



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 11:29 am BST

PDB ID : 8R4F / pdb_00008r4f
Title : Crystal structure of the native copper efflux oxidase (CueO) from Hafnia alvei
Authors : Leone, P.; Contaldo, U.
Deposited on : 2023-11-13
Resolution : 3.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

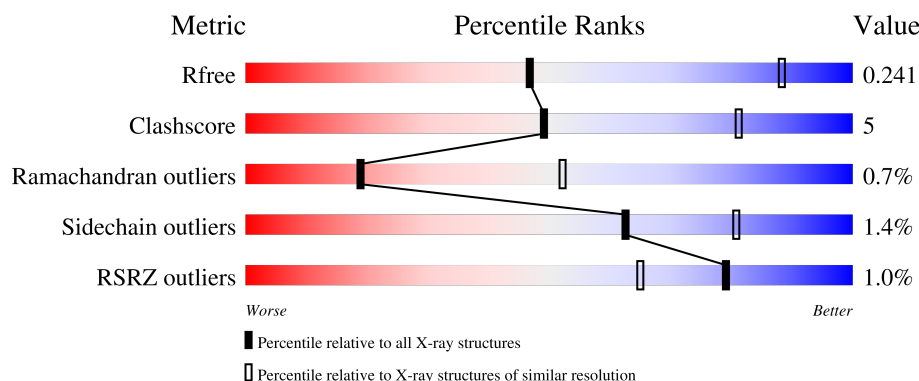
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.19 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}	164625	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	522	 78% 12% 10%
1	B	522	 78% 12% 9%
1	C	522	 80% 10% 10%
1	D	522	 3% 78% 12% 9%
1	E	522	 3% 77% 13% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18593 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 Copper efflux oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3648	2318	634	661	35			
1	B	473	Total	C	N	O	S	0	0	0
			3656	2323	635	662	36			
1	C	472	Total	C	N	O	S	0	0	0
			3648	2318	634	661	35			
1	D	473	Total	C	N	O	S	0	0	0
			3656	2323	635	662	36			
1	E	473	Total	C	N	O	S	0	0	0
			3656	2323	635	662	36			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	513	SER	-	expression tag	UNP A0A377PPH3
A	514	ALA	-	expression tag	UNP A0A377PPH3
A	515	TRP	-	expression tag	UNP A0A377PPH3
A	516	SER	-	expression tag	UNP A0A377PPH3
A	517	HIS	-	expression tag	UNP A0A377PPH3
A	518	PRO	-	expression tag	UNP A0A377PPH3
A	519	GLN	-	expression tag	UNP A0A377PPH3
A	520	PHE	-	expression tag	UNP A0A377PPH3
A	521	GLU	-	expression tag	UNP A0A377PPH3
A	522	LYS	-	expression tag	UNP A0A377PPH3
B	513	SER	-	expression tag	UNP A0A377PPH3
B	514	ALA	-	expression tag	UNP A0A377PPH3
B	515	TRP	-	expression tag	UNP A0A377PPH3
B	516	SER	-	expression tag	UNP A0A377PPH3
B	517	HIS	-	expression tag	UNP A0A377PPH3
B	518	PRO	-	expression tag	UNP A0A377PPH3
B	519	GLN	-	expression tag	UNP A0A377PPH3
B	520	PHE	-	expression tag	UNP A0A377PPH3
B	521	GLU	-	expression tag	UNP A0A377PPH3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	522	LYS	-	expression tag	UNP A0A377PPH3
C	513	SER	-	expression tag	UNP A0A377PPH3
C	514	ALA	-	expression tag	UNP A0A377PPH3
C	515	TRP	-	expression tag	UNP A0A377PPH3
C	516	SER	-	expression tag	UNP A0A377PPH3
C	517	HIS	-	expression tag	UNP A0A377PPH3
C	518	PRO	-	expression tag	UNP A0A377PPH3
C	519	GLN	-	expression tag	UNP A0A377PPH3
C	520	PHE	-	expression tag	UNP A0A377PPH3
C	521	GLU	-	expression tag	UNP A0A377PPH3
C	522	LYS	-	expression tag	UNP A0A377PPH3
D	513	SER	-	expression tag	UNP A0A377PPH3
D	514	ALA	-	expression tag	UNP A0A377PPH3
D	515	TRP	-	expression tag	UNP A0A377PPH3
D	516	SER	-	expression tag	UNP A0A377PPH3
D	517	HIS	-	expression tag	UNP A0A377PPH3
D	518	PRO	-	expression tag	UNP A0A377PPH3
D	519	GLN	-	expression tag	UNP A0A377PPH3
D	520	PHE	-	expression tag	UNP A0A377PPH3
D	521	GLU	-	expression tag	UNP A0A377PPH3
D	522	LYS	-	expression tag	UNP A0A377PPH3
E	513	SER	-	expression tag	UNP A0A377PPH3
E	514	ALA	-	expression tag	UNP A0A377PPH3
E	515	TRP	-	expression tag	UNP A0A377PPH3
E	516	SER	-	expression tag	UNP A0A377PPH3
E	517	HIS	-	expression tag	UNP A0A377PPH3
E	518	PRO	-	expression tag	UNP A0A377PPH3
E	519	GLN	-	expression tag	UNP A0A377PPH3
E	520	PHE	-	expression tag	UNP A0A377PPH3
E	521	GLU	-	expression tag	UNP A0A377PPH3
E	522	LYS	-	expression tag	UNP A0A377PPH3

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Cu	0	0
			2	2		
2	E	2	Total	Cu	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		

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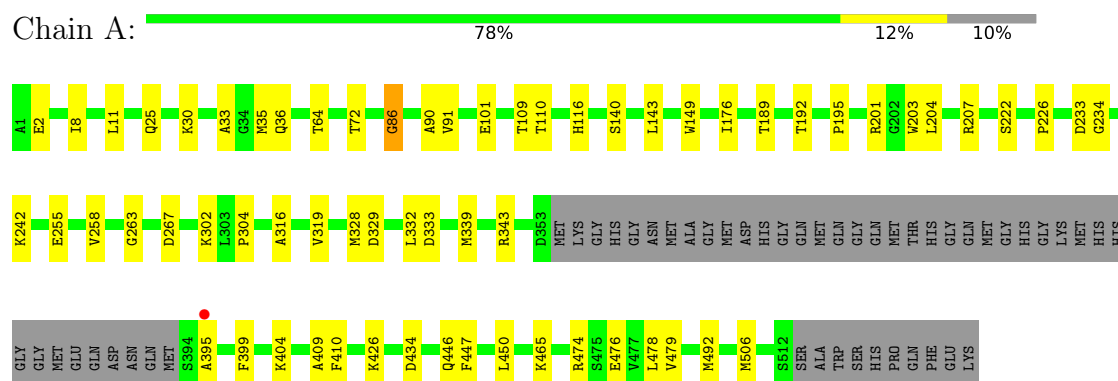
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	69	Total 69	O 69	0	0
4	C	66	Total 66	O 66	0	0
4	D	56	Total 56	O 56	0	0
4	E	53	Total 53	O 53	0	0

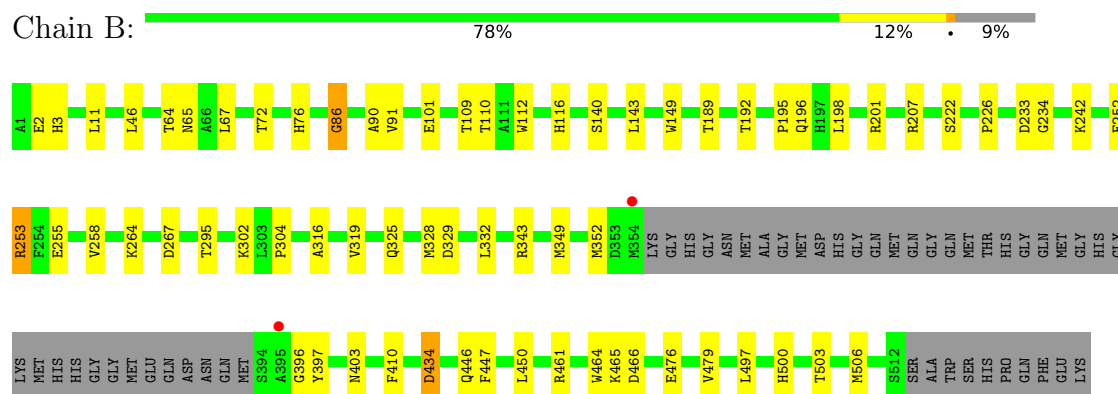
3 Residue-property plots

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.

