



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:25 AM UTC

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

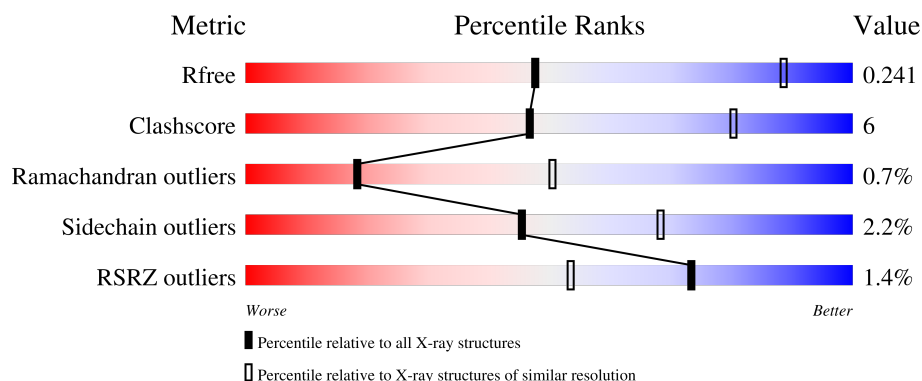
1 Overall quality at a glance

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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (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	
1	B	522	
1	C	522	
1	D	522	
1	E	522	

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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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

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.

Chain A:

76% 13% 10%

ALA TRP SER HIS PRO GLN PHE GLU LYS MET GLY HIS LYS MET GLY GLY MET GLN ASP ASN MET GLN MET SER S394 A395 G396 F399 N403 K404 A409 F410 K414 K426 D434 Q446 F447 L450 K455 W473 R474 S475 E476 V477 L478 V479 K480 M492 L497 M505 M506 S512 S52

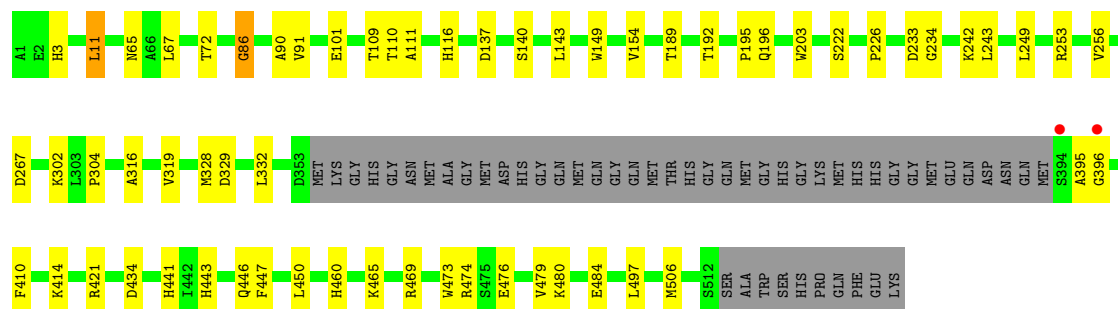
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

S222 S226 D233 G234 K242 E255 V256 L257 V258 G263 D267 K302 L303 P304 A316 V319 M328 D329 L332 D333 M334 M335 M339 D353 MET LYS GLY HIS ASN MET A1A E476 MET ASP HIS GLN MET GLN GLY MET THR HIS GLN

