



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 22, 2021 – 10:09 PM JST

PDB ID : 7EK7
Title : prawn ferritin to coordinate with heavy metal ions
Authors : Wang, Y.; Zang, J.
Deposited on : 2021-04-04
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.25
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)	:	2.25

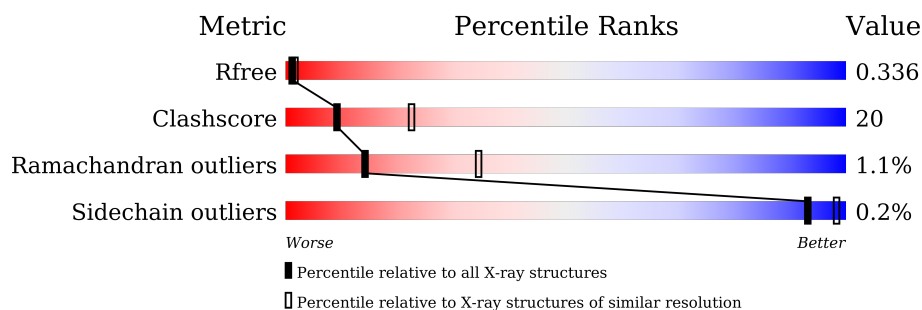
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	169	<div> <div>50%</div> <div>48%</div> <div>.</div> </div>
1	B	169	<div> <div>58%</div> <div>41%</div> <div>.</div> </div>
1	C	169	<div> <div>63%</div> <div>37%</div> <div>.</div> </div>
1	D	169	<div> <div>59%</div> <div>40%</div> <div>.</div> </div>
1	E	169	<div> <div>57%</div> <div>43%</div> <div>.</div> </div>
1	F	169	<div> <div>61%</div> <div>37%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8354 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	169	Total	C	N	O	S	0	0	0
			1361	853	230	271	7			
1	F	169	Total	C	N	O	S	3	2	0
			1370	860	231	272	7			
1	A	169	Total	C	N	O	S	0	1	0
			1368	858	232	271	7			
1	B	169	Total	C	N	O	S	0	1	0
			1367	858	231	271	7			
1	D	169	Total	C	N	O	S	0	6	0
			1391	875	233	276	7			
1	E	169	Total	C	N	O	S	0	1	0
			1367	857	230	273	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	89	ARG	GLN	engineered mutation	UNP T2B7E1
F	89	ARG	GLN	engineered mutation	UNP T2B7E1
A	89	ARG	GLN	engineered mutation	UNP T2B7E1
B	89	ARG	GLN	engineered mutation	UNP T2B7E1
D	89	ARG	GLN	engineered mutation	UNP T2B7E1
E	89	ARG	GLN	engineered mutation	UNP T2B7E1

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Hg	0	0
			1	1		
2	A	1	Total	Hg	0	0
			1	1		
2	D	1	Total	Hg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Hg	0	0
			1	1		

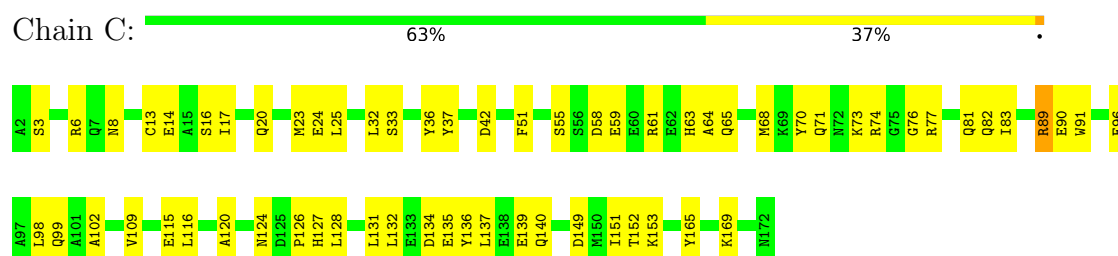
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	23	Total	O	0	0
			23	23		
3	F	21	Total	O	0	0
			21	21		
3	A	24	Total	O	0	0
			24	24		
3	B	21	Total	O	0	0
			21	21		
3	D	17	Total	O	0	0
			17	17		
3	E	20	Total	O	0	0
			20	20		

