Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 02:49 PM JST

PDB ID	:	7CPI
Title	:	His-Mediated Reversible Self-assembly of Ferritin Nanocage with Zn binding
Authors	:	Gu, C.; Zhang, T.; Zhao, G.
Deposited on	:	2020-08-07
Resolution	:	2.60 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 (i) 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 (1)) were used in the production of this report:

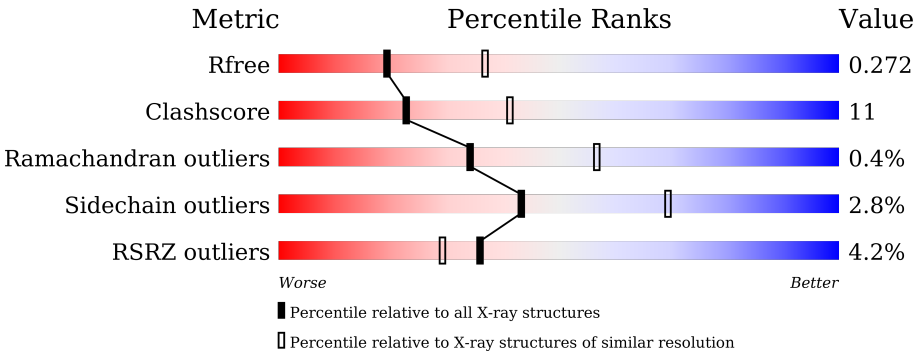
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	169	5% 82% 15%
1	B	169	5% 72% 24%
1	C	169	3% 71% 26%
1	D	169	3% 78% 20%
1	E	169	4% 79% 18%
1	F	169	5% 74% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16133 atoms, of which 7866 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 Ferritin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	167	Total	C	H	N	O	S	0	0	0
			2683	859	1311	238	268	7			
1	A	167	Total	C	H	N	O	S	0	0	0
			2683	859	1311	238	268	7			
1	B	167	Total	C	H	N	O	S	0	0	0
			2683	859	1311	238	268	7			
1	C	167	Total	C	H	N	O	S	0	0	0
			2683	859	1311	238	268	7			
1	D	167	Total	C	H	N	O	S	0	0	0
			2683	859	1311	238	268	7			
1	F	167	Total	C	H	N	O	S	0	0	0
			2683	859	1311	238	268	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	89	ARG	GLN	engineered mutation	UNP T2B7E1
E	157	HIS	-	expression tag	UNP T2B7E1
E	158	HIS	-	expression tag	UNP T2B7E1
E	159	HIS	-	expression tag	UNP T2B7E1
E	160	HIS	-	expression tag	UNP T2B7E1
E	161	HIS	-	expression tag	UNP T2B7E1
E	162	HIS	-	expression tag	UNP T2B7E1
E	163	GLU	-	expression tag	UNP T2B7E1
E	164	TYR	-	expression tag	UNP T2B7E1
E	165	MET	-	expression tag	UNP T2B7E1
E	166	PHE	-	expression tag	UNP T2B7E1
E	167	ASP	-	expression tag	UNP T2B7E1
E	168	LYS	-	expression tag	UNP T2B7E1
E	169	GLU	-	expression tag	UNP T2B7E1
E	170	LEU	-	expression tag	UNP T2B7E1
E	171	ASN	-	expression tag	UNP T2B7E1
A	89	ARG	GLN	engineered mutation	UNP T2B7E1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	157	HIS	-	expression tag	UNP T2B7E1
A	158	HIS	-	expression tag	UNP T2B7E1
A	159	HIS	-	expression tag	UNP T2B7E1
A	160	HIS	-	expression tag	UNP T2B7E1
A	161	HIS	-	expression tag	UNP T2B7E1
A	162	HIS	-	expression tag	UNP T2B7E1
A	163	GLU	-	expression tag	UNP T2B7E1
A	164	TYR	-	expression tag	UNP T2B7E1
A	165	MET	-	expression tag	UNP T2B7E1
A	166	PHE	-	expression tag	UNP T2B7E1
A	167	ASP	-	expression tag	UNP T2B7E1
A	168	LYS	-	expression tag	UNP T2B7E1
A	169	GLU	-	expression tag	UNP T2B7E1
A	170	LEU	-	expression tag	UNP T2B7E1
A	171	ASN	-	expression tag	UNP T2B7E1
B	89	ARG	GLN	engineered mutation	UNP T2B7E1
B	157	HIS	-	expression tag	UNP T2B7E1
B	158	HIS	-	expression tag	UNP T2B7E1
B	159	HIS	-	expression tag	UNP T2B7E1
B	160	HIS	-	expression tag	UNP T2B7E1
B	161	HIS	-	expression tag	UNP T2B7E1
B	162	HIS	-	expression tag	UNP T2B7E1
B	163	GLU	-	expression tag	UNP T2B7E1
B	164	TYR	-	expression tag	UNP T2B7E1
B	165	MET	-	expression tag	UNP T2B7E1
B	166	PHE	-	expression tag	UNP T2B7E1
B	167	ASP	-	expression tag	UNP T2B7E1
B	168	LYS	-	expression tag	UNP T2B7E1
B	169	GLU	-	expression tag	UNP T2B7E1
B	170	LEU	-	expression tag	UNP T2B7E1
B	171	ASN	-	expression tag	UNP T2B7E1
C	89	ARG	GLN	engineered mutation	UNP T2B7E1
C	157	HIS	-	expression tag	UNP T2B7E1
C	158	HIS	-	expression tag	UNP T2B7E1
C	159	HIS	-	expression tag	UNP T2B7E1
C	160	HIS	-	expression tag	UNP T2B7E1
C	161	HIS	-	expression tag	UNP T2B7E1
C	162	HIS	-	expression tag	UNP T2B7E1
C	163	GLU	-	expression tag	UNP T2B7E1
C	164	TYR	-	expression tag	UNP T2B7E1
C	165	MET	-	expression tag	UNP T2B7E1
C	166	PHE	-	expression tag	UNP T2B7E1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	167	ASP	-	expression tag	UNP T2B7E1
C	168	LYS	-	expression tag	UNP T2B7E1
C	169	GLU	-	expression tag	UNP T2B7E1
C	170	LEU	-	expression tag	UNP T2B7E1
C	171	ASN	-	expression tag	UNP T2B7E1
D	89	ARG	GLN	engineered mutation	UNP T2B7E1
D	157	HIS	-	expression tag	UNP T2B7E1
D	158	HIS	-	expression tag	UNP T2B7E1
D	159	HIS	-	expression tag	UNP T2B7E1
D	160	HIS	-	expression tag	UNP T2B7E1
D	161	HIS	-	expression tag	UNP T2B7E1
D	162	HIS	-	expression tag	UNP T2B7E1
D	163	GLU	-	expression tag	UNP T2B7E1
D	164	TYR	-	expression tag	UNP T2B7E1
D	165	MET	-	expression tag	UNP T2B7E1
D	166	PHE	-	expression tag	UNP T2B7E1
D	167	ASP	-	expression tag	UNP T2B7E1
D	168	LYS	-	expression tag	UNP T2B7E1
D	169	GLU	-	expression tag	UNP T2B7E1
D	170	LEU	-	expression tag	UNP T2B7E1
D	171	ASN	-	expression tag	UNP T2B7E1
F	89	ARG	GLN	engineered mutation	UNP T2B7E1
F	157	HIS	-	expression tag	UNP T2B7E1
F	158	HIS	-	expression tag	UNP T2B7E1
F	159	HIS	-	expression tag	UNP T2B7E1
F	160	HIS	-	expression tag	UNP T2B7E1
F	161	HIS	-	expression tag	UNP T2B7E1
F	162	HIS	-	expression tag	UNP T2B7E1
F	163	GLU	-	expression tag	UNP T2B7E1
F	164	TYR	-	expression tag	UNP T2B7E1
F	165	MET	-	expression tag	UNP T2B7E1
F	166	PHE	-	expression tag	UNP T2B7E1
F	167	ASP	-	expression tag	UNP T2B7E1
F	168	LYS	-	expression tag	UNP T2B7E1
F	169	GLU	-	expression tag	UNP T2B7E1
F	170	LEU	-	expression tag	UNP T2B7E1
F	171	ASN	-	expression tag	UNP T2B7E1

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Fe 2 2	0	0
2	A	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	F	2	Total Fe 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Zn 1 1	0	0
3	A	2	Total Zn 2 2	0	0
3	C	1	Total Zn 1 1	0	0
3	D	2	Total Zn 2 2	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is water.

