wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2024 – 03:39 pm GMT

PDB ID	:	7BDZ
Title	:	X-ray structure of Hen Egg White Lysozyme with dirhodium tetraacetate (1)
Authors	:	Loreto, D.; Merlino, A.; Ferraro, G.
Deposited on	:	2020-12-22
Resolution	:	1.94 Å(reported)

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

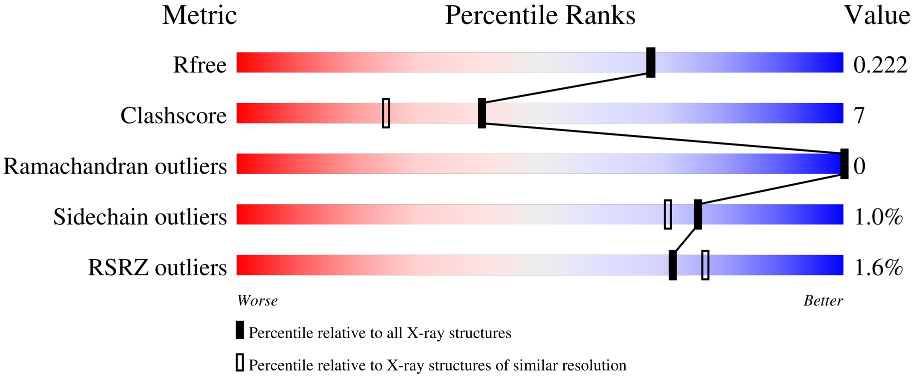
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

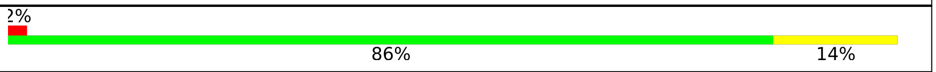
The reported resolution of this entry is 1.94 Å.

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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	129	

2 Entry composition (i)

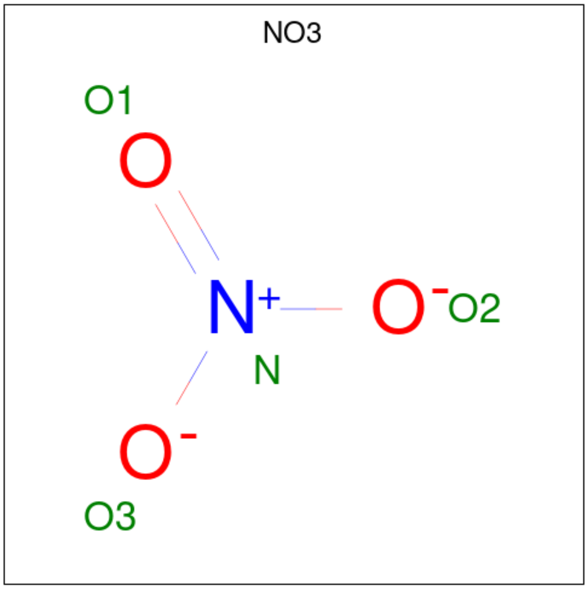
There are 6 unique types of molecules in this entry. The entry contains 1220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	129	1017	621	197	189	10	0	2	0

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
2	AAA	1	4	1	3	0	0
2	AAA	1	4	1	3	0	0
2	AAA	1	4	1	3	0	0
2	AAA	1	4	1	3	0	0
2	AAA	1	4	1	3	0	0

