63:PRO:O	1:G:66:VAL:HG22	2.04	0.58
1:P:70:MET:HE1	1:R:167:ARG:HB3	1.85	0.58
1:I:106:ILE:HD11	1:I:185:PHE:CZ	2.39	0.57
1:O:63:PRO:O	1:O:66:VAL:HG22	2.04	0.57
1:R:13:ILE:N	1:R:13:ILE:HD12	2.20	0.57
1:H:181:VAL:HG21	1:H:192:ARG:HH12	1.69	0.57
1:D:19:GLN:NE2	1:D:19:GLN:H	2.02	0.57
1:C:52:TYR:HD2	1:F:28:LEU:HD11	1.70	0.57
1:C:145:MET:HE2	1:C:182:ARG:HB3	1.86	0.57
1:G:154:ILE:HD13	1:G:181:VAL:CG1	2.34	0.57
1:L:72:ASP:OD2	1:L:72:ASP:C	2.48	0.56
1:K:145:MET:HE3	1:K:182:ARG:CB	2.35	0.56
1:K:146:LYS:HE3	1:K:147:LYS:HE3	1.87	0.56
1:A:52:TYR:CE2	1:D:28:LEU:HD21	2.39	0.56
1:P:196:LEU:O	1:P:200:LEU:HD23	2.06	0.56
1:O:194:GLU:O	1:O:198:LEU:HD12	2.06	0.56
1:R:54:GLU:O	1:R:128:LYS:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PRO:O	1:A:66:VAL:HG22	2.05	0.56
1:A:70:MET:HE1	1:I:167:ARG:HB3	1.87	0.56
1:N:81:VAL:CG1	1:N:116:LEU:HD22	2.36	0.56
1:T:14:ARG:HD2	1:T:59:LEU:HB3	1.87	0.56
1:A:52:TYR:HE2	1:D:28:LEU:HD21	1.71	0.56
1:F:70:MET:HE1	1:H:167:ARG:HB3	1.88	0.56
1:O:38:ARG:O	1:O:42:VAL:HG23	2.06	0.56
1:M:52:TYR:HE2	1:P:28:LEU:HD21	1.67	0.55
1:R:184:LEU:HD23	1:R:184:LEU:O	2.05	0.55
1:H:54:GLU:O	1:H:128:LYS:HD3	2.07	0.55
1:H:38:ARG:O	1:H:42:VAL:HG23	2.07	0.55
1:B:81:VAL:HG22	1:B:116:LEU:CD1	2.37	0.54
1:C:28:LEU:HD21	1:F:52:TYR:CZ	2.43	0.54
1:B:63:PRO:O	1:B:66:VAL:HG22	2.08	0.54
1:C:188:ASN:HB3	1:C:191:SER:OG	2.07	0.54
1:S:63:PRO:O	1:S:66:VAL:HG22	2.08	0.54
1:A:110:ASP:CG	1:A:112:ARG:HD2	2.32	0.54
1:B:81:VAL:CG1	1:B:116:LEU:HD12	2.36	0.54
1:L:78:LEU:HD21	1:L:80:LEU:HD13	1.90	0.54
1:L:196:LEU:HD13	1:L:200:LEU:HD23	1.90	0.54
1:Q:168:GLY:C	1:S:116:LEU:HD23	2.33	0.54
1:C:52:TYR:HE2	1:F:28:LEU:HD21	1.71	0.53
1:R:63:PRO:O	1:R:66:VAL:HG22	2.08	0.53
1:I:78:LEU:HD12	1:I:79:VAL:N	2.24	0.53
1:S:166:MET:HE3	1:S:166:MET:HA	1.90	0.53
1:C:67:LEU:HD21	1:C:122:LEU:CD1	2.38	0.53
1:A:116:LEU:HD22	1:I:168:GLY:O	2.09	0.53
1:M:167:ARG:HB3	1:O:70:MET:HE1	1.89	0.53
1:L:164:MET:HE3	1:T:72:ASP:HA	1.90	0.53
1:O:54:GLU:O	1:O:128:LYS:HD3	2.09	0.53
1:B:169:VAL:HG23	1:J:70:MET:HE1	1.90	0.53
1:J:164:MET:CE	1:J:167:ARG:HD2	2.39	0.53
1:I:64:ASP:HB3	1:I:147:LYS:HE3	1.91	0.53
1:N:19:GLN:H	1:N:19:GLN:NE2	2.06	0.53
1:C:43:ALA:HB3	1:C:47:ARG:HH12	1.74	0.52
1:M:154:ILE:HG13	1:M:181:VAL:HG12	1.91	0.52
1:P:194:GLU:O	1:P:198:LEU:HD23	2.09	0.52
1:D:78:LEU:HD21	1:D:80:LEU:HD13	1.91	0.52
1:N:63:PRO:O	1:N:66:VAL:HG22	2.10	0.52
1:I:63:PRO:O	1:I:66:VAL:HG22	2.10	0.52
1:L:140:ILE:HG22	1:L:155:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:191:SER:O	1:O:194:GLU:HG2	2.08	0.52
1:R:70:MET:HE1	1:T:167:ARG:HB3	1.91	0.52
1:A:167:ARG:HH21	1:D:51:SER:HB3	1.73	0.52
1:B:70:MET:CE	1:D:169:VAL:CG2	2.88	0.52
1:H:163:CYS:O	1:H:166:MET:HG2	2.10	0.52
1:J:78:LEU:HD13	1:J:185:PHE:HZ	1.75	0.52
1:K:121:ARG:HG2	1:K:121:ARG:HH11	1.74	0.52
1:D:184:LEU:HD23	1:D:184:LEU:O	2.09	0.52
1:C:52:TYR:CD2	1:F:28:LEU:HD11	2.45	0.51
1:K:194:GLU:O	1:K:198:LEU:HD12	2.10	0.51
1:E:28:LEU:HD21	1:H:52:TYR:CE2	2.45	0.51
1:N:34:GLU:CG	1:N:41:LEU:HD11	2.40	0.51
1:P:63:PRO:O	1:P:66:VAL:HG22	2.10	0.51
1:K:145:MET:HE3	1:K:182:ARG:HB2	1.92	0.51
1:Q:28:LEU:HD21	1:T:52:TYR:CE2	2.45	0.51
1:A:38:ARG:O	1:A:42:VAL:HG23	2.11	0.51
1:F:149:ASP:N	1:F:150:PRO:HD3	2.26	0.51
1:H:154:ILE:HD11	1:H:196:LEU:CD2	2.41	0.51
1:L:81:VAL:HG11	1:L:84:ILE:HD11	1.93	0.51
1:N:81:VAL:HG13	1:N:116:LEU:HD22	1.93	0.51
1:G:20:ARG:NH1	1:J:30:TYR:HB3	2.25	0.50
1:K:165:ALA:HB1	1:N:87:TYR:CZ	2.45	0.50
1:M:170:ARG:NH1	1:O:77:GLU:HG3	2.26	0.50
1:I:184:LEU:HD23	1:I:184:LEU:O	2.11	0.50
1:D:38:ARG:O	1:D:42:VAL:HG13	2.12	0.50
1:A:33:GLY:O	1:D:14:ARG:HD2	2.11	0.50
1:J:184:LEU:O	1:J:184:LEU:HD23	2.11	0.50
1:B:114:THR:HG23	1:B:119:ILE:CD1	2.42	0.50
1:D:81:VAL:HG13	1:D:116:LEU:CD1	2.41	0.50
1:N:106:ILE:HD11	1:N:185:PHE:CZ	2.47	0.50
1:C:63:PRO:O	1:C:66:VAL:HG22	2.11	0.50
1:D:184:LEU:HD23	1:D:184:LEU:C	2.36	0.50
1:A:115:GLY:HA2	1:I:168:GLY:O	2.12	0.50
1:B:72:ASP:OD2	1:D:164:MET:HE3	2.12	0.50
1:C:169:VAL:HG11	1:E:113:VAL:HG21	1.94	0.50
1:E:154:ILE:HG13	1:E:181:VAL:HG12	1.92	0.50
1:Q:194:GLU:O	1:Q:198:LEU:HD23	2.12	0.50
1:N:164:MET:SD	1:N:169:VAL:HB	2.52	0.49
1:B:115:GLY:HA2	1:D:168:GLY:O	2.11	0.49
1:C:28:LEU:HD21	1:F:52:TYR:CE2	2.48	0.49
1:D:164:MET:HG3	1:D:169:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:GLY:O	1:L:186:LYS:HG2	2.12	0.49
1:D:149:ASP:N	1:D:150:PRO:HD3	2.26	0.49
1:K:52:TYR:HA	1:K:55:MET:HG2	1.94	0.49
1:G:184:LEU:HD13	1:G:184:LEU:O	2.13	0.49
1:L:66:VAL:O	1:L:118:LYS:HD2	2.12	0.49
1:L:124:ASP:O	1:L:128:LYS:HD3	2.13	0.49
1:B:70:MET:HE1	1:D:169:VAL:HG23	1.95	0.49
1:D:81:VAL:HG13	1:D:116:LEU:HD11	1.95	0.49
1:C:44:THR:CG2	1:C:45:PRO:HD3	2.40	0.49
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.28	0.49
1:H:188:ASN:HB3	1:H:191:SER:HB2	1.94	0.49
1:L:20:ARG:HE	1:S:27:GLU:HG2	1.78	0.49
1:R:145:MET:HE1	1:R:152:GLY:HA2	1.94	0.49
1:M:145:MET:HE1	1:M:152:GLY:HA2	1.95	0.48
1:E:74:ASP:HB2	1:E:75:HIS:ND1	2.28	0.48
1:N:58:GLY:HA3	1:N:125:LEU:O	2.13	0.48
1:K:146:LYS:HE3	1:K:147:LYS:HE2	1.92	0.48
1:A:124:ASP:O	1:A:128:LYS:HG2	2.13	0.48
1:Q:165:ALA:HB1	1:T:87:TYR:CE2	2.48	0.48
1:I:114:THR:HG22	1:I:119:ILE:HD11	1.96	0.48
1:F:38:ARG:O	1:F:42:VAL:HG23	2.13	0.48
1:I:184:LEU:HD23	1:I:184:LEU:C	2.39	0.48
1:F:17:ASP:C	1:F:17:ASP:OD1	2.57	0.48
1:O:53:ARG:HB2	1:O:53:ARG:NH1	2.27	0.48
1:Q:63:PRO:O	1:Q:122:LEU:HD12	2.14	0.48
1:C:21:ALA:O	1:C:25:VAL:HG23	2.14	0.47
1:F:106:ILE:HD12	1:F:184:LEU:HD23	1.96	0.47
1:R:13:ILE:C	1:R:14:ARG:HD2	2.39	0.47
1:A:116:LEU:HD22	1:I:168:GLY:C	2.40	0.47
1:F:188:ASN:HB3	1:F:191:SER:HB2	1.97	0.47
1:Q:164:MET:HE3	1:S:72:ASP:HA	1.97	0.47
1:D:58:GLY:HA3	1:D:125:LEU:O	2.14	0.47
1:N:78:LEU:HD13	1:N:106:ILE:CD1	2.44	0.47
1:I:34:GLU:HG2	1:I:41:LEU:CD1	2.45	0.47
1:J:35:ASP:O	1:J:38:ARG:HG2	2.15	0.47
1:M:28:LEU:HD21	1:P:52:TYR:CE2	2.44	0.47
1:B:58:GLY:HA3	1:B:125:LEU:O	2.15	0.47
1:J:116:LEU:HD12	1:J:116:LEU:H	1.80	0.47
1:O:164:MET:HE3	1:Q:72:ASP:HA	1.97	0.47
1:P:188:ASN:HB3	1:P:191:SER:HB2	1.97	0.47
1:S:84:ILE:HD12	1:S:101:ALA:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ASP:HB3	1:K:190:ALA:HB2	1.98	0.46
1:E:145:MET:HE2	1:E:153:VAL:HG23	1.97	0.46
1:M:82:LYS:HB3	1:M:83:GLU:OE1	2.14	0.46
1:L:188:ASN:OD1	1:L:190:ALA:N	2.49	0.46
1:L:200:LEU:N	1:L:200:LEU:HD22	2.30	0.46
1:Q:169:VAL:C	1:S:116:LEU:HD21	2.40	0.46
1:S:58:GLY:HA3	1:S:125:LEU:O	2.15	0.46
1:B:168:GLY:C	1:J:116:LEU:CD1	2.88	0.46
1:P:110:ASP:OD2	1:P:112:ARG:HG3	2.16	0.46
1:A:81:VAL:HG22	1:A:116:LEU:HD12	1.96	0.46
1:O:102:HIS:CB	1:O:199:ILE:HD12	2.45	0.46
1:L:145:MET:SD	1:L:153:VAL:HG23	2.55	0.46
1:D:63:PRO:O	1:D:66:VAL:HG22	2.15	0.46
1:R:184:LEU:HD23	1:R:184:LEU:C	2.41	0.46
1:H:112:ARG:HG3	1:H:148:LEU:HD23	1.97	0.46
1:H:124:ASP:OD2	1:H:128:LYS:HE3	2.15	0.46
1:K:149:ASP:N	1:K:150:PRO:HD3	2.31	0.46
1:M:21:ALA:O	1:M:25:VAL:HG23	2.16	0.46
1:R:145:MET:SD	1:R:153:VAL:HG23	2.56	0.46
1:T:185:PHE:O	1:T:192:ARG:NH1	2.49	0.46
1:G:164:MET:HE3	1:I:72:ASP:HA	1.97	0.45
1:S:72:ASP:OD1	1:S:75:HIS:O	2.33	0.45
1:C:67:LEU:HD22	1:C:67:LEU:H	1.80	0.45
1:F:63:PRO:O	1:F:122:LEU:HD12	2.16	0.45
1:S:117:SER:O	1:S:121:ARG:CD	2.64	0.45
1:S:121:ARG:NH2	1:T:117:SER:HB2	2.31	0.45
1:B:169:VAL:CG2	1:J:70:MET:CE	2.94	0.45
1:F:196:LEU:O	1:F:200:LEU:CD2	2.63	0.45
1:H:82:LYS:NZ	1:H:199:ILE:O	2.49	0.45
1:P:164:MET:HB3	1:P:170:ARG:HG3	1.98	0.45
1:A:164:MET:HE3	1:C:72:ASP:HA	1.98	0.45
1:C:145:MET:SD	1:C:153:VAL:HG23	2.56	0.45
1:I:149:ASP:N	1:I:150:PRO:HD3	2.32	0.45
1:R:109:ASP:N	1:R:151:ARG:HH21	2.14	0.45
1:B:118:LYS:N	1:B:118:LYS:HD2	2.31	0.45
1:C:48:VAL:HG21	1:F:94:LEU:HD12	1.98	0.45
1:I:196:LEU:O	1:I:200:LEU:CD2	2.65	0.45
1:L:79:VAL:O	1:L:104:GLY:HA2	2.17	0.45
1:P:66:VAL:HG11	1:P:121:ARG:HG2	1.99	0.45
1:S:151:ARG:C	1:S:184:LEU:HD13	2.42	0.45
1:K:188:ASN:C	1:K:188:ASN:HD22	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:63:PRO:HB2	1:P:126:TYR:CE2	2.52	0.45
1:J:63:PRO:O	1:J:66:VAL:HG22	2.16	0.45
1:F:82:LYS:HB3	1:F:83:GLU:OE1	2.17	0.44
1:O:94:LEU:HD23	1:R:48:VAL:HG22	2.00	0.44
1:O:162:LEU:HD22	1:R:87:TYR:CE2	2.49	0.44
1:H:149:ASP:N	1:H:150:PRO:HD3	2.31	0.44
1:I:67:LEU:HD12	1:I:147:LYS:HG3	1.98	0.44
1:B:28:LEU:HD21	1:I:52:TYR:CE2	2.52	0.44
1:H:145:MET:HE2	1:H:150:PRO:HG2	2.00	0.44
1:S:54:GLU:HA	1:S:54:GLU:OE1	2.17	0.44
1:H:184:LEU:HD23	1:H:184:LEU:O	2.17	0.44
1:L:188:ASN:OD1	1:L:188:ASN:C	2.61	0.44
1:T:52:TYR:CE1	1:T:55:MET:HE1	2.53	0.44
1:K:184:LEU:HD23	1:K:184:LEU:C	2.43	0.44
1:O:38:ARG:NH1	1:O:41:LEU:HD11	2.33	0.44
1:G:200:LEU:HD23	1:G:200:LEU:N	2.33	0.44
1:H:186:LYS:HE2	1:K:109:ASP:O	2.17	0.44
1:K:63:PRO:HB3	1:K:125:LEU:HB2	2.00	0.44
1:L:78:LEU:HA	1:L:106:ILE:HD13	1.99	0.44
1:T:81:VAL:CG2	1:T:116:LEU:HD23	2.47	0.44
1:C:66:VAL:O	1:C:118:LYS:HD2	2.18	0.43
1:B:169:VAL:HG23	1:J:70:MET:CE	2.49	0.43
1:K:172:PRO:CB	1:N:87:TYR:OH	2.66	0.43
1:S:21:ALA:O	1:S:25:VAL:HG23	2.18	0.43
1:I:196:LEU:O	1:I:200:LEU:HD22	2.19	0.43
1:K:63:PRO:O	1:K:66:VAL:HG22	2.18	0.43
1:L:184:LEU:O	1:L:184:LEU:HD23	2.18	0.43
1:R:196:LEU:HG	1:R:200:LEU:CD1	2.49	0.43
1:E:18:GLN:HE21	1:E:53:ARG:HH22	1.65	0.43
1:F:47:ARG:HG2	1:F:50:ARG:HH22	1.82	0.43
1:J:38:ARG:O	1:J:42:VAL:HG23	2.18	0.43
1:J:149:ASP:N	1:J:150:PRO:HD3	2.34	0.43
1:K:145:MET:HE3	1:K:182:ARG:HB3	2.00	0.43
1:L:87:TYR:CD2	1:L:98:HIS:HB2	2.53	0.43
1:T:35:ASP:O	1:T:38:ARG:HG2	2.19	0.43
1:B:116:LEU:HD21	1:D:169:VAL:C	2.43	0.43
1:G:38:ARG:CG	3:G:502:CL:CL	3.03	0.43
1:K:116:LEU:HD11	1:S:169:VAL:C	2.43	0.43
1:K:115:GLY:HA2	1:S:168:GLY:O	2.18	0.43
1:O:184:LEU:C	1:O:184:LEU:HD23	2.44	0.43
1:S:81:VAL:HG13	1:S:116:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:CD2	1:D:169:VAL:C	2.92	0.43
1:C:53:ARG:HD2	1:C:53:ARG:O	2.18	0.43
1:D:145:MET:SD	1:D:150:PRO:HD2	2.58	0.43
1:O:25:VAL:HG11	1:O:45:PRO:HA	2.00	0.43
1:O:28:LEU:HD11	1:R:52:TYR:CD2	2.54	0.43
1:P:76:ASP:OD1	1:P:151:ARG:NH2	2.52	0.43
1:F:73:GLU:OE1	1:F:73:GLU:HA	2.19	0.43
1:J:184:LEU:HD23	1:J:184:LEU:C	2.43	0.43
1:F:148:LEU:HB2	1:F:150:PRO:HG3	2.01	0.43
1:G:171:LYS:HG2	1:I:80:LEU:O	2.18	0.43
1:H:63:PRO:O	1:H:66:VAL:HG22	2.19	0.43
1:Q:167:ARG:O	1:Q:168:GLY:C	2.60	0.43
1:Q:172:PRO:HB3	1:T:87:TYR:OH	2.18	0.43
1:G:169:VAL:HG11	1:I:113:VAL:HG21	2.01	0.43
1:S:103:VAL:HG22	1:S:155:VAL:HG13	1.99	0.42
1:J:50:ARG:CZ	1:J:53:ARG:HH21	2.32	0.42
1:C:27:GLU:HG2	1:F:24:ALA:HB2	2.01	0.42
1:G:94:LEU:HD12	1:J:48:VAL:HG21	2.01	0.42
1:O:169:VAL:C	1:Q:116:LEU:HD11	2.45	0.42
1:Q:184:LEU:C	1:Q:184:LEU:HD23	2.44	0.42
1:D:21:ALA:O	1:D:25:VAL:HG23	2.19	0.42
1:M:35:ASP:O	1:M:38:ARG:HG2	2.20	0.42
1:B:96:ALA:HB2	1:I:166:MET:HE3	2.00	0.42
1:C:38:ARG:O	1:C:42:VAL:HG23	2.19	0.42
1:C:68:ASN:O	1:C:112:ARG:NH2	2.52	0.42
1:C:149:ASP:N	1:C:150:PRO:HD3	2.34	0.42
1:I:135:ARG:HG2	1:I:139:GLN:NE2	2.34	0.42
1:F:72:ASP:HA	1:H:164:MET:HE3	2.01	0.42
1:K:196:LEU:O	1:K:200:LEU:CD2	2.68	0.42
1:L:145:MET:SD	1:L:153:VAL:CG2	3.07	0.42
1:B:164:MET:HE2	1:B:164:MET:HA	2.01	0.42
1:L:81:VAL:HG22	1:L:116:LEU:CD2	2.48	0.42
1:P:113:VAL:HG21	1:R:169:VAL:HG11	2.02	0.42
1:P:185:PHE:O	1:P:192:ARG:HB2	2.20	0.42
1:C:25:VAL:HG11	1:C:48:VAL:HB	2.02	0.42
1:K:164:MET:HE3	1:M:72:ASP:HA	2.02	0.42
1:K:198:LEU:O	1:K:201:ARG:HG2	2.20	0.42
1:M:122:LEU:HD22	1:M:144:LEU:HD21	2.02	0.42
1:M:145:MET:SD	1:M:153:VAL:CG2	3.07	0.42
1:R:16:PHE:HB2	1:R:60:TYR:CZ	2.55	0.42
1:F:58:GLY:HA3	1:F:125:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ALA:HB1	1:J:87:TYR:OH	2.19	0.42
1:B:168:GLY:O	1:J:115:GLY:HA2	2.19	0.42
1:E:164:MET:CE	1:E:169:VAL:HG21	2.49	0.42
1:K:63:PRO:O	1:K:122:LEU:HD12	2.20	0.42
1:L:166:MET:HE3	1:L:167:ARG:HG3	2.01	0.42
1:N:112:ARG:NH1	1:N:113:VAL:O	2.52	0.42
1:O:194:GLU:O	1:O:198:LEU:CD1	2.67	0.42
1:S:72:ASP:OD1	1:S:72:ASP:C	2.62	0.42
1:S:185:PHE:O	1:S:192:ARG:CG	2.68	0.42
1:B:52:TYR:CE2	1:I:28:LEU:HD21	2.56	0.41
1:C:87:TYR:CZ	1:F:165:ALA:HB1	2.55	0.41
1:G:52:TYR:CE2	1:J:28:LEU:HD21	2.55	0.41
1:K:196:LEU:O	1:K:200:LEU:HD22	2.20	0.41
1:R:44:THR:N	1:R:45:PRO:CD	2.83	0.41
1:T:47:ARG:HG2	1:T:50:ARG:NH2	2.35	0.41
1:T:149:ASP:N	1:T:150:PRO:HD3	2.35	0.41
1:L:67:LEU:HD23	1:L:118:LYS:HB3	2.01	0.41
1:A:149:ASP:N	1:A:150:PRO:HD3	2.35	0.41
1:B:186:LYS:O	1:B:192:ARG:NH2	2.53	0.41
1:N:91:GLU:CD	1:N:135:ARG:HH22	2.29	0.41
1:B:121:ARG:HA	1:B:121:ARG:NE	2.34	0.41
1:B:168:GLY:O	1:J:116:LEU:HD12	2.21	0.41
1:D:81:VAL:CG1	1:D:116:LEU:CD1	2.98	0.41
1:L:167:ARG:HB3	1:T:70:MET:HE1	2.03	0.41
1:R:118:LYS:HA	1:R:118:LYS:HD3	1.82	0.41
1:C:194:GLU:HG3	1:C:195:ALA:N	2.34	0.41
1:G:166:MET:HE1	1:J:51:SER:HB2	2.01	0.41
1:I:197:ASP:O	1:I:201:ARG:HG2	2.20	0.41
1:L:15:VAL:O	1:L:15:VAL:HG23	2.19	0.41
1:O:194:GLU:CG	1:O:195:ALA:N	2.83	0.41
1:P:183:GLY:O	1:P:187:THR:HG23	2.21	0.41
1:A:70:MET:CE	1:I:167:ARG:HB3	2.50	0.41
1:P:149:ASP:N	1:P:150:PRO:HD3	2.36	0.41
1:S:35:ASP:O	1:S:38:ARG:HG2	2.21	0.41
1:G:81:VAL:HG22	1:G:116:LEU:HD22	2.02	0.41
1:L:72:ASP:HA	1:N:164:MET:HE3	2.03	0.41
1:L:124:ASP:OD2	1:L:128:LYS:CE	2.69	0.41
1:B:72:ASP:OD2	1:D:164:MET:SD	2.78	0.41
1:B:114:THR:CG2	1:B:119:ILE:HD11	2.51	0.41
1:C:47:ARG:HE	1:D:73:GLU:CD	2.28	0.41
1:C:112:ARG:HD2	1:C:113:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:PHE:HB3	1:F:59:LEU:HD12	2.02	0.41
1:H:82:LYS:HE3	1:H:82:LYS:HB3	1.75	0.41
1:I:70:MET:CE	1:J:54:GLU:OE1	2.69	0.41
1:I:70:MET:HE1	1:J:54:GLU:OE1	2.21	0.41
1:O:102:HIS:HB3	1:O:199:ILE:HD12	2.03	0.41
1:R:108:GLY:HA2	1:R:151:ARG:NE	2.36	0.41
1:T:15:VAL:HG12	1:T:16:PHE:N	2.35	0.41
1:A:172:PRO:HB3	1:D:87:TYR:OH	2.21	0.41
1:B:64:ASP:HB3	1:B:147:LYS:HE3	2.03	0.41
1:G:87:TYR:HE2	1:J:162:LEU:HD22	1.86	0.41
1:M:175:VAL:O	1:M:175:VAL:HG13	2.21	0.41
1:O:29:LEU:HD12	1:O:41:LEU:CD1	2.50	0.41
1:S:117:SER:O	1:S:121:ARG:HD2	2.21	0.41
1:D:82:LYS:HB3	1:D:83:GLU:OE1	2.21	0.40
1:G:149:ASP:N	1:G:150:PRO:HD3	2.36	0.40
1:I:34:GLU:HG2	1:I:41:LEU:HD11	2.03	0.40
1:L:147:LYS:N	1:L:147:LYS:HD2	2.36	0.40
1:T:78:LEU:HD13	1:T:185:PHE:HZ	1.85	0.40
1:C:29:LEU:HD11	1:C:44:THR:HG23	2.02	0.40
1:F:66:VAL:O	1:F:118:LYS:HD2	2.21	0.40
1:K:64:ASP:HA	1:K:122:LEU:CD1	2.51	0.40
1:O:149:ASP:N	1:O:150:PRO:HD3	2.37	0.40
1:Q:168:GLY:C	1:S:116:LEU:CD2	2.93	0.40
1:S:70:MET:C	1:S:71:PHE:CD1	2.99	0.40
1:T:184:LEU:C	1:T:184:LEU:HD13	2.46	0.40
1:C:78:LEU:HD13	1:C:185:PHE:HZ	1.85	0.40
1:M:55:MET:SD	1:P:166:MET:HE1	2.61	0.40
1:N:34:GLU:CG	1:N:41:LEU:CD1	2.99	0.40
1:D:35:ASP:O	1:D:38:ARG:HG2	2.21	0.40
1:E:149:ASP:N	1:E:150:PRO:HD3	2.36	0.40
1:S:66:VAL:O	1:S:118:LYS:HD2	2.21	0.40
1:F:116:LEU:HD11	1:H:169:VAL:C	2.47	0.40
1:R:95:VAL:HG21	1:R:166:MET:HE1	2.02	0.40
1:S:63:PRO:O	1:S:122:LEU:HD12	2.22	0.40
1:S:181:VAL:HG23	1:S:186:LYS:HG2	2.04	0.40