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

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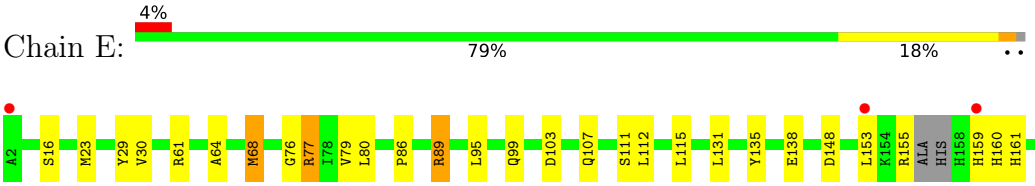
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

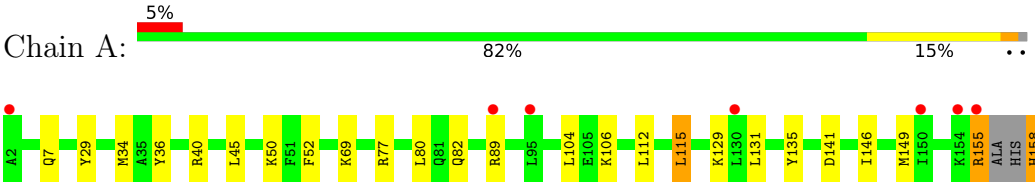
• Molecule 1: Ferritin

Chain E:



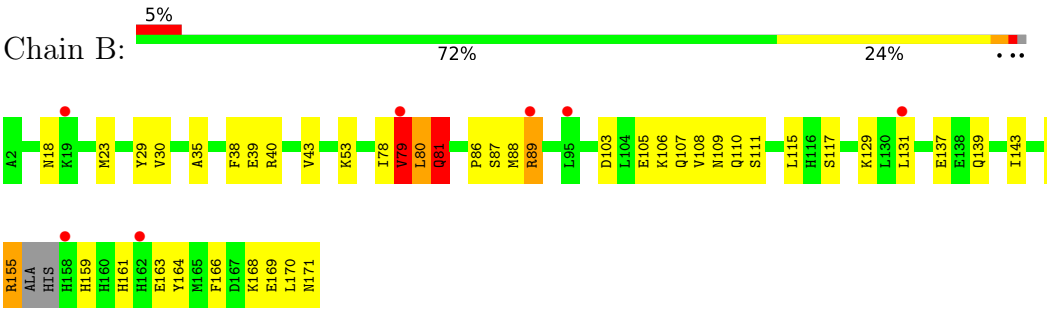
• Molecule 1: Ferritin

Chain A:



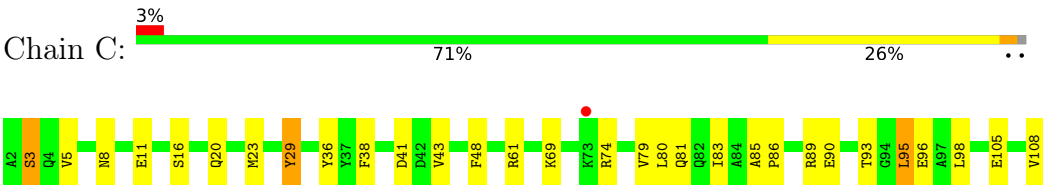
• Molecule 1: Ferritin

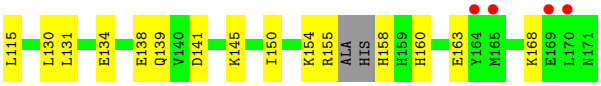
Chain B:



• Molecule 1: Ferritin

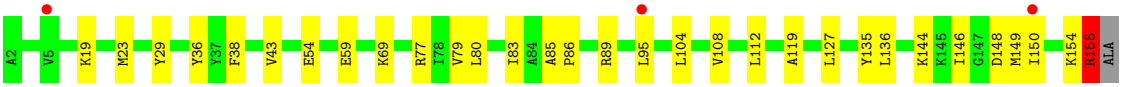
Chain C:

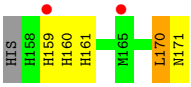




• Molecule 1: Ferritin

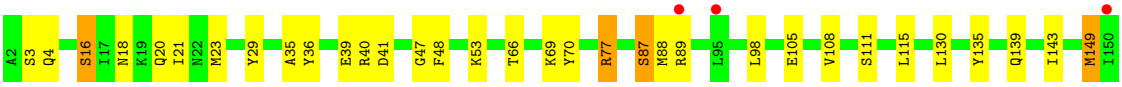
Chain D:

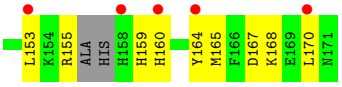




• Molecule 1: Ferritin

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	126.37Å 126.37Å 177.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.11 – 2.60 34.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.11-2.60) 99.9 (34.11-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.194 , 0.272 0.194 , 0.272	Depositor DCC
R_{free} test set	2027 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 20.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.034 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.038 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.044 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.136 for -h,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16133	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: FE, 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	0.61	0/1399	0.78	5/1878 (0.3%)
1	B	0.77	1/1399 (0.1%)	0.90	9/1878 (0.5%)
1	C	0.65	0/1399	0.75	2/1878 (0.1%)
1	D	0.61	0/1399	0.83	3/1878 (0.2%)
1	E	0.93	4/1399 (0.3%)	1.43	9/1878 (0.5%)
1	F	0.63	0/1399	0.76	1/1878 (0.1%)
All	All	0.71	5/8394 (0.1%)	0.94	29/11268 (0.3%)

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	B	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	89	ARG	CZ-NH2	18.68	1.57	1.33
1	B	81	GLN	CD-OE1	-10.98	0.99	1.24
1	E	89	ARG	CZ-NH1	8.70	1.44	1.33
1	E	89	ARG	CD-NE	-8.66	1.31	1.46
1	E	89	ARG	CB-CG	-5.30	1.38	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	89	ARG	NE-CZ-NH1	-45.31	97.65	120.30
1	E	89	ARG	NH1-CZ-NH2	17.52	138.68	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	155	ARG	NE-CZ-NH2	14.07	127.33	120.30
1	E	89	ARG	CG-CD-NE	-13.48	83.49	111.80
1	B	81	GLN	OE1-CD-NE2	-10.88	96.86	121.90
1	B	89	ARG	NE-CZ-NH1	-10.77	114.92	120.30
1	E	89	ARG	CB-CG-CD	-8.63	89.16	111.60
1	D	155	ARG	NE-CZ-NH1	-8.39	116.10	120.30
1	E	61	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	89	ARG	CG-CD-NE	-7.55	95.95	111.80
1	E	80	LEU	CB-CG-CD1	7.28	123.37	111.00
1	B	79	VAL	CG1-CB-CG2	-7.11	99.52	110.90
1	E	68	MET	CG-SD-CE	6.95	111.32	100.20
1	C	95	LEU	CB-CG-CD1	6.48	122.01	111.00
1	A	104	LEU	CB-CG-CD1	6.32	121.75	111.00
1	B	40	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	E	89	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	F	149	MET	CG-SD-CE	5.87	109.59	100.20
1	A	104	LEU	CB-CG-CD2	-5.84	101.08	111.00
1	B	79	VAL	N-CA-CB	-5.72	98.91	111.50
1	C	95	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	A	141	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	79	VAL	N-CA-C	5.64	126.23	111.00
1	A	45	LEU	CB-CG-CD2	5.61	120.53	111.00
1	B	89	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	E	61	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	23	MET	CG-SD-CE	5.34	108.75	100.20
1	B	79	VAL	C-N-CA	5.24	134.81	121.70
1	A	45	LEU	CB-CG-CD1	-5.11	102.31	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	78	ILE	Peptide
1	B	79	VAL	Peptide
1	B	81	GLN	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	1372	1311	1311	36	2
1	B	1372	1311	1311	37	6
1	C	1372	1311	1311	53	0
1	D	1372	1311	1311	34	1
1	E	1372	1311	1311	29	3
1	F	1372	1311	1311	40	3
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	1
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	4	0	0	1	0
4	B	2	0	0	4	0
4	C	2	0	0	1	0
4	D	2	0	0	0	0
4	E	3	0	0	2	0
4	F	3	0	0	0	0
All	All	8267	7866	7866	185	10

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 11.