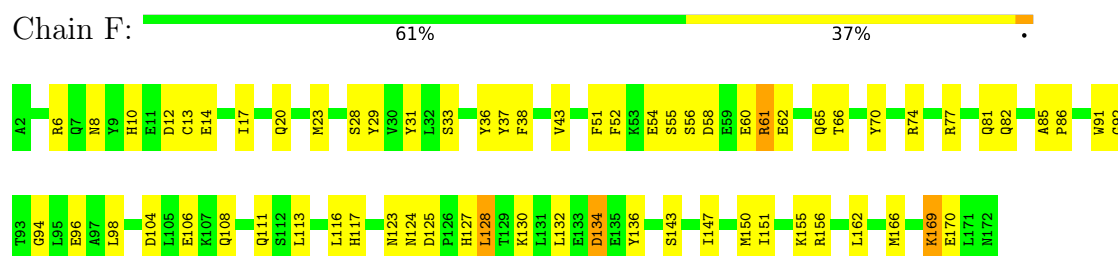
3 Residue-property plots [i](#)

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. 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. 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.

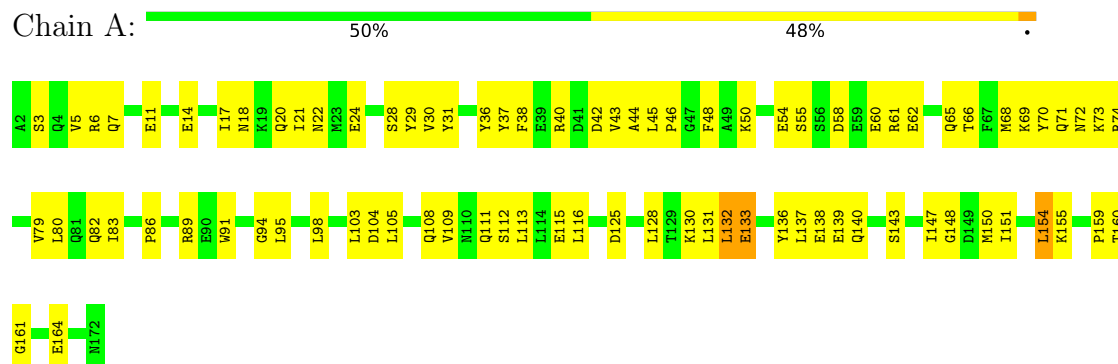
• Molecule 1: Ferritin



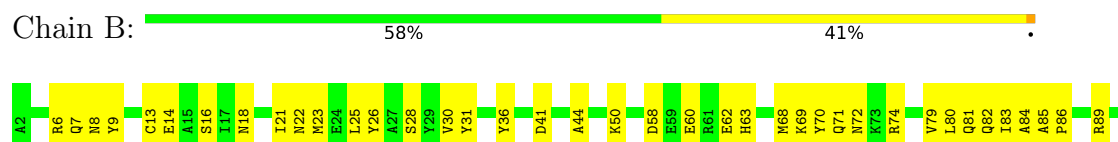
• Molecule 1: Ferritin



• Molecule 1: Ferritin



• Molecule 1: Ferritin

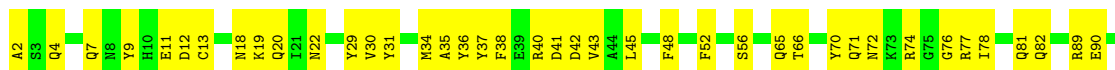




• Molecule 1: Ferritin



• Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	126.28Å 126.28Å 177.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 2.70 30.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.02-2.70) 99.9 (30.02-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.254 , 0.336 0.254 , 0.336	Depositor DCC
R_{free} test set	2056 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 11.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.116 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.115 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.097 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.096 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.447 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8354	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/1396	0.76	3/1876 (0.2%)
1	B	0.52	0/1394	0.68	1/1872 (0.1%)
1	C	0.49	0/1385	0.63	0/1861
1	D	0.58	3/1433 (0.2%)	0.77	3/1923 (0.2%)
1	E	0.52	0/1394	0.70	2/1873 (0.1%)
1	F	0.59	2/1400 (0.1%)	0.71	3/1880 (0.2%)
All	All	0.54	5/8402 (0.1%)	0.71	12/11285 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	13	CYS	CB-SG	10.60	2.00	1.82
1	D	145	LYS	CD-CE	-6.96	1.33	1.51
1	D	145	LYS	CB-CG	-5.67	1.37	1.52
1	D	145	LYS	CG-CD	-5.32	1.34	1.52
1	F	169	LYS	CE-NZ	5.02	1.61	1.49