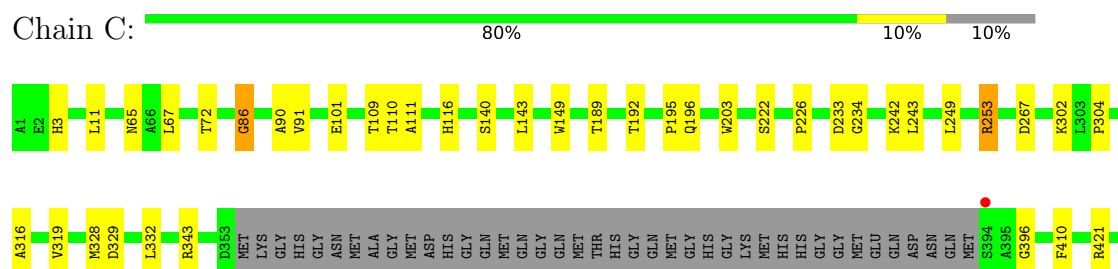
• Molecule 1: Copper efflux oxidase



• Molecule 1: Copper efflux oxidase

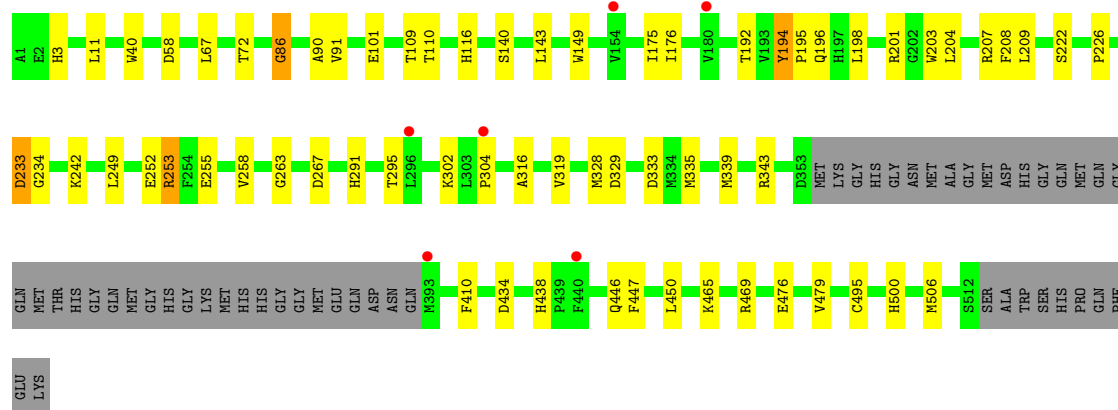
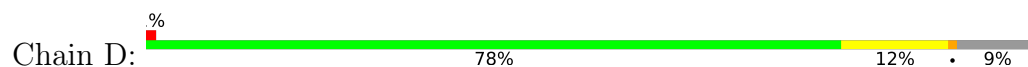


• Molecule 1: Copper efflux oxidase

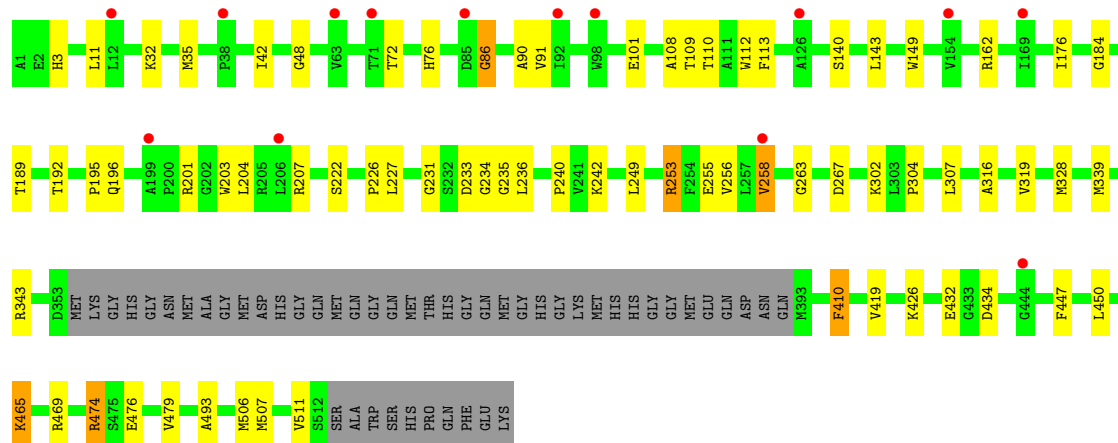
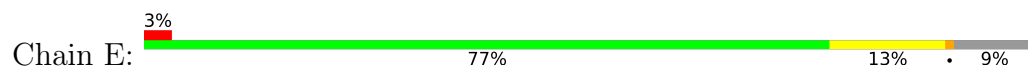




• Molecule 1: Copper efflux oxidase



• Molecule 1: Copper efflux oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.53Å 167.28Å 229.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.56 – 3.19 46.56 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.56-3.19) 99.9 (46.56-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.216 , 0.246 0.216 , 0.241	Depositor DCC
R_{free} test set	2995 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18593	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: CU, 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	A	0.35	0/3743	0.54	0/5079
1	B	0.33	0/3751	0.54	0/5089
1	C	0.33	0/3743	0.54	0/5079
1	D	0.32	0/3751	0.54	0/5089
1	E	0.33	0/3751	0.53	0/5089
All	All	0.33	0/18739	0.54	0/25425

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	3648	0	3629	35	0
1	B	3656	0	3638	39	0
1	C	3648	0	3629	33	0
1	D	3656	0	3639	42	0
1	E	3656	0	3638	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	1	0
2	E	2	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	1	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
3	E	4	0	6	0	0
4	A	51	0	0	1	0
4	B	69	0	0	0	0
4	C	66	0	0	0	0
4	D	56	0	0	0	0
4	E	53	0	0	2	0
All	All	18593	0	18209	192	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 5.