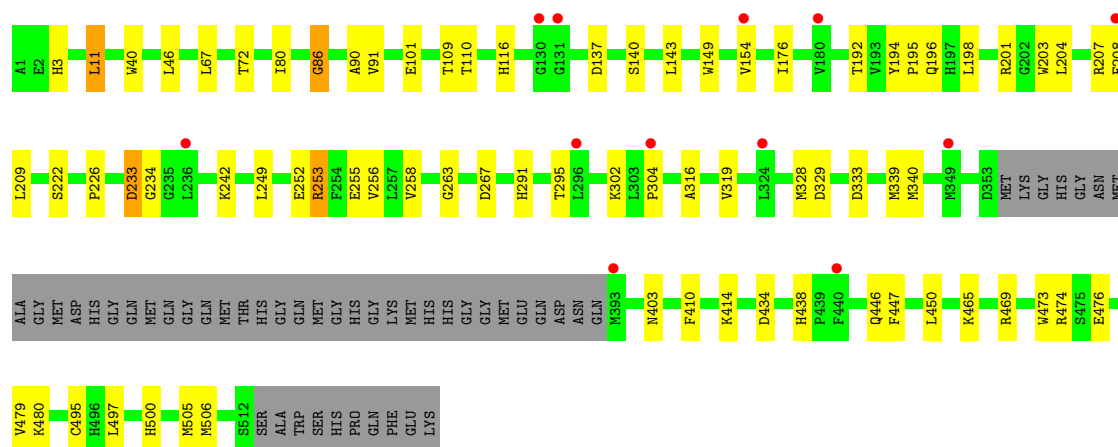
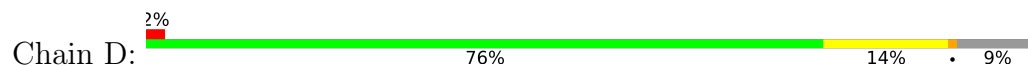
A1 E2 I8 L11 Q25 K30 A33 G34 K35 Q36 T64 T72 G86 A90 V91 E101 T109 T110 H116 D137 S140 L143 W149 V154 H169 I175 I176 T189 T192 P195 R201 G202 W203 L204 R207

Chain B:

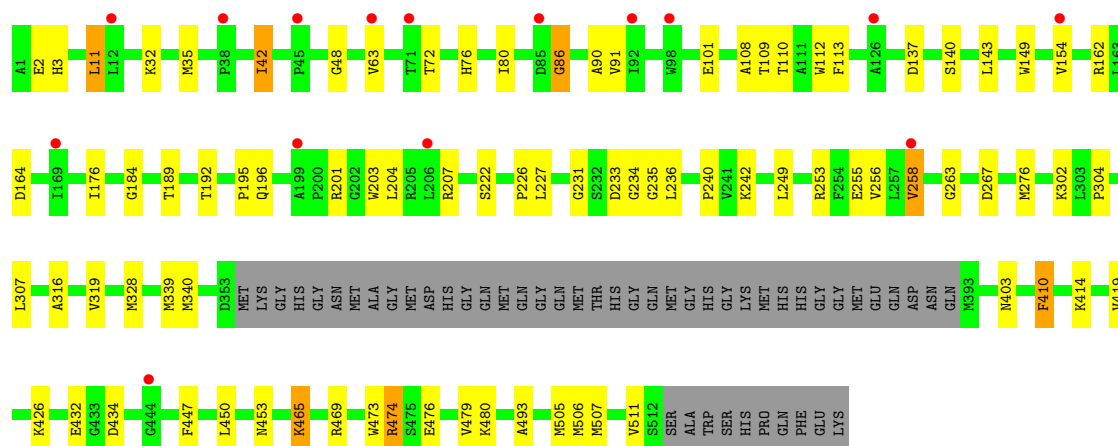
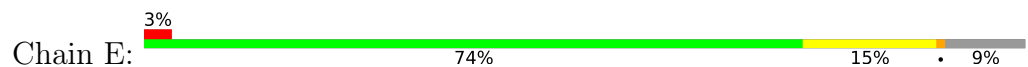
Chain C: 79% 11% 10%



• 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	2993 reflections (5.06%)	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