All (185) 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:B:105:GLU:O	1:B:139:GLN:NE2	1.76	1.19
1:A:115:LEU:HD23	1:A:131:LEU:HD11	1.32	1.10
1:C:80:LEU:HB3	1:D:29:TYR:OH	1.63	0.96
1:E:23:MET:HE1	1:E:111:SER:HB3	1.47	0.95
1:B:39:GLU:OE2	1:B:53:LYS:NZ	2.02	0.93
1:F:39:GLU:OE2	1:F:53:LYS:NZ	2.02	0.91
1:A:115:LEU:HD23	1:A:131:LEU:CD1	2.01	0.91
1:D:159:HIS:ND1	1:D:161:HIS:HB3	1.89	0.86
1:A:115:LEU:CD2	1:A:131:LEU:HD11	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:ARG:HD3	1:C:160:HIS:HB3	1.59	0.83
1:C:80:LEU:O	1:D:89:ARG:NH1	2.13	0.82
1:C:105:GLU:OE1	1:C:139:GLN:NE2	2.14	0.80
1:B:155:ARG:HA	1:B:155:ARG:HE	1.47	0.80
1:E:23:MET:HE1	1:E:111:SER:CB	2.13	0.78
1:F:16:SER:HB3	1:F:115:LEU:HD13	1.68	0.76
1:E:16:SER:HB3	1:E:115:LEU:HD13	1.67	0.76
1:A:34:MET:HE3	1:A:52:PHE:CZ	2.22	0.75
1:E:23:MET:CE	1:E:111:SER:HB3	2.19	0.72
1:A:115:LEU:HD22	1:A:131:LEU:HD21	1.71	0.71
1:B:155:ARG:O	4:B:301:HOH:O	2.08	0.71
1:B:109:ASN:HB2	1:B:139:GLN:HG3	1.73	0.71
1:A:34:MET:HE3	1:A:52:PHE:CE1	2.27	0.70
1:C:80:LEU:H	1:D:89:ARG:NH2	1.89	0.69
1:B:169:GLU:HG3	1:F:168:LYS:HZ2	1.57	0.69
1:A:155:ARG:HH21	1:A:158:HIS:CE1	2.12	0.67
1:D:144:LYS:NZ	1:D:148:ASP:OD1	2.28	0.66
1:C:80:LEU:HB3	1:D:29:TYR:CZ	2.31	0.65
1:A:69:LYS:HG3	1:F:36:TYR:HE2	1.61	0.65
1:F:48:PHE:HZ	1:F:153:LEU:HD11	1.62	0.65
1:B:18:ASN:ND2	1:B:79:VAL:H	1.94	0.65
1:A:80:LEU:H	1:F:89:ARG:HE	1.42	0.64
1:F:89:ARG:CZ	1:F:89:ARG:HB2	2.26	0.64
1:A:146:ILE:HA	1:A:149:MET:HE3	1.80	0.64
1:C:80:LEU:H	1:D:89:ARG:HH22	1.46	0.63
1:C:90:GLU:OE1	1:D:77:ARG:NH1	2.32	0.63
1:C:23:MET:HE1	1:C:111:SER:HB3	1.81	0.62
1:E:76:GLY:C	1:E:77:ARG:HD2	2.20	0.62
1:E:155:ARG:CD	1:C:160:HIS:HB3	2.29	0.61
1:D:89:ARG:NH2	1:D:89:ARG:HG3	2.16	0.60
1:A:40:ARG:NE	1:F:77:ARG:NH1	2.50	0.59
1:A:146:ILE:HA	1:A:149:MET:CE	2.31	0.59
1:B:109:ASN:HB2	1:B:139:GLN:CG	2.31	0.59
1:A:89:ARG:NH2	1:F:77:ARG:HB3	2.18	0.59
1:C:80:LEU:HD13	1:D:29:TYR:CE1	2.38	0.59
1:C:29:TYR:CE1	1:D:80:LEU:HD13	2.37	0.59
1:E:155:ARG:HD3	1:C:160:HIS:CB	2.28	0.59
1:A:36:TYR:HE2	1:F:69:LYS:HG3	1.66	0.59
1:B:153:LEU:HD11	1:B:163:GLU:HA	1.83	0.59
1:B:115:LEU:HD22	1:B:131:LEU:HD21	1.84	0.59
1:B:155:ARG:HE	1:B:155:ARG:CA	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TYR:HE2	1:D:69:LYS:HG3	1.67	0.58
1:F:105:GLU:OE1	1:F:139:GLN:NE2	2.36	0.58
1:C:158:HIS:CE1	4:C:301:HOH:O	2.56	0.58
1:A:80:LEU:H	1:F:89:ARG:NE	2.02	0.57
1:E:155:ARG:HD3	1:C:160:HIS:CG	2.39	0.57
1:B:153:LEU:HD13	1:B:166:PHE:CG	2.40	0.57
1:B:23:MET:HE1	1:B:111:SER:HB3	1.85	0.57
1:E:155:ARG:HD3	1:C:160:HIS:ND1	2.19	0.57
1:C:154:LYS:O	1:C:155:ARG:HB2	2.05	0.56
1:B:18:ASN:CG	1:B:79:VAL:H	2.09	0.56
1:E:155:ARG:NH1	1:C:163:GLU:OE1	2.39	0.56
1:C:29:TYR:CD2	1:C:86:PRO:HD3	2.40	0.56
1:D:159:HIS:CE1	1:D:161:HIS:HB3	2.41	0.56
1:A:34:MET:CE	1:A:52:PHE:CE1	2.88	0.56
1:C:29:TYR:OH	1:D:80:LEU:HB3	2.06	0.55
1:F:48:PHE:CZ	1:F:153:LEU:HD11	2.41	0.55
1:E:77:ARG:HD2	1:E:77:ARG:N	2.22	0.55
1:A:155:ARG:NE	1:A:158:HIS:ND1	2.44	0.55
1:F:165:MET:HE3	1:F:168:LYS:HE2	1.89	0.55
1:E:30:VAL:HG22	1:E:86:PRO:HB3	1.89	0.54
1:C:115:LEU:HG	1:C:131:LEU:HD11	1.88	0.54
1:A:77:ARG:HA	1:F:40:ARG:HH12	1.71	0.54
1:C:38:PHE:HA	1:C:43:VAL:HG11	1.90	0.54
1:C:8:ASN:O	1:C:74:ARG:NH2	2.41	0.53
1:A:165:MET:SD	1:A:168:LYS:HE2	2.48	0.53
1:E:64:ALA:O	1:E:68:MET:HG3	2.09	0.53
1:B:159:HIS:NE2	4:B:302:HOH:O	2.34	0.52
1:F:89:ARG:HH21	1:F:89:ARG:CG	2.23	0.52
1:E:95:LEU:O	1:E:99:GLN:HG3	2.11	0.51
1:B:106:LYS:HG3	1:B:143:ILE:HD13	1.93	0.51
1:B:103:ASP:O	1:B:107:GLN:HG3	2.10	0.51
1:A:34:MET:CE	1:A:52:PHE:CD1	2.94	0.51
1:D:29:TYR:CD2	1:D:86:PRO:HD3	2.46	0.51
1:E:23:MET:CE	1:E:111:SER:CB	2.83	0.51
1:E:103:ASP:O	1:E:107:GLN:HG3	2.11	0.51
1:E:16:SER:CB	1:E:115:LEU:HD13	2.40	0.51
1:B:159:HIS:CE1	4:B:302:HOH:O	2.64	0.51
1:C:130:LEU:O	1:C:134:GLU:HB2	2.10	0.51
1:A:115:LEU:CD2	1:A:131:LEU:HD21	2.41	0.51
1:B:155:ARG:HA	1:B:155:ARG:NE	2.19	0.51
1:F:20:GLN:HE22	1:F:23:MET:CE	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG22	1:B:86:PRO:HB3	1.93	0.50
1:F:35:ALA:HB1	1:F:53:LYS:HG3	1.92	0.50
1:C:3:SER:HB3	1:C:5:VAL:H	1.77	0.50
1:A:149:MET:HB3	1:A:166:PHE:HZ	1.76	0.50
1:E:165:MET:O	1:E:168:LYS:HB3	2.11	0.50
1:F:98:LEU:HD12	1:F:153:LEU:HD12	1.94	0.50
1:A:166:PHE:O	1:A:169:GLU:HB3	2.12	0.49