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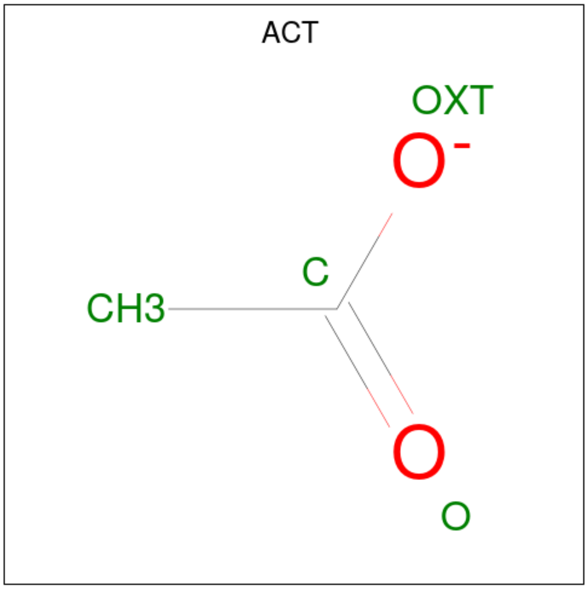
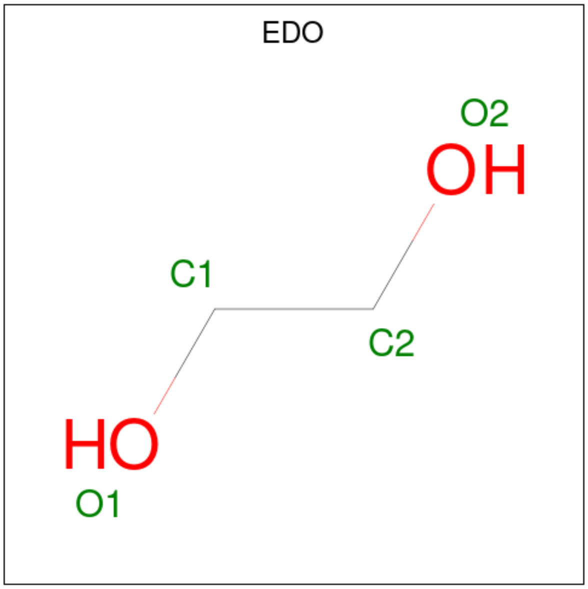
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total N O 4 1 3	0	0
2	AAA	1	Total N O 4 1 3	0	0
2	AAA	1	Total N O 4 1 3	0	0
2	AAA	1	Total N O 4 1 3	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0

- Molecule 5 is Rhodium (three-letter code: RH) (formula: Rh) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	4	Total Rh 4 4	0	1

- Molecule 6 is water.

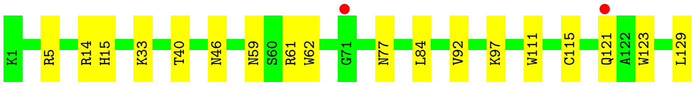
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	125	Total O 127 127	0	3

3 Residue-property plots ⓘ

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

- Molecule 1: Lysozyme

Chain AAA:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.96Å 77.96Å 37.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.48 – 1.94 25.47 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.48-1.94) 99.2 (25.47-1.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.156 , 0.217 0.165 , 0.222	Depositor DCC
R_{free} test set	430 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1220	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: ACT, RH, NO3, EDO

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	AAA	0.74	0/1037	0.81	0/1401

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	AAA	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	62	TRP	Peptide

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	AAA	1017	0	968	13	1
2	AAA	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	28	0	21	3	0
4	AAA	8	0	12	0	0
5	AAA	4	0	0	0	0
6	AAA	127	0	0	5	1
All	All	1220	0	1001	15	2

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.

The worst 5 of 15 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:AAA:14:ARG:NH2	6:AAA:301:HOH:O	2.07	0.81
3:AAA:214:ACT:H1	6:AAA:309:HOH:O	1.90	0.70
1:AAA:5:ARG:HB2	3:AAA:211:ACT:H2	1.78	0.64
1:AAA:46:ASN:ND2	1:AAA:59[B]:ASN:ND2	2.45	0.64
1:AAA:15:HIS:HB3	1:AAA:92:VAL:HG11	1.80	0.63

All (2) 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:AAA:129:LEU:OXT	1:AAA:129:LEU:OXT[7_554]	2.10	0.10
6:AAA:308:HOH:O	6:AAA:321:HOH:O[3_455]	2.13	0.07

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	AAA	129/129 (100%)	126 (98%)	3 (2%)	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	AAA	107/105 (102%)	106 (99%)	1 (1%)	78 75

