WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2023 – 12:30 PM EST

PDB ID	:	8U8R
Title	:	Y229F/V290N/S292F Streptomyces coelicolor Laccase
Authors	:	Wang, J.-X.; Lu, Y.
Deposited on	:	2023-09-18
Resolution	:	2.86 Å(reported)

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

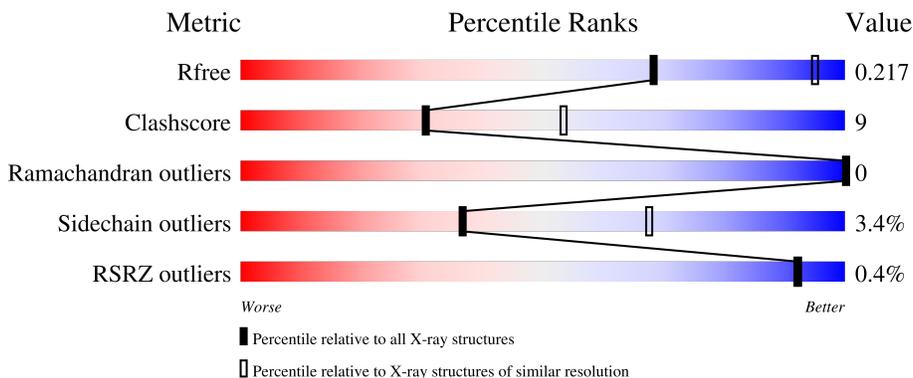|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.86 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	Percentile Ranks	Value
Rfree		0.217
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		3.4%
RSRZ outliers		0.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	351	63% 16% • 21%
1	B	351	62% 16% • 21%
1	C	351	63% 16% • 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLY	A	406	-	X	-	-
4	GLY	A	409	-	X	-	-
4	GLY	B	406	-	X	-	-
4	GLY	C	406	-	X	-	-

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 7090 atoms, of which 258 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 Copper oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2155	1349	393	402	11			
1	B	278	Total	C	N	O	S	0	0	0
			2155	1349	393	402	11			
1	C	278	Total	C	N	O	S	0	0	0
			2155	1349	393	402	11			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	PHE	TYR	engineered mutation	UNP Q9XAL8
A	290	ASN	VAL	engineered mutation	UNP Q9XAL8
A	292	PHE	SER	engineered mutation	UNP Q9XAL8
A	344	LEU	-	expression tag	UNP Q9XAL8
A	345	GLU	-	expression tag	UNP Q9XAL8
A	346	HIS	-	expression tag	UNP Q9XAL8
A	347	HIS	-	expression tag	UNP Q9XAL8
A	348	HIS	-	expression tag	UNP Q9XAL8
A	349	HIS	-	expression tag	UNP Q9XAL8
A	350	HIS	-	expression tag	UNP Q9XAL8
A	351	HIS	-	expression tag	UNP Q9XAL8
B	229	PHE	TYR	engineered mutation	UNP Q9XAL8
B	290	ASN	VAL	engineered mutation	UNP Q9XAL8
B	292	PHE	SER	engineered mutation	UNP Q9XAL8
B	344	LEU	-	expression tag	UNP Q9XAL8
B	345	GLU	-	expression tag	UNP Q9XAL8
B	346	HIS	-	expression tag	UNP Q9XAL8
B	347	HIS	-	expression tag	UNP Q9XAL8
B	348	HIS	-	expression tag	UNP Q9XAL8
B	349	HIS	-	expression tag	UNP Q9XAL8
B	350	HIS	-	expression tag	UNP Q9XAL8
B	351	HIS	-	expression tag	UNP Q9XAL8
C	229	PHE	TYR	engineered mutation	UNP Q9XAL8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	290	ASN	VAL	engineered mutation	UNP Q9XAL8
C	292	PHE	SER	engineered mutation	UNP Q9XAL8
C	344	LEU	-	expression tag	UNP Q9XAL8
C	345	GLU	-	expression tag	UNP Q9XAL8
C	346	HIS	-	expression tag	UNP Q9XAL8
C	347	HIS	-	expression tag	UNP Q9XAL8
C	348	HIS	-	expression tag	UNP Q9XAL8
C	349	HIS	-	expression tag	UNP Q9XAL8
C	350	HIS	-	expression tag	UNP Q9XAL8
C	351	HIS	-	expression tag	UNP Q9XAL8

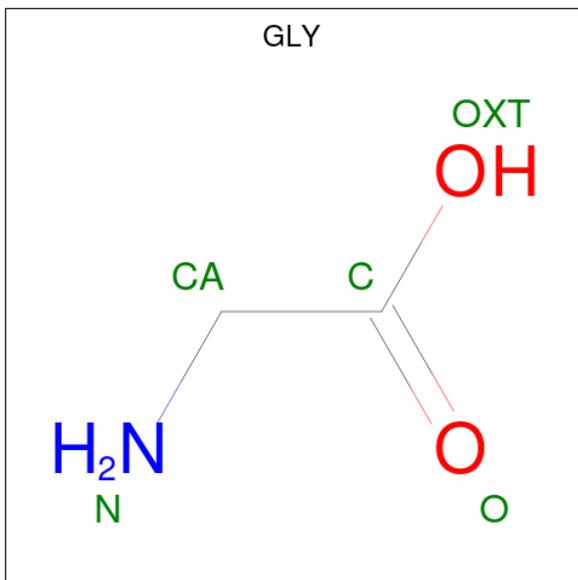- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Cu 4	0	0
2	B	4	Total 4	Cu 4	0	0
2	C	4	Total 4	Cu 4	0	0

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO) (labeled as "Ligand of Interest" by depositor).

OH

HO⁻ₒ
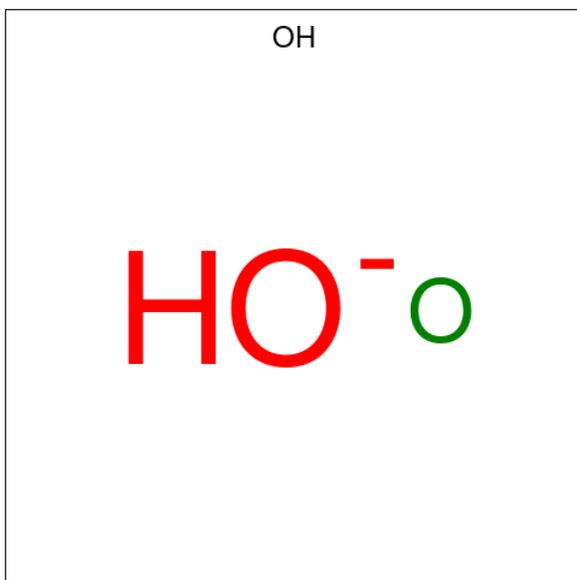
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	1	Total 1	O 1	0	0
3	C	1	Total 1	O 1	0	0

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	A	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	A	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	A	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	A	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	B	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	B	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	B	1	Total 10	C 2	H 5	N 1	O 2	0	0
4	B	1	Total 10	C 2	H 5	N 1	O 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
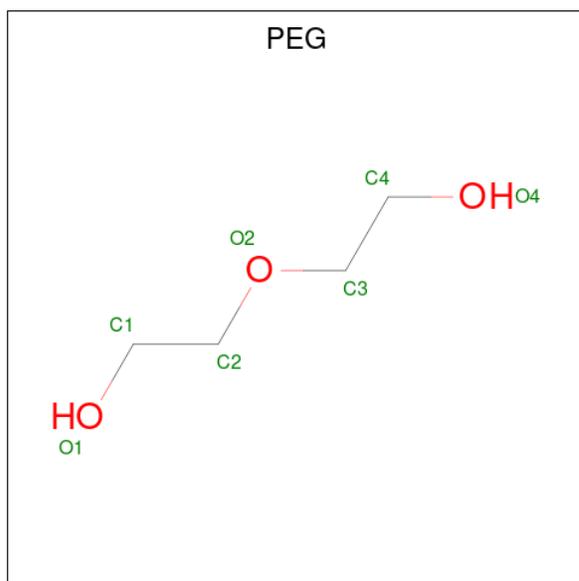
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
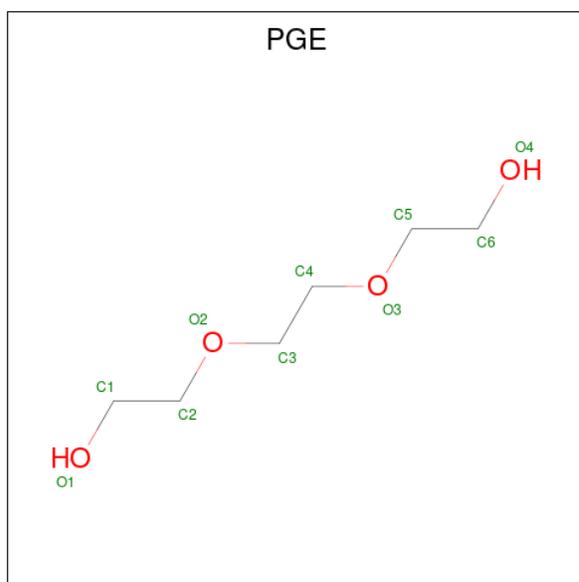
PGE