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	187/223 (84%)	185 (99%)	2 (1%)	0	100	100
1	B	187/223 (84%)	185 (99%)	2 (1%)	0	100	100
1	C	187/223 (84%)	185 (99%)	2 (1%)	0	100	100
1	D	187/223 (84%)	183 (98%)	4 (2%)	0	100	100
1	E	187/223 (84%)	183 (98%)	4 (2%)	0	100	100
1	F	186/223 (83%)	183 (98%)	3 (2%)	0	100	100
1	G	185/223 (83%)	183 (99%)	2 (1%)	0	100	100
1	H	188/223 (84%)	185 (98%)	3 (2%)	0	100	100
1	I	187/223 (84%)	185 (99%)	2 (1%)	0	100	100
1	J	187/223 (84%)	184 (98%)	3 (2%)	0	100	100
1	K	186/223 (83%)	184 (99%)	2 (1%)	0	100	100
1	L	184/223 (82%)	182 (99%)	2 (1%)	0	100	100
1	M	184/223 (82%)	181 (98%)	3 (2%)	0	100	100
1	N	188/223 (84%)	185 (98%)	3 (2%)	0	100	100
1	O	182/223 (82%)	179 (98%)	3 (2%)	0	100	100
1	P	186/223 (83%)	183 (98%)	3 (2%)	0	100	100
1	Q	186/223 (83%)	183 (98%)	3 (2%)	0	100	100
1	R	181/223 (81%)	180 (99%)	1 (1%)	0	100	100
1	S	185/223 (83%)	182 (98%)	3 (2%)	0	100	100
1	T	187/223 (84%)	184 (98%)	3 (2%)	0	100	100
All	All	3717/4460 (83%)	3664 (99%)	53 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	153/184 (83%)	151 (99%)	2 (1%)	61	75
1	B	156/184 (85%)	156 (100%)	0	100	100
1	C	155/184 (84%)	154 (99%)	1 (1%)	78	87
1	D	156/184 (85%)	156 (100%)	0	100	100
1	E	156/184 (85%)	155 (99%)	1 (1%)	78	87
1	F	153/184 (83%)	153 (100%)	0	100	100
1	G	153/184 (83%)	151 (99%)	2 (1%)	61	75
1	H	157/184 (85%)	156 (99%)	1 (1%)	78	87
1	I	156/184 (85%)	156 (100%)	0	100	100
1	J	156/184 (85%)	154 (99%)	2 (1%)	61	75
1	K	154/184 (84%)	154 (100%)	0	100	100
1	L	154/184 (84%)	154 (100%)	0	100	100
1	M	154/184 (84%)	154 (100%)	0	100	100
1	N	157/184 (85%)	157 (100%)	0	100	100
1	O	149/184 (81%)	149 (100%)	0	100	100
1	P	155/184 (84%)	155 (100%)	0	100	100
1	Q	156/184 (85%)	156 (100%)	0	100	100
1	R	150/184 (82%)	150 (100%)	0	100	100
1	S	153/184 (83%)	151 (99%)	2 (1%)	61	75
1	T	155/184 (84%)	155 (100%)	0	100	100
All	All	3088/3680 (84%)	3077 (100%)	11 (0%)	84	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	67	LEU
1	C	196	LEU