5.1 Standard geometry

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	0.63	1/3743 (0.0%)	0.96	5/5079 (0.1%)
1	B	0.61	1/3751 (0.0%)	0.96	2/5089 (0.0%)
1	C	0.62	1/3743 (0.0%)	0.96	3/5079 (0.1%)
1	D	0.60	0/3751	0.96	4/5089 (0.1%)
1	E	0.62	0/3751	0.97	6/5089 (0.1%)
All	All	0.62	3/18739 (0.0%)	0.96	20/25425 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	ALA	CA-C	8.70	1.64	1.52
1	C	395	ALA	CA-C	6.22	1.60	1.53
1	B	395	ALA	CA-C	5.12	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	VAL	N-CA-C	7.28	115.83	107.89
1	E	154	VAL	N-CA-C	7.24	115.78	107.89
1	C	154	VAL	N-CA-C	7.18	115.72	107.89
1	D	154	VAL	N-CA-C	7.12	115.65	107.89
1	B	154	VAL	N-CA-C	7.01	115.53	107.89
1	E	164	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	137	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	137	ASP	CA-CB-CG	5.64	118.24	112.60
1	C	137	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	137	ASP	CA-CB-CG	5.58	118.18	112.60
1	E	137	ASP	CA-CB-CG	5.57	118.17	112.60
1	E	63	VAL	CA-C-N	5.55	129.81	122.42
1	E	63	VAL	C-N-CA	5.55	129.81	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	LEU	N-CA-C	-5.42	98.14	108.17
1	D	497	LEU	N-CA-C	-5.20	98.56	108.17
1	D	80	ILE	N-CA-CB	-5.19	107.26	111.67
1	E	80	ILE	N-CA-CB	-5.07	107.36	111.67
1	C	497	LEU	N-CA-C	-5.02	98.89	108.17
1	A	332	LEU	CA-C-N	5.00	127.24	120.38
1	A	332	LEU	C-N-CA	5.00	127.24	120.38

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	3648	0	3629	39	0
1	B	3656	0	3638	46	0
1	C	3648	0	3629	34	0
1	D	3656	0	3639	43	0
1	E	3656	0	3638	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	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	208	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 6.

All (208) 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:327:MET:HE2	1:D:339:MET:HE1	1.39	1.03
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:B:112:TRP:CD1	1:B:253:ARG:HH11	2.01	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: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
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:A:403:ASN:HB3	1:A:505:MET:HE3	1.85	0.57
1:D:403:ASN:HB3	1:D:505:MET:HE3	1.85	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:A:175:ILE:HG12	1:A:335:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ILE:HD12	1:E:113:PHE:HE2	1.73	0.54
1:A:35:MET:HE2	1:A:168:HIS:CD2	2.43	0.53
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:B:403:ASN:HB3	1:B:505:MET:HE3	1.91	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:473:TRP:CG	1:A:474:ARG:H	2.28	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:350:ALA:HB3	1:B:352:MET:HE2	1.93	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: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
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:D:109:THR:HG22	1:D:110:THR:N	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:473:TRP:CG	1:D:474:ARG:H	2.31	0.48
1:D:72:THR:HG22	1:D:91:VAL:HA	1.96	0.48
1:E:473:TRP:CG	1:E:474:ARG:H	2.32	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
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:C:473:TRP:CG	1:C:474:ARG:H	2.35	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:340:MET:HE2	1:B:340:MET:HB3	1.92	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:B:334:MET:HE3	1:B:334:MET:HB2	1.84	0.44
1:D:11:LEU:HD13	1:D:149:TRP:CE2	2.53	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:B:473:TRP:CG	1:B:474:ARG:H	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:276:MET:HG2	1:E:340:MET:HE1	2.02	0.41
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:173:LEU:HD23	1:B:400:MET:HE1	2.01	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:E:403:ASN:HB3	1:E:505:MET:HE3	2.03	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:D:340:MET:HE2	1:D:340:MET:HB3	1.92	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	45
1	B	469/522 (90%)	437 (93%)	27 (6%)	5 (1%)	11	41
1	C	468/522 (90%)	437 (93%)	28 (6%)	3 (1%)	21	53
1	D	469/522 (90%)	441 (94%)	25 (5%)	3 (1%)	21	53
1	E	469/522 (90%)	438 (93%)	29 (6%)	2 (0%)	30	60
All	All	2343/2610 (90%)	2191 (94%)	135 (6%)	17 (1%)	18	50

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%)	379 (98%)	9 (2%)	44	68
1	B	389/426 (91%)	378 (97%)	11 (3%)	38	64
1	C	388/426 (91%)	383 (99%)	5 (1%)	61	75
1	D	389/426 (91%)	381 (98%)	8 (2%)	47	69
1	E	389/426 (91%)	379 (97%)	10 (3%)	40	66
All	All	1943/2130 (91%)	1900 (98%)	43 (2%)	45	68