All (192) 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:112:TRP:HD1	1:B:253:ARG:HH11	1.12	0.94
1:D:495:CYS:HG	2:D:602:CU:CU	0.65	0.94
1:E:233:ASP:HB2	1:E:465:LYS:HA	1.62	0.81
1:D:201:ARG:HE	1:D:263:GLY:HA3	1.50	0.74
1:C:233:ASP:HB2	1:C:465:LYS:HA	1.70	0.73
1:E:32:LYS:HB3	1:E:35:MET:HB2	1.74	0.69
1:C:111:ALA:HA	1:C:253:ARG:HH11	1.58	0.68
1:A:233:ASP:HB2	1:A:465:LYS:HA	1.77	0.67
1:E:450:LEU:HD12	1:E:476:GLU:HG2	1.77	0.67
1:B:65:ASN:OD1	1:B:67:LEU:HB2	1.95	0.66
1:B:325:GLN:HG2	1:D:339:MET:HE3	1.80	0.64
1:A:35:MET:HG3	1:A:36:GLN:N	2.13	0.64
1:D:267:ASP:OD1	1:D:291:HIS:ND1	2.30	0.63
1:A:11:LEU:HD13	1:A:149:TRP:CD1	2.35	0.62
1:C:11:LEU:HD13	1:C:149:TRP:CD1	2.35	0.62
1:D:11:LEU:HD13	1:D:149:TRP:CD1	2.35	0.61
1:E:3:HIS:HB2	1:E:196:GLN:HB2	1.82	0.61
1:D:192:THR:HB	1:D:195:PRO:HG3	1.83	0.61
1:E:192:THR:HB	1:E:195:PRO:HG3	1.83	0.61
1:D:208:PHE:O	1:D:253:ARG:HB2	2.00	0.60
1:B:11:LEU:HD13	1:B:149:TRP:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ARG:HE	1:D:263:GLY:CA	2.15	0.59
1:D:233:ASP:HB2	1:D:465:LYS:HA	1.84	0.59
1:E:11:LEU:HD13	1:E:149:TRP:CD1	2.38	0.59
1:B:192:THR:HB	1:B:195:PRO:HG3	1.85	0.59
1:A:192:THR:HB	1:A:195:PRO:HG3	1.85	0.58
1:C:192:THR:HB	1:C:195:PRO:HG3	1.85	0.58
1:E:109:THR:HG21	1:E:234:GLY:HA2	1.85	0.57
1:E:204:LEU:HB3	1:E:258:VAL:HG23	1.86	0.57
1:B:3:HIS:HB2	1:B:196:GLN:HB2	1.87	0.56
1:A:201:ARG:HE	1:A:263:GLY:HA3	1.71	0.55
1:B:112:TRP:HD1	1:B:253:ARG:NH1	1.92	0.55
1:C:3:HIS:HB2	1:C:196:GLN:HB2	1.89	0.55
1:E:42:ILE:HD12	1:E:113:PHE:HE2	1.73	0.54
1:B:234:GLY:HA3	1:B:446:GLN:HG2	1.90	0.53
1:C:11:LEU:HD13	1:C:149:TRP:NE1	2.24	0.53
1:D:450:LEU:HD12	1:D:476:GLU:HG2	1.91	0.53
1:B:233:ASP:HB2	1:B:465:LYS:HA	1.91	0.53
1:B:497:LEU:HD22	1:B:500:HIS:CD2	2.44	0.53
1:A:329:ASP:O	1:A:333:ASP:HB2	2.09	0.53
1:C:110:THR:O	1:C:253:ARG:HD2	2.09	0.52
1:B:201:ARG:HD2	1:B:295:THR:O	2.08	0.52
1:E:109:THR:CG2	1:E:234:GLY:HA2	2.39	0.52
1:E:112:TRP:CD1	1:E:253:ARG:HD2	2.44	0.52
1:C:111:ALA:HA	1:C:253:ARG:NH1	2.24	0.52
1:D:208:PHE:O	1:D:253:ARG:CB	2.57	0.52
1:E:201:ARG:HE	1:E:263:GLY:HA2	1.74	0.52
1:D:11:LEU:HD13	1:D:149:TRP:NE1	2.26	0.51
1:A:11:LEU:HD13	1:A:149:TRP:NE1	2.25	0.51
1:A:201:ARG:HE	1:A:263:GLY:CA	2.23	0.51
1:E:256:VAL:HB	4:E:703:HOH:O	2.11	0.51
1:A:72:THR:HG22	1:A:91:VAL:HA	1.94	0.50
1:C:441:HIS:CD2	1:C:443:HIS:CD2	2.99	0.50
1:B:109:THR:HG22	1:B:110:THR:N	2.27	0.50
1:C:450:LEU:HD12	1:C:476:GLU:HG2	1.94	0.50
1:E:222:SER:HB3	1:E:267:ASP:HB2	1.93	0.50
1:B:450:LEU:HD12	1:B:476:GLU:HG2	1.94	0.49
1:A:109:THR:HG22	1:A:110:THR:N	2.26	0.49
1:B:72:THR:HG22	1:B:91:VAL:HA	1.94	0.49
1:D:109:THR:HG22	1:D:110:THR:N	2.27	0.49
1:E:72:THR:HG22	1:E:91:VAL:HA	1.94	0.49
1:B:11:LEU:HD13	1:B:149:TRP:NE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ARG:HE	1:E:263:GLY:CA	2.24	0.49
1:B:222:SER:HB3	1:B:267:ASP:HB2	1.93	0.49
1:E:11:LEU:HD13	1:E:149:TRP:NE1	2.27	0.49
1:A:86:GLY:HA2	1:A:90:ALA:HB3	1.94	0.49
1:A:450:LEU:HD12	1:A:476:GLU:HG2	1.95	0.49
1:C:109:THR:HG22	1:C:110:THR:N	2.27	0.49
1:D:222:SER:HB3	1:D:267:ASP:HB2	1.94	0.49
1:C:222:SER:HB3	1:C:267:ASP:HB2	1.95	0.48
1:E:176:ILE:HG12	1:E:339:MET:HB3	1.94	0.48
1:A:204:LEU:HB3	1:A:258:VAL:HG12	1.94	0.48
1:A:222:SER:HB3	1:A:267:ASP:HB2	1.95	0.48
1:B:316:ALA:HB1	1:B:319:VAL:HG11	1.96	0.48
1:E:86:GLY:HA2	1:E:90:ALA:HB3	1.95	0.48
1:D:72:THR:HG22	1:D:91:VAL:HA	1.96	0.48
1:C:72:THR:HG22	1:C:91:VAL:HA	1.95	0.48
1:E:76:HIS:CD2	1:E:253:ARG:NH1	2.82	0.48
1:B:198:LEU:HB3	1:B:295:THR:CG2	2.44	0.47
1:C:11:LEU:CD1	1:C:149:TRP:CE2	2.97	0.47
1:A:426:LYS:HD3	4:A:734:HOH:O	2.13	0.47
1:C:86:GLY:HA2	1:C:90:ALA:HB3	1.97	0.47
1:A:234:GLY:HA3	1:A:446:GLN:HG2	1.97	0.47
1:E:493:ALA:HB3	1:E:507:MET:SD	2.55	0.47
1:E:109:THR:HG22	1:E:110:THR:N	2.30	0.47
1:D:40:TRP:CE2	1:D:67:LEU:HD22	2.50	0.47
1:D:86:GLY:HA2	1:D:90:ALA:HB3	1.97	0.47
1:D:204:LEU:HB3	1:D:258:VAL:HG12	1.96	0.47
1:A:11:LEU:CD1	1:A:149:TRP:CE2	2.98	0.47
1:E:162:ARG:HB2	1:E:184:GLY:HA2	1.96	0.47
1:C:65:ASN:OD1	1:C:67:LEU:HB2	2.15	0.47
1:D:176:ILE:CG1	1:D:339:MET:HB3	2.45	0.47
1:E:419:VAL:HB	1:E:511:VAL:HG22	1.95	0.47
1:B:11:LEU:CD1	1:B:149:TRP:CE2	2.98	0.46
1:C:243:LEU:HD11	1:C:460:HIS:CE1	2.49	0.46
1:D:116:HIS:HE1	1:D:506:MET:SD	2.37	0.46
1:E:11:LEU:CD1	1:E:149:TRP:CE2	2.98	0.46
1:A:316:ALA:HB1	1:A:319:VAL:HG11	1.97	0.46
1:D:316:ALA:HB1	1:D:319:VAL:HG11	1.97	0.46
1:A:30:LYS:HE3	1:A:33:ALA:HA	1.96	0.46
1:B:86:GLY:HA2	1:B:90:ALA:HB3	1.97	0.46
1:E:432:GLU:OE1	1:E:474:ARG:NH1	2.49	0.46
1:D:11:LEU:CD1	1:D:149:TRP:CE2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ALA:HB1	1:C:319:VAL:HG11	1.97	0.46
1:E:42:ILE:O	1:E:48:GLY:HA2	2.15	0.46
1:B:464:TRP:CZ3	3:B:603:EDO:H11	2.51	0.46
1:A:328:MET:SD	1:A:434:ASP:OD1	2.75	0.45
1:C:465:LYS:HB3	1:C:465:LYS:HE3	1.80	0.45
1:D:234:GLY:HA3	1:D:446:GLN:HG2	1.99	0.45
1:E:240:PRO:HG3	1:E:307:LEU:HD21	1.99	0.45
1:B:403:ASN:ND2	1:B:503:THR:OG1	2.47	0.45
1:C:116:HIS:HE1	1:C:506:MET:SD	2.40	0.45
1:B:329:ASP:HB3	1:B:332:LEU:HB2	1.99	0.45
1:D:209:LEU:HD13	1:D:253:ARG:HD3	1.99	0.45
1:B:189:THR:HB	1:B:195:PRO:CD	2.47	0.44
1:A:8:ILE:H	1:B:264:LYS:NZ	2.14	0.44
1:C:329:ASP:HB3	1:C:332:LEU:HB2	1.99	0.44
1:E:316:ALA:HB1	1:E:319:VAL:HG11	1.98	0.44
1:B:11:LEU:HD13	1:B:149:TRP:CE2	2.53	0.44
1:A:189:THR:HB	1:A:195:PRO:CD	2.48	0.44
1:D:11:LEU:HD13	1:D:149:TRP:CE2	2.53	0.44
1:D:175:ILE:HD11	1:D:335:MET:HE3	1.99	0.44
1:A:332:LEU:HD13	1:A:399:PHE:HA	1.99	0.43
1:D:226:PRO:HG3	1:D:242:LYS:HE3	2.00	0.43
1:E:11:LEU:HD13	1:E:149:TRP:CE2	2.53	0.43
1:E:447:PHE:HB3	1:E:479:VAL:HG12	2.00	0.43
1:B:253:ARG:NH2	1:B:466:ASP:OD2	2.51	0.43
1:C:140:SER:HA	1:C:143:LEU:HD12	2.00	0.43
1:E:227:LEU:HD23	1:E:258:VAL:HG13	1.99	0.43
1:B:316:ALA:HB1	1:B:319:VAL:CG1	2.48	0.43
1:C:421:ARG:HD3	1:C:484:GLU:HG3	2.01	0.43
1:B:349:MET:O	1:B:352:MET:HG2	2.18	0.43
1:C:234:GLY:HA3	1:C:446:GLN:HG2	1.99	0.43
1:C:11:LEU:HD13	1:C:149:TRP:CE2	2.53	0.43
1:D:3:HIS:HB3	1:D:194:TYR:O	2.18	0.43
1:A:11:LEU:HD13	1:A:149:TRP:CE2	2.54	0.43
1:B:302:LYS:O	1:B:304:PRO:HD3	2.18	0.43
1:C:189:THR:HB	1:C:195:PRO:CD	2.48	0.43
1:A:226:PRO:HG3	1:A:242:LYS:HE3	2.01	0.43
1:C:249:LEU:HD11	1:C:469:ARG:HB2	2.01	0.43
1:D:329:ASP:O	1:D:333:ASP:HB2	2.18	0.43
1:A:116:HIS:HE1	1:A:506:MET:SD	2.41	0.42
1:C:226:PRO:HG3	1:C:242:LYS:HE3	2.01	0.42
1:D:302:LYS:O	1:D:304:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:HIS:HD2	1:B:253:ARG:NH1	2.17	0.42
1:B:116:HIS:HE1	1:B:506:MET:SD	2.42	0.42
1:C:302:LYS:O	1:C:304:PRO:HD3	2.19	0.42
1:C:328:MET:SD	1:C:434:ASP:OD1	2.78	0.42
1:E:189:THR:HB	1:E:195:PRO:CD	2.49	0.42
1:A:302:LYS:O	1:A:304:PRO:HD3	2.20	0.42
1:B:140:SER:HA	1:B:143:LEU:HD12	2.00	0.42
1:A:140:SER:HA	1:A:143:LEU:HD12	2.01	0.42
1:D:339:MET:HB2	1:D:339:MET:HE2	1.98	0.42
1:E:108:ALA:O	1:E:235:GLY:HA2	2.20	0.42
1:A:207:ARG:HG2	1:A:255:GLU:HG2	2.02	0.42
1:B:226:PRO:HG3	1:B:242:LYS:HE3	2.02	0.42
1:D:140:SER:HA	1:D:143:LEU:HD12	2.02	0.42
1:E:249:LEU:HD11	1:E:469:ARG:HB2	2.02	0.42
1:B:207:ARG:HG2	1:B:255:GLU:HG2	2.02	0.42
1:D:207:ARG:HG2	1:D:255:GLU:HG2	2.02	0.42
1:D:447:PHE:HB3	1:D:479:VAL:HG12	2.01	0.42
1:E:226:PRO:HG3	1:E:242:LYS:HE3	2.00	0.42
1:E:316:ALA:HB1	1:E:319:VAL:CG1	2.50	0.41
1:A:203:TRP:CD1	1:A:302:LYS:HA	2.55	0.41
1:B:447:PHE:HB3	1:B:479:VAL:HG12	2.01	0.41
1:C:203:TRP:CD1	1:C:302:LYS:HA	2.55	0.41
1:C:447:PHE:HB3	1:C:479:VAL:HG12	2.03	0.41
1:D:316:ALA:HB1	1:D:319:VAL:CG1	2.50	0.41
1:B:109:THR:CG2	1:B:233:ASP:O	2.69	0.41
1:B:252:GLU:OE1	1:B:461:ARG:NH2	2.52	0.41
1:E:140:SER:HA	1:E:143:LEU:HD12	2.01	0.41
1:A:447:PHE:HB3	1:A:479:VAL:HG12	2.02	0.41
1:E:203:TRP:CD1	1:E:302:LYS:HA	2.55	0.41
1:D:198:LEU:HB3	1:D:295:THR:CG2	2.51	0.41
1:E:328:MET:SD	1:E:434:ASP:OD1	2.78	0.41
1:B:328:MET:SD	1:B:434:ASP:OD1	2.79	0.41
1:C:316:ALA:HB1	1:C:319:VAL:CG1	2.51	0.41
1:D:438:HIS:CE1	1:D:500:HIS:CE1	3.08	0.41
1:E:410:PHE:HB2	1:E:506:MET:HB3	2.03	0.41
1:A:316:ALA:HB1	1:A:319:VAL:CG1	2.51	0.41
1:E:426:LYS:HE3	4:E:708:HOH:O	2.21	0.41
1:D:203:TRP:CD1	1:D:302:LYS:HA	2.56	0.40
1:D:434:ASP:OD2	1:D:438:HIS:NE2	2.48	0.40
1:D:249:LEU:HD11	1:D:469:ARG:HB2	2.03	0.40
1:E:231:GLY:HA2	1:E:236:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LEU:O	1:D:252:GLU:HB2	2.22	0.40
1:E:207:ARG:HG2	1:E:255:GLU:HG2	2.02	0.40
1:E:302:LYS:O	1:E:304:PRO:HD3	2.22	0.40
1:A:404:LYS:HG2	1:A:409:ALA:HB2	2.03	0.40
1:A:450:LEU:HD21	1:A:478:LEU:HB2	2.04	0.40
1:A:176:ILE:HG12	1:A:339:MET:HB3	2.04	0.40
1:D:328:MET:SD	1:D:434:ASP:OD1	2.79	0.40