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Mol	Chain	Res	Type
1	E	18	GLN
1	G	167	ARG
1	G	184	LEU
1	H	61	THR
1	J	71	PHE
1	J	112	ARG
1	S	27	GLU
1	S	158	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	19	GLN
1	E	18	GLN
1	F	18	GLN
1	J	75	HIS
1	K	98	HIS
1	K	188	ASN
1	N	18	GLN
1	N	19	GLN
1	N	133	GLN
1	P	75	HIS
1	Q	19	GLN
1	R	75	HIS
1	S	98	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 23 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, 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	189/223 (84%)	0.22	6 (3%) 50 48	34, 58, 91, 126	0
1	B	189/223 (84%)	0.47	9 (4%) 35 35	40, 67, 117, 147	0
1	C	189/223 (84%)	0.69	16 (8%) 16 17	49, 73, 114, 147	0
1	D	189/223 (84%)	0.25	7 (3%) 45 43	35, 54, 95, 136	0
1	E	189/223 (84%)	0.17	5 (2%) 57 54	34, 52, 83, 134	0
1	F	188/223 (84%)	0.26	7 (3%) 45 43	31, 51, 101, 125	0
1	G	187/223 (83%)	0.23	5 (2%) 56 53	37, 55, 93, 106	0
1	H	190/223 (85%)	0.14	2 (1%) 78 77	34, 54, 102, 124	0
1	I	189/223 (84%)	0.37	8 (4%) 40 39	40, 61, 100, 128	0
1	J	189/223 (84%)	0.20	4 (2%) 63 60	38, 58, 90, 98	0
1	K	188/223 (84%)	0.25	6 (3%) 50 48	35, 56, 91, 139	0
1	L	186/223 (83%)	0.59	12 (6%) 25 24	43, 72, 128, 167	0
1	M	186/223 (83%)	0.41	4 (2%) 62 59	46, 69, 100, 113	0
1	N	190/223 (85%)	0.21	4 (2%) 63 60	36, 59, 105, 130	0
1	O	184/223 (82%)	0.35	8 (4%) 40 38	34, 52, 91, 113	0
1	P	188/223 (84%)	0.31	5 (2%) 56 53	37, 59, 94, 107	0
1	Q	188/223 (84%)	0.21	5 (2%) 56 53	35, 58, 93, 127	0
1	R	185/223 (82%)	0.54	20 (10%) 11 10	35, 59, 105, 190	0
1	S	187/223 (83%)	0.49	11 (5%) 28 28	41, 66, 103, 126	0
1	T	189/223 (84%)	0.20	3 (1%) 70 68	36, 59, 91, 116	0
All	All	3759/4460 (84%)	0.33	147 (3%) 43 41	31, 60, 105, 190	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	ILE	5.2
1	C	33	GLY	4.6
1	M	15	VAL	4.2
1	L	15	VAL	4.1
1	R	45	PRO	3.9
1	D	75	HIS	3.8
1	B	202	LYS	3.7
1	R	32	ILE	3.6
1	K	75	HIS	3.6
1	L	60	TYR	3.5
1	R	29	LEU	3.3
1	I	87	TYR	3.3
1	B	63	PRO	3.2
1	B	15	VAL	3.1
1	S	125	LEU	3.1
1	R	168	GLY	3.1
1	D	76	ASP	3.0
1	F	15	VAL	3.0
1	L	63	PRO	3.0
1	S	70	MET	3.0
1	R	25	VAL	3.0
1	R	75	HIS	2.9
1	N	200	LEU	2.9
1	C	63	PRO	2.9
1	R	13	ILE	2.9
1	M	169	VAL	2.9
1	S	108	GLY	2.9
1	Q	42	VAL	2.9
1	S	200	LEU	2.9
1	C	30	TYR	2.8
1	R	36	PRO	2.8
1	S	63	PRO	2.8
1	L	200	LEU	2.8
1	J	15	VAL	2.8
1	M	63	PRO	2.8
1	K	76	ASP	2.8
1	P	75	HIS	2.8
1	N	170	ARG	2.8
1	B	125	LEU	2.8
1	B	200	LEU	2.8
1	C	29	LEU	2.8
1	M	200	LEU	2.7
1	O	51	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	25	VAL	2.7
1	R	34	GLU	2.7
1	D	200	LEU	2.7
1	S	170	ARG	2.7
1	D	202	LYS	2.7
1	I	166	MET	2.7
1	B	14	ARG	2.7
1	A	171	LYS	2.7
1	L	74	ASP	2.7
1	Q	76	ASP	2.7
1	B	75	HIS	2.6
1	K	60	TYR	2.6
1	D	125	LEU	2.6
1	F	75	HIS	2.6
1	L	75	HIS	2.6
1	E	73	GLU	2.6
1	I	61	THR	2.6
1	O	74	ASP	2.6
1	P	76	ASP	2.6
1	R	35	ASP	2.6
1	K	15	VAL	2.6
1	P	167	ARG	2.6
1	R	37	ASP	2.5
1	F	19	GLN	2.5
1	C	55	MET	2.5
1	R	169	VAL	2.5
1	S	69	THR	2.5
1	S	75	HIS	2.5
1	F	16	PHE	2.5
1	A	148	LEU	2.4
1	R	76	ASP	2.4
1	D	63	PRO	2.4
1	C	48	VAL	2.4
1	P	169	VAL	2.4
1	D	69	THR	2.4
1	N	171	LYS	2.4
1	R	19	GLN	2.4
1	C	14	ARG	2.4
1	R	30	TYR	2.4
1	L	116	LEU	2.4
1	B	183	GLY	2.4
1	P	16	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	134	GLU	2.3
1	E	171	LYS	2.3
1	Q	171	LYS	2.3
1	O	28	LEU	2.3
1	C	44	THR	2.3
1	R	170	ARG	2.3
1	E	202	LYS	2.3
1	H	76	ASP	2.3
1	L	66	VAL	2.3
1	K	125	LEU	2.3
1	Q	166	MET	2.3
1	I	70	MET	2.2
1	A	151	ARG	2.2
1	C	15	VAL	2.2
1	L	125	LEU	2.2
1	G	60	TYR	2.2
1	C	36	PRO	2.2
1	J	200	LEU	2.2
1	C	66	VAL	2.2
1	I	13	ILE	2.2
1	G	201	ARG	2.2
1	F	76	ASP	2.2
1	S	76	ASP	2.2
1	Q	170	ARG	2.2
1	J	164	MET	2.2
1	G	75	HIS	2.2
1	T	75	HIS	2.2
1	O	23	ALA	2.1
1	L	67	LEU	2.1
1	O	200	LEU	2.1
1	H	75	HIS	2.1
1	T	15	VAL	2.1
1	R	171	LYS	2.1
1	R	18	GLN	2.1
1	L	199	ILE	2.1
1	C	46	SER	2.1
1	S	167	ARG	2.1
1	O	61	THR	2.1
1	N	164	MET	2.1
1	R	166	MET	2.1
1	I	125	LEU	2.1
1	S	111	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	66	VAL	2.1
1	I	79	VAL	2.1
1	T	76	ASP	2.1
1	J	194	GLU	2.1
1	G	164	MET	2.1
1	I	75	HIS	2.1
1	A	76	ASP	2.0
1	C	49	ALA	2.0
1	O	27	GLU	2.0
1	K	168	GLY	2.0
1	C	42	VAL	2.0
1	E	66	VAL	2.0
1	G	169	VAL	2.0
1	O	48	VAL	2.0
1	A	14	ARG	2.0
1	C	26	ARG	2.0
1	E	112	ARG	2.0
1	R	26	ARG	2.0
1	F	200	LEU	2.0
1	L	87	TYR	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 oligosaccharides 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, 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
3	CL	G	502	1/1	0.92	0.08	67,67,67,67	0
3	CL	J	502	1/1	0.92	0.22	79,79,79,79	0
3	CL	F	502	1/1	0.93	0.10	70,70,70,70	0

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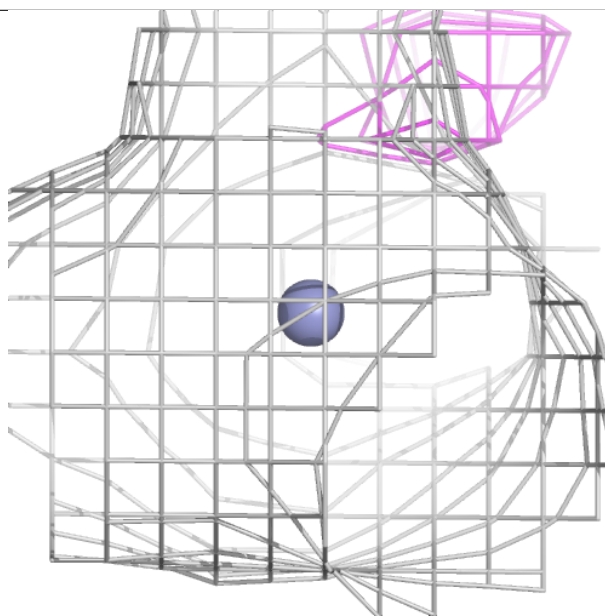
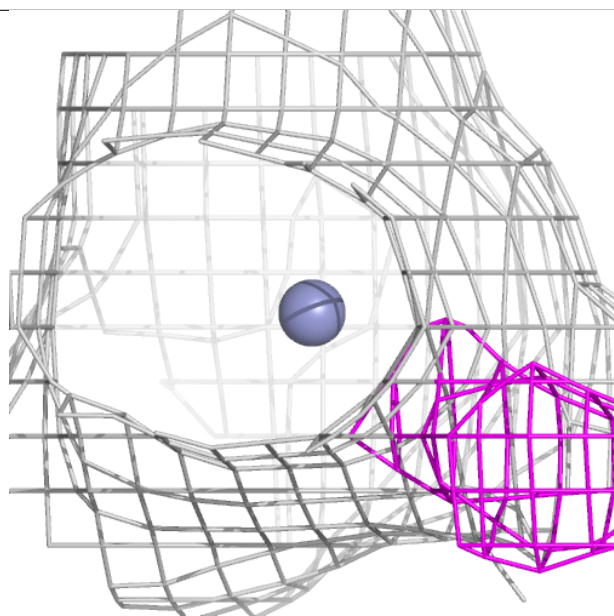
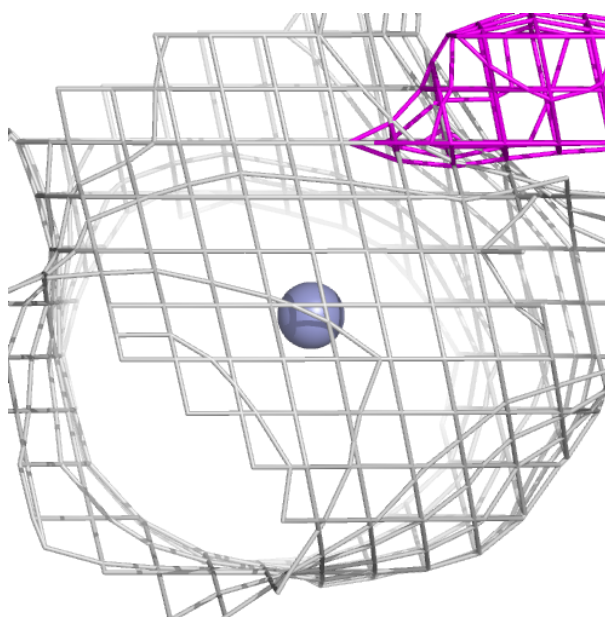
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	M	501	1/1	0.98	0.04	61,61,61,61	0
2	ZN	S	501	1/1	0.98	0.05	57,57,57,57	0
2	ZN	A	501	1/1	0.98	0.12	82,82,82,82	0
2	ZN	C	501	1/1	0.98	0.04	66,66,66,66	0
2	ZN	H	501	1/1	0.98	0.11	74,74,74,74	0
2	ZN	K	501	1/1	0.99	0.02	38,38,38,38	0
2	ZN	D	501	1/1	0.99	0.04	58,58,58,58	0
2	ZN	N	501	1/1	0.99	0.03	58,58,58,58	0
2	ZN	O	501	1/1	0.99	0.03	65,65,65,65	0
2	ZN	P	501	1/1	0.99	0.03	44,44,44,44	0
2	ZN	Q	501	1/1	0.99	0.02	44,44,44,44	0
2	ZN	R	501	1/1	0.99	0.03	57,57,57,57	0
2	ZN	F	501	1/1	0.99	0.03	44,44,44,44	0
2	ZN	T	501	1/1	0.99	0.04	53,53,53,53	0
2	ZN	B	501	1/1	0.99	0.05	61,61,61,61	0
2	ZN	I	501	1/1	0.99	0.03	42,42,42,42	0
2	ZN	J	501	1/1	0.99	0.12	65,65,65,65	0
2	ZN	L	501	1/1	1.00	0.02	46,46,46,46	0
2	ZN	E	501	1/1	1.00	0.04	37,37,37,37	0
2	ZN	G	501	1/1	1.00	0.02	60,60,60,60	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.