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	25	GLN
1	A	64	THR
1	A	101	GLU
1	A	256	VAL
1	A	414	LYS
1	A	474	ARG
1	A	480	LYS
1	A	492	MET

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Mol	Chain	Res	Type
1	B	2	GLU
1	B	11	LEU
1	B	46	LEU
1	B	64	THR
1	B	101	GLU
1	B	201	ARG
1	B	253	ARG
1	B	258	VAL
1	B	297	LYS
1	B	414	LYS
1	B	480	LYS
1	C	11	LEU
1	C	101	GLU
1	C	256	VAL
1	C	414	LYS
1	C	480	LYS
1	D	11	LEU
1	D	46	LEU
1	D	101	GLU
1	D	196	GLN
1	D	253	ARG
1	D	256	VAL
1	D	414	LYS
1	D	480	LYS
1	E	2	GLU
1	E	11	LEU
1	E	42	ILE
1	E	101	GLU
1	E	258	VAL
1	E	414	LYS
1	E	453	ASN
1	E	465	LYS
1	E	474	ARG
1	E	480	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	B	168	HIS
1	B	318	ASN
1	B	338	GLN

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Mol	Chain	Res	Type
1	C	168	HIS
1	D	23	ASN
1	D	168	HIS
1	D	342	GLN
1	E	196	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	603	-	3,3,3	0.40	0	2,2,2	0.09	0
3	EDO	B	604	-	3,3,3	0.30	0	2,2,2	0.21	0
3	EDO	A	603	-	3,3,3	0.25	0	2,2,2	0.30	0
3	EDO	B	603	-	3,3,3	0.42	0	2,2,2	0.07	0
3	EDO	E	603	-	3,3,3	0.36	0	2,2,2	0.25	0
3	EDO	D	603	-	3,3,3	0.34	0	2,2,2	0.10	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	C	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	E	603	-	-	1/1/1/1	-
3	EDO	D	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	604	EDO	O1-C1-C2-O2
3	B	603	EDO	O1-C1-C2-O2
3	D	603	EDO	O1-C1-C2-O2
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%)	-0.14	2 (0%)	88 78	48, 74, 99, 111	0
1	B	473/522 (90%)	-0.07	2 (0%)	88 78	56, 75, 90, 108	0
1	C	472/522 (90%)	-0.18	2 (0%)	88 78	57, 74, 90, 103	0
1	D	473/522 (90%)	0.35	12 (2%)	58 37	55, 89, 107, 120	0
1	E	473/522 (90%)	0.49	15 (3%)	50 30	51, 94, 126, 135	0
All	All	2363/2610 (90%)	0.09	33 (1%)	73 53	48, 78, 111, 135	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	154	VAL	3.2
1	E	92	ILE	3.0
1	D	440	PHE	2.9
1	E	444	GLY	2.7
1	E	63	VAL	2.6
1	E	126	ALA	2.6
1	B	354	MET	2.6
1	E	169	ILE	2.6
1	E	154	VAL	2.6
1	E	199	ALA	2.5
1	E	71	THR	2.5
1	E	12	LEU	2.5
1	A	395	ALA	2.4
1	E	85	ASP	2.4
1	C	394	SER	2.4
1	B	395	ALA	2.3
1	E	38	PRO	2.3
1	E	98	TRP	2.2
1	E	258	VAL	2.2
1	D	296	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	393	MET	2.2
1	D	304	PRO	2.2
1	D	180	VAL	2.2
1	E	206	LEU	2.2
1	D	349	MET	2.1
1	A	396	GLY	2.1
1	D	131	GLY	2.1
1	E	45	PRO	2.1
1	D	208	PHE	2.1
1	D	324	LEU	2.1
1	C	396	GLY	2.1
1	D	236	LEU	2.0
1	D	130	GLY	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 oligosaccharides 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(Å 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