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	468/522 (90%)	438 (94%)	26 (6%)	4 (1%)	14	47
1	B	469/522 (90%)	437 (93%)	27 (6%)	5 (1%)	12	42
1	C	468/522 (90%)	437 (93%)	28 (6%)	3 (1%)	22	55
1	D	469/522 (90%)	441 (94%)	25 (5%)	3 (1%)	22	55
1	E	469/522 (90%)	438 (93%)	29 (6%)	2 (0%)	30	62
All	All	2343/2610 (90%)	2191 (94%)	135 (6%)	17 (1%)	19	52

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLY
1	A	410	PHE
1	B	86	GLY
1	B	396	GLY
1	B	397	TYR
1	B	410	PHE
1	B	434	ASP

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Mol	Chain	Res	Type
1	C	86	GLY
1	C	410	PHE
1	D	86	GLY
1	D	410	PHE
1	E	86	GLY
1	E	410	PHE
1	A	2	GLU
1	A	395	ALA
1	D	233	ASP
1	C	396	GLY

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	388/426 (91%)	382 (98%)	6 (2%)	60	79
1	B	389/426 (91%)	382 (98%)	7 (2%)	54	75
1	C	388/426 (91%)	385 (99%)	3 (1%)	79	89
1	D	389/426 (91%)	383 (98%)	6 (2%)	60	79
1	E	389/426 (91%)	383 (98%)	6 (2%)	60	79
All	All	1943/2130 (91%)	1915 (99%)	28 (1%)	62	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	64	THR
1	A	101	GLU
1	A	343	ARG
1	A	474	ARG
1	A	492	MET
1	B	2	GLU
1	B	46	LEU
1	B	64	THR

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Mol	Chain	Res	Type
1	B	101	GLU
1	B	253	ARG
1	B	258	VAL
1	B	343	ARG
1	C	101	GLU
1	C	253	ARG
1	C	343	ARG
1	D	58	ASP
1	D	101	GLU
1	D	194	TYR
1	D	196	GLN
1	D	253	ARG
1	D	343	ARG
1	E	101	GLU
1	E	253	ARG
1	E	258	VAL
1	E	343	ARG
1	E	465	LYS
1	E	474	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	$\# Z > 2$
3	EDO	D	603	-	3,3,3	0.37	0	2,2,2	0.05	0
3	EDO	E	603	-	3,3,3	0.40	0	2,2,2	0.20	0
3	EDO	B	604	-	3,3,3	0.33	0	2,2,2	0.18	0
3	EDO	A	603	-	3,3,3	0.27	0	2,2,2	0.26	0
3	EDO	B	603	-	3,3,3	0.46	0	2,2,2	0.14	0
3	EDO	C	603	-	3,3,3	0.44	0	2,2,2	0.08	0

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
3	EDO	D	603	-	-	1/1/1/1	-
3	EDO	E	603	-	-	1/1/1/1	-
3	EDO	B	604	-	-	1/1/1/1	-
3	EDO	A	603	-	-	1/1/1/1	-
3	EDO	B	603	-	-	1/1/1/1	-
3	EDO	C	603	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	EDO	O1-C1-C2-O2
3	B	603	EDO	O1-C1-C2-O2
3	B	604	EDO	O1-C1-C2-O2
3	D	603	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	E	603	EDO	O1-C1-C2-O2
3	C	603	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	EDO	1	0

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, 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	472/522 (90%)	-0.29	1 (0%) 92 87	48, 74, 99, 111	0
1	B	473/522 (90%)	-0.22	2 (0%) 89 81	56, 75, 90, 108	0
1	C	472/522 (90%)	-0.33	1 (0%) 92 87	57, 74, 90, 103	0
1	D	473/522 (90%)	0.20	6 (1%) 74 59	55, 89, 107, 120	0
1	E	473/522 (90%)	0.34	14 (2%) 52 36	51, 94, 126, 135	0
All	All	2363/2610 (90%)	-0.06	24 (1%) 79 65	48, 78, 111, 135	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	154	VAL	3.1
1	E	92	ILE	2.8
1	D	440	PHE	2.7
1	E	444	GLY	2.5
1	E	126	ALA	2.5
1	E	63	VAL	2.5
1	B	354	MET	2.5
1	E	169	ILE	2.4
1	E	154	VAL	2.4
1	E	199	ALA	2.4
1	E	71	THR	2.3
1	E	12	LEU	2.3
1	A	395	ALA	2.3
1	B	395	ALA	2.2
1	E	85	ASP	2.2
1	C	394	SER	2.2
1	E	38	PRO	2.1
1	E	258	VAL	2.1
1	D	296	LEU	2.1
1	D	393	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	180	VAL	2.1
1	E	206	LEU	2.0
1	D	304	PRO	2.0
1	E	98	TRP	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.