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NO3	AAA	205	-	1,3,3	0.06	0	0,3,3	-	-
4	EDO	AAA	217	-	3,3,3	0.23	0	2,2,2	0.12	0
3	ACT	AAA	211	-	3,3,3	0.95	0	3,3,3	0.81	0
3	ACT	AAA	215	-	3,3,3	1.12	0	3,3,3	0.97	0
3	ACT	AAA	213	5	3,3,3	0.96	0	3,3,3	0.70	0
2	NO3	AAA	201	-	1,3,3	0.83	0	0,3,3	-	-
2	NO3	AAA	208	-	1,3,3	0.23	0	0,3,3	-	-
3	ACT	AAA	216	5	3,3,3	0.87	0	3,3,3	0.76	0
2	NO3	AAA	203	-	1,3,3	0.94	0	0,3,3	-	-
3	ACT	AAA	210	-	3,3,3	1.12	0	3,3,3	0.60	0
2	NO3	AAA	202	-	1,3,3	0.16	0	0,3,3	-	-
2	NO3	AAA	204	-	1,3,3	0.02	0	0,3,3	-	-
2	NO3	AAA	206	-	1,3,3	0.06	0	0,3,3	-	-
3	ACT	AAA	214	-	3,3,3	0.94	0	3,3,3	1.00	0
2	NO3	AAA	209	-	1,3,3	0.31	0	0,3,3	-	-
3	ACT	AAA	212	-	3,3,3	1.09	0	3,3,3	0.72	0
4	EDO	AAA	218	-	3,3,3	0.21	0	2,2,2	0.06	0
2	NO3	AAA	207	-	1,3,3	0.30	0	0,3,3	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	217	-	-	0/1/1/1	-
4	EDO	AAA	218	-	-	0/1/1/1	-

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	211	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	215	ACT	1	0
3	AAA	214	ACT	1	0

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	AAA	129/129 (100%)	0.09	2 (1%)	72	77	13, 19, 32, 43	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	121	GLN	3.7
1	AAA	71	GLY	3.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	RH	AAA	222	1/1	0.71	0.17	67,67,67,67	1
3	ACT	AAA	216	4/4	0.81	0.20	38,38,39,46	0
2	NO3	AAA	206	4/4	0.85	0.21	39,41,43,43	0
5	RH	AAA	221	1/1	0.86	0.14	75,75,75,75	1
2	NO3	AAA	207	4/4	0.87	0.24	29,31,34,42	0