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	LYS	CD-CE-NZ	-14.61	78.09	111.70
1	D	145	LYS	CB-CG-CD	-8.36	89.88	111.60
1	D	107	LYS	CD-CE-NZ	-7.03	95.53	111.70
1	B	130	LYS	CD-CE-NZ	6.97	127.74	111.70
1	E	130	LYS	CD-CE-NZ	-6.48	96.81	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1368	0	1322	75	3
1	B	1367	0	1329	64	0
1	C	1361	0	1315	48	1
1	D	1391	0	1365	61	3
1	E	1367	0	1320	57	1
1	F	1370	0	1334	60	1
2	A	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
3	A	24	0	0	6	0
3	B	21	0	0	4	0
3	C	23	0	0	5	0
3	D	17	0	0	5	0
3	E	20	0	0	5	0
3	F	21	0	0	8	0
All	All	8354	0	7985	323	5

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 20.

The worst 5 of 323 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:13:CYS:SG	1:B:123:ASN:ND2	2.27	1.05
1:D:53:LYS:NZ	3:D:301:HOH:O	1.94	1.00
1:A:138:GLU:OE2	3:A:301:HOH:O	1.81	0.97
1:A:154:LEU:HB2	3:A:302:HOH:O	1.75	0.85
1:F:123:ASN:ND2	3:F:201:HOH:O	2.06	0.85

All (5) 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:A:7:GLN:OE1	1:D:107:LYS:NZ[6_444]	1.85	0.35
1:A:72:ASN:O	1:D:145:LYS:NZ[6_444]	1.99	0.21
1:A:130:LYS:NZ	1:D:133:GLU:O[6_444]	2.02	0.18
1:E:43:VAL:O	1:E:156:ARG:NH2[3_455]	2.02	0.18
1:C:134:ASP:OD1	1:F:130:LYS:NZ[3_555]	2.10	0.10

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	168/169 (99%)	153 (91%)	13 (8%)	2 (1%)	13	32
1	B	168/169 (99%)	155 (92%)	10 (6%)	3 (2%)	8	21
1	C	167/169 (99%)	156 (93%)	9 (5%)	2 (1%)	13	32
1	D	173/169 (102%)	163 (94%)	9 (5%)	1 (1%)	25	50
1	E	168/169 (99%)	154 (92%)	12 (7%)	2 (1%)	13	32
1	F	169/169 (100%)	160 (95%)	8 (5%)	1 (1%)	25	50
All	All	1013/1014 (100%)	941 (93%)	61 (6%)	11 (1%)	14	34

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	171	LEU
1	C	115	GLU
1	F	134	ASP
1	A	132	LEU
1	B	138	GLU

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	146/145 (101%)	146 (100%)	0	100	100
1	B	146/145 (101%)	146 (100%)	0	100	100
1	C	145/145 (100%)	144 (99%)	1 (1%)	84	94
1	D	151/145 (104%)	150 (99%)	1 (1%)	84	94
1	E	146/145 (101%)	146 (100%)	0	100	100
1	F	147/145 (101%)	147 (100%)	0	100	100
All	All	881/870 (101%)	879 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	89	ARG
1	D	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	110	ASN
1	E	4	GLN
1	E	140	GLN
1	A	82	GLN
1	B	71	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