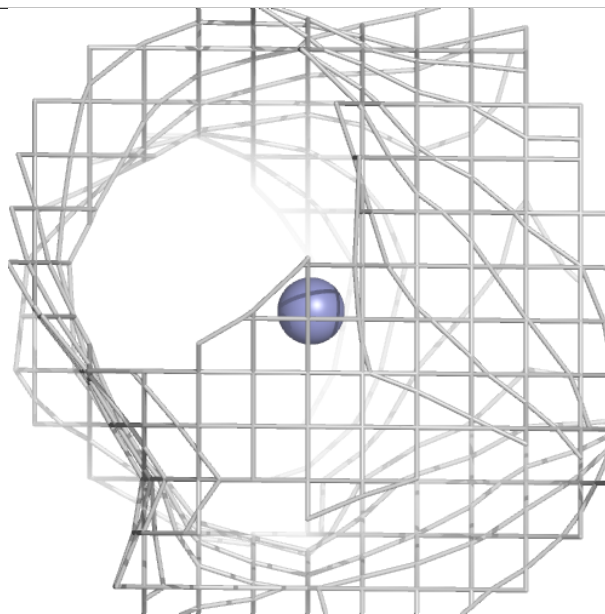
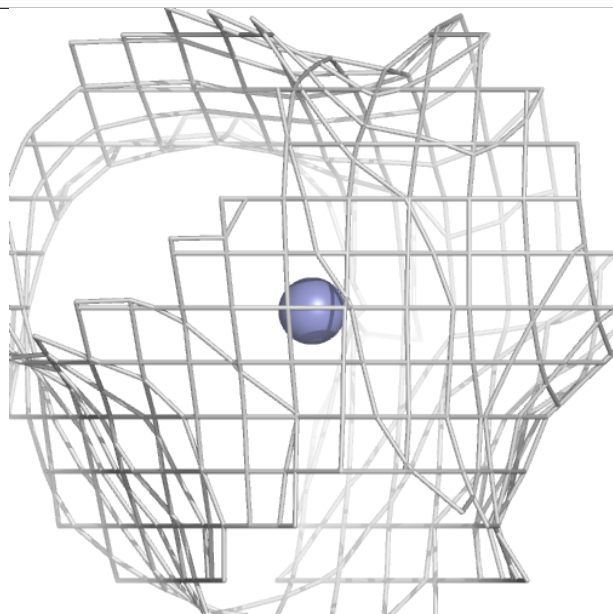
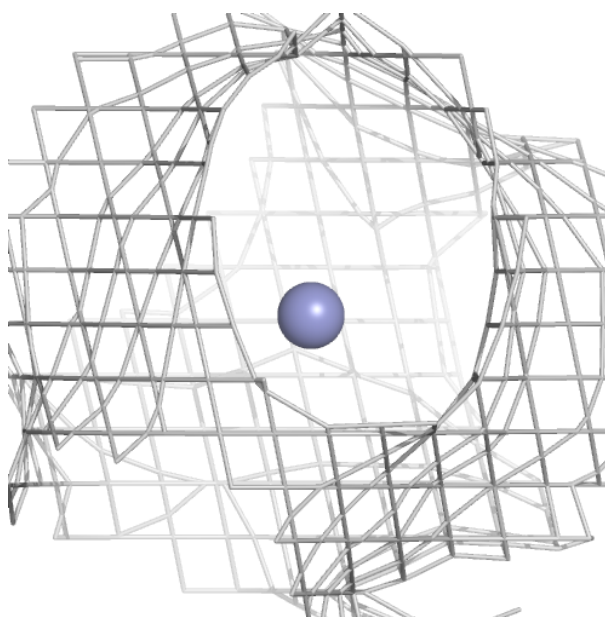
Electron density around ZN M 501:

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



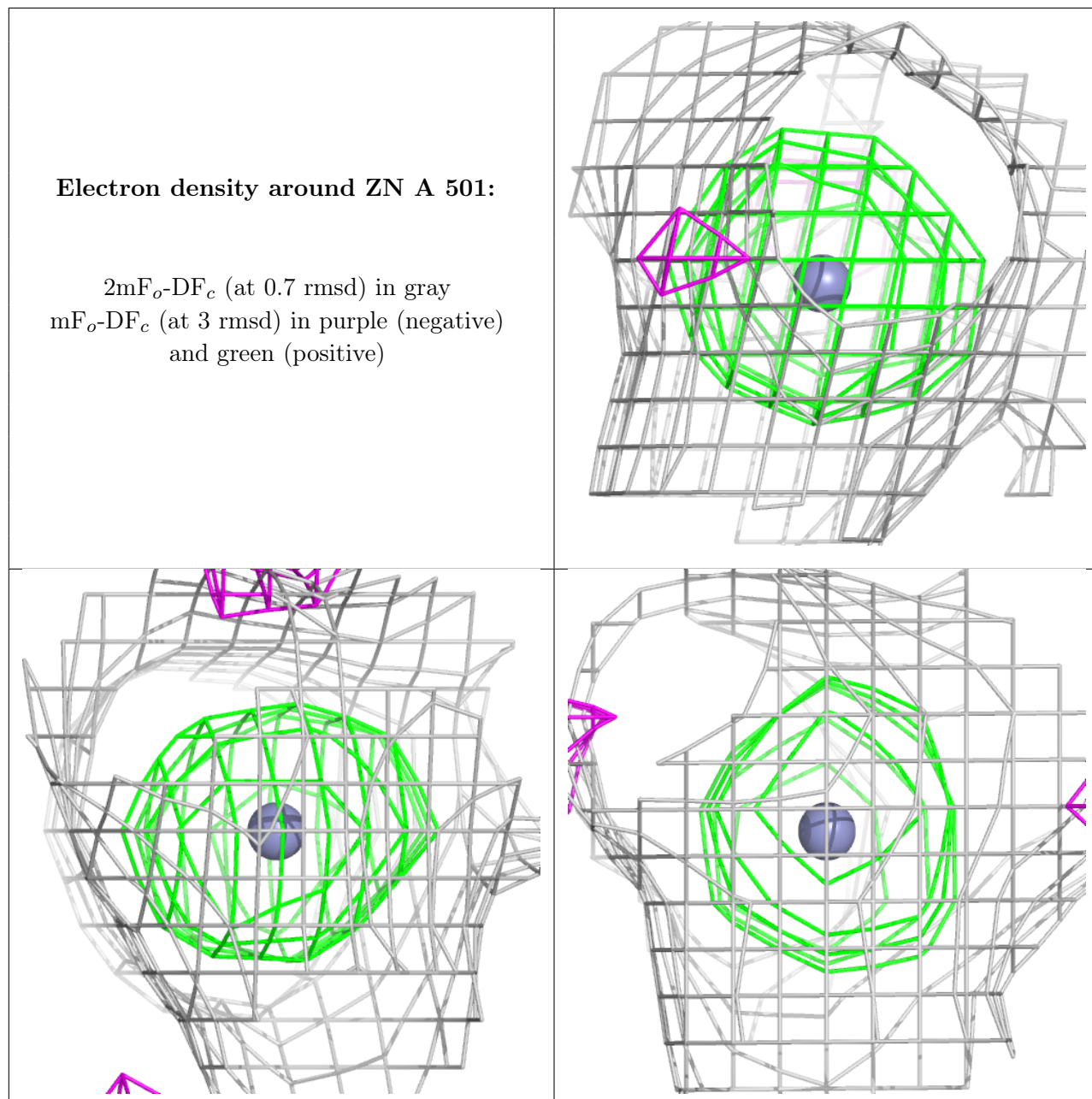
Electron density around ZN S 501:

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and green (positive)



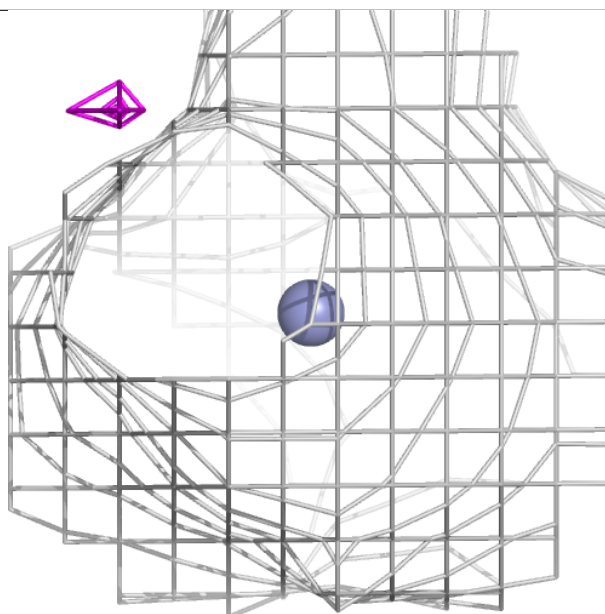
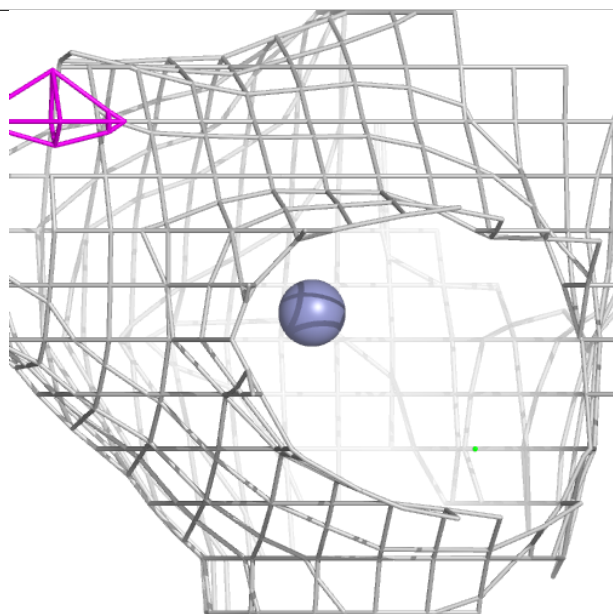
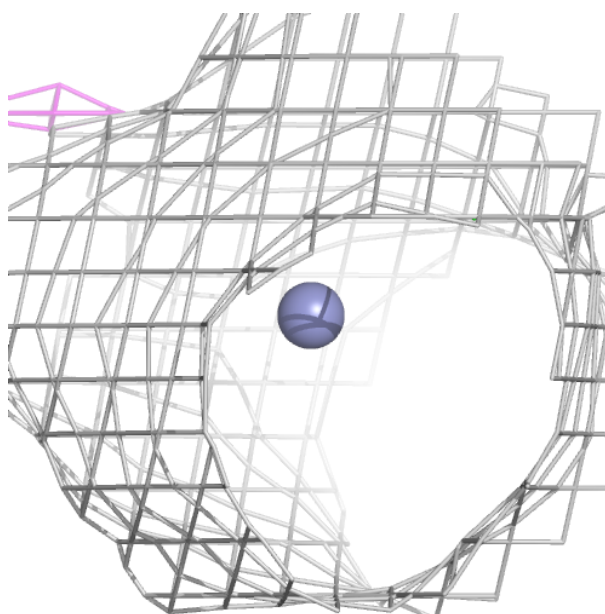
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and green (positive)