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			24	6	14	4		
6	B	1	Total	C	H	O	0	0
			24	6	14	4		
6	C	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
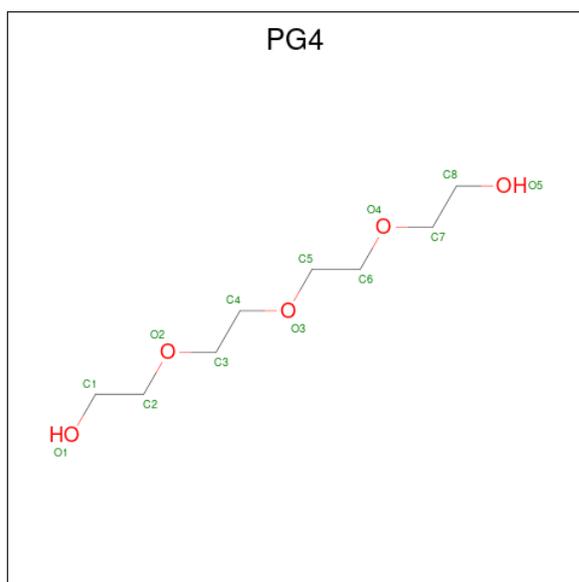
PG4

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			31	8	18	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 31	C 8	H 18	O 5	0	0
7	B	1	Total 31	C 8	H 18	O 5	0	0
7	B	1	Total 31	C 8	H 18	O 5	0	0
7	C	1	Total 31	C 8	H 18	O 5	0	0
7	C	1	Total 31	C 8	H 18	O 5	0	0

- Molecule 8 is BORIC ACID (three-letter code: BO3) (formula: BH_3O_3).
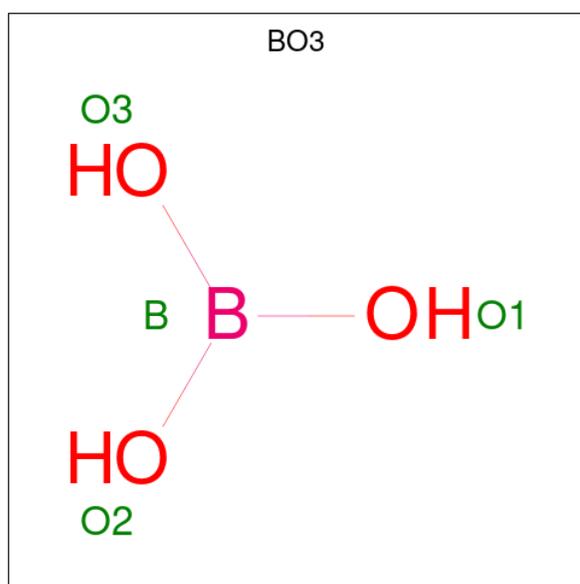
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 7	B 1	H 3	O 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	50	Total 50	O 50	0	0
9	B	52	Total 52	O 52	0	0
9	C	42	Total 42	O 42	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Copper oxidase

Chain A:

- Molecule 1: Copper oxidase

Chain B:

- Molecule 1: Copper oxidase

Chain C:

D121 R128 T129 Y130 R133 P137 G138 R139 R146 P147 G148 W153 V159 N171 G172 L173 V179 I193 V194 R203 H206 T207 G208 P209 T214 V215 I221 V222 M223 I224 Y230 H231 T232 R239 W240 A241 R244 T245 G246 T249 D252 D253

P254 S255 G264 D267 M285 Y286 H287 C288 G297 M298 V299 G300 D308 G309 T310 Y314 GLU PRO HIS GLU HIS GLY GLY ALA THR ALA LYS SER GLY GLU SER GLY GLU PRO THR GLY GLY ALA ALA ALA HIS GLU HIS GLU HIS LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	177.35Å 177.35Å 176.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.70 – 2.86 72.38 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.70-2.86) 87.0 (72.38-2.65)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.48 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.181 , 0.214 0.184 , 0.217	Depositor DCC
R_{free} test set	4048 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.457 for -h,-l,-k 0.457 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7090	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BO3, PG4, PEG, PGE, CU, OH

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	0.40	0/2218	0.66	0/3009
1	B	0.39	0/2218	0.65	0/3009
1	C	0.40	0/2218	0.66	0/3009
All	All	0.40	0/6654	0.65	0/9027

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (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	2155	0	2036	40	0
1	B	2155	0	2036	41	0
1	C	2155	0	2036	42	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	25	25	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	25	25	10	0	0
4	C	25	25	10	1	0
5	A	7	10	10	0	0
5	B	7	10	10	0	0
5	C	7	10	10	1	0
6	A	10	14	14	1	0
6	B	10	14	14	0	0
6	C	10	14	14	1	0
7	A	26	36	36	7	0
7	B	26	36	36	4	0
7	C	26	36	36	4	0
8	A	4	3	3	0	0
9	A	50	0	0	0	0
9	B	52	0	0	1	0
9	C	42	0	0	0	0
All	All	6832	258	6321	119	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 9.

The worst 5 of 119 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:C:249:THR:HG23	1:C:253:ASP:OD2	1.76	0.85
1:A:249:THR:HG23	1:A:253:ASP:OD2	1.83	0.79
1:C:60:ASP:OD1	1:C:62:GLN:HG3	1.84	0.76
1:B:249:THR:HG23	1:B:253:ASP:OD2	1.86	0.76
1:B:53:MET:HE3	1:B:89:ILE:HG21	1.68	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	276/351 (79%)	262 (95%)	14 (5%)	0	100	100
1	B	276/351 (79%)	265 (96%)	11 (4%)	0	100	100
1	C	276/351 (79%)	262 (95%)	14 (5%)	0	100	100
All	All	828/1053 (79%)	789 (95%)	39 (5%)	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	223/270 (83%)	215 (96%)	8 (4%)	35	66
1	B	223/270 (83%)	217 (97%)	6 (3%)	44	74
1	C	223/270 (83%)	214 (96%)	9 (4%)	31	62
All	All	669/810 (83%)	646 (97%)	23 (3%)	37	67

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	53	MET
1	C	133	ARG
1	C	120	SER
1	C	139	ARG
1	A	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	B	164	HIS
1	C	287	HIS
1	C	82	ASN
1	B	62	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 43 ligands modelled in this entry, 12 are monoatomic and 3 are modelled with single atom - leaving 28 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	#$|Z| > 2$
4	GLY	B	406	-	4,4,4	0.99	0	3,4,4	1.69	2 (66%)
4	GLY	C	408	-	4,4,4	0.94	0	3,4,4	2.08	1 (33%)
7	PG4	A	413	-	12,12,12	0.19	0	11,11,11	0.63	0
5	PEG	B	410	-	6,6,6	0.38	0	5,5,5	0.24	0
4	GLY	A	415	-	4,4,4	1.17	1 (25%)	3,4,4	1.68	1 (33%)
4	GLY	B	407	-	4,4,4	1.22	1 (25%)	3,4,4	1.30	0
4	GLY	C	406	-	4,4,4	1.18	1 (25%)	3,4,4	1.48	1 (33%)
4	GLY	B	414	-	4,4,4	1.11	0	3,4,4	1.16	0
4	GLY	A	407	-	4,4,4	1.18	0	3,4,4	0.94	0
7	PG4	B	412	-	12,12,12	0.25	0	11,11,11	0.52	0
6	PGE	B	411	-	9,9,9	0.37	0	8,8,8	0.35	0
4	GLY	C	410	-	4,4,4	1.07	1 (25%)	3,4,4	1.52	1 (33%)
4	GLY	B	409	-	4,4,4	1.05	0	3,4,4	1.80	1 (33%)
6	PGE	C	411	-	9,9,9	0.42	0	8,8,8	0.32	0
8	BO3	A	414	-	3,3,3	0.46	0	3,3,3	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	PG4	C	413	-	12,12,12	0.29	0	11,11,11	0.78	0
6	PGE	A	411	-	9,9,9	0.32	0	8,8,8	0.47	0
4	GLY	B	408	-	4,4,4	1.22	1 (25%)	3,4,4	1.27	0
4	GLY	C	407	-	4,4,4	1.11	1 (25%)	3,4,4	1.46	0
7	PG4	A	412	-	12,12,12	0.29	0	11,11,11	0.53	0
4	GLY	C	409	-	4,4,4	1.20	1 (25%)	3,4,4	1.46	0
4	GLY	A	409	-	4,4,4	1.06	0	3,4,4	1.79	2 (66%)
4	GLY	A	408	-	4,4,4	1.15	1 (25%)	3,4,4	1.51	0
7	PG4	B	413	-	12,12,12	0.22	0	11,11,11	0.60	0
5	PEG	A	410	-	6,6,6	0.32	0	5,5,5	0.29	0
7	PG4	C	414	-	12,12,12	0.23	0	11,11,11	0.70	0
5	PEG	C	412	-	6,6,6	0.33	0	5,5,5	0.19	0
4	GLY	A	406	-	4,4,4	1.19	1 (25%)	3,4,4	1.57	1 (33%)