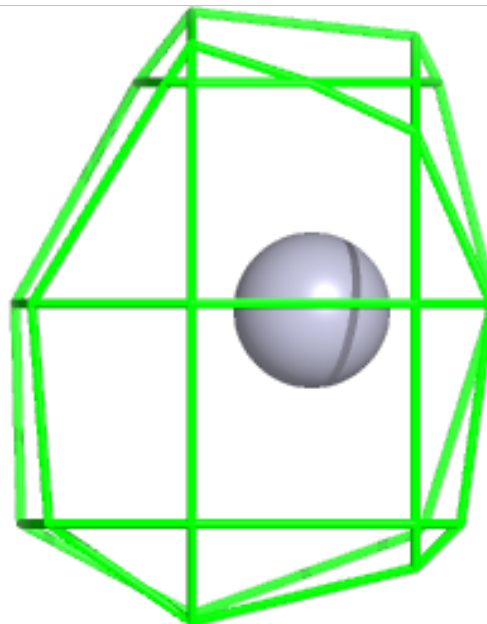
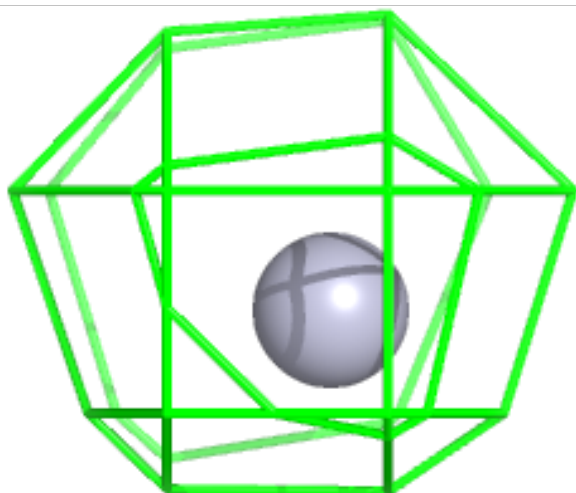
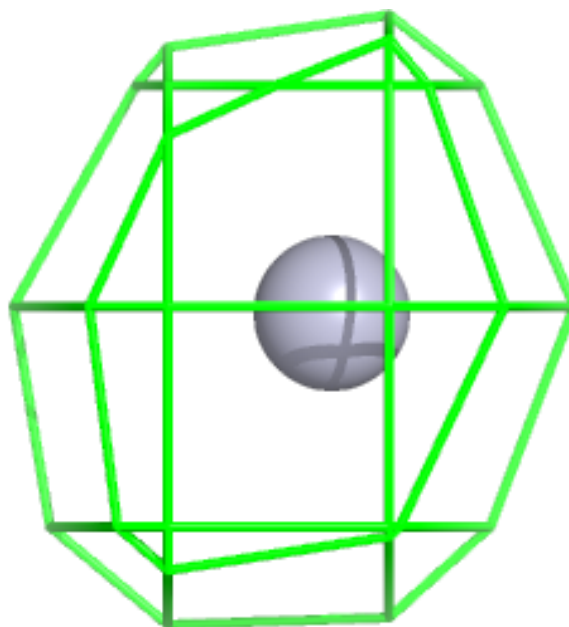
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

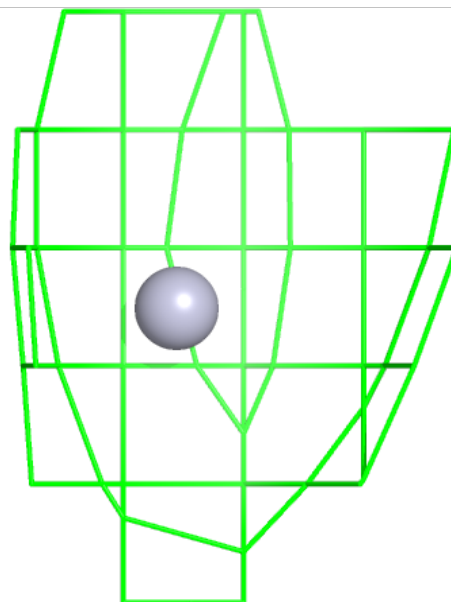
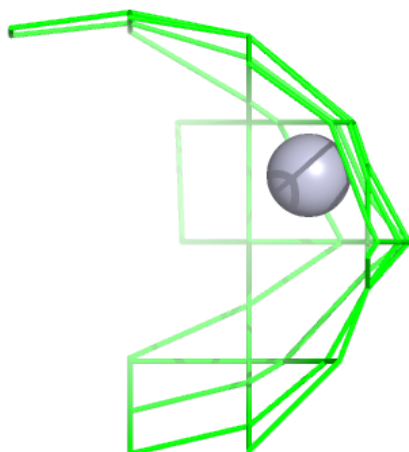
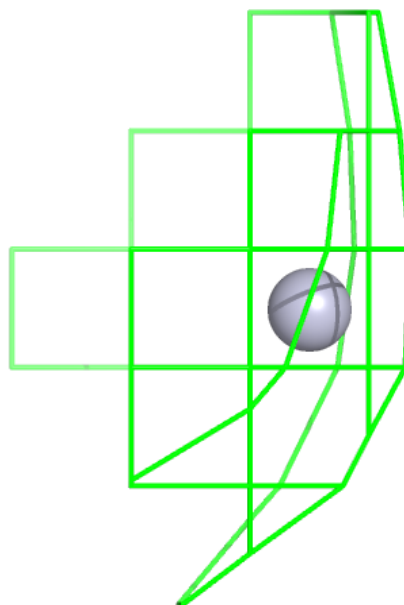
Electron density around HG C 201:

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



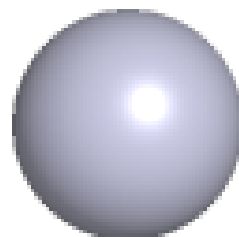
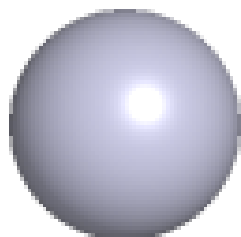
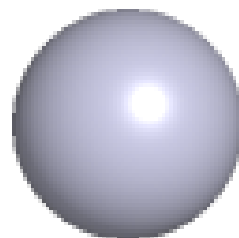
Electron density around HG A 201:

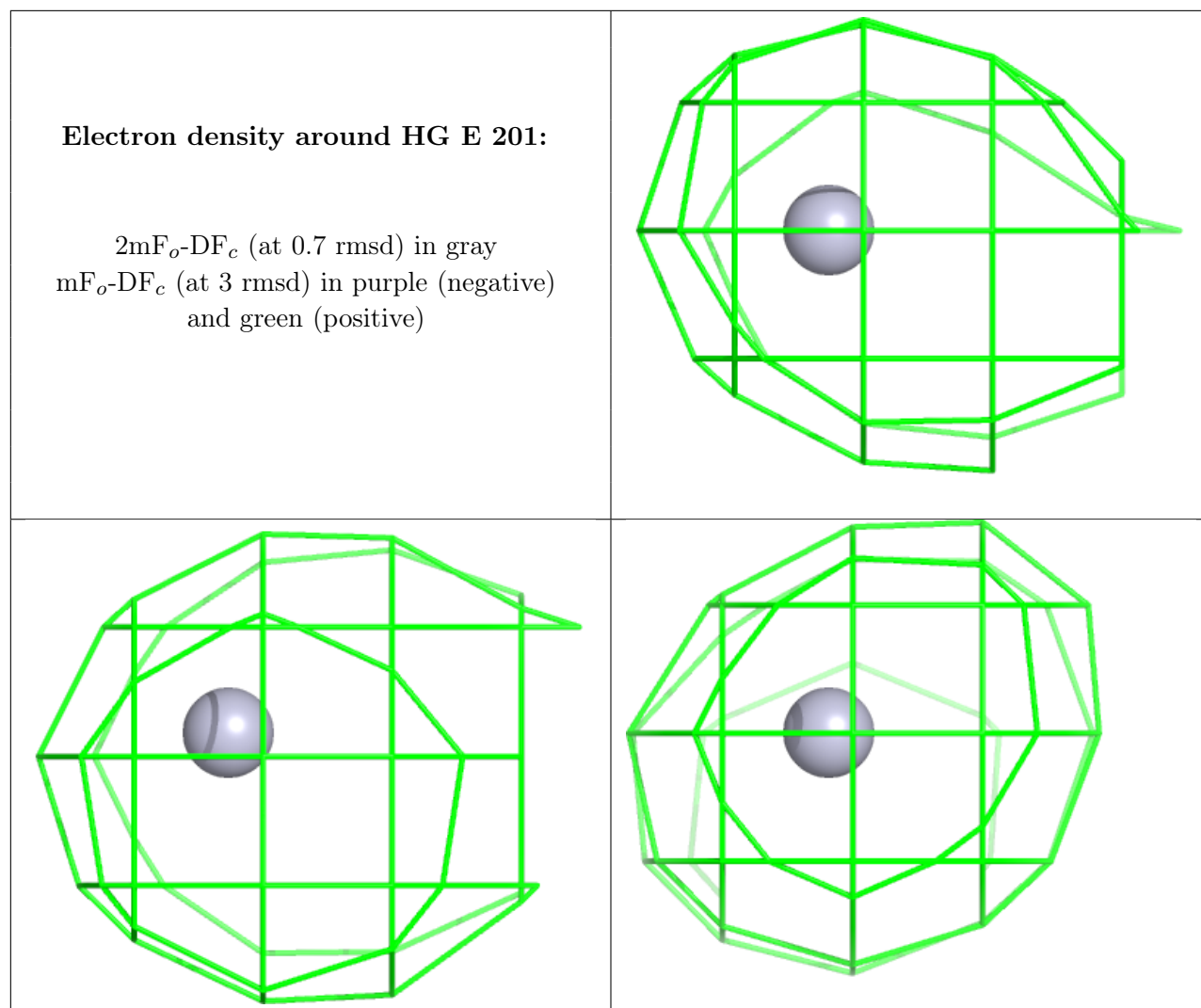
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HG D 201:

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





6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.