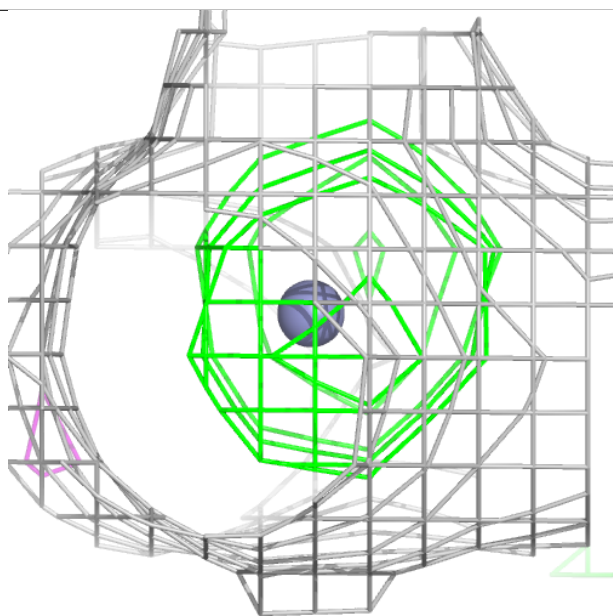
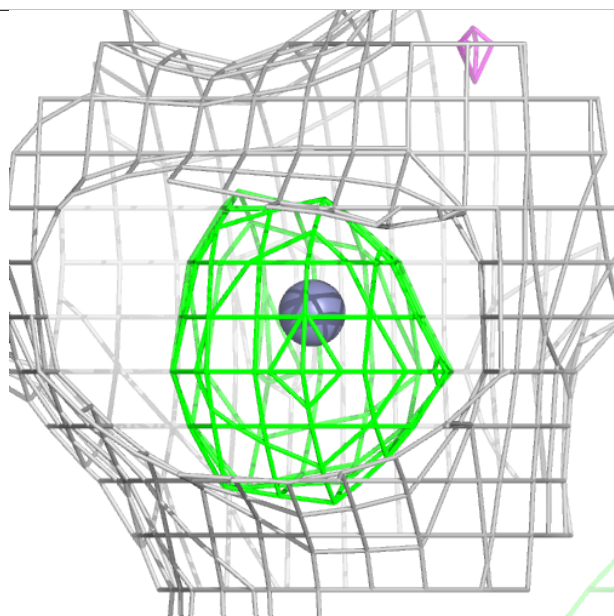
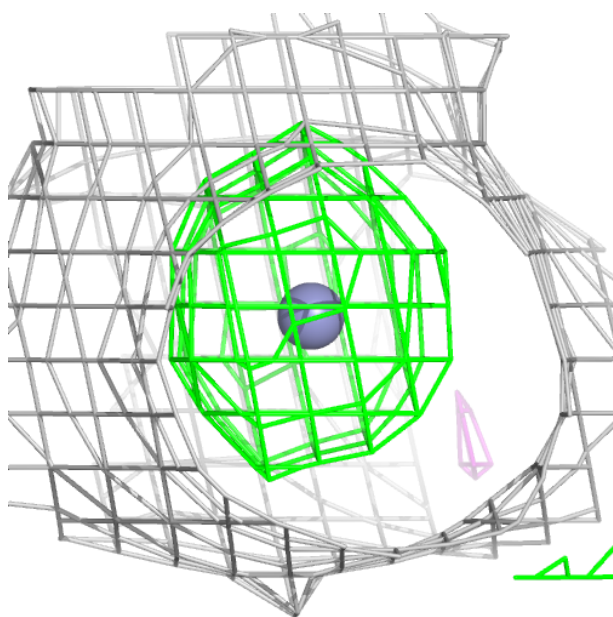
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and green (positive)



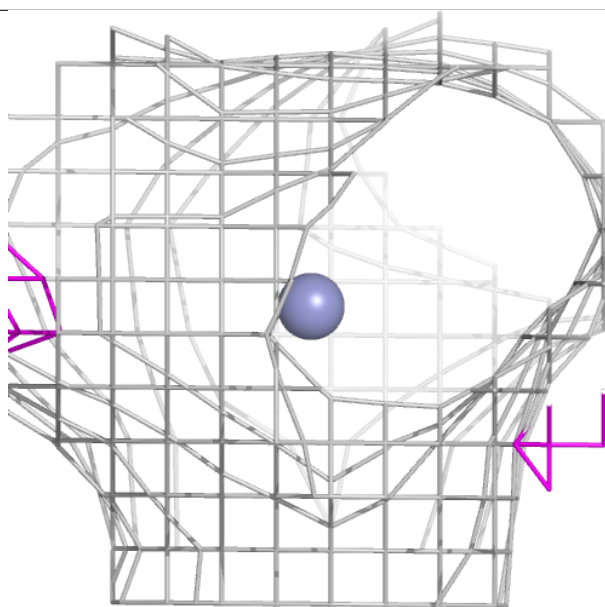
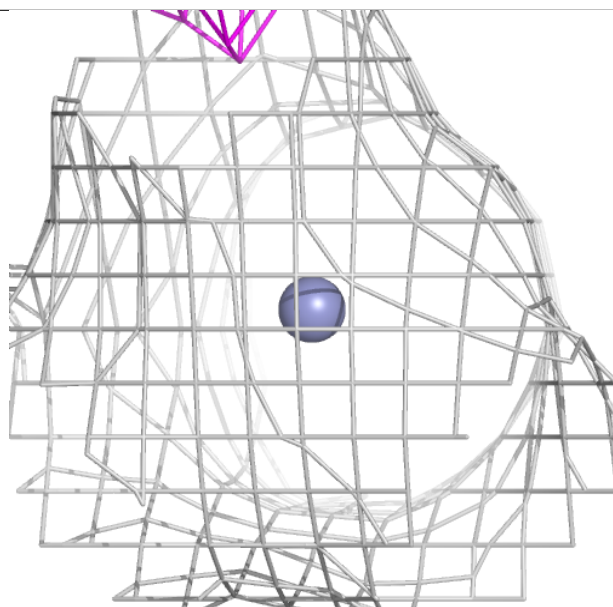
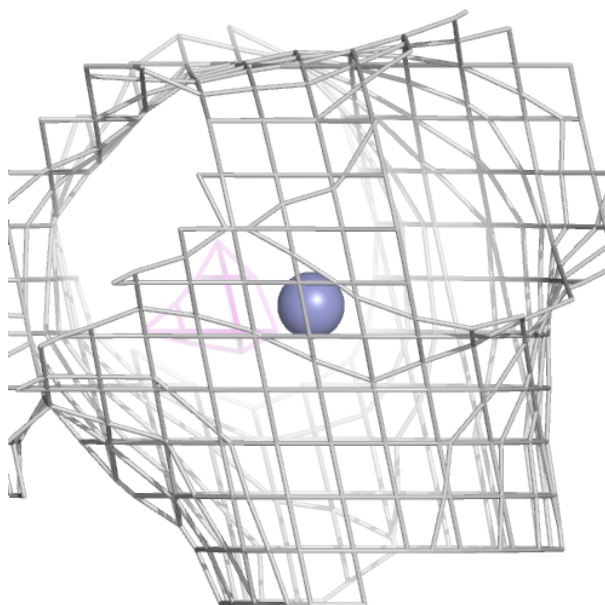
Electron density around ZN H 501:

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and green (positive)



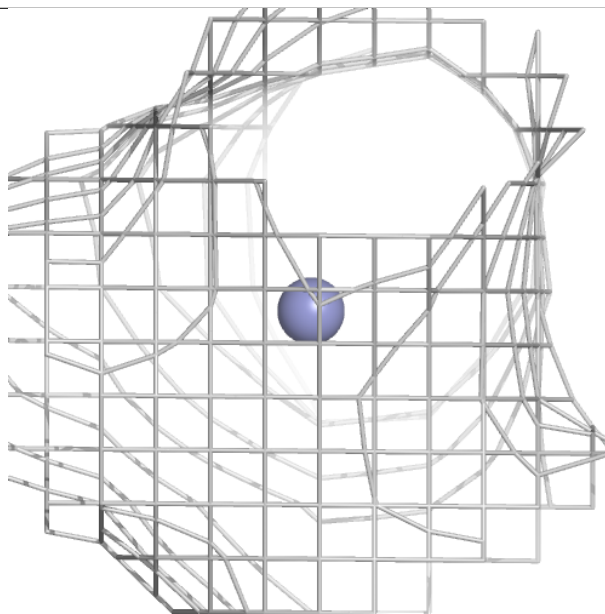
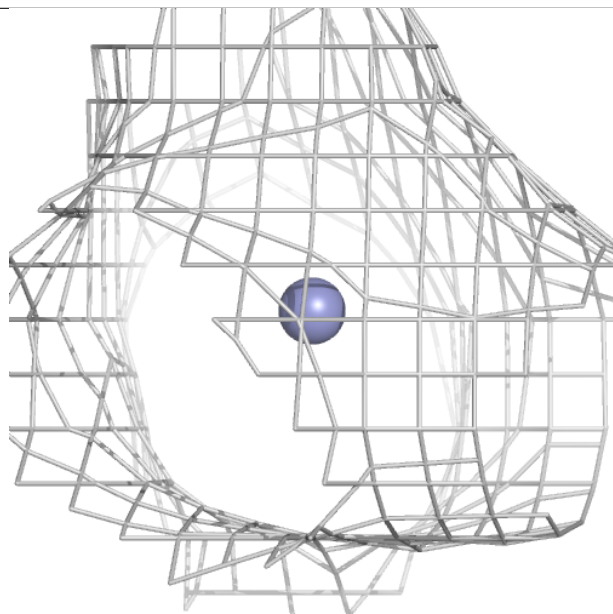
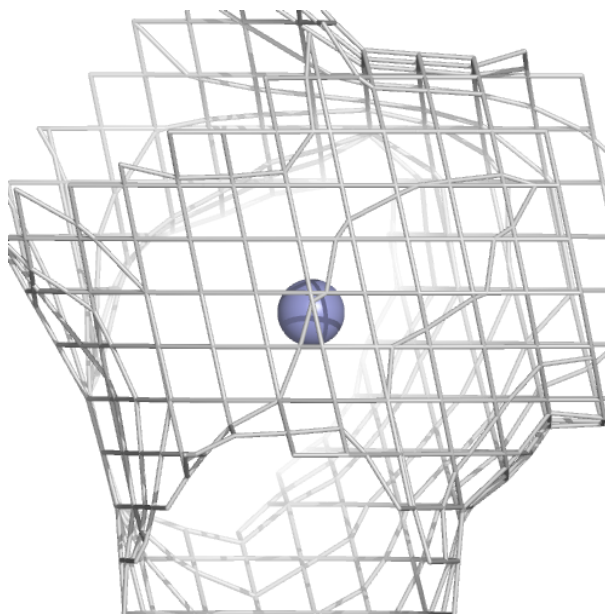
Electron density around ZN K 501:

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and green (positive)



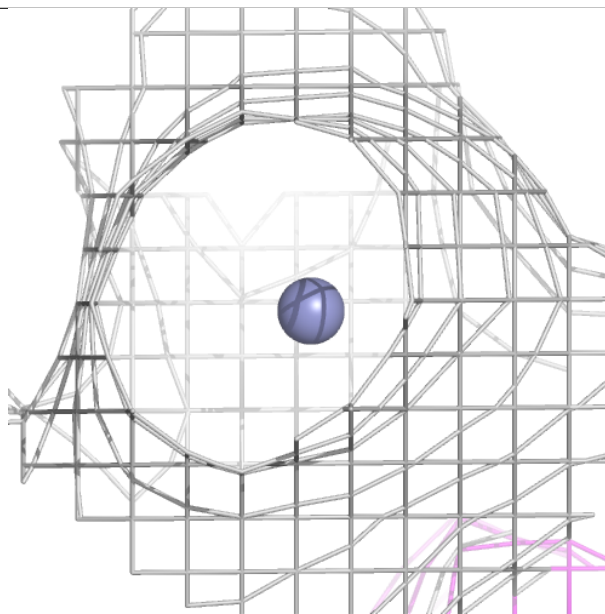
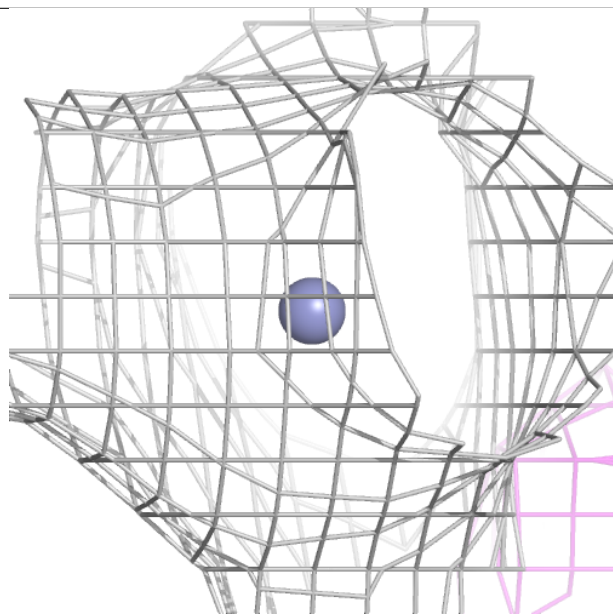
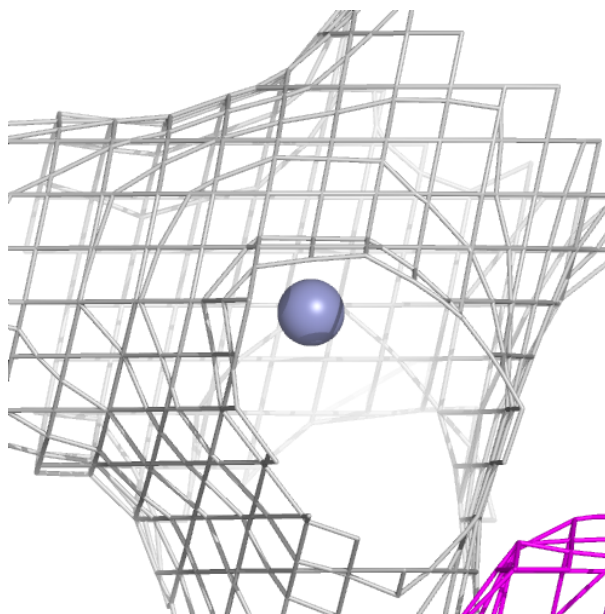
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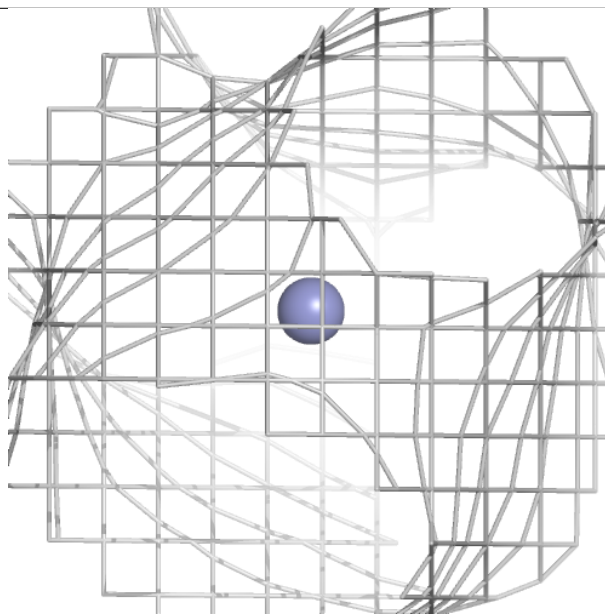
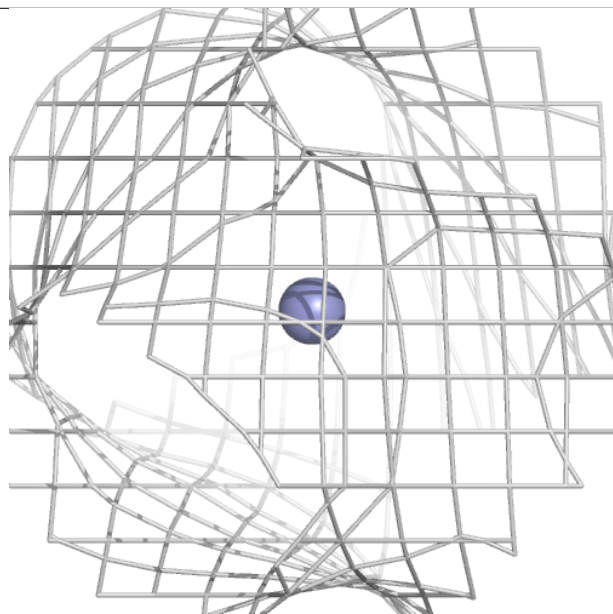
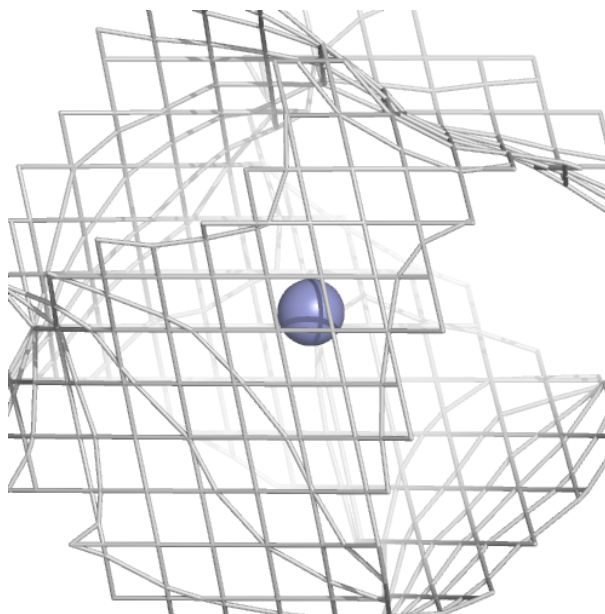
Electron density around ZN N 501:

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and green (positive)



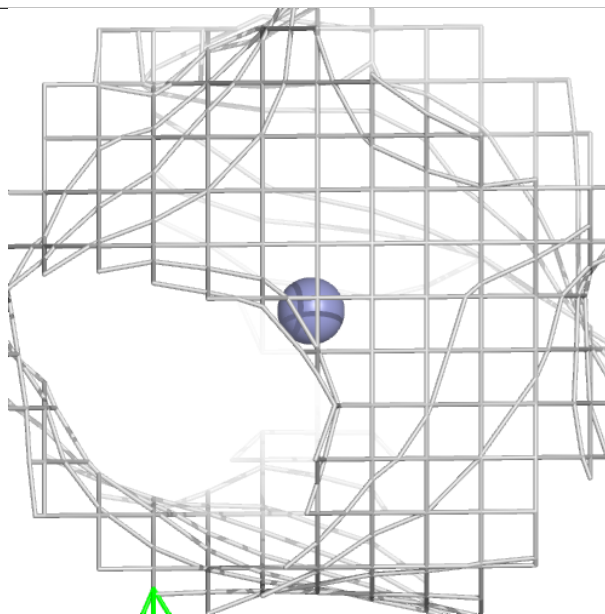
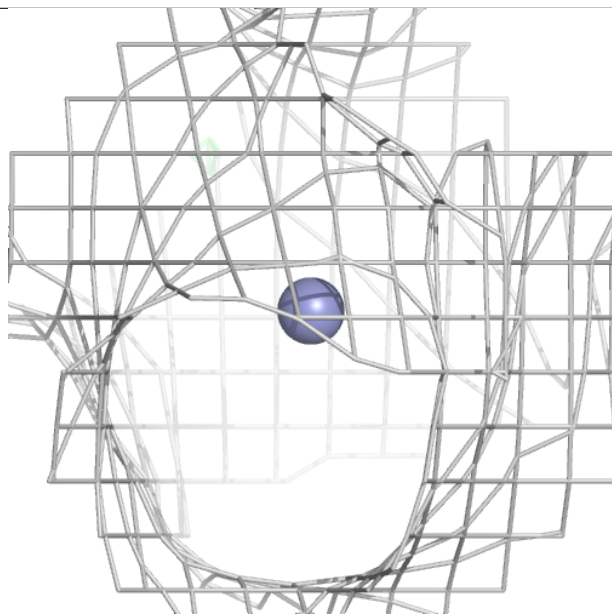
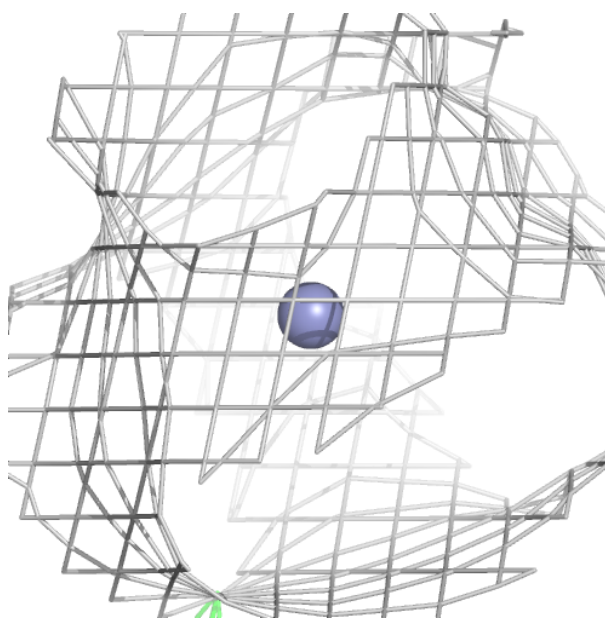
Electron density around ZN O 501:

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and green (positive)



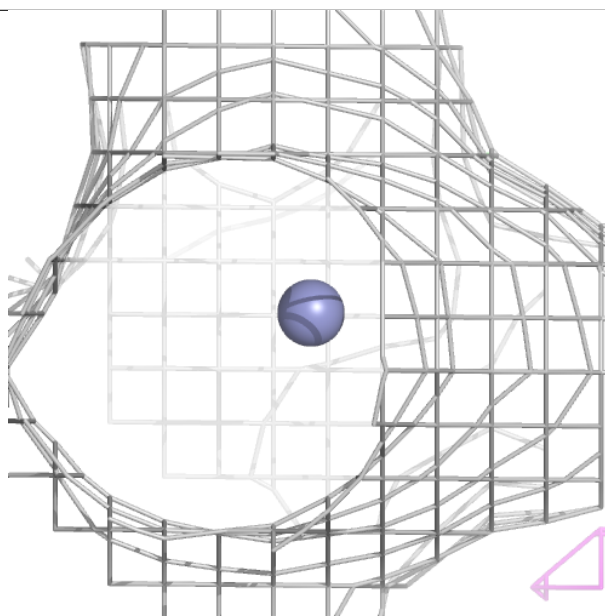
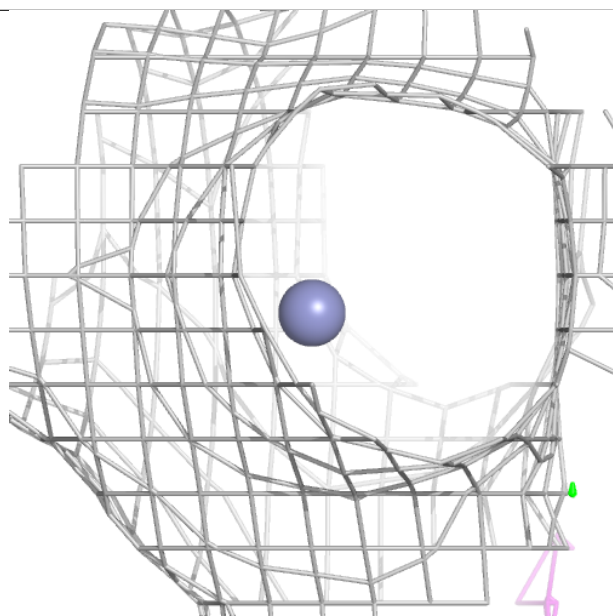
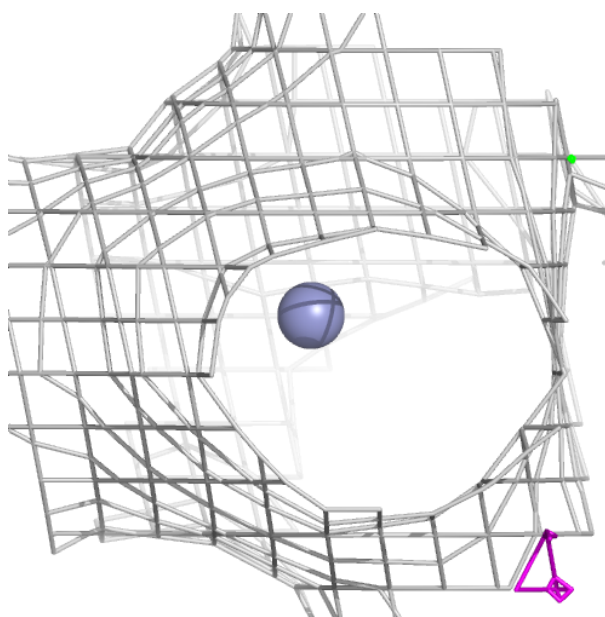
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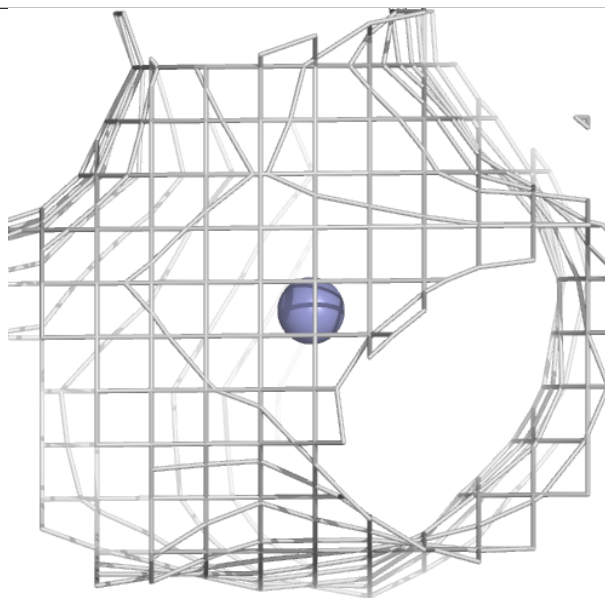
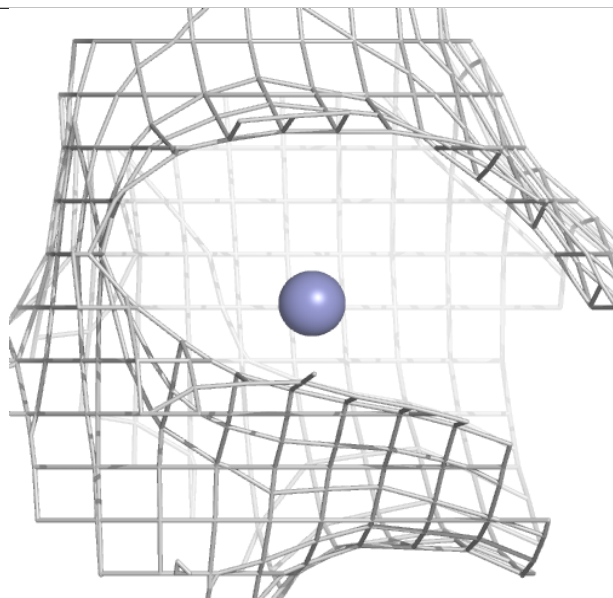
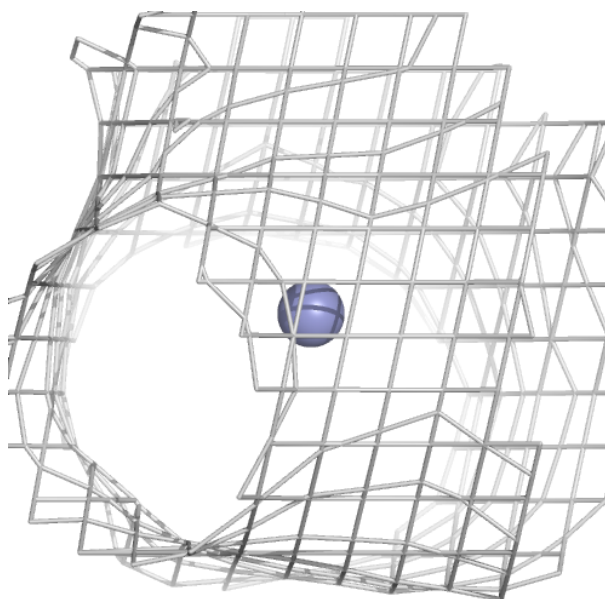
Electron density around ZN Q 501:

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and green (positive)