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	GLY	B	406	-	-	2/2/2/2	-
4	GLY	C	408	-	-	0/2/2/2	-
7	PG4	A	413	-	-	8/10/10/10	-
5	PEG	B	410	-	-	4/4/4/4	-
4	GLY	A	415	-	-	0/2/2/2	-
4	GLY	B	407	-	-	2/2/2/2	-
4	GLY	C	406	-	-	2/2/2/2	-
4	GLY	B	414	-	-	0/2/2/2	-
4	GLY	A	407	-	-	2/2/2/2	-
7	PG4	B	412	-	-	7/10/10/10	-
6	PGE	B	411	-	-	3/7/7/7	-
4	GLY	C	410	-	-	0/2/2/2	-
4	GLY	B	409	-	-	0/2/2/2	-
6	PGE	C	411	-	-	4/7/7/7	-
7	PG4	C	413	-	-	6/10/10/10	-
6	PGE	A	411	-	-	5/7/7/7	-
4	GLY	B	408	-	-	2/2/2/2	-
4	GLY	C	407	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	A	412	-	-	4/10/10/10	-
4	GLY	C	409	-	-	2/2/2/2	-
4	GLY	A	409	-	-	2/2/2/2	-
4	GLY	A	408	-	-	2/2/2/2	-
7	PG4	B	413	-	-	6/10/10/10	-
5	PEG	A	410	-	-	1/4/4/4	-
7	PG4	C	414	-	-	6/10/10/10	-
5	PEG	C	412	-	-	0/4/4/4	-
4	GLY	A	406	-	-	2/2/2/2	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	409	GLY	OXT-C	-2.23	1.23	1.30
4	B	407	GLY	OXT-C	-2.20	1.23	1.30
4	A	406	GLY	OXT-C	-2.20	1.23	1.30
4	B	408	GLY	OXT-C	-2.19	1.23	1.30
4	A	415	GLY	OXT-C	-2.18	1.23	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	408	GLY	OXT-C-CA	2.75	124.38	113.45
4	A	415	GLY	OXT-C-O	-2.32	117.52	123.30
4	B	409	GLY	OXT-C-CA	2.28	122.53	113.45
4	A	409	GLY	OXT-C-O	-2.21	117.78	123.30
4	C	410	GLY	OXT-C-O	-2.21	117.78	123.30

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	GLY	O-C-CA-N
4	A	406	GLY	OXT-C-CA-N
4	A	407	GLY	OXT-C-CA-N
4	A	408	GLY	O-C-CA-N
4	A	408	GLY	OXT-C-CA-N

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	413	PG4	4	0
4	A	407	GLY	1	0
6	C	411	PGE	1	0
7	C	413	PG4	2	0
6	A	411	PGE	1	0
4	C	407	GLY	1	0
7	A	412	PG4	3	0
7	B	413	PG4	4	0
7	C	414	PG4	2	0
5	C	412	PEG	1	0
4	A	406	GLY	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	A	278/351 (79%)	0.06	1 (0%)	92	92	39, 51, 71, 99	0
1	B	278/351 (79%)	0.10	1 (0%)	92	92	36, 52, 71, 105	0
1	C	278/351 (79%)	0.10	1 (0%)	92	92	39, 52, 70, 102	0
All	All	834/1053 (79%)	0.09	3 (0%)	92	92	36, 52, 71, 105	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	ILE	4.4
1	C	37	ILE	2.9
1	A	37	ILE	2.3