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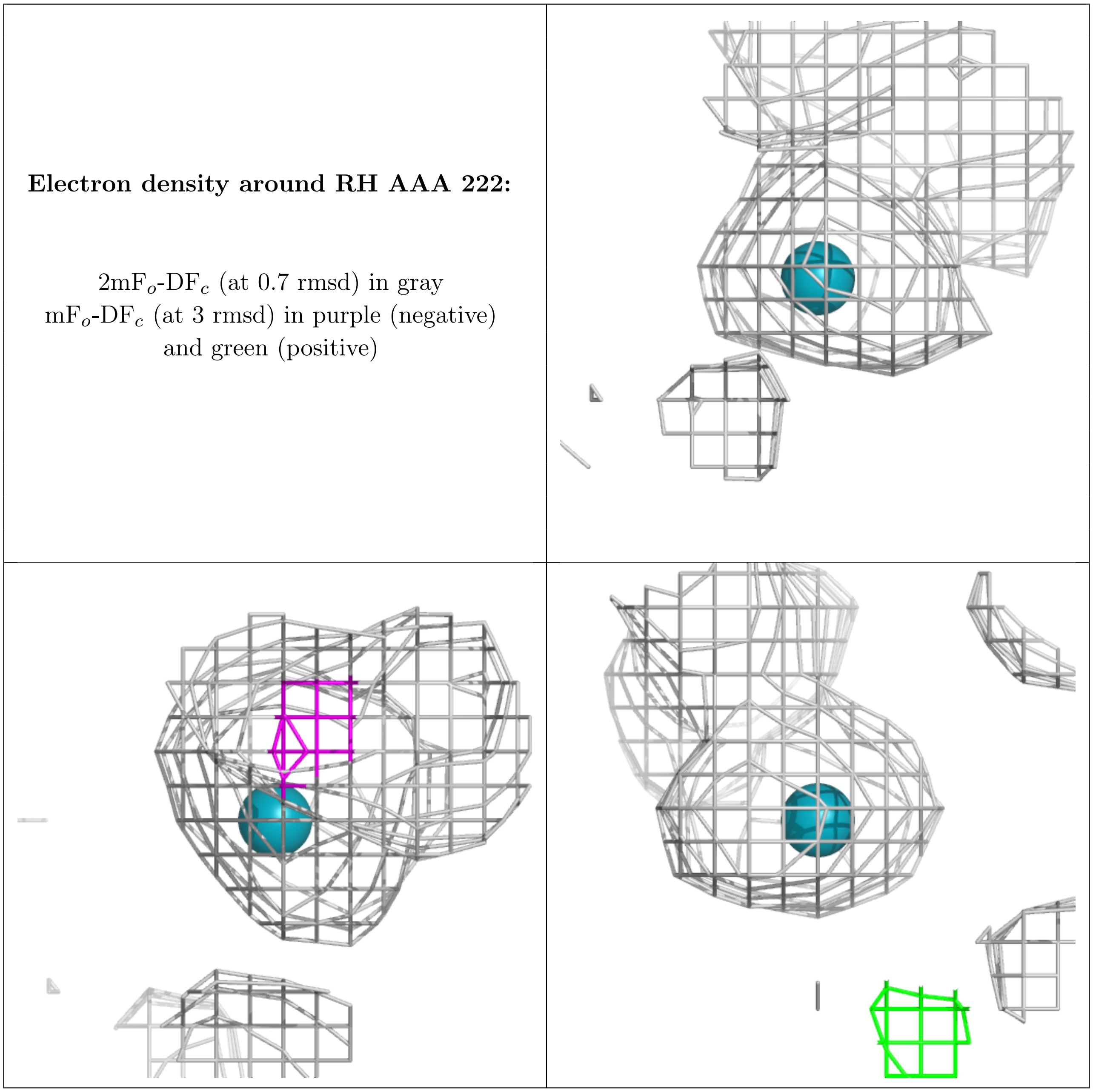
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
2	NO3	AAA	201	4/4	0.87	0.18	29,35,40,40	0
3	ACT	AAA	212	4/4	0.88	0.28	50,50,52,53	0
2	NO3	AAA	205	4/4	0.88	0.15	29,39,42,45	0
3	ACT	AAA	214	4/4	0.89	0.14	18,19,21,23	0
3	ACT	AAA	211	4/4	0.90	0.15	35,37,41,43	0
2	NO3	AAA	208	4/4	0.90	0.30	45,56,58,60	0
3	ACT	AAA	213	4/4	0.92	0.23	31,32,33,34	4
3	ACT	AAA	215	4/4	0.94	0.15	25,28,33,36	0
2	NO3	AAA	204	4/4	0.95	0.14	23,23,28,32	0
4	EDO	AAA	217	4/4	0.95	0.13	22,23,23,24	0
3	ACT	AAA	210	4/4	0.96	0.14	28,29,30,33	0
2	NO3	AAA	209	4/4	0.96	0.32	32,38,39,42	0
2	NO3	AAA	202	4/4	0.97	0.14	22,25,26,28	0
2	NO3	AAA	203	4/4	0.97	0.17	33,33,35,40	0
5	RH	AAA	220	1/1	0.98	0.05	31,31,31,31	1
4	EDO	AAA	218	4/4	0.98	0.13	20,20,20,20	4
5	RH	AAA	219[B]	1/1	0.98	0.04	33,33,33,33	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.