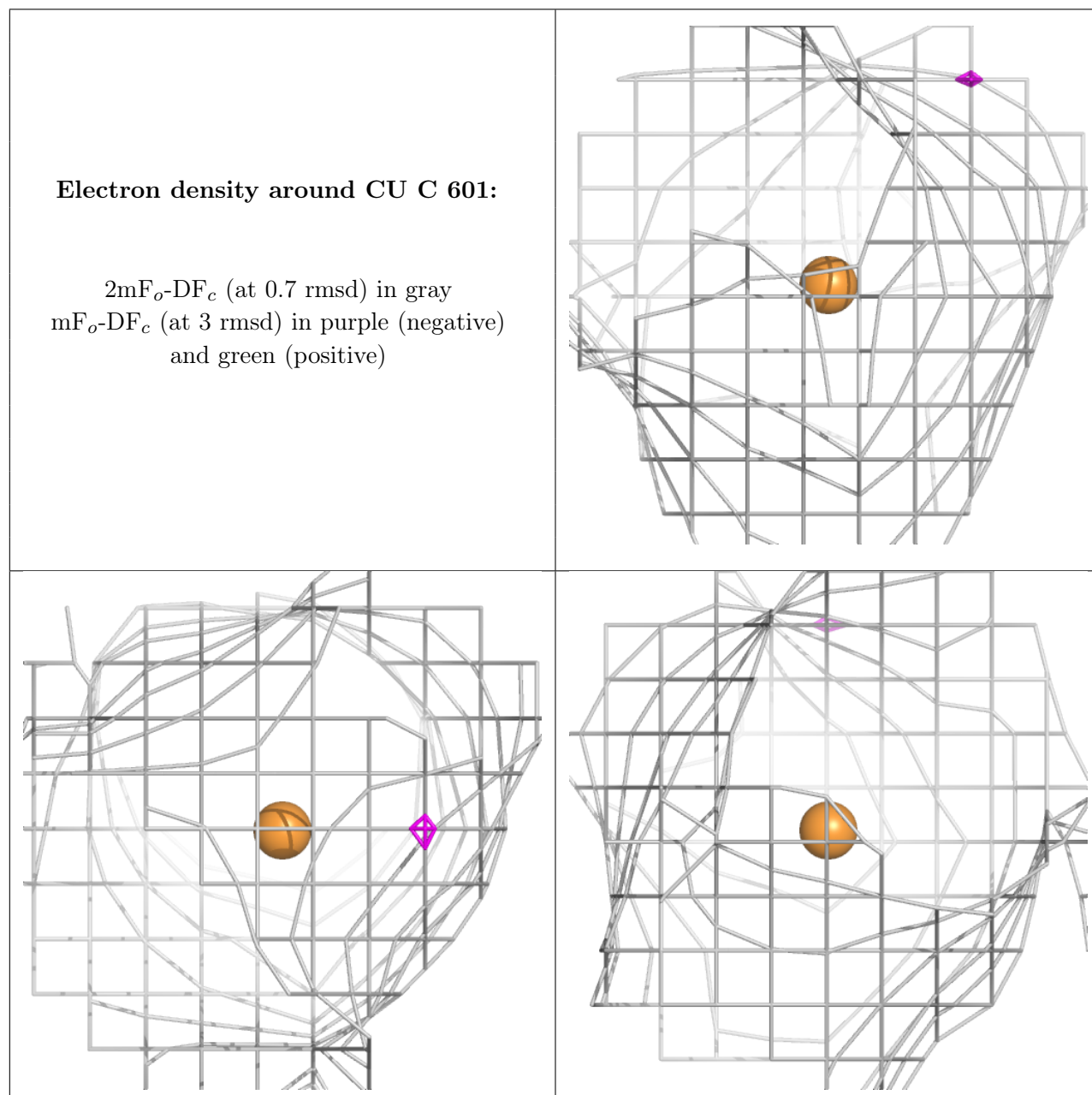
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
3	EDO	D	603	4/4	0.20	0.26	93,93,93,93	0
3	EDO	A	603	4/4	0.37	0.21	68,68,68,68	0
3	EDO	E	603	4/4	0.38	0.28	79,80,80,80	0
3	EDO	B	604	4/4	0.46	0.22	81,81,81,81	0
3	EDO	B	603	4/4	0.51	0.29	87,87,87,87	0
3	EDO	C	603	4/4	0.58	0.16	82,82,82,82	0
2	CU	C	601	1/1	0.98	0.04	84,84,84,84	0
2	CU	A	602	1/1	0.99	0.02	61,61,61,61	0
2	CU	B	601	1/1	0.99	0.02	86,86,86,86	0
2	CU	A	601	1/1	0.99	0.04	82,82,82,82	0
2	CU	D	601	1/1	0.99	0.05	79,79,79,79	0
2	CU	D	602	1/1	0.99	0.02	65,65,65,65	0
2	CU	E	601	1/1	0.99	0.03	93,93,93,93	0
2	CU	C	602	1/1	1.00	0.02	65,65,65,65	0
2	CU	B	602	1/1	1.00	0.01	52,52,52,52	0
2	CU	E	602	1/1	1.00	0.02	69,69,69,69	0

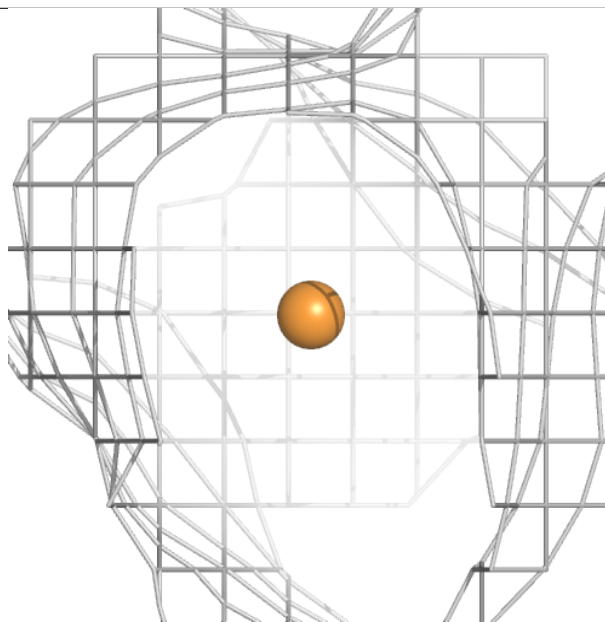
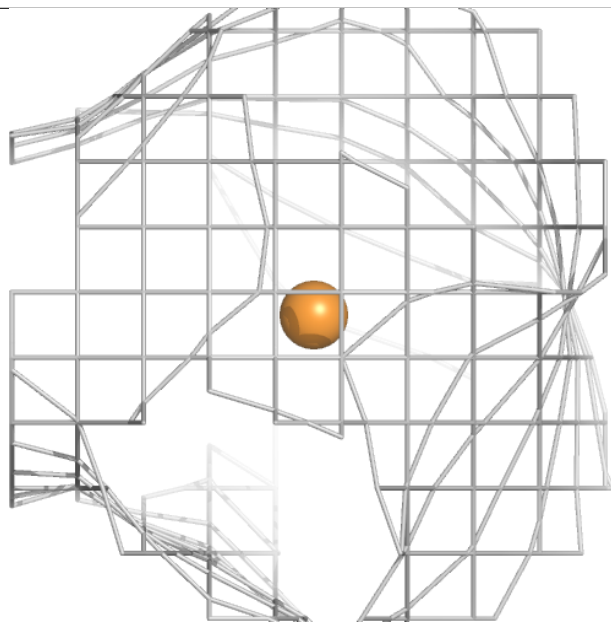
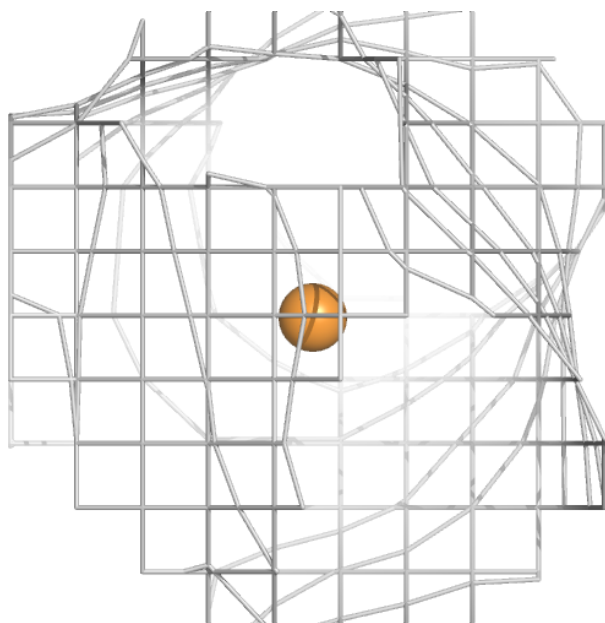
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



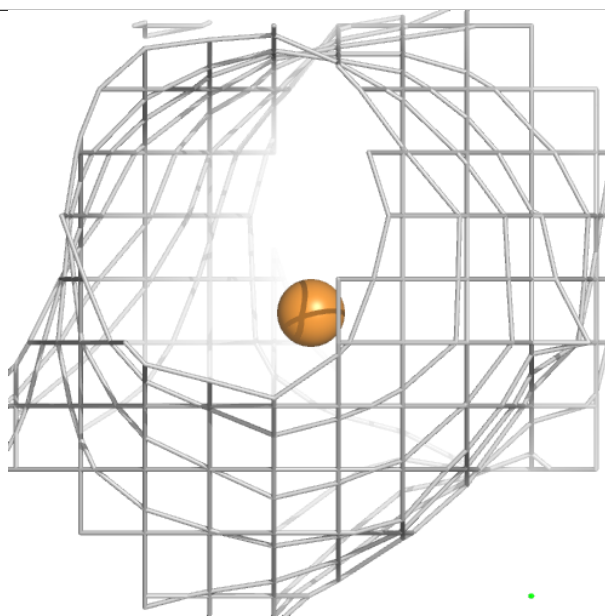
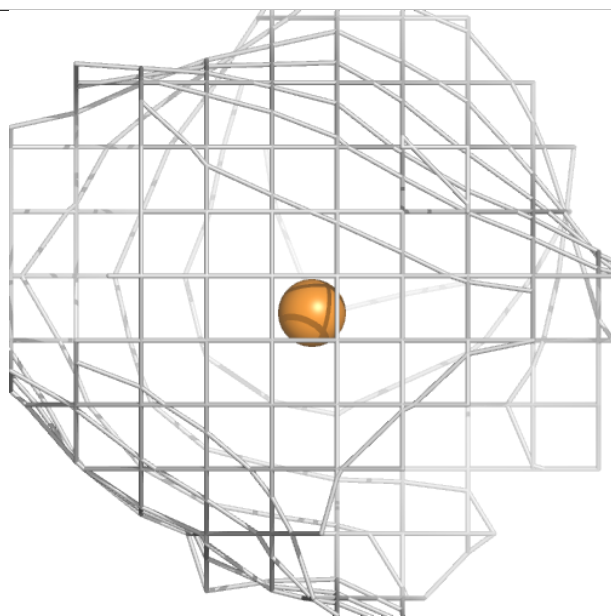
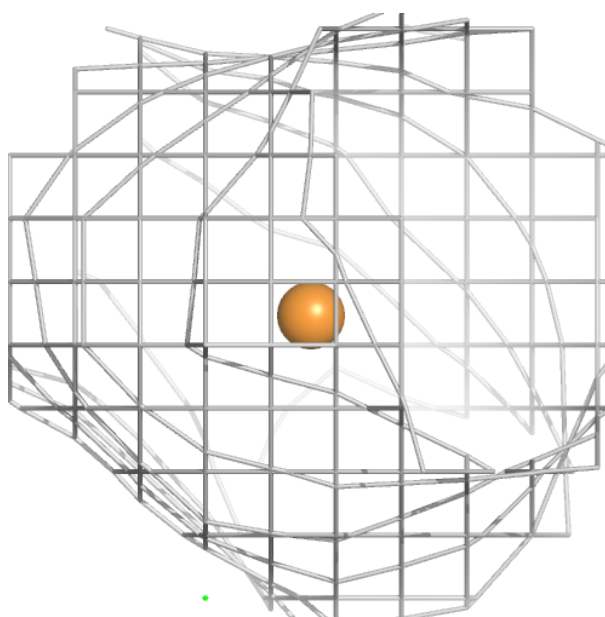
Electron density around CU A 602:

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



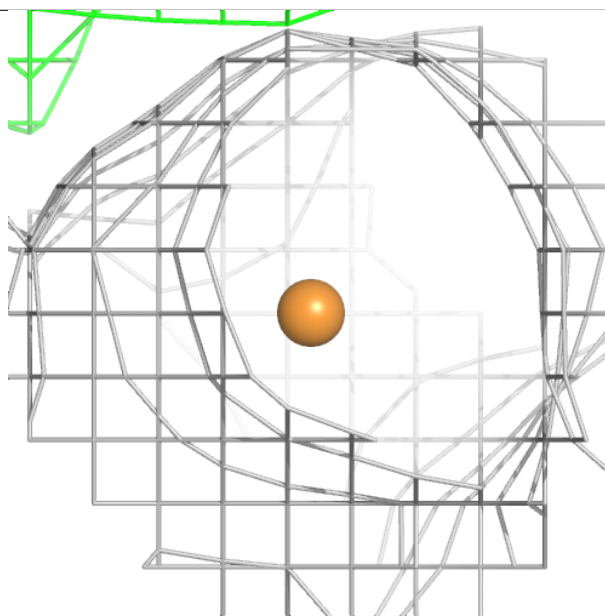
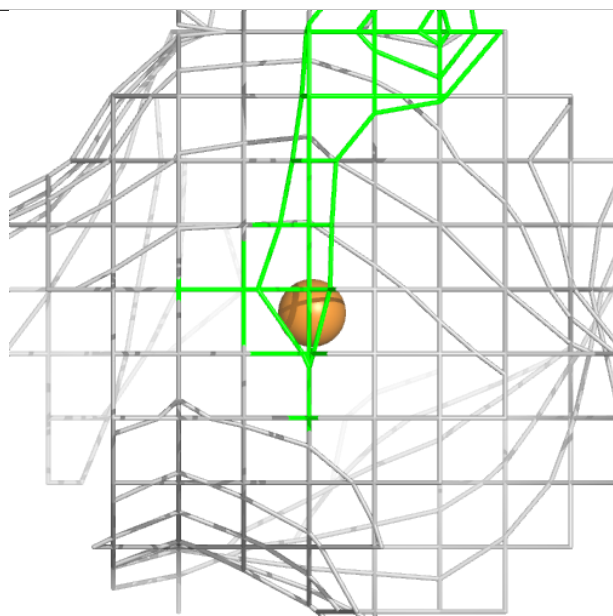
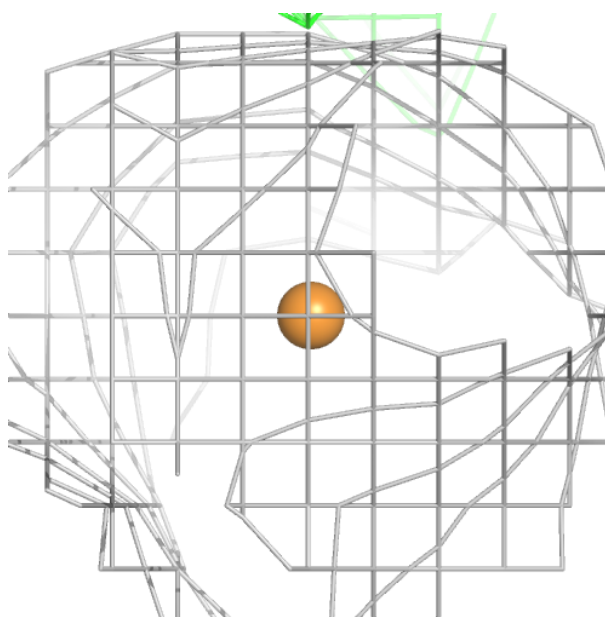
Electron density around CU B 601:

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



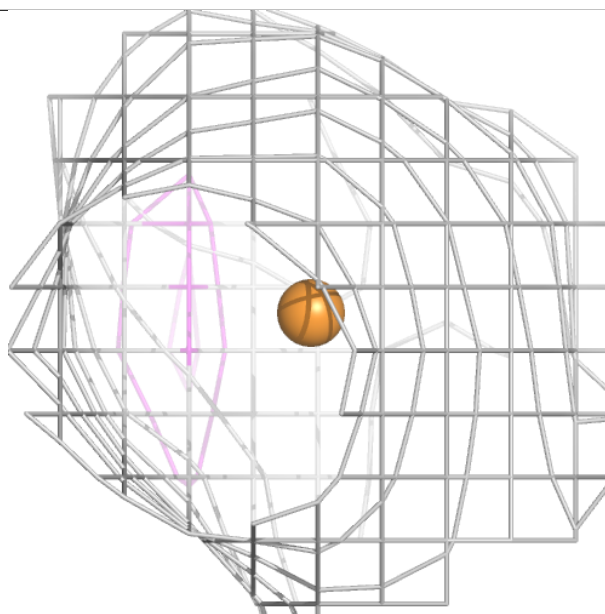
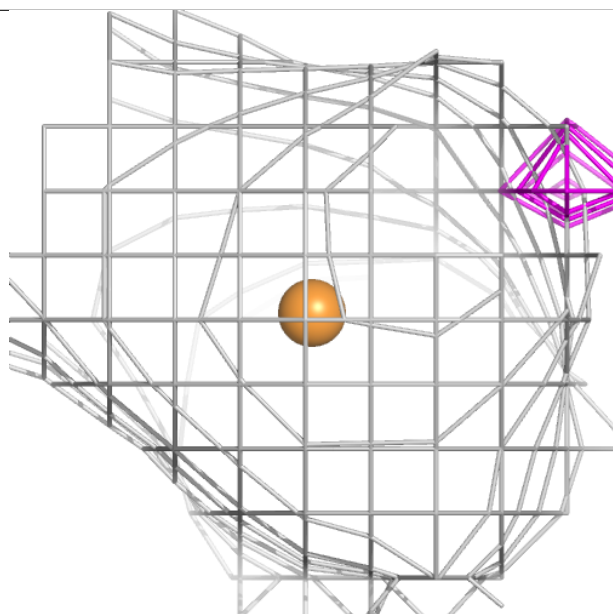
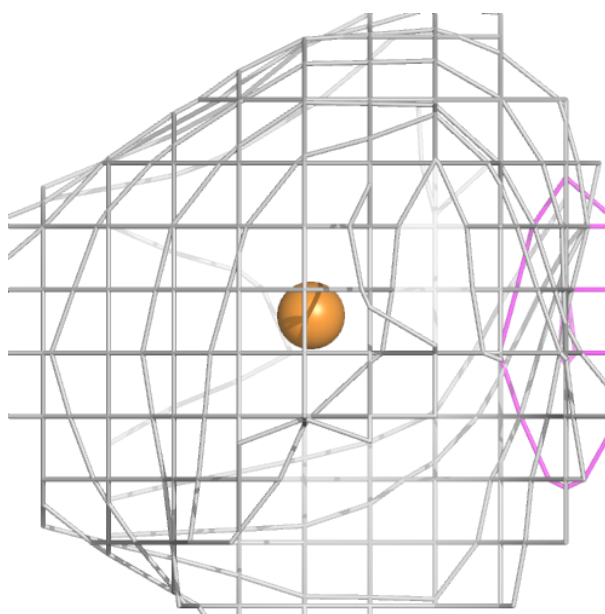
Electron density around CU A 601:

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



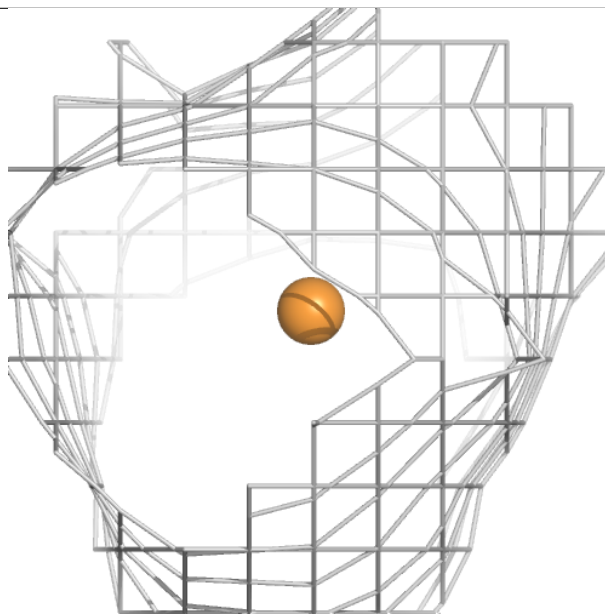
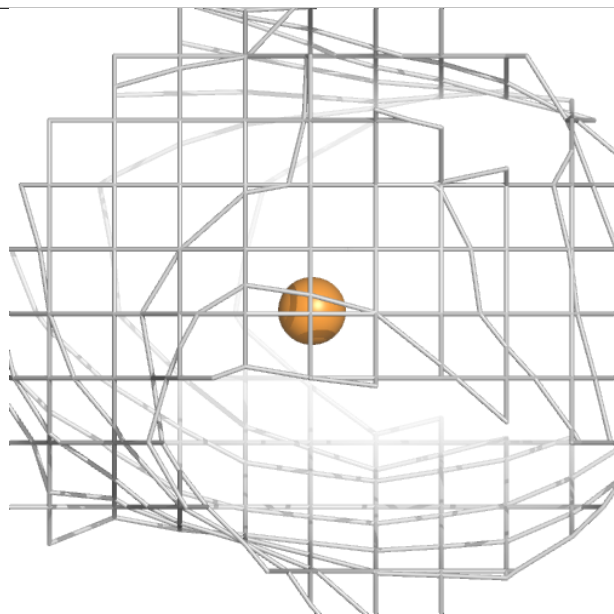
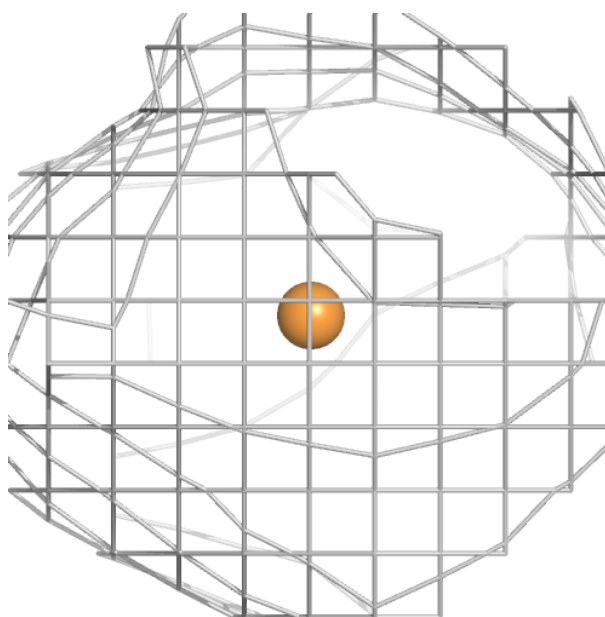
Electron density around CU D 601:

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



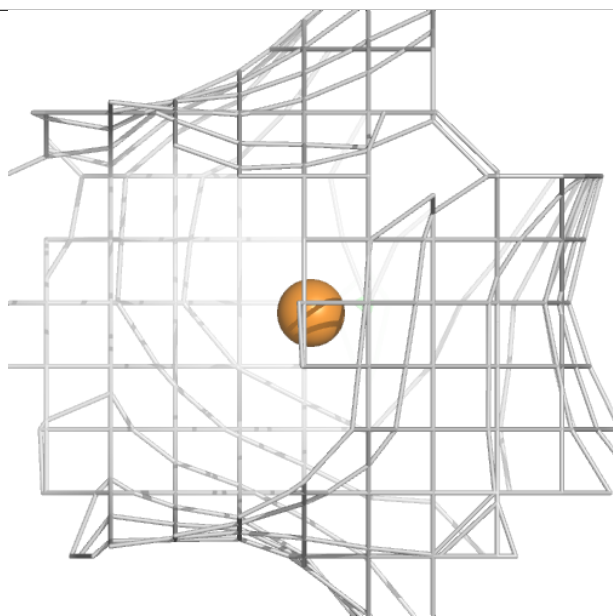
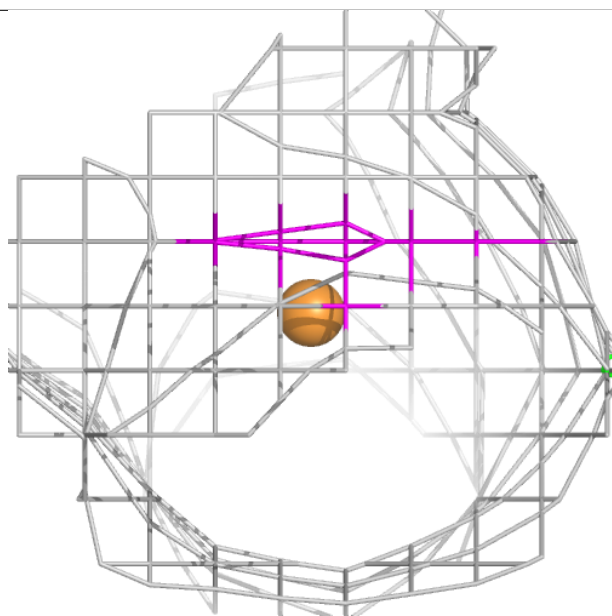
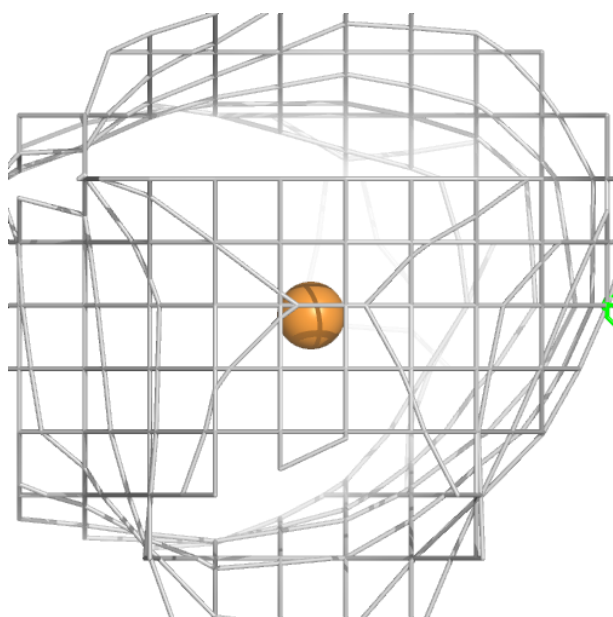
Electron density around CU D 602:

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



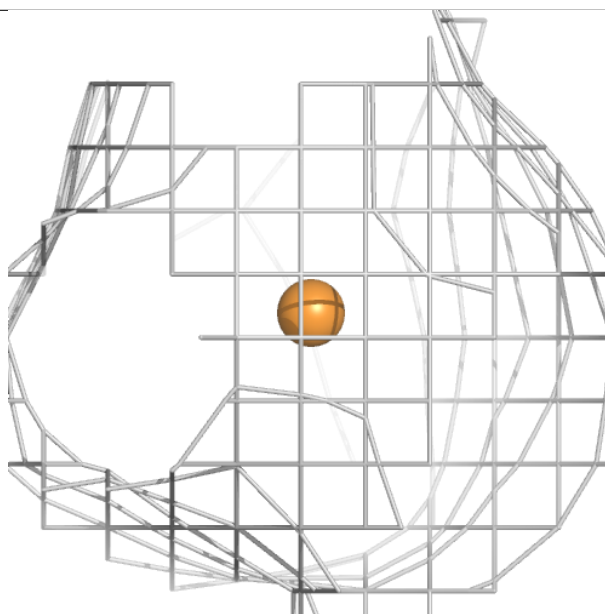
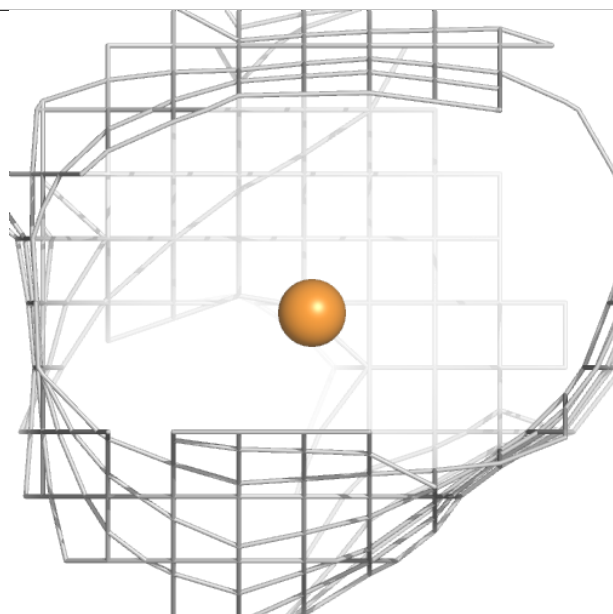
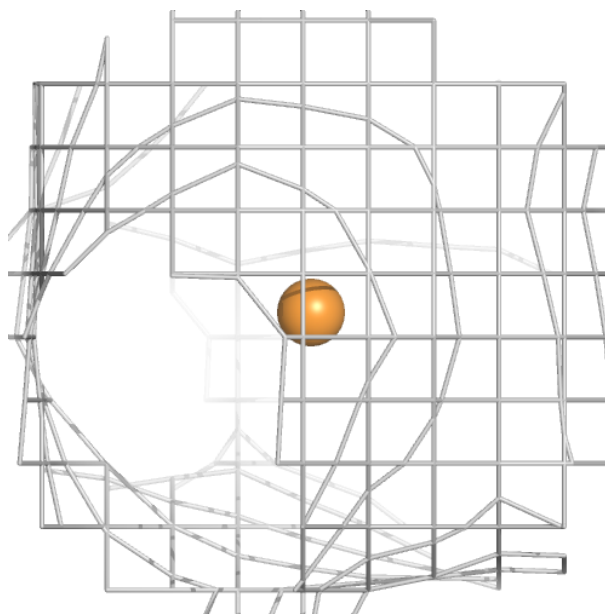
Electron density around CU E 601:

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



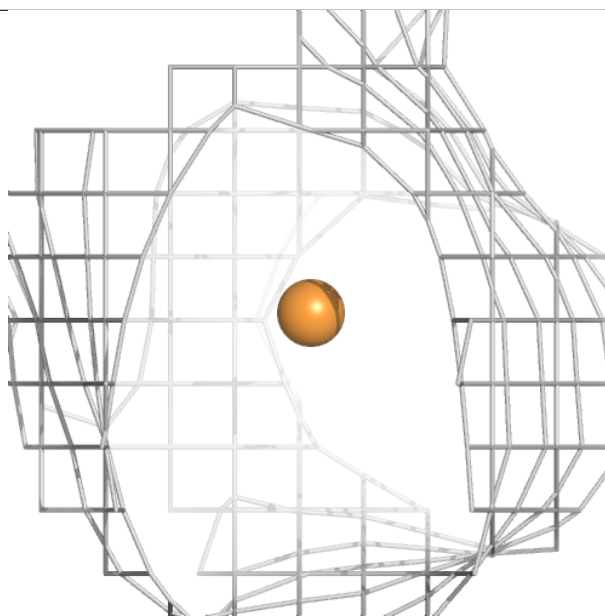
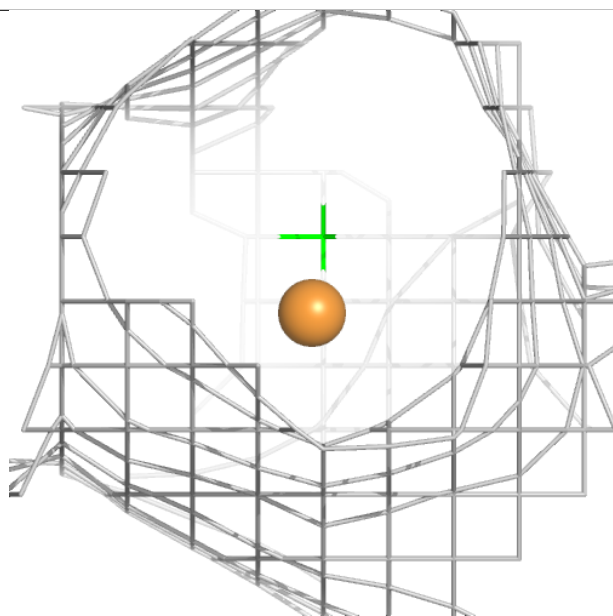
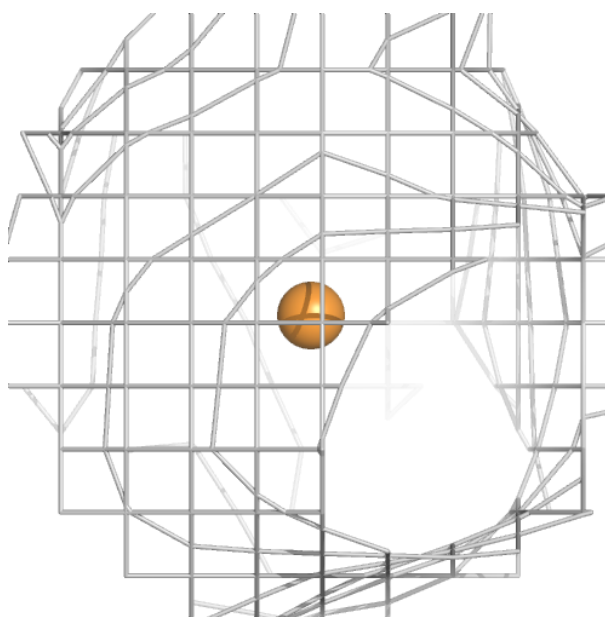
Electron density around CU C 602:

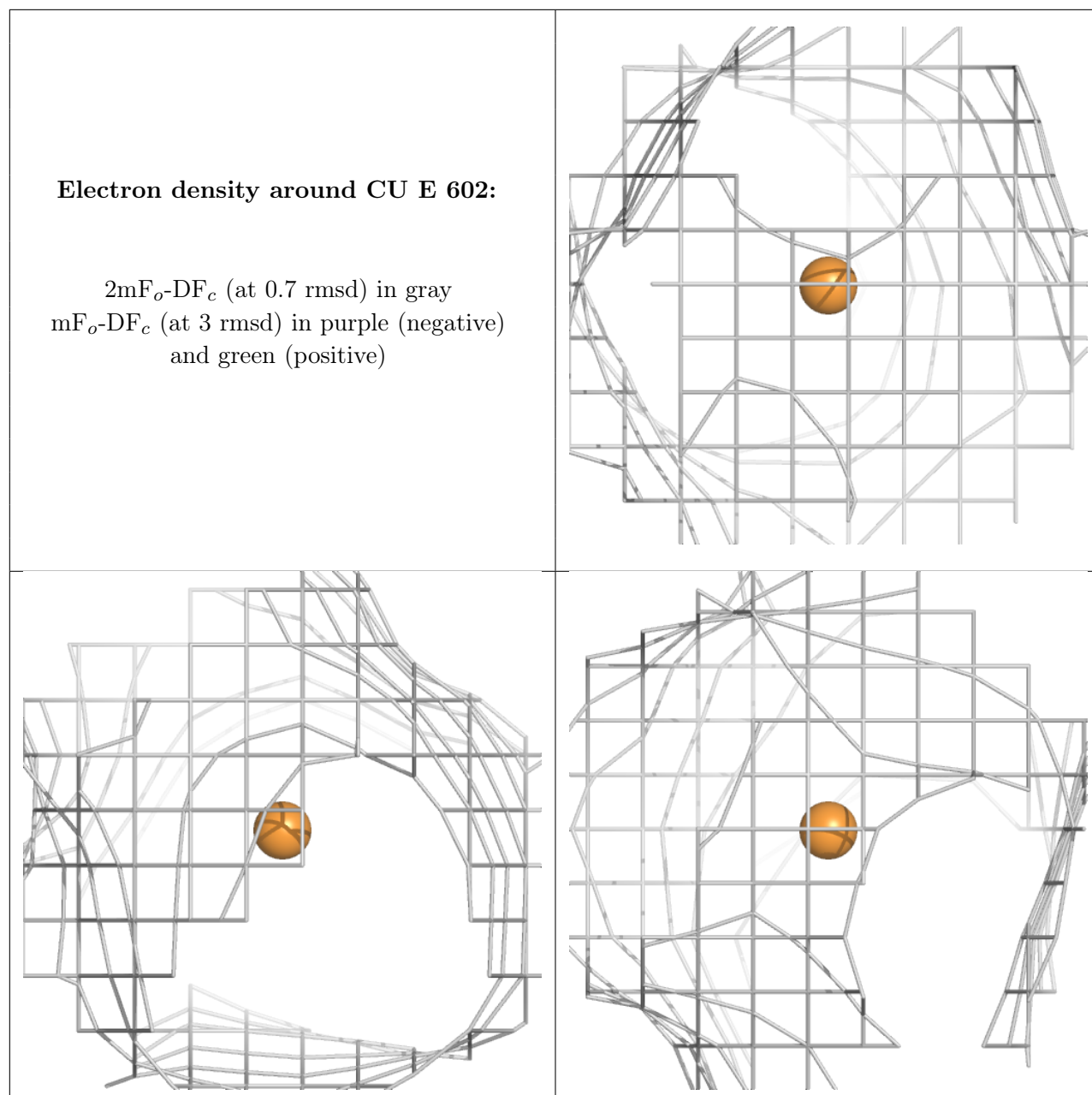
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU B 602:

$2mF_o-DF_c$ (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.