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	PEG	B	410	7/7	0.63	0.37	72,99,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	A	410	7/7	0.75	0.25	65,98,123,123	0
5	PEG	C	412	7/7	0.76	0.36	71,94,114,114	0
6	PGE	A	411	10/10	0.81	0.30	73,103,124,124	0
6	PGE	C	411	10/10	0.81	0.28	66,100,123,127	0
7	PG4	C	413	13/13	0.86	0.31	65,91,111,112	0
7	PG4	A	413	13/13	0.87	0.24	68,89,107,122	0
7	PG4	B	412	13/13	0.89	0.24	67,92,112,119	0
6	PGE	B	411	10/10	0.89	0.36	71,101,116,116	0
7	PG4	A	412	13/13	0.90	0.27	67,88,112,116	0
7	PG4	B	413	13/13	0.91	0.24	73,90,104,108	0
4	GLY	A	409	5/5	0.91	0.26	72,86,94,94	0
7	PG4	C	414	13/13	0.91	0.29	66,94,113,120	0
4	GLY	C	410	5/5	0.92	0.23	65,79,99,99	0
4	GLY	B	409	5/5	0.93	0.29	71,85,102,102	0
4	GLY	B	408	5/5	0.93	0.22	65,78,92,94	0
4	GLY	C	409	5/5	0.94	0.25	64,81,97,97	0
4	GLY	A	408	5/5	0.95	0.22	70,80,87,87	0
4	GLY	B	406	5/5	0.95	0.20	52,63,70,78	0
4	GLY	A	415	5/5	0.96	0.24	42,50,66,81	0
4	GLY	C	407	5/5	0.97	0.25	53,63,74,80	0
4	GLY	C	408	5/5	0.97	0.21	51,62,77,82	0
3	OH	C	405	1/1	0.97	0.46	49,49,49,49	1
4	GLY	A	407	5/5	0.97	0.27	49,58,66,74	0
4	GLY	B	407	5/5	0.98	0.26	47,56,82,88	0
3	OH	B	405	1/1	0.98	0.35	49,49,49,49	1
2	CU	C	403	1/1	0.98	0.81	49,49,49,49	1
4	GLY	B	414	5/5	0.98	0.19	37,52,71,73	0
4	GLY	C	406	5/5	0.98	0.22	39,47,62,72	0
4	GLY	A	406	5/5	0.98	0.20	55,66,68,76	0
3	OH	A	405	1/1	0.98	0.51	54,54,54,54	0
8	BO3	A	414	4/4	0.98	0.19	50,60,70,72	0
2	CU	A	402	1/1	0.99	0.14	52,52,52,52	1
2	CU	A	403	1/1	0.99	0.36	54,54,54,54	1
2	CU	A	404	1/1	0.99	0.18	50,50,50,50	1
2	CU	B	404	1/1	0.99	0.21	41,41,41,41	1
2	CU	B	402	1/1	0.99	0.12	55,55,55,55	1
2	CU	B	403	1/1	0.99	0.49	48,48,48,48	1
2	CU	C	404	1/1	0.99	0.21	44,44,44,44	1
2	CU	C	402	1/1	0.99	0.15	50,50,50,50	1
2	CU	B	401	1/1	1.00	0.20	55,55,55,55	0
2	CU	A	401	1/1	1.00	0.19	56,56,56,56	0