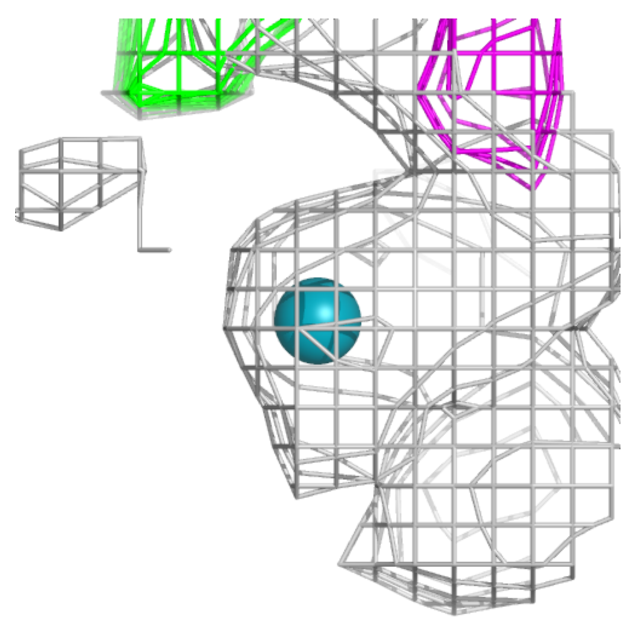


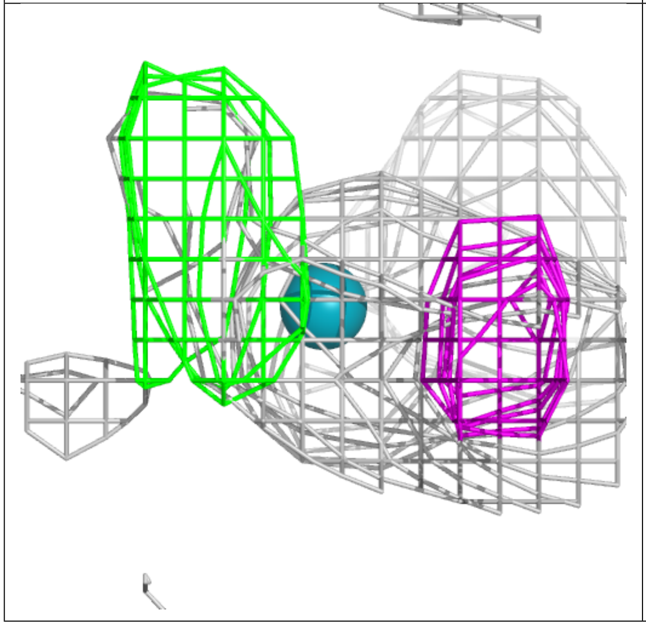
Electron density around RH AAA 222:

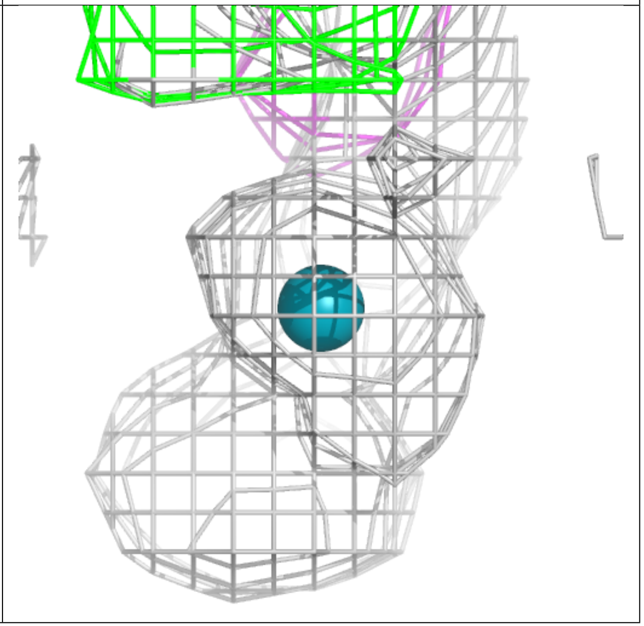
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