4:B:301:HOH:O	1:F:159:HIS:CE1	2.65	0.49
1:C:11:GLU:H	1:C:11:GLU:CD	2.14	0.49
1:C:16:SER:HB3	1:C:115:LEU:HD13	1.95	0.49
1:F:89:ARG:HH21	1:F:89:ARG:HG3	1.76	0.49
1:A:40:ARG:HB3	1:F:77:ARG:HH12	1.77	0.49
1:C:109:ASN:HB2	1:C:139:GLN:HG3	1.95	0.49
1:D:89:ARG:HG3	1:D:89:ARG:HH21	1.77	0.49
1:E:155:ARG:HB3	1:C:160:HIS:CB	2.43	0.49
1:B:164:TYR:CZ	1:B:168:LYS:HD2	2.48	0.49
1:F:70:TYR:CD1	1:F:130:LEU:HD22	2.47	0.49
1:C:89:ARG:HD3	1:D:79:VAL:HA	1.94	0.49
1:A:89:ARG:HH22	1:F:77:ARG:HB3	1.78	0.49
1:B:109:ASN:CB	1:B:139:GLN:HG3	2.42	0.49
1:A:40:ARG:NE	1:F:77:ARG:HH11	2.10	0.48
1:F:23:MET:HE1	1:F:111:SER:HB3	1.95	0.48
1:A:40:ARG:HB3	1:F:77:ARG:NH1	2.29	0.48
1:E:155:ARG:HB3	1:C:160:HIS:HB3	1.95	0.48
1:C:29:TYR:CE2	1:C:85:ALA:HA	2.49	0.48
1:C:29:TYR:CE2	1:C:86:PRO:HD3	2.49	0.48
1:D:29:TYR:CE2	1:D:85:ALA:HA	2.49	0.47
1:B:23:MET:HE1	1:B:111:SER:CB	2.44	0.47
1:C:69:LYS:HG3	1:D:36:TYR:HE2	1.79	0.47
1:C:80:LEU:N	1:D:89:ARG:HH22	2.09	0.47
1:F:87:SER:OG	1:F:88:MET:N	2.46	0.47
1:C:141:ASP:O	1:C:145:LYS:HG2	2.14	0.47
1:B:23:MET:HE1	1:B:108:VAL:HA	1.97	0.47
1:D:54:GLU:O	1:D:59:GLU:HG3	2.14	0.47
1:C:48:PHE:HE1	1:C:98:LEU:HD11	1.80	0.46
1:F:18:ASN:HA	1:F:21:ILE:HD12	1.97	0.46
1:A:89:ARG:O	1:A:89:ARG:HD2	2.16	0.46
1:C:93:THR:HG23	1:C:96:GLU:OE2	2.15	0.46
1:A:7:GLN:NE2	1:B:110:GLN:OE1	2.48	0.46
1:B:148:ASP:OD1	1:F:41:ASP:HA	2.16	0.46
1:E:153:LEU:HD13	1:E:166:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HB3	1:C:61:ARG:NH2	2.31	0.46
1:C:29:TYR:CZ	1:D:80:LEU:HB3	2.51	0.45
1:D:112:LEU:HD13	1:D:135:TYR:HB3	1.97	0.45
1:B:35:ALA:HB1	1:B:53:LYS:HG3	1.97	0.45
1:F:139:GLN:O	1:F:143:ILE:HG13	2.16	0.45
1:B:109:ASN:CB	1:B:139:GLN:CG	2.95	0.45
1:B:155:ARG:HD3	1:F:160:HIS:ND1	2.32	0.45
1:C:83:ILE:HD12	1:D:83:ILE:HB	1.99	0.45
1:A:158:HIS:HD2	4:A:303:HOH:O	2.00	0.45
1:D:119:ALA:HB2	1:D:127:LEU:HD23	1.99	0.45
1:E:89:ARG:HD3	1:E:89:ARG:HA	1.22	0.44
1:D:149:MET:HE3	1:D:170:LEU:HD21	1.98	0.44
1:C:138:GLU:H	1:C:138:GLU:CD	2.20	0.44
1:A:129:LYS:HE2	1:B:137:GLU:OE1	2.18	0.44
1:B:115:LEU:CD2	1:B:131:LEU:HD11	2.48	0.44
1:A:112:LEU:HD13	1:A:135:TYR:HB3	1.99	0.44
1:E:115:LEU:HG	1:E:131:LEU:HD11	1.99	0.44
1:B:169:GLU:CG	1:F:168:LYS:HZ2	2.29	0.44
1:F:149:MET:CE	1:F:170:LEU:HD11	2.47	0.44
1:E:112:LEU:HD13	1:E:135:TYR:HB3	2.00	0.44
1:B:170:LEU:O	1:B:171:ASN:O	2.36	0.43
1:B:115:LEU:HD22	1:B:131:LEU:HD11	2.00	0.43
1:D:104:LEU:O	1:D:108:VAL:HG23	2.17	0.43
1:A:115:LEU:HD22	1:A:131:LEU:CD2	2.44	0.43
1:E:148:ASP:OD1	1:C:41:ASP:HA	2.19	0.43
1:C:20:GLN:HE22	1:C:23:MET:CE	2.32	0.43
1:F:164:TYR:CZ	1:F:168:LYS:HD2	2.53	0.43
1:F:89:ARG:HB2	1:F:89:ARG:NH2	2.33	0.43
1:A:149:MET:HB3	1:A:166:PHE:CZ	2.54	0.43
1:F:66:THR:HB	1:F:135:TYR:OH	2.19	0.43
1:A:82:GLN:HB2	1:C:81:GLN:OE1	2.19	0.43
1:D:155:ARG:HE	1:D:155:ARG:HB3	1.60	0.43
1:C:95:LEU:HD11	1:C:150:ILE:HG23	2.00	0.42
1:C:145:LYS:N	1:C:145:LYS:HD3	2.33	0.42
1:D:38:PHE:HA	1:D:43:VAL:HG11	2.01	0.42
1:E:153:LEU:HD13	1:E:166:PHE:CG	2.55	0.42
1:E:161:HIS:CD2	4:E:302:HOH:O	2.73	0.42
1:E:159:HIS:CD2	4:E:301:HOH:O	2.71	0.42
1:A:69:LYS:HE3	1:F:36:TYR:OH	2.20	0.42
1:C:168:LYS:HA	1:C:168:LYS:HD3	1.91	0.42
1:C:79:VAL:HA	1:D:89:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PHE:HA	1:B:43:VAL:HG11	2.02	0.41
1:C:23:MET:HE1	1:C:108:VAL:HA	2.02	0.41
1:F:23:MET:HE1	1:F:108:VAL:HA	2.03	0.41
1:F:47:GLY:N	1:F:167:ASP:OD1	2.53	0.41
1:B:88:MET:O	1:B:89:ARG:HG2	2.21	0.41
1:D:95:LEU:HD11	1:D:150:ILE:HG23	2.03	0.41
1:D:135:TYR:O	1:D:136:LEU:C	2.58	0.41
1:C:150:ILE:O	1:C:154:LYS:HG3	2.22	0.40
1:D:155:ARG:HH11	1:D:155:ARG:HD2	1.56	0.40
1:C:38:PHE:HA	1:C:43:VAL:CG1	2.50	0.40
1:D:146:ILE:O	1:D:150:ILE:HG13	2.22	0.40
1:B:105:GLU:C	1:B:139:GLN:NE2	2.66	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:CD	1:B:81:GLN:OE1[2_655]	0.99	1.21
1:B:81:GLN:CD	1:B:81:GLN:CD[2_655]	1.54	0.66
1:E:79:VAL:HA	1:B:89:ARG:HH22[7_545]	1.13	0.47
1:B:81:GLN:OE1	1:B:81:GLN:NE2[2_655]	1.78	0.42
1:E:89:ARG:HH22	1:B:80:LEU:HD12[7_545]	1.28	0.32
1:D:155:ARG:HH22	1:D:160:HIS:H[4_655]	1.34	0.26
1:E:160:HIS:ND1	1:F:155:ARG:NH1[6_545]	2.07	0.13
1:A:106:LYS:NZ	1:F:4:GLN:O[3_555]	2.07	0.13
1:A:106:LYS:HZ2	1:F:4:GLN:O[3_555]	1.49	0.11
1:B:161:HIS:HE2	3:C:203:ZN:ZN[6_544]	1.59	0.01