2	CU	C	401	1/1	1.00	0.20	56,56,56,56	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 OH C 405:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
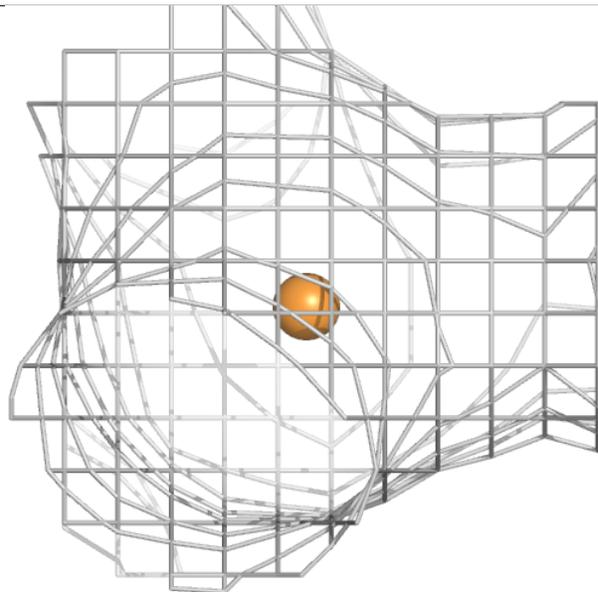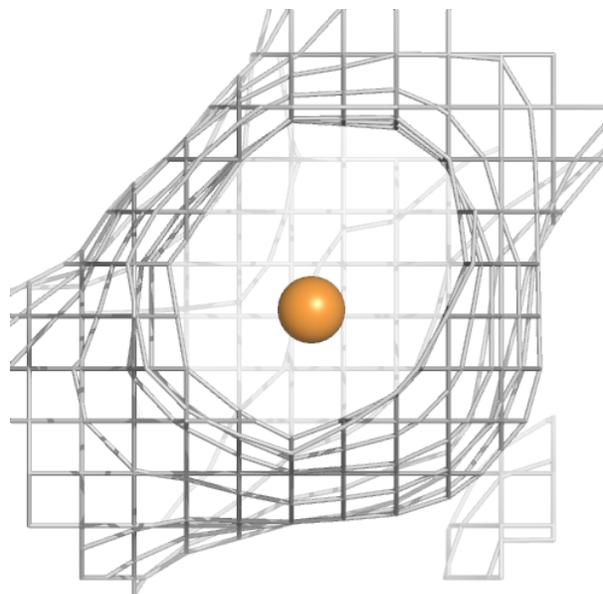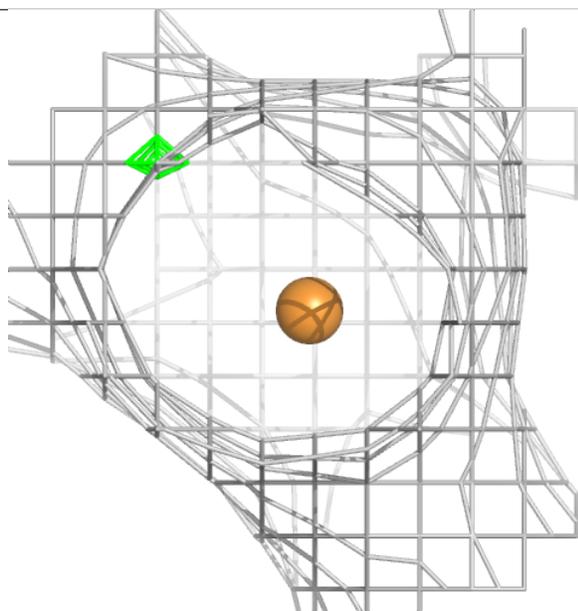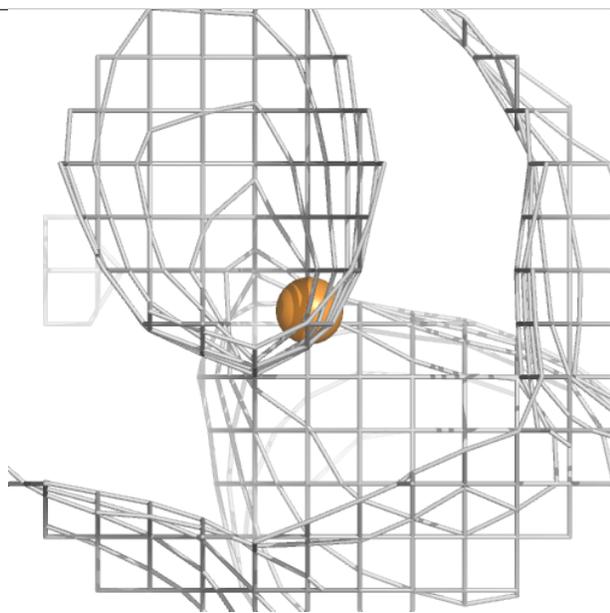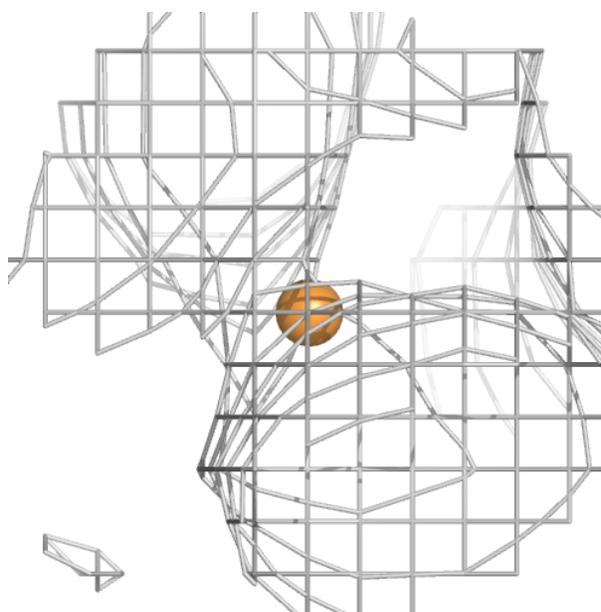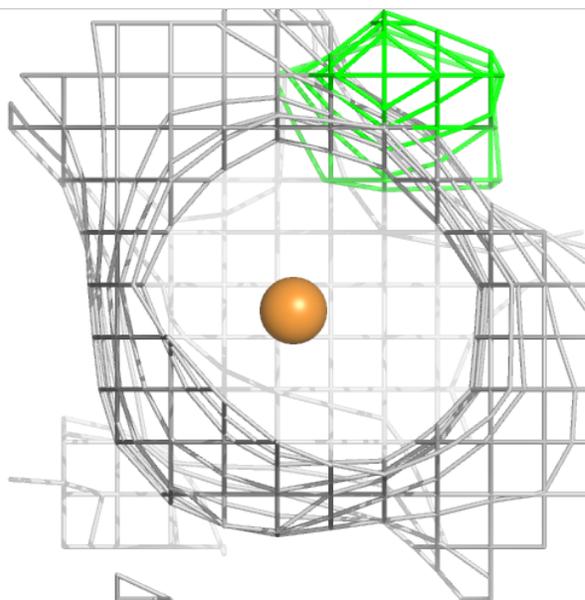$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
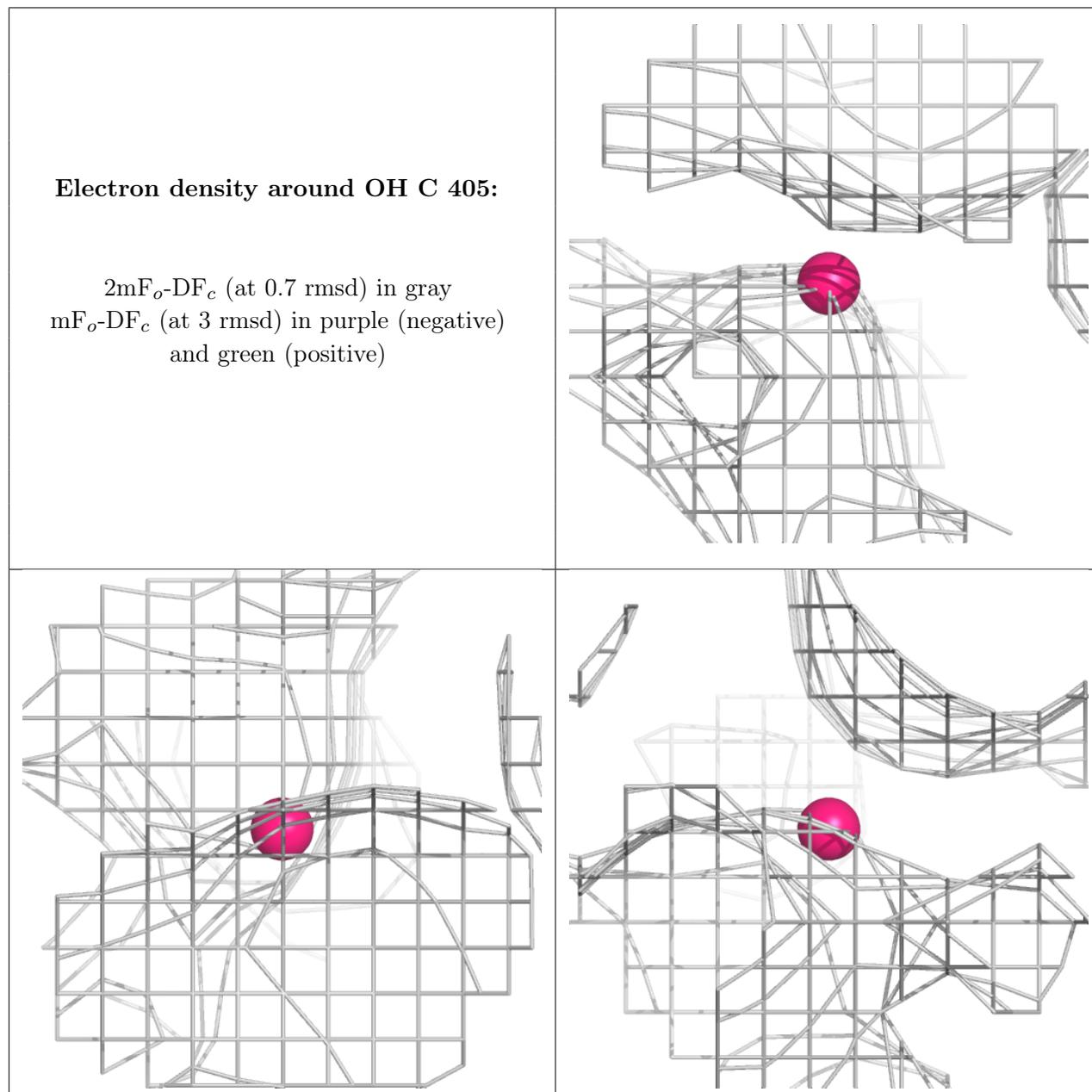
Electron density around OH B 405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
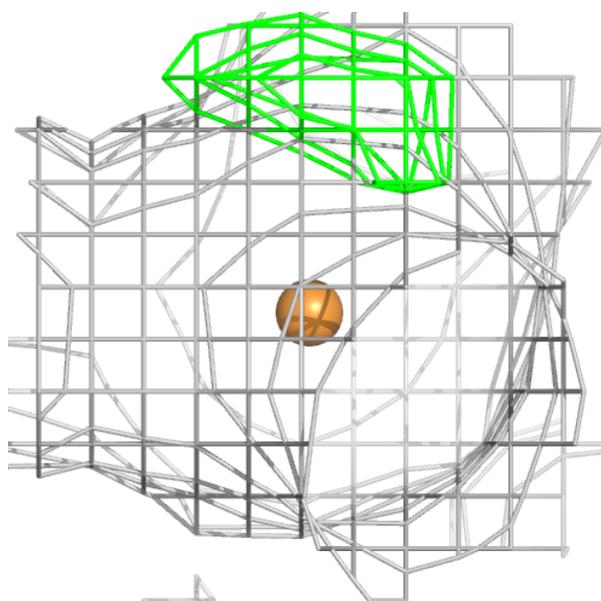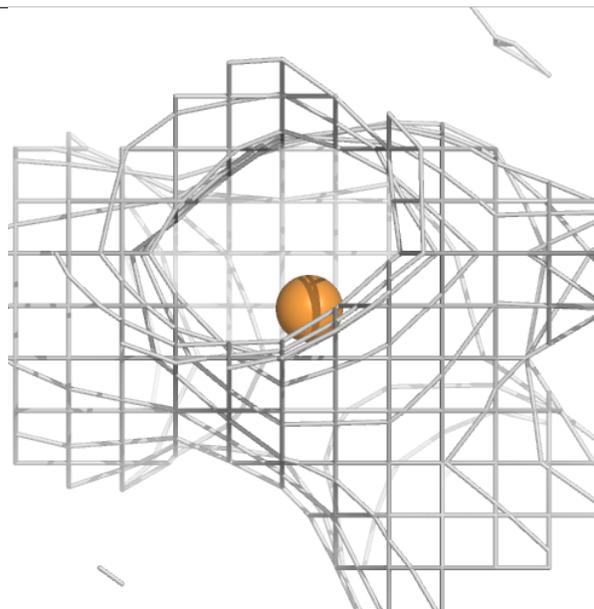mF_o-DF_c (at 3 rmsd) in purple (negative)
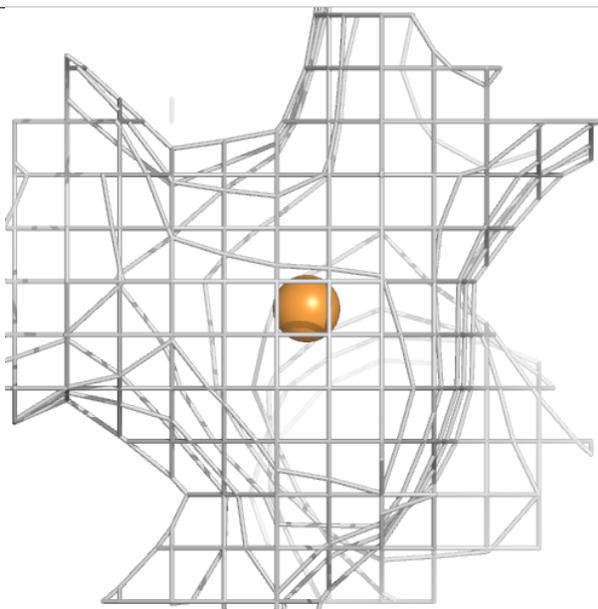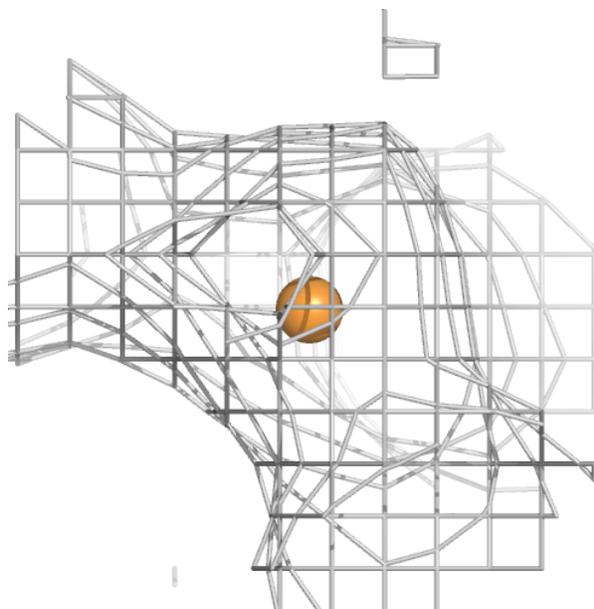and green (positive)
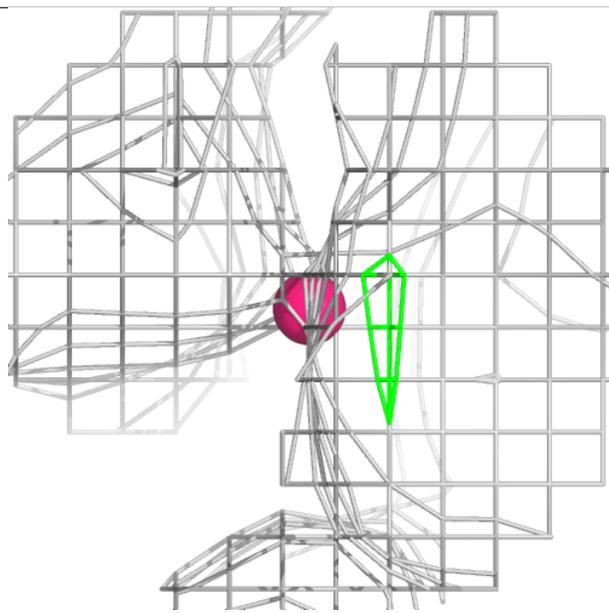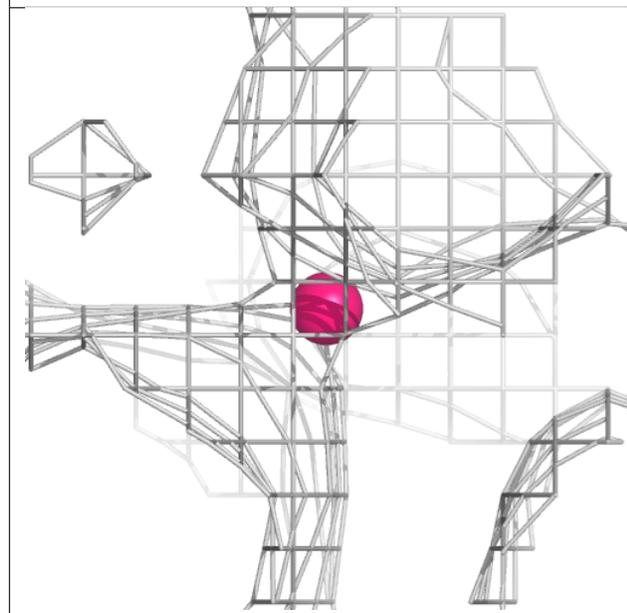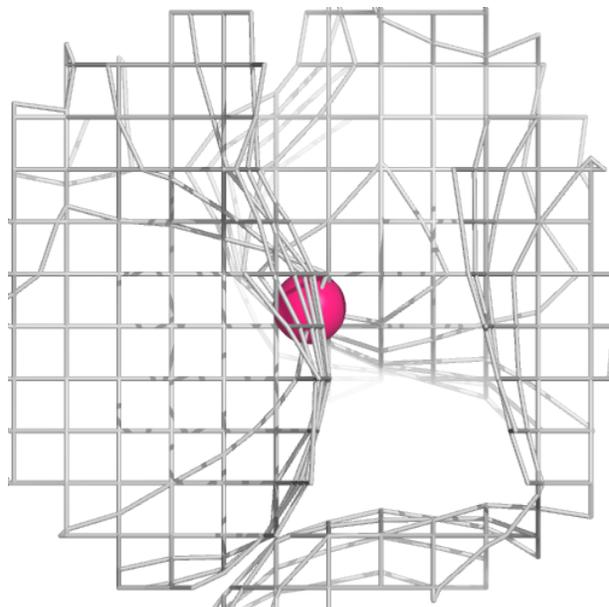
Electron density around CU C 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
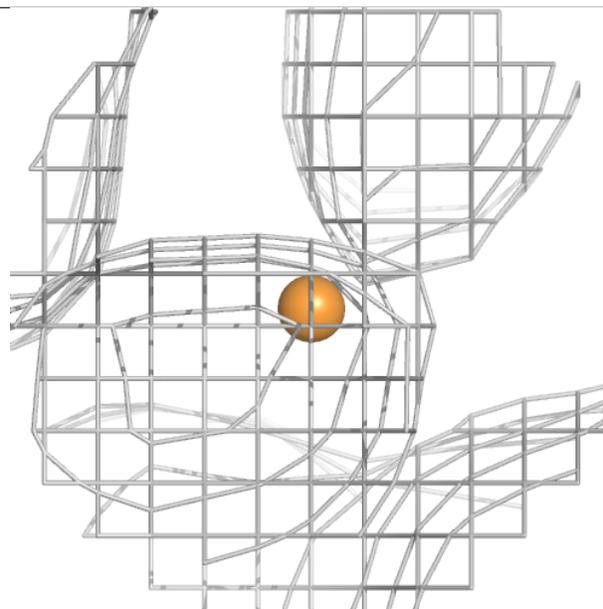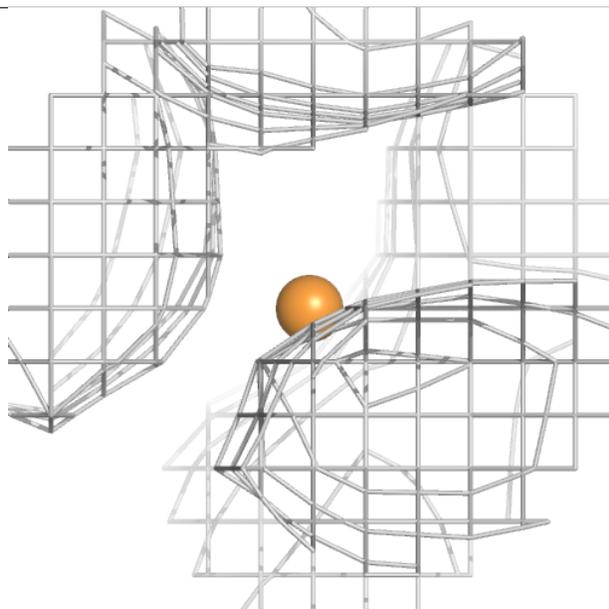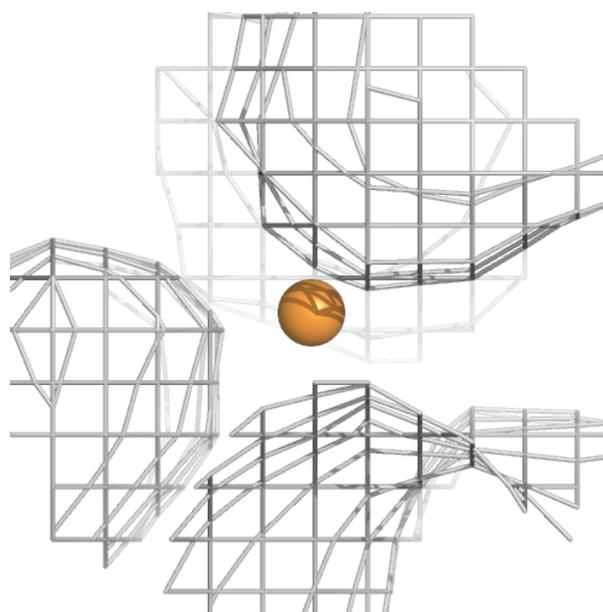
Electron density around OH A 405:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
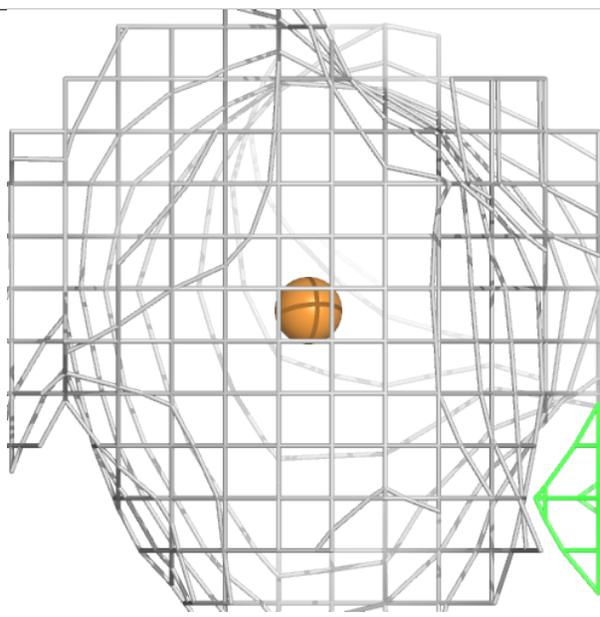and green (positive)
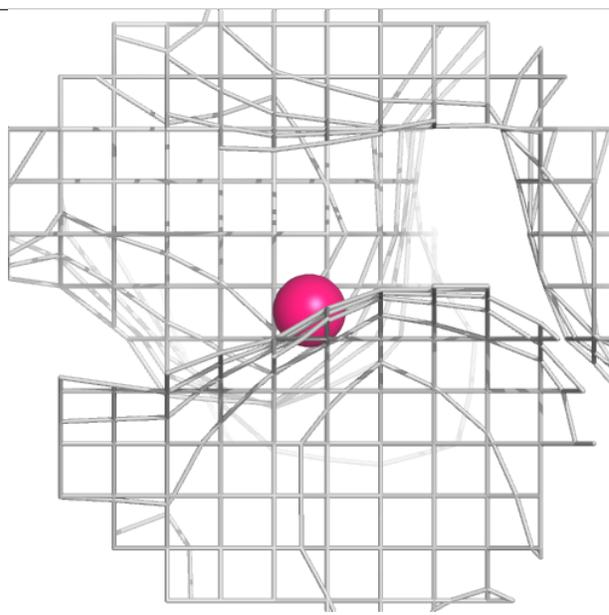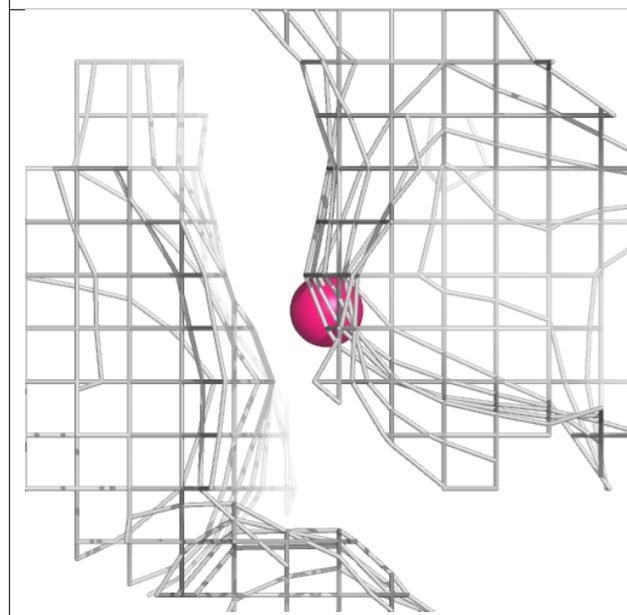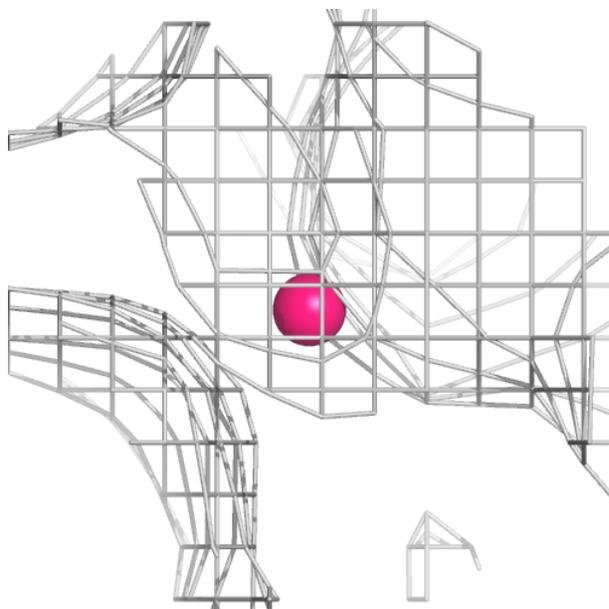
Electron density around CU A 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
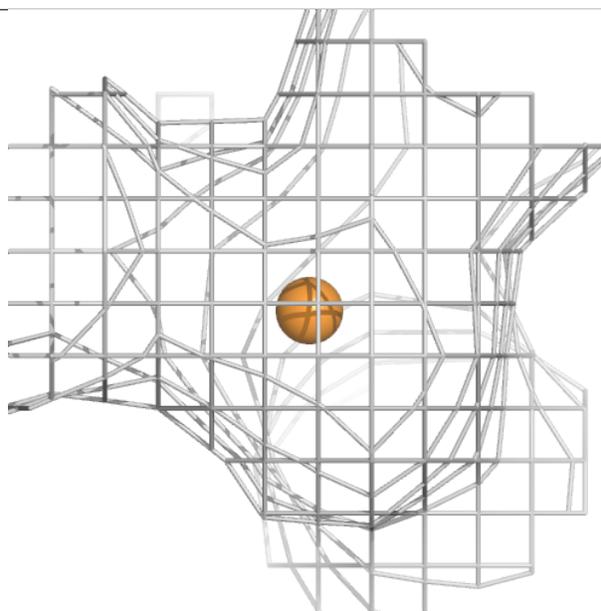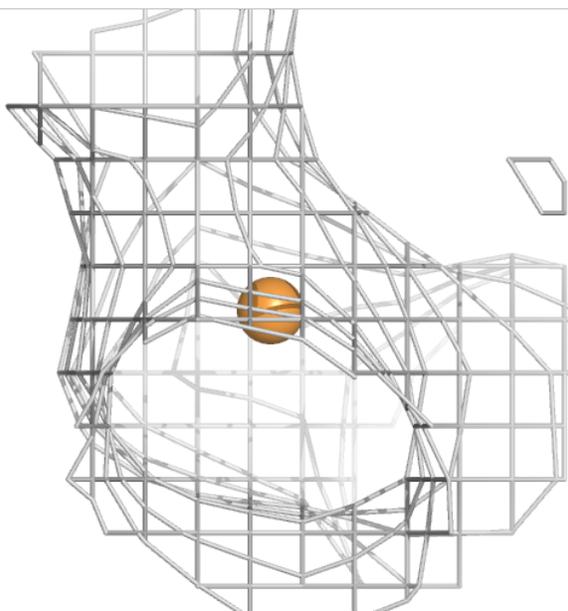
Electron density around CU A 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
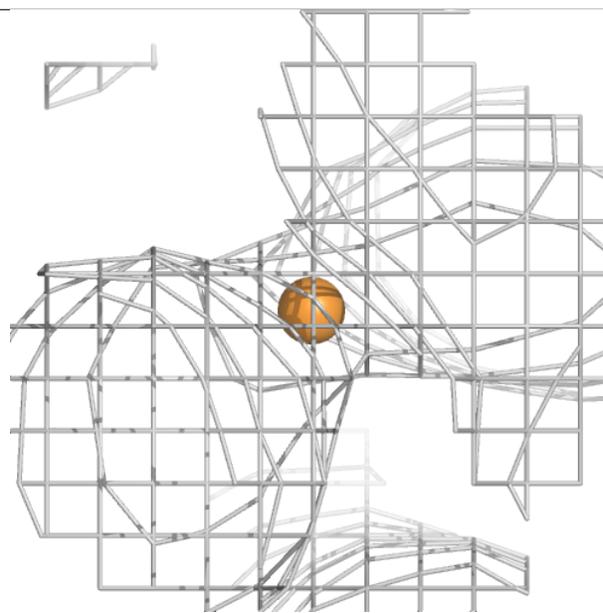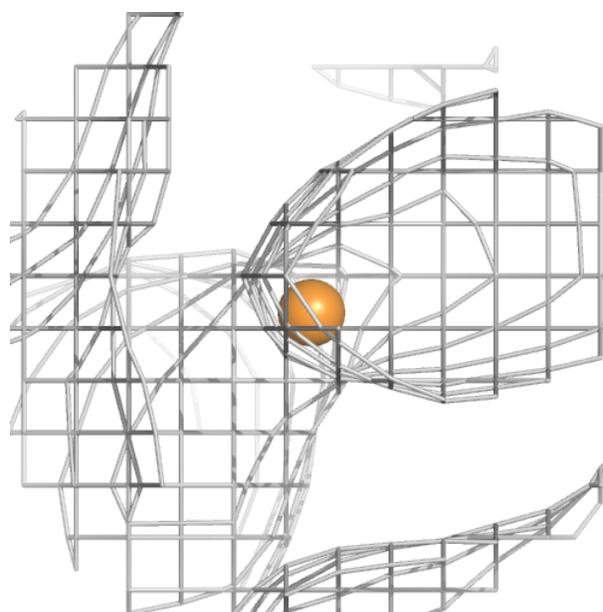
Electron density around CU A 404:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
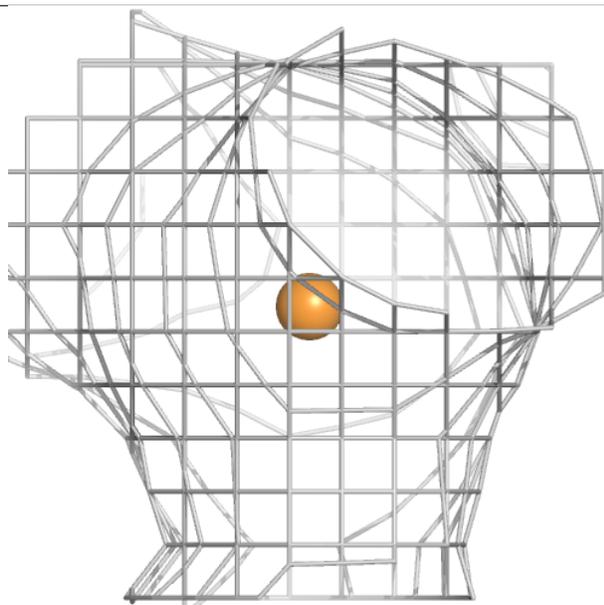
Electron density around CU B 404:

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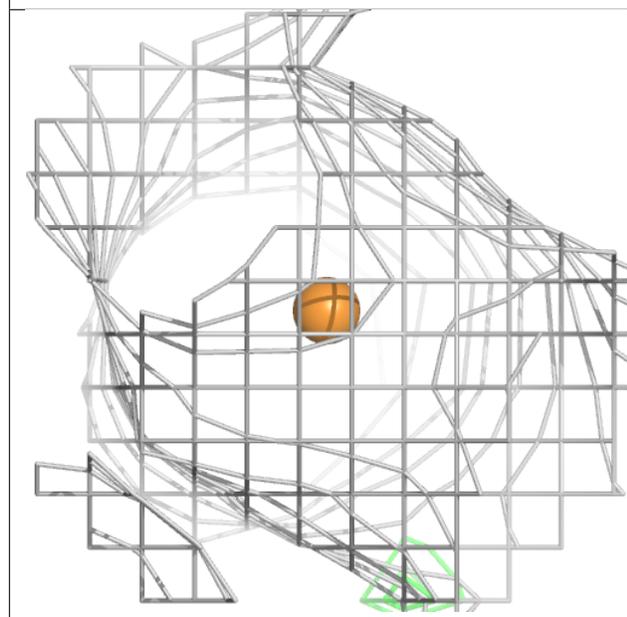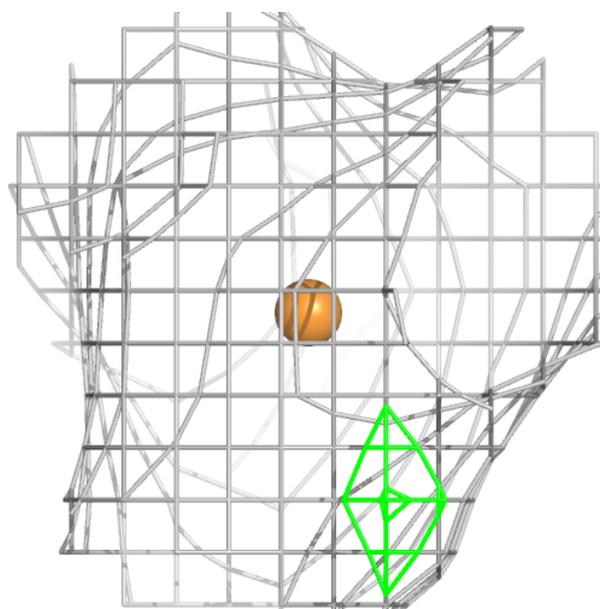$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
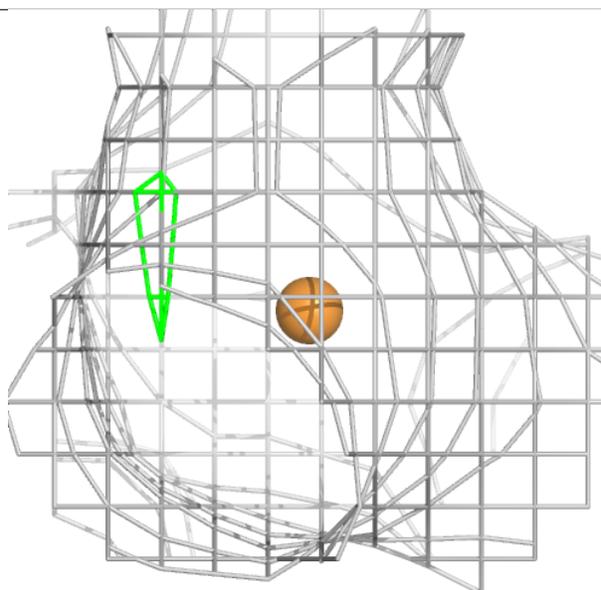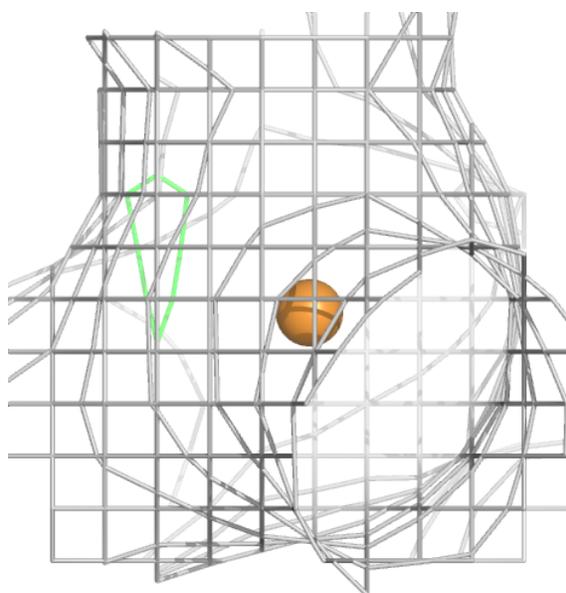
Electron density around CU B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
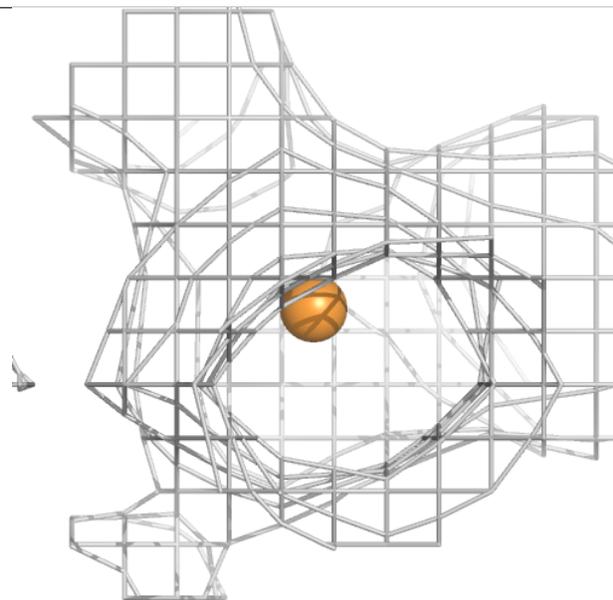
Electron density around CU B 403:

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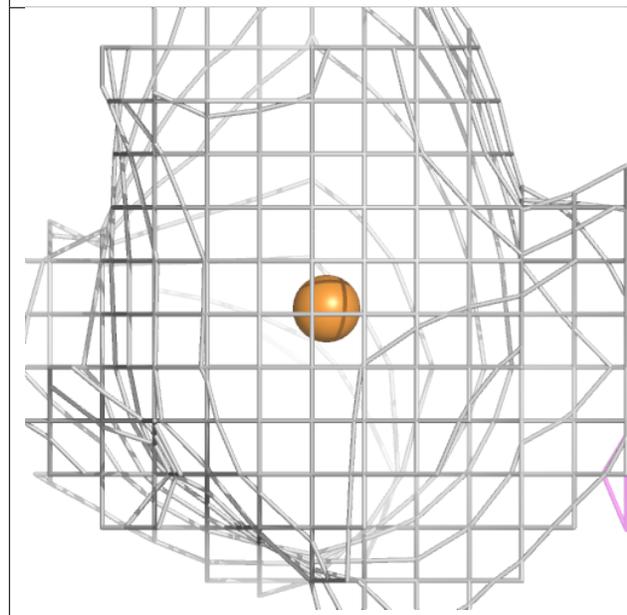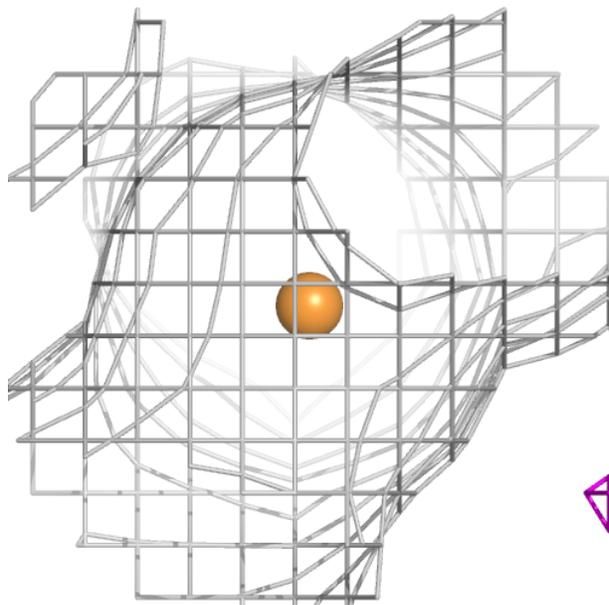and green (positive)