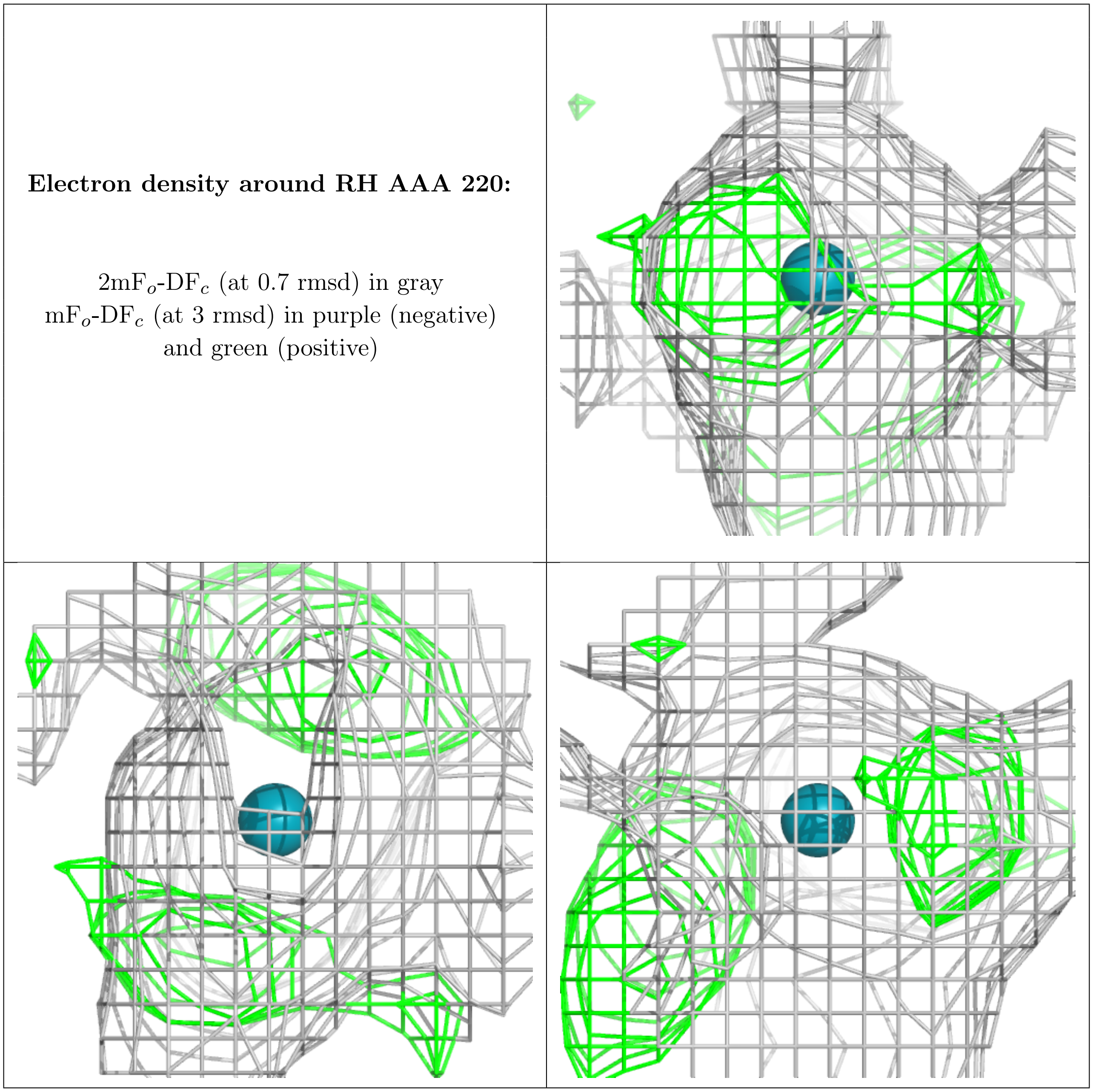
Electron density around RH AAA 221:

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







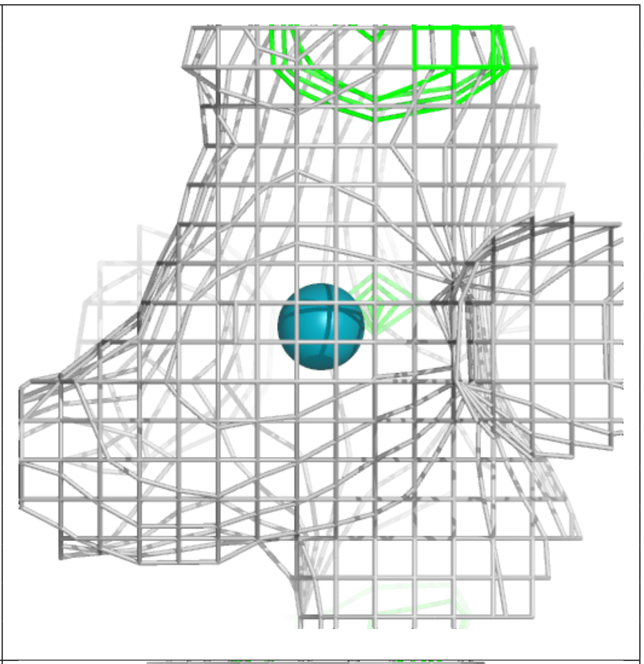


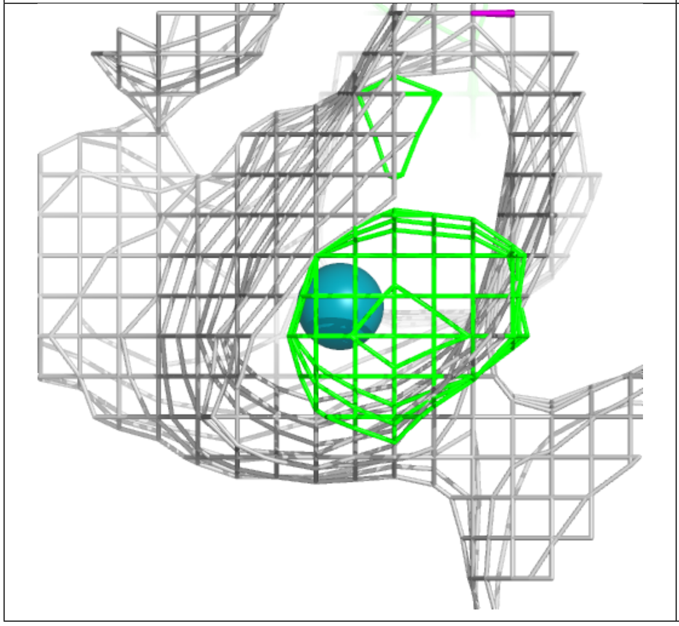
Electron density around RH AAA 220:

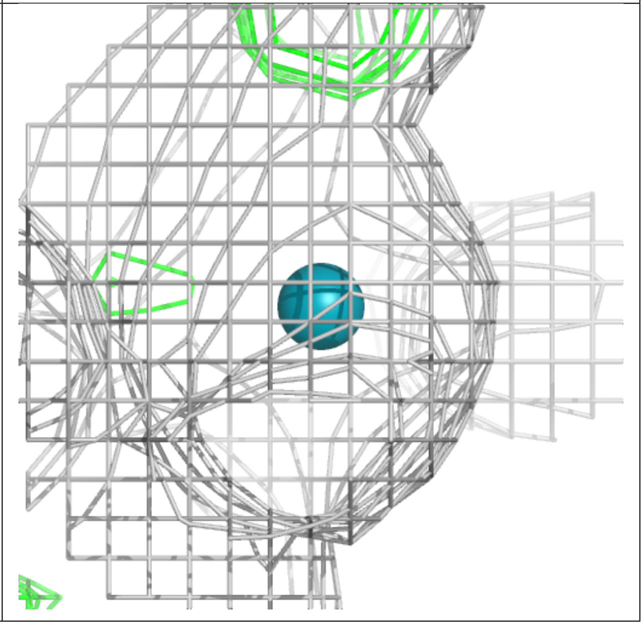
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around RH AAA 219 (B):

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.