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	163/169 (96%)	157 (96%)	6 (4%)	0	100	100
1	B	163/169 (96%)	153 (94%)	8 (5%)	2 (1%)	13	27
1	C	163/169 (96%)	156 (96%)	7 (4%)	0	100	100
1	D	163/169 (96%)	160 (98%)	2 (1%)	1 (1%)	25	47
1	E	163/169 (96%)	160 (98%)	3 (2%)	0	100	100
1	F	163/169 (96%)	158 (97%)	4 (2%)	1 (1%)	25	47
All	All	978/1014 (96%)	944 (96%)	30 (3%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	87	SER
1	B	87	SER
1	B	80	LEU
1	D	154	LYS

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	147/148 (99%)	141 (96%)	6 (4%)	30	56
1	B	147/148 (99%)	143 (97%)	4 (3%)	44	71
1	C	147/148 (99%)	145 (99%)	2 (1%)	67	85
1	D	147/148 (99%)	143 (97%)	4 (3%)	44	71
1	E	147/148 (99%)	142 (97%)	5 (3%)	37	63
1	F	147/148 (99%)	143 (97%)	4 (3%)	44	71
All	All	882/888 (99%)	857 (97%)	25 (3%)	43	69

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	29	TYR

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Mol	Chain	Res	Type
1	E	77	ARG
1	E	138	GLU
1	E	170	LEU
1	E	171	ASN
1	A	29	TYR
1	A	50	LYS
1	A	115	LEU
1	A	155	ARG
1	A	158	HIS
1	A	168	LYS
1	B	29	TYR
1	B	117	SER
1	B	129	LYS
1	B	155	ARG
1	C	3	SER
1	C	29	TYR
1	D	19	LYS
1	D	155	ARG
1	D	170	LEU
1	D	171	ASN
1	F	3	SER
1	F	16	SER
1	F	29	TYR
1	F	77	ARG

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

Mol	Chain	Res	Type
1	A	107	GLN
1	D	139	GLN
1	D	171	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 19 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	167/169 (98%)	0.51	9 (5%)	25	20	39, 47, 67, 84	0
1	B	167/169 (98%)	0.51	8 (4%)	30	24	39, 48, 69, 90	0
1	C	167/169 (98%)	0.47	5 (2%)	50	43	38, 47, 65, 79	0
1	D	167/169 (98%)	0.44	5 (2%)	50	43	36, 47, 66, 84	0
1	E	167/169 (98%)	0.48	7 (4%)	36	29	37, 47, 64, 84	0
1	F	167/169 (98%)	0.46	8 (4%)	30	24	36, 48, 66, 90	0
All	All	1002/1014 (98%)	0.48	42 (4%)	36	29	36, 47, 68, 90	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	158	HIS	4.1
1	F	150	ILE	3.9
1	B	153	LEU	3.8
1	A	89	ARG	3.7
1	A	164	TYR	3.3
1	B	79	VAL	3.3
1	C	164	TYR	3.1
1	A	150	ILE	3.0
1	D	159	HIS	2.9
1	E	164	TYR	2.9
1	C	73	LYS	2.8
1	E	170	LEU	2.8
1	F	95	LEU	2.7
1	C	170	LEU	2.7
1	A	2	ALA	2.6
1	A	95	LEU	2.5
1	A	130	LEU	2.5
1	D	165	MET	2.5
1	A	154	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	171	ASN	2.5
1	C	169	GLU	2.4
1	B	95	LEU	2.4
1	D	5	VAL	2.4
1	E	159	HIS	2.3
1	F	89	ARG	2.3
1	B	19	LYS	2.3
1	C	165	MET	2.3
1	B	158	HIS	2.2
1	E	153	LEU	2.2
1	F	160	HIS	2.2
1	B	89	ARG	2.2
1	F	170	LEU	2.2
1	E	168	LYS	2.1
1	E	171	ASN	2.1
1	B	162	HIS	2.1
1	F	164	TYR	2.1
1	D	150	ILE	2.1
1	D	95	LEU	2.1
1	F	153	LEU	2.1
1	A	155	ARG	2.1
1	E	2	ALA	2.1
1	B	131	LEU	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.

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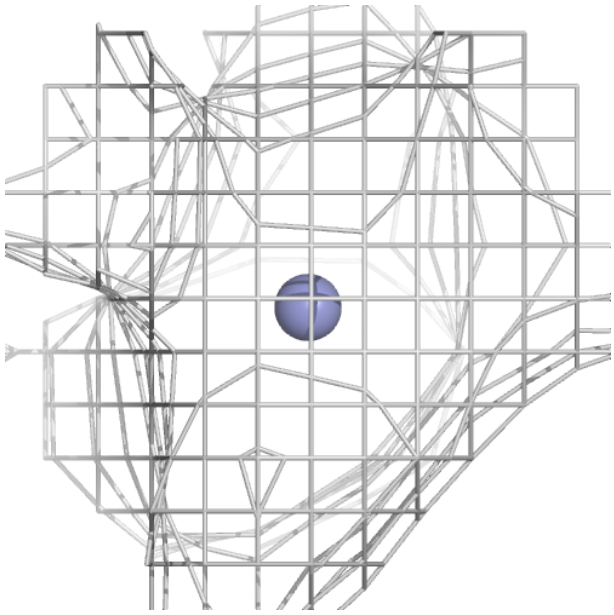
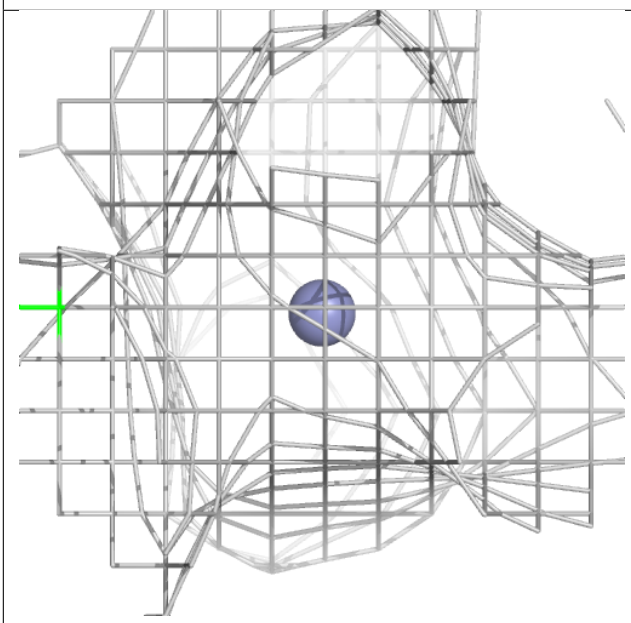
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	F	203	1/1	0.85	0.07	115,115,115,115	0
3	ZN	D	203	1/1	0.86	0.18	67,67,67,67	1
3	ZN	A	203	1/1	0.95	0.27	59,59,59,59	1
2	FE	C	202	1/1	0.95	0.27	41,41,41,41	0
3	ZN	E	203	1/1	0.95	0.14	97,97,97,97	0
2	FE	A	202	1/1	0.96	0.30	44,44,44,44	0
2	FE	C	201	1/1	0.97	0.29	38,38,38,38	0
2	FE	E	202	1/1	0.97	0.25	42,42,42,42	0
2	FE	D	201	1/1	0.97	0.29	41,41,41,41	0
2	FE	F	202	1/1	0.97	0.27	44,44,44,44	0
2	FE	B	201	1/1	0.98	0.29	41,41,41,41	0
2	FE	D	202	1/1	0.98	0.31	43,43,43,43	0
3	ZN	C	203	1/1	0.98	0.18	60,60,60,60	0
2	FE	F	201	1/1	0.98	0.31	41,41,41,41	0
2	FE	B	202	1/1	0.98	0.27	43,43,43,43	0
2	FE	A	201	1/1	0.99	0.30	38,38,38,38	0
2	FE	E	201	1/1	0.99	0.31	36,36,36,36	0
3	ZN	D	204	1/1	0.99	0.22	102,102,102,102	1
3	ZN	A	204	1/1	0.99	0.28	92,92,92,92	1