Electron density around CU C 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
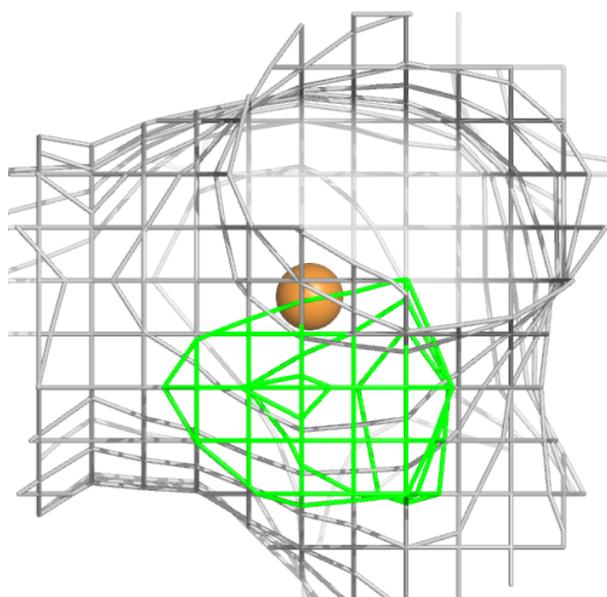
Electron density around CU C 402:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
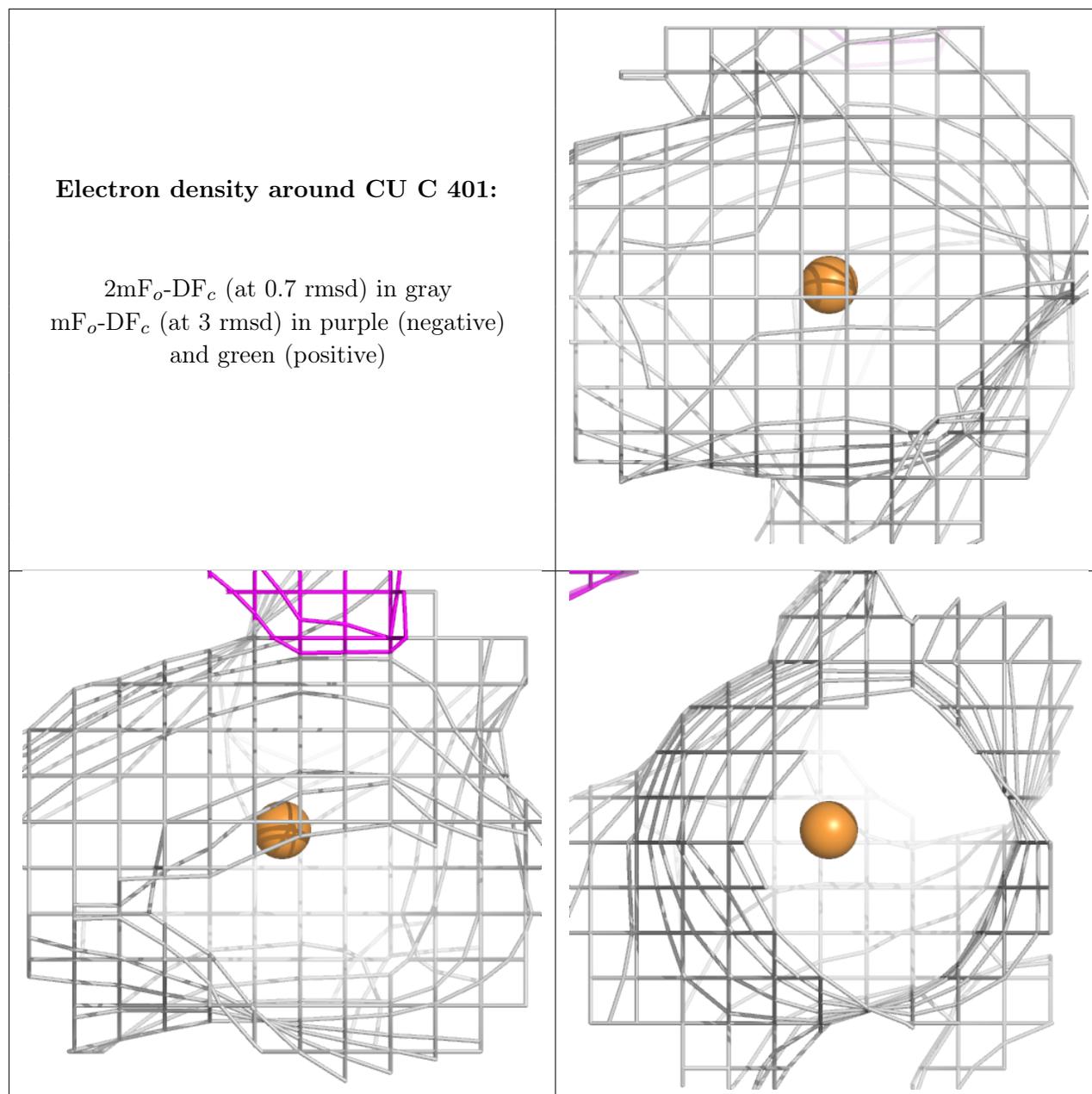
Electron density around CU B 401:

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

Electron density around CU A 401:

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

Electron density around CU C 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.