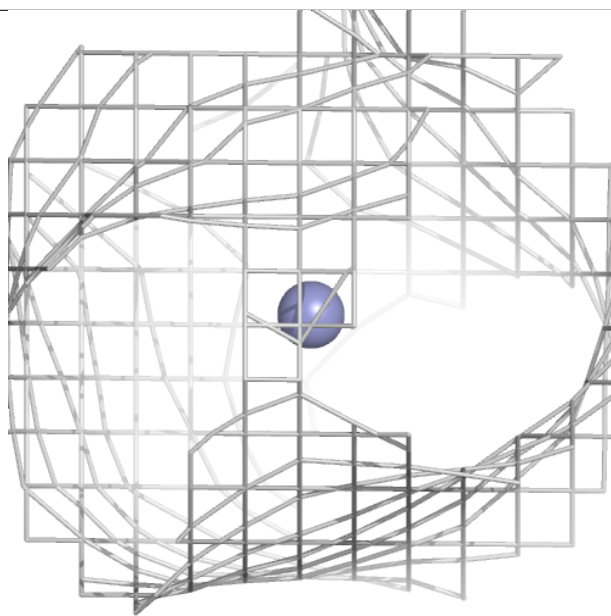
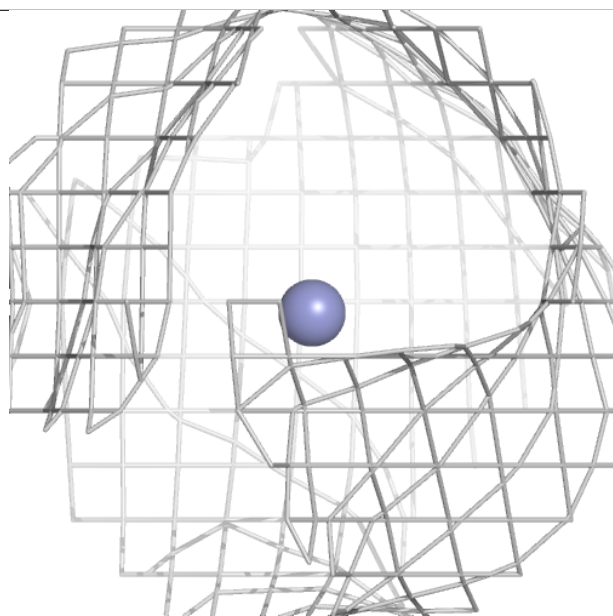
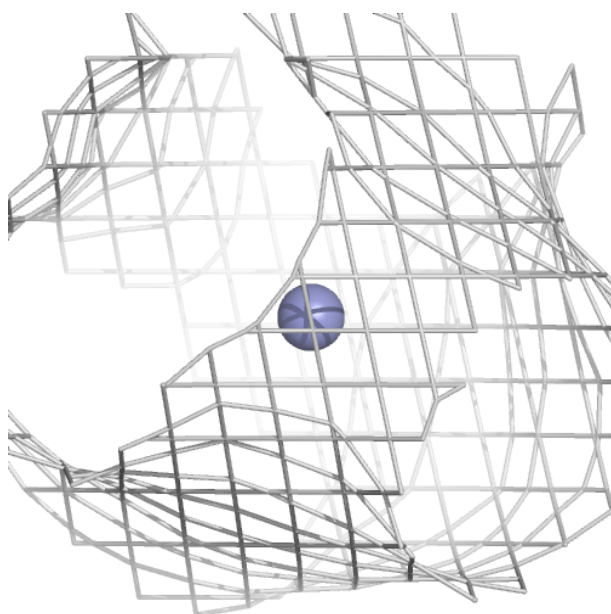
Electron density around ZN R 501:

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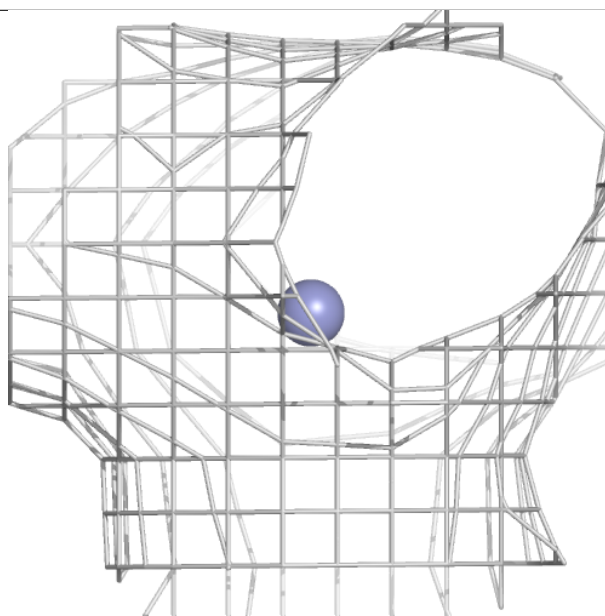
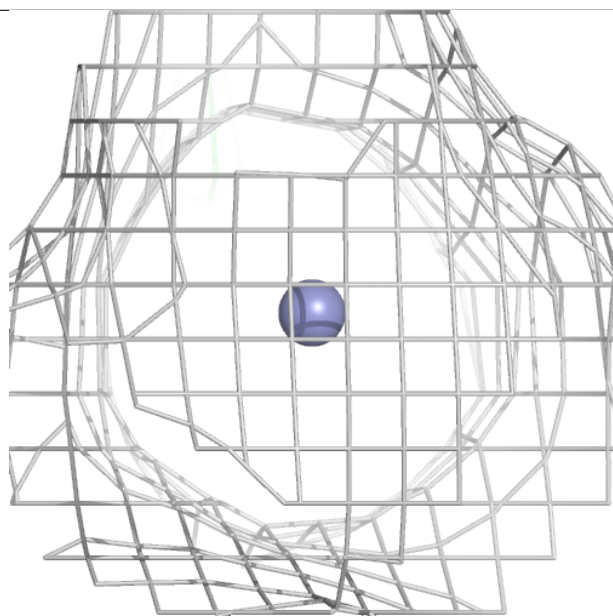
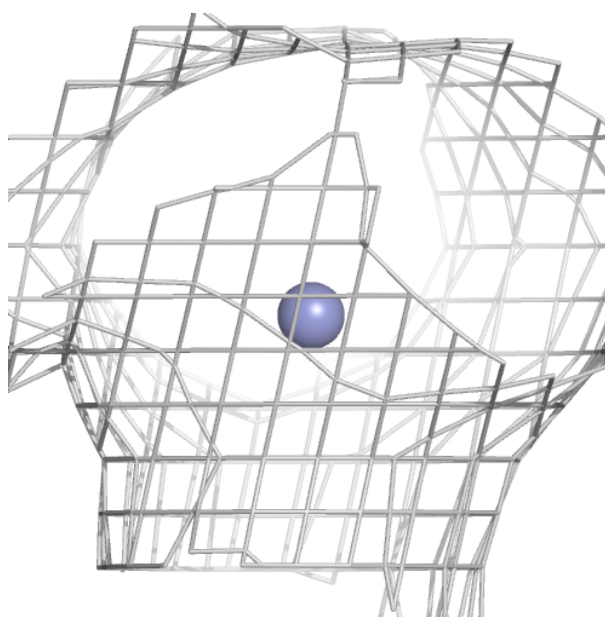
Electron density around ZN F 501:

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



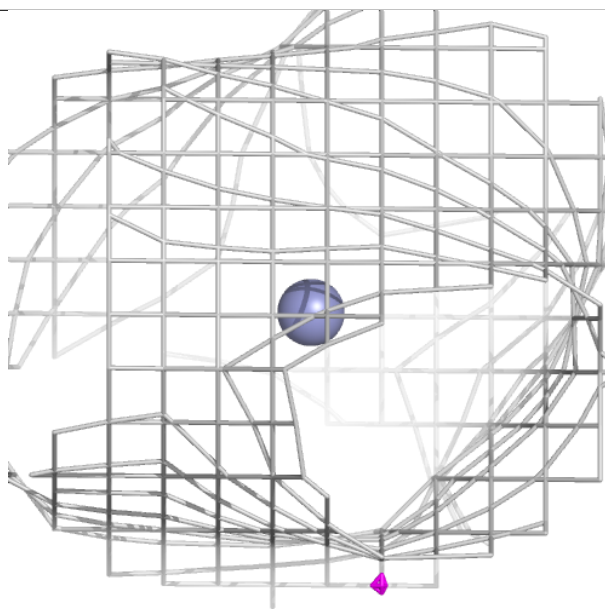
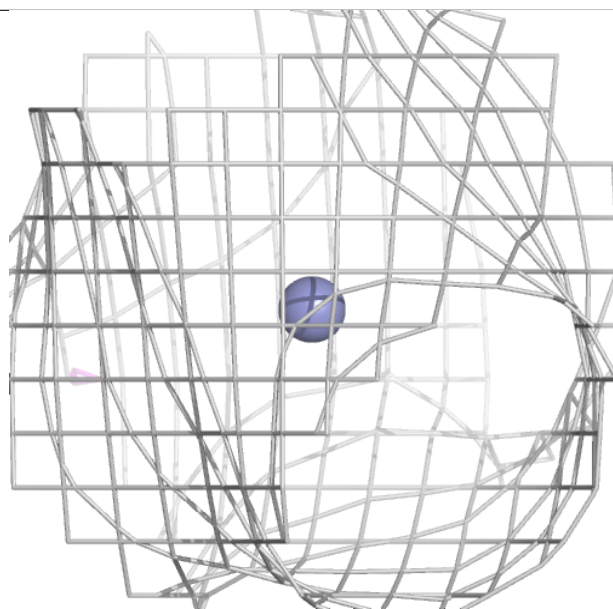
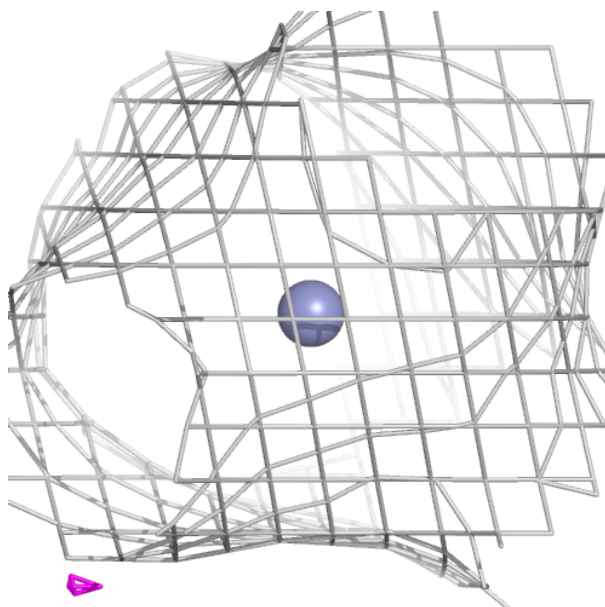
Electron density around ZN T 501:

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



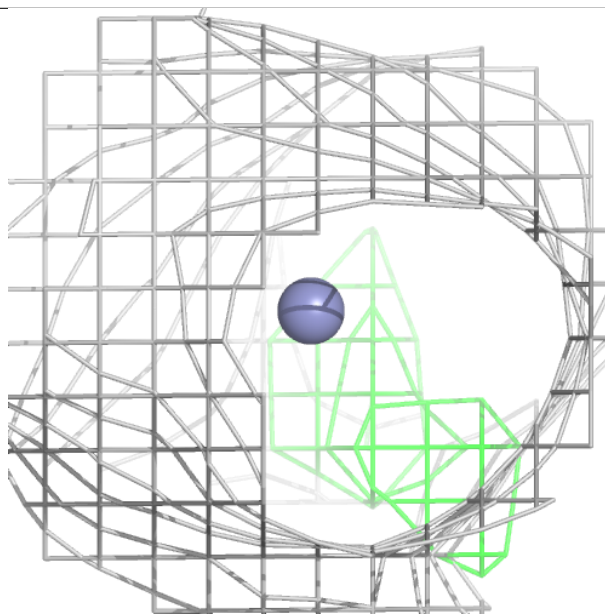
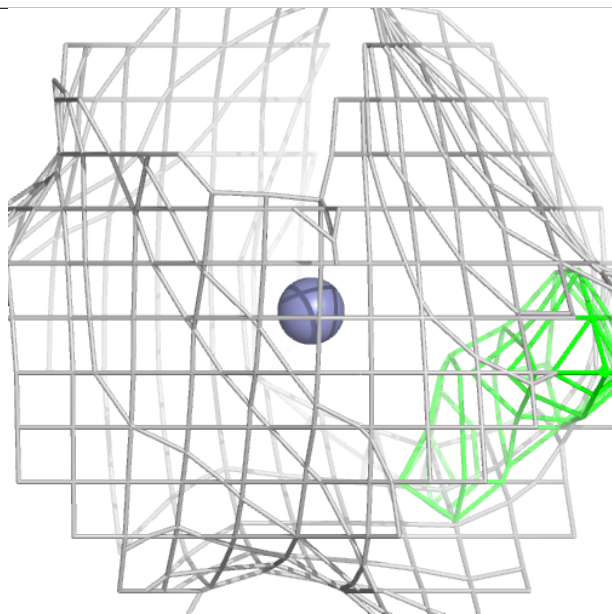
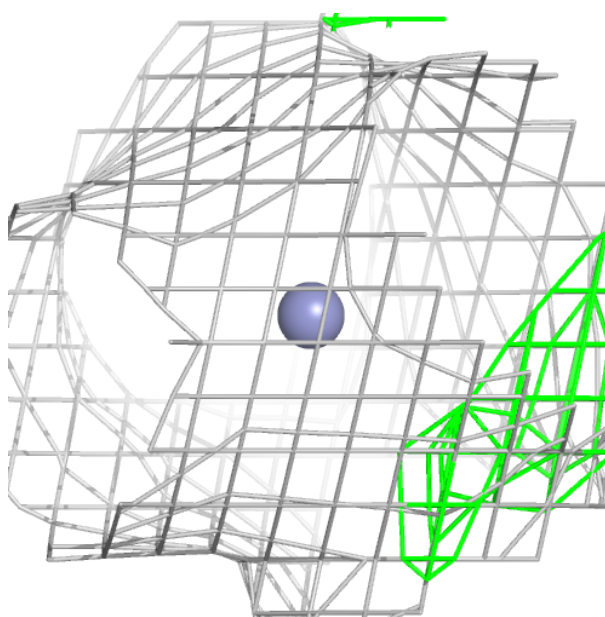
Electron density around ZN B 501:

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



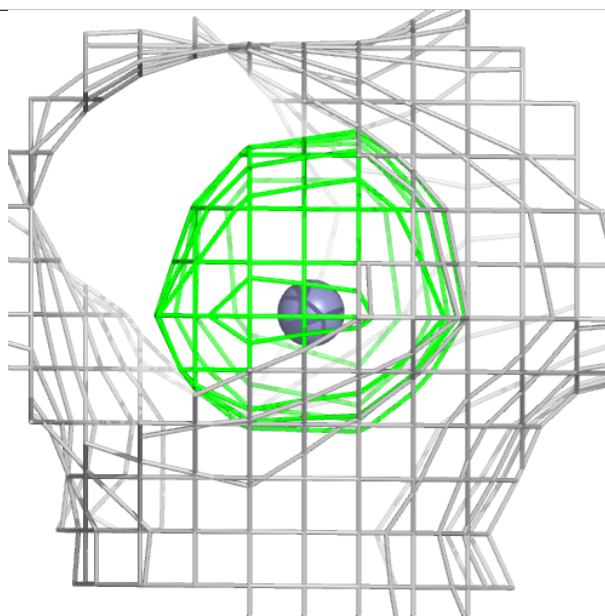
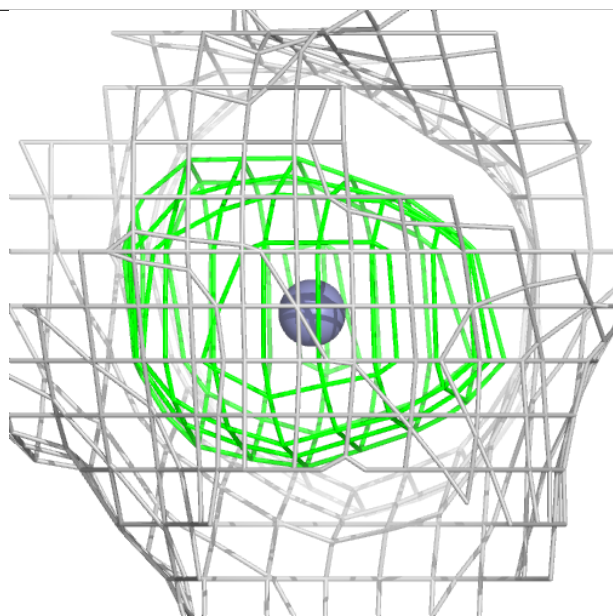
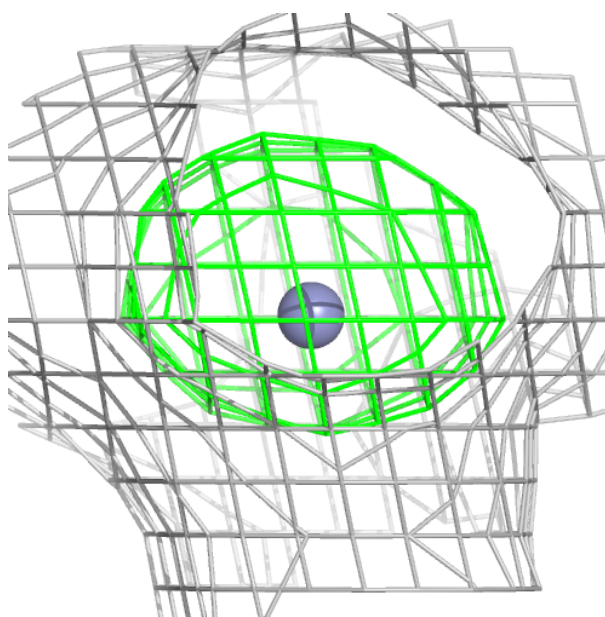
Electron density around ZN I 501:

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



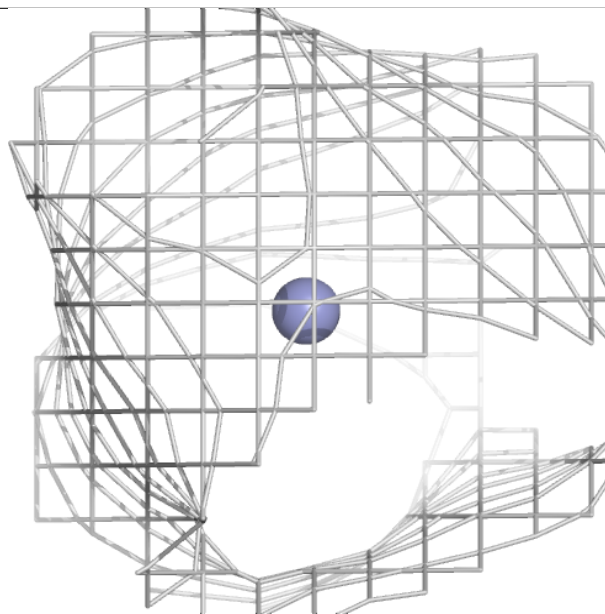
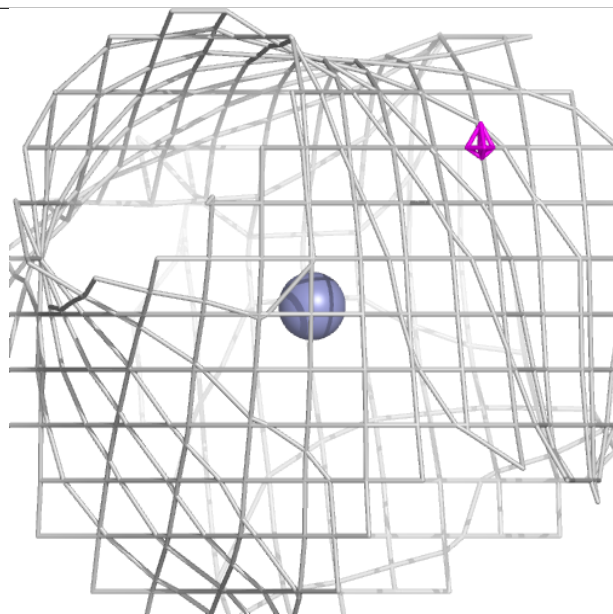
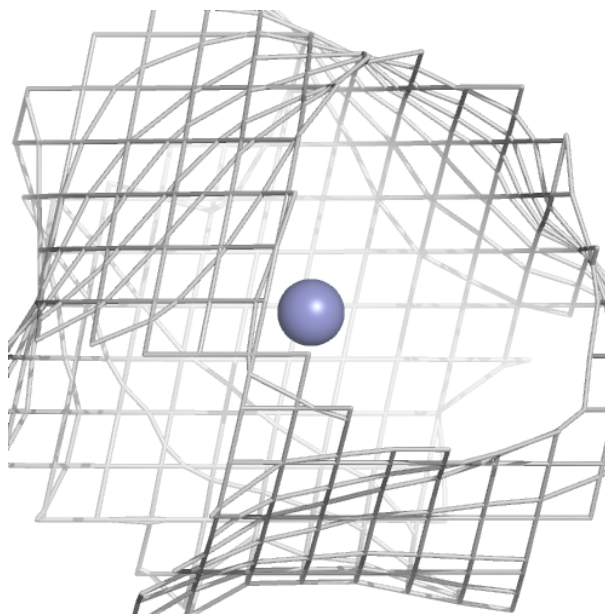
Electron density around ZN J 501:

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



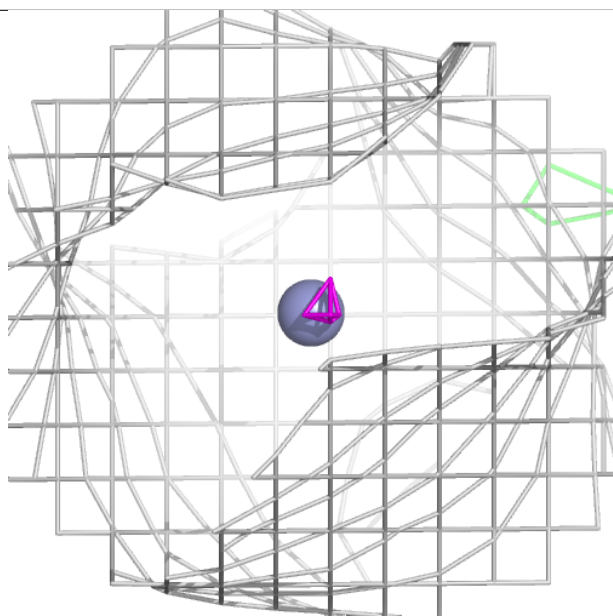
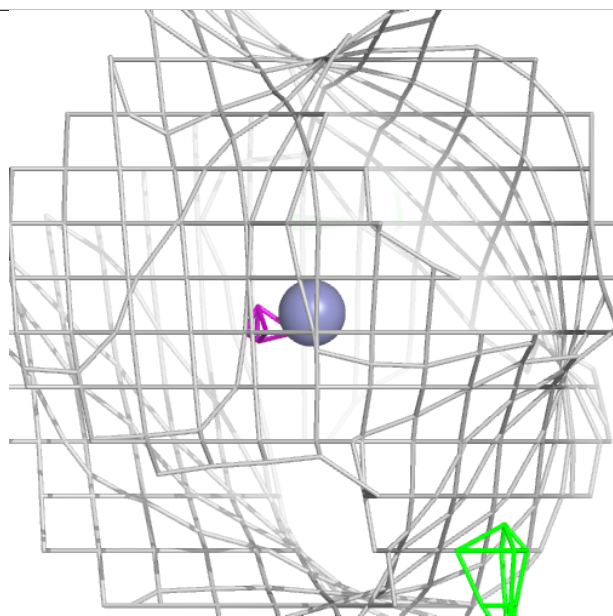
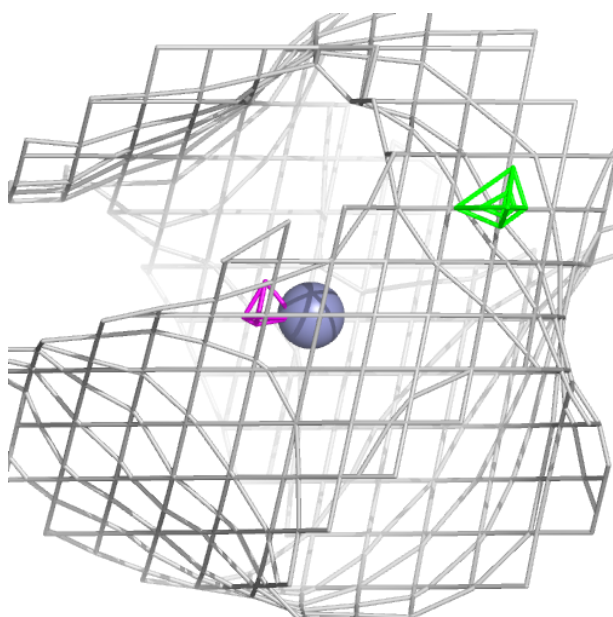
Electron density around ZN L 501:

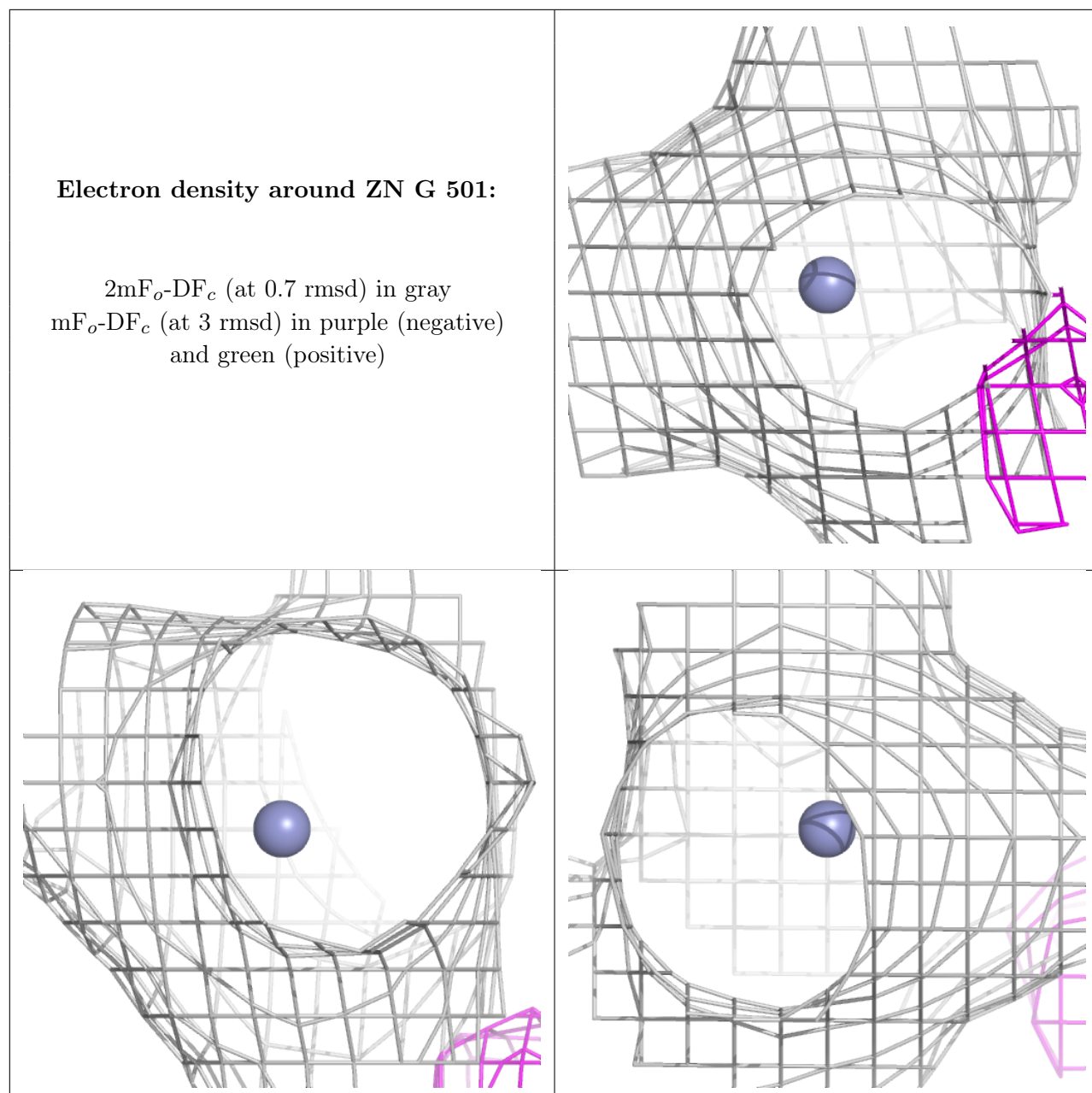
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.