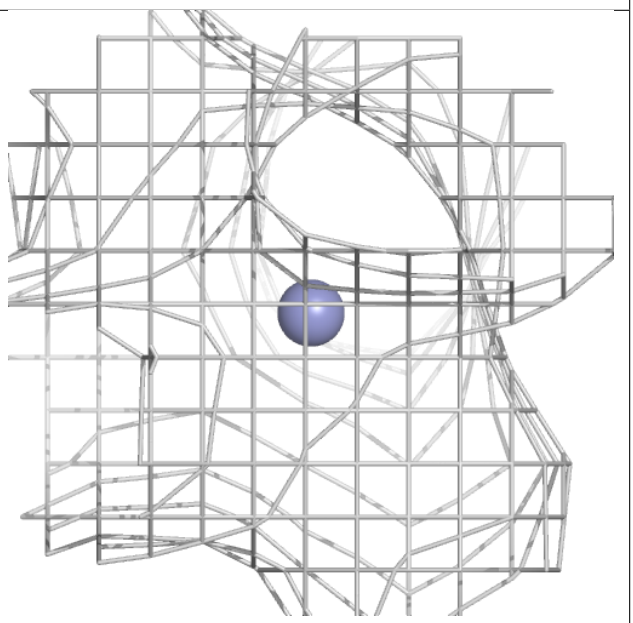
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN F 203:

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

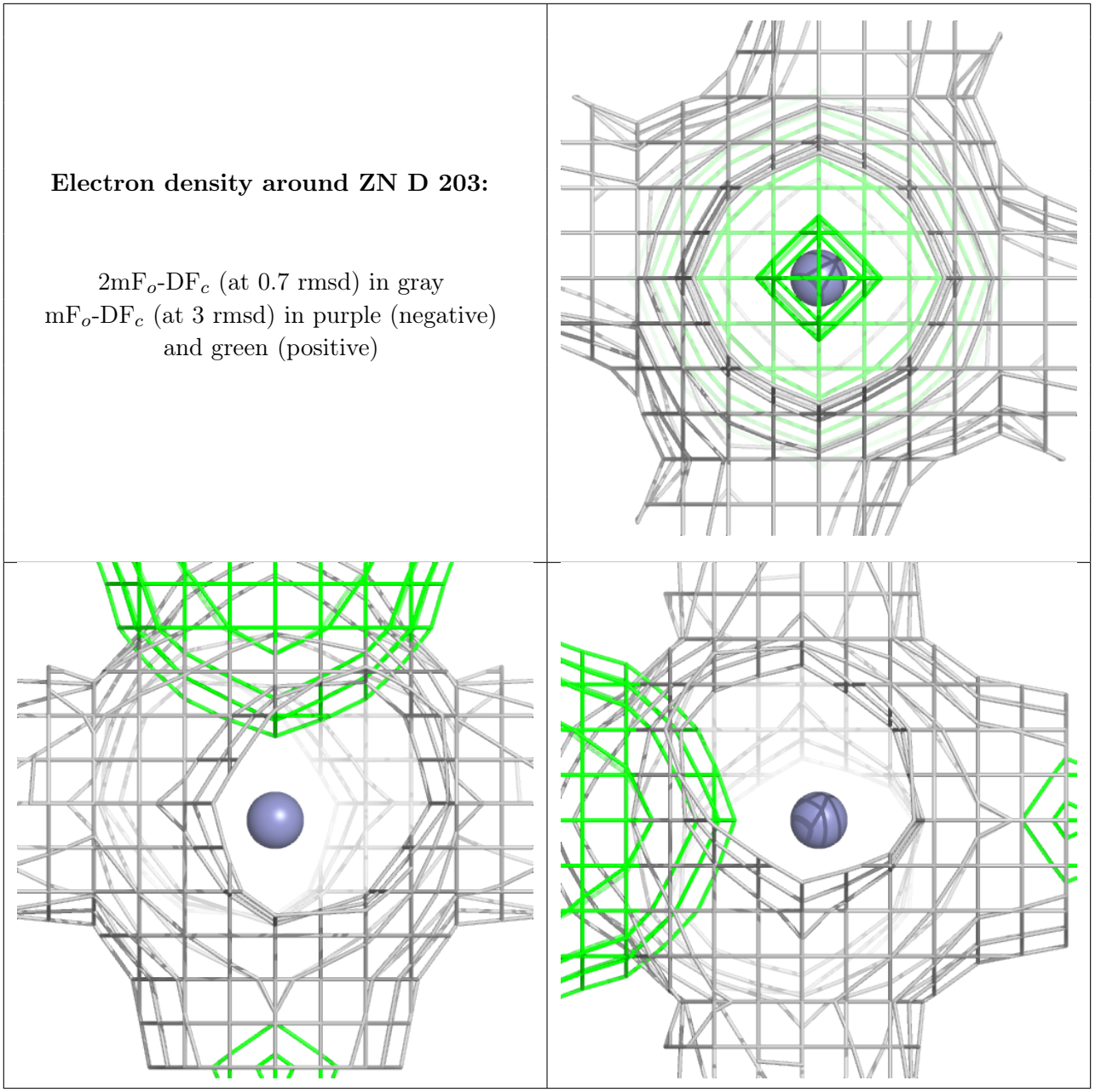






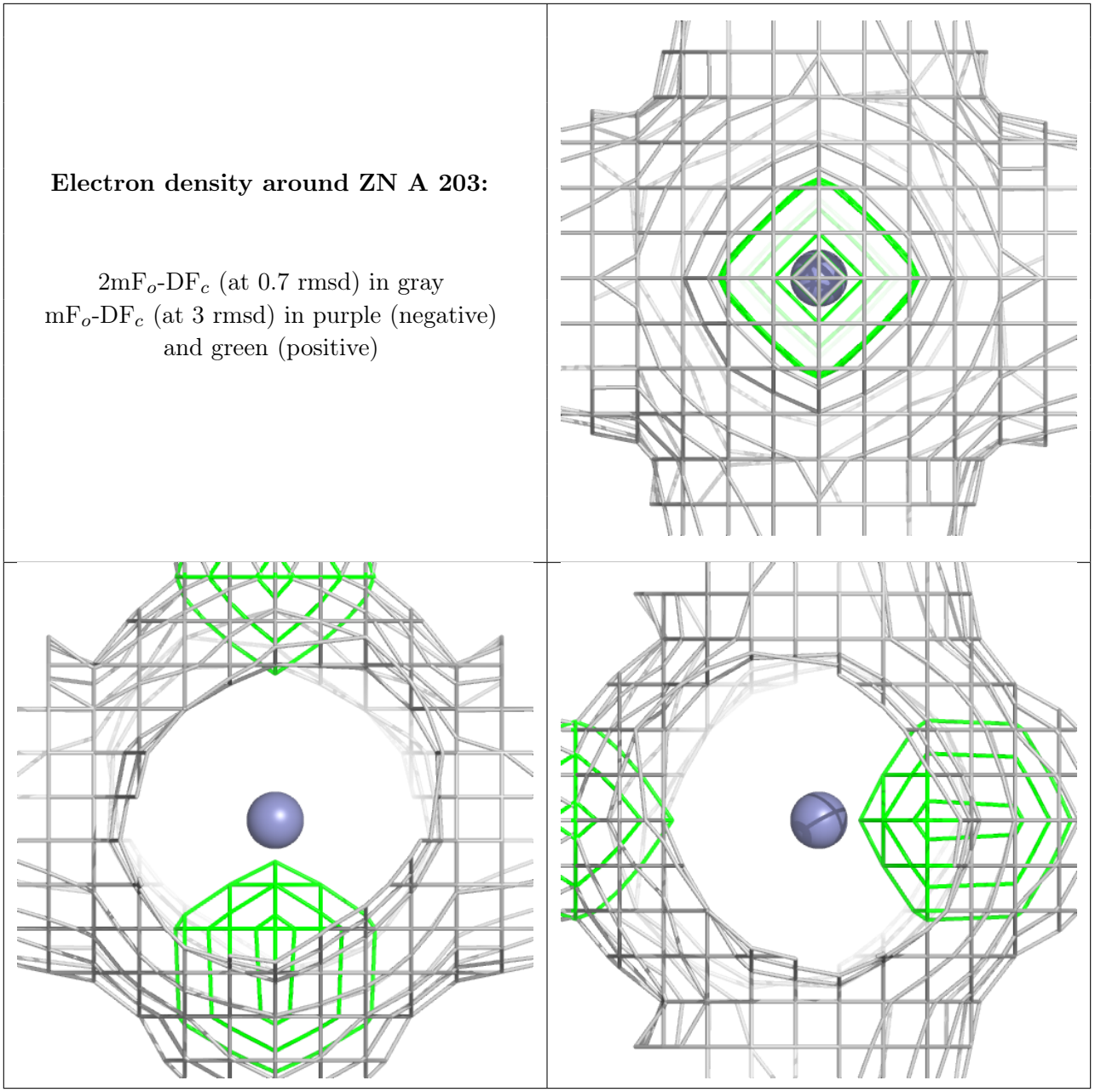
Electron density around ZN D 203:

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



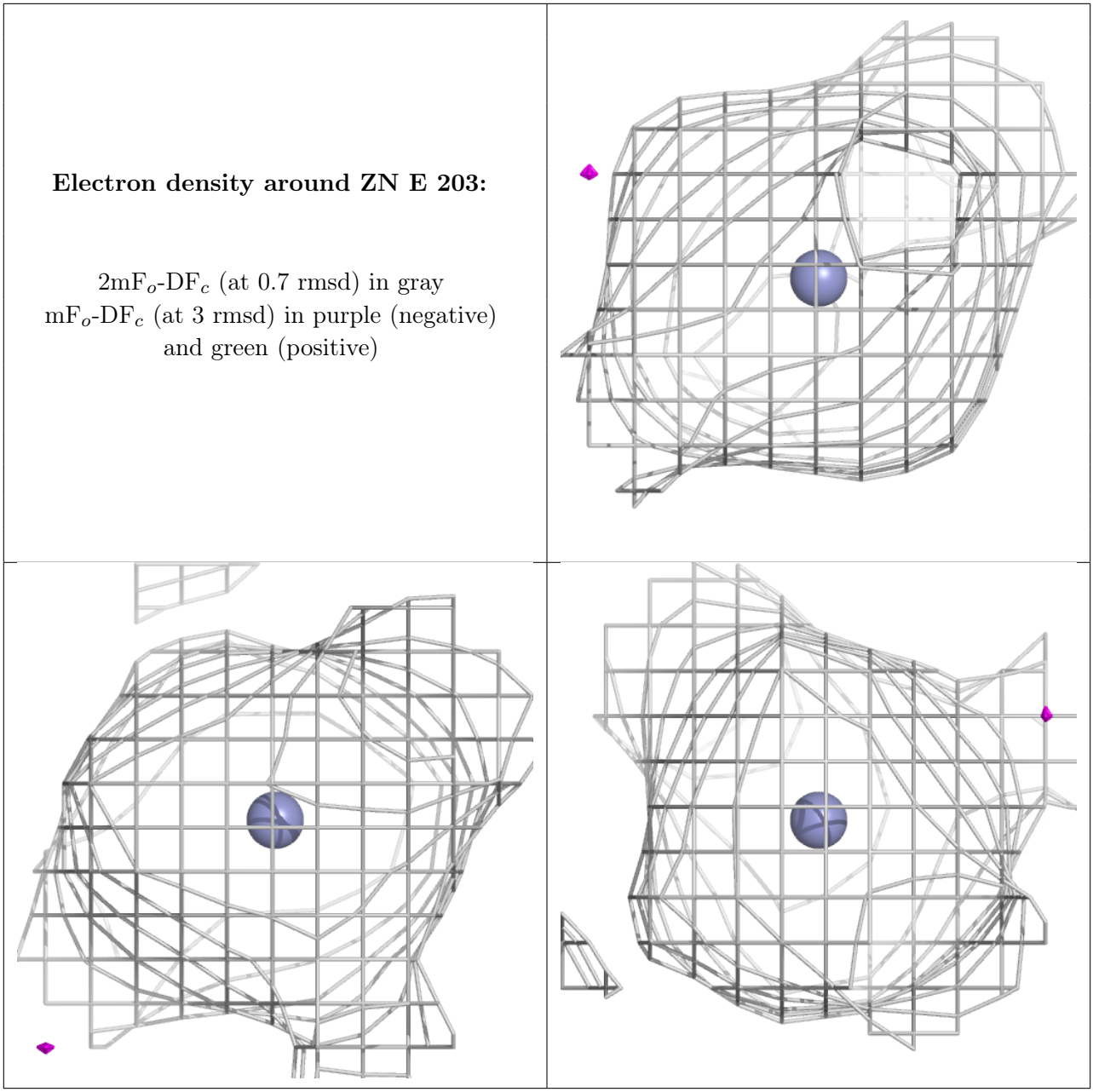
Electron density around ZN A 203:

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



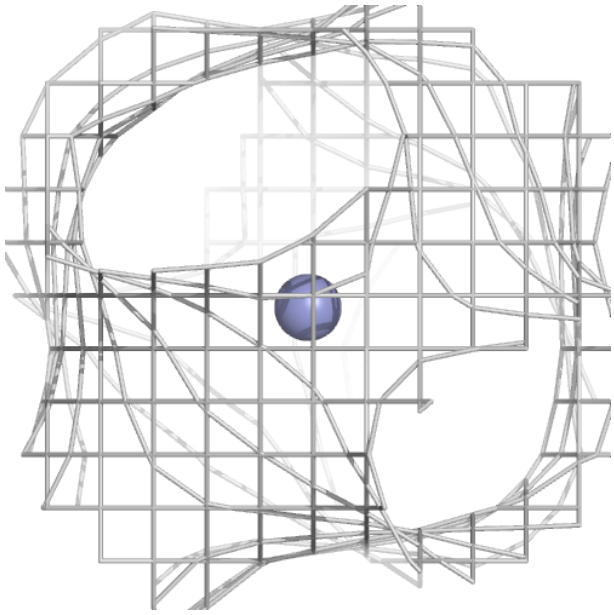
Electron density around ZN E 203:

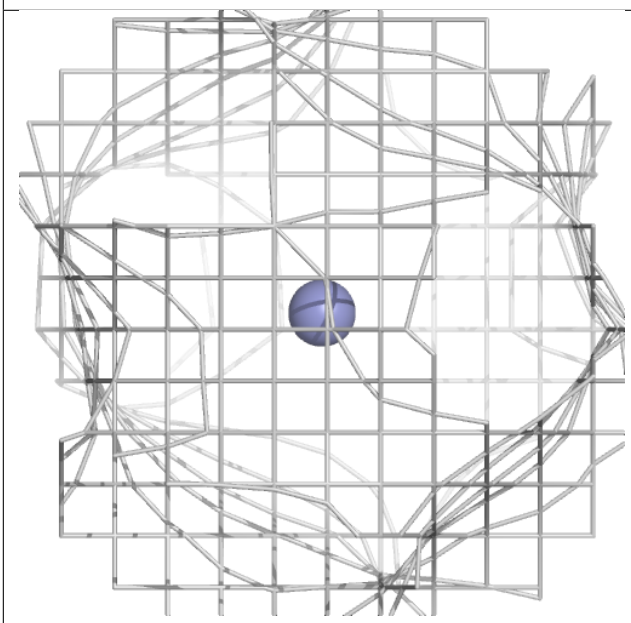
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

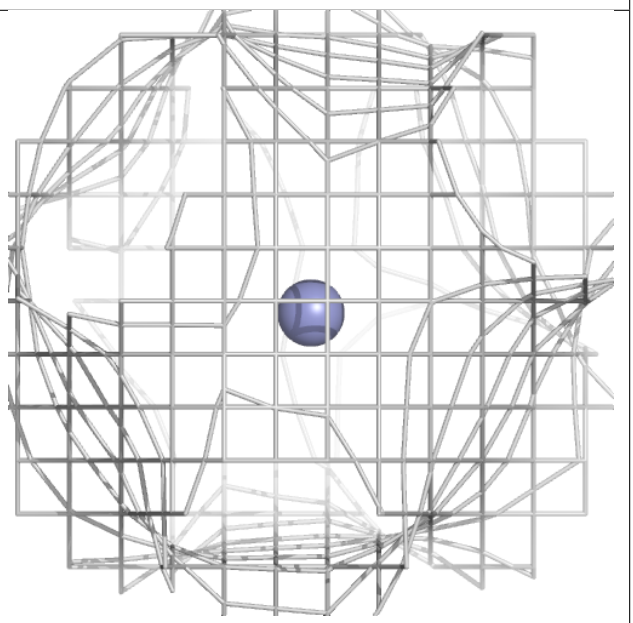


Electron density around ZN C 203:

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

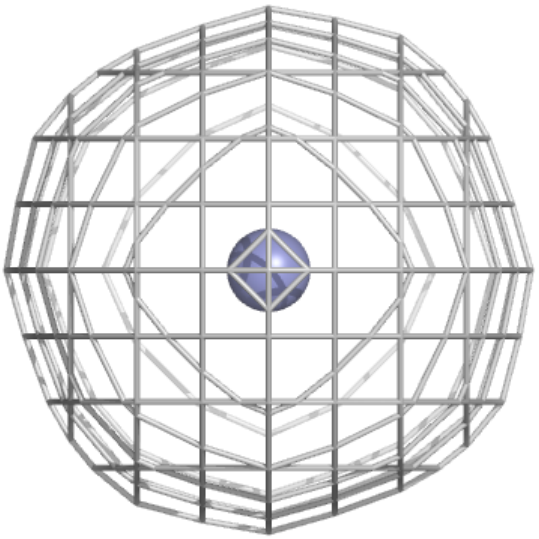


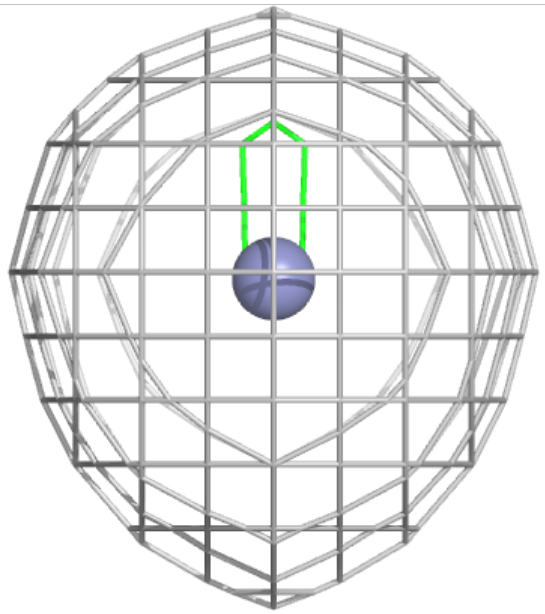


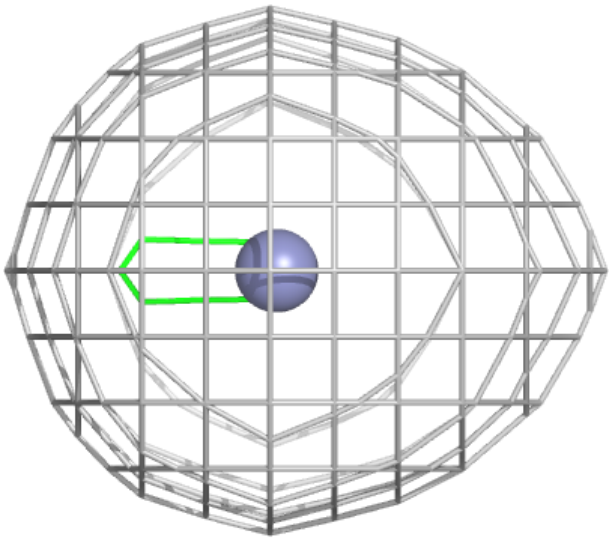


Electron density around ZN D 204:

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

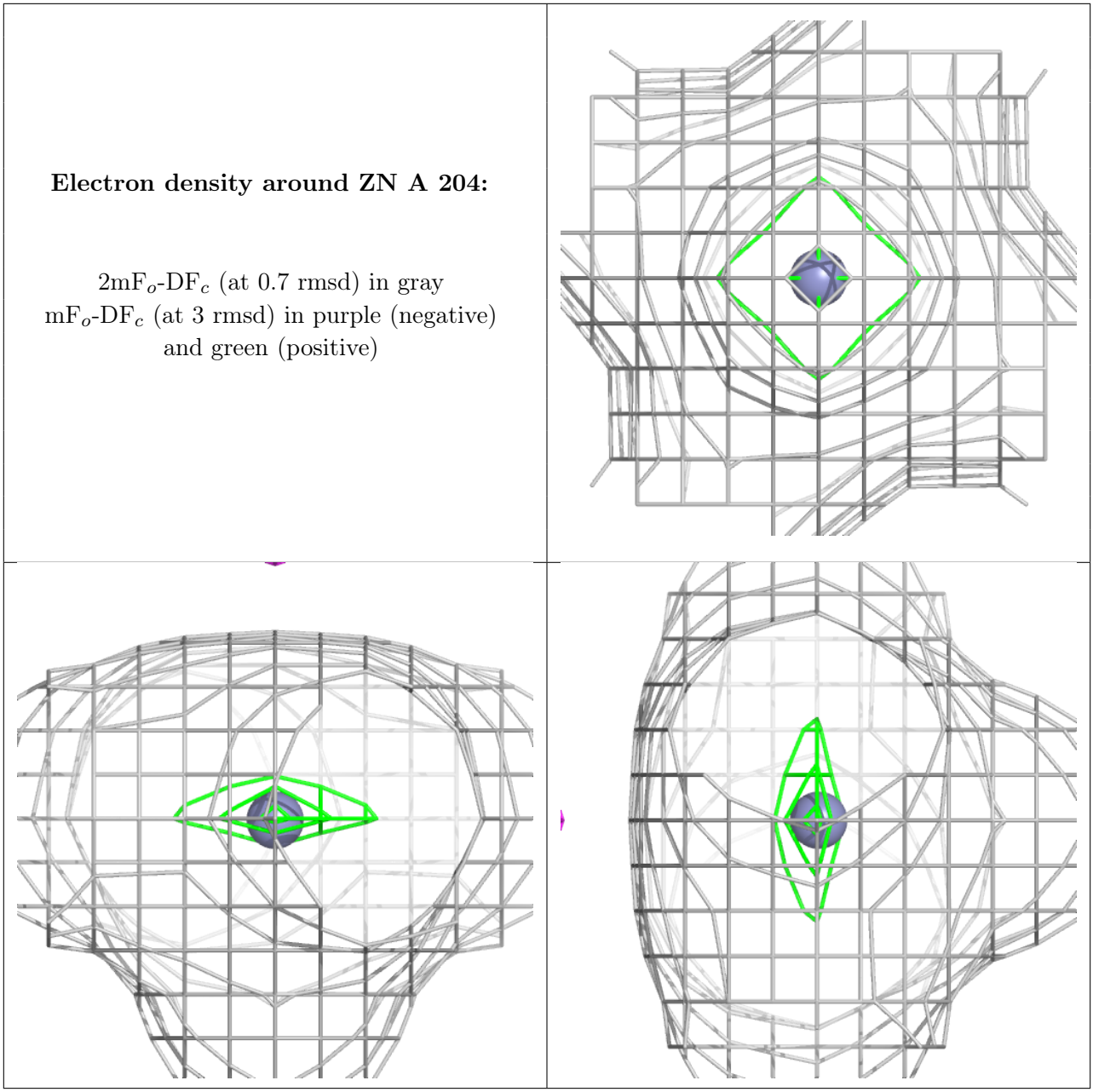






Electron density around ZN A 204:

$2mF_o$-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.