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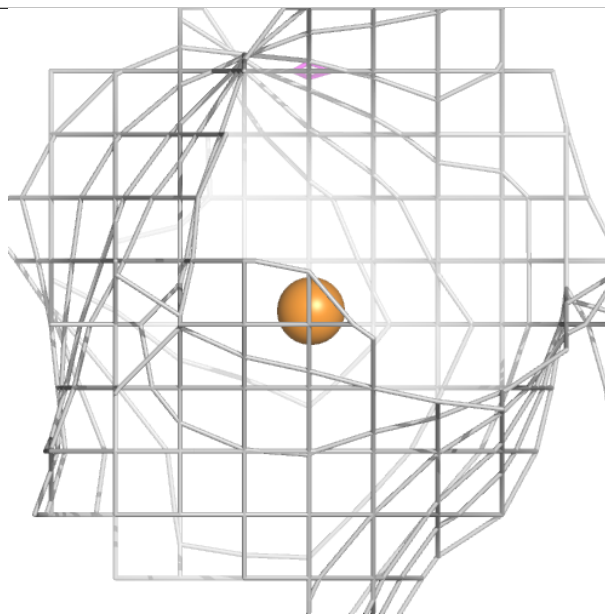
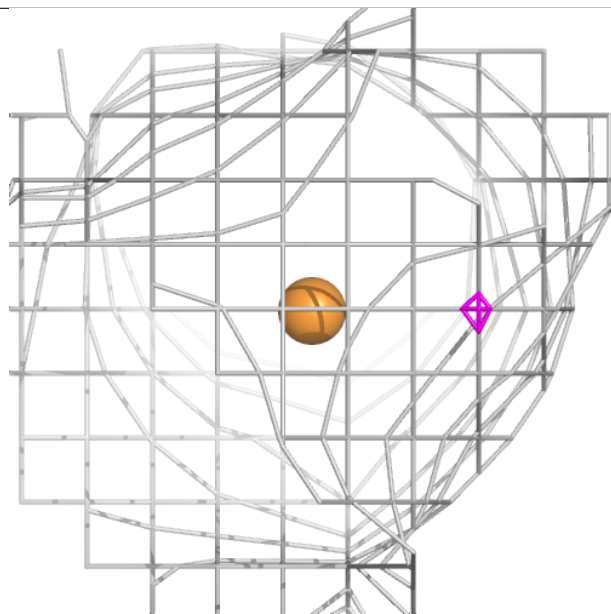
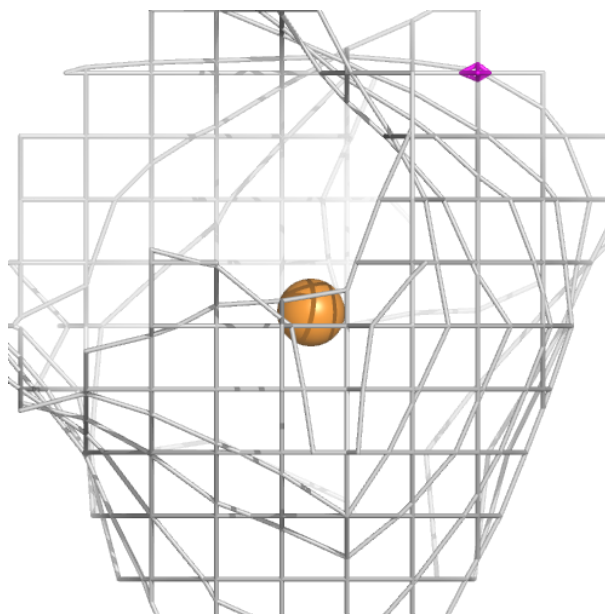
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	D	601	1/1	0.99	0.05	79,79,79,79	0
2	CU	D	602	1/1	0.99	0.02	65,65,65,65	0
2	CU	E	601	1/1	0.99	0.03	93,93,93,93	0
2	CU	C	602	1/1	1.00	0.02	65,65,65,65	0
2	CU	B	602	1/1	1.00	0.01	52,52,52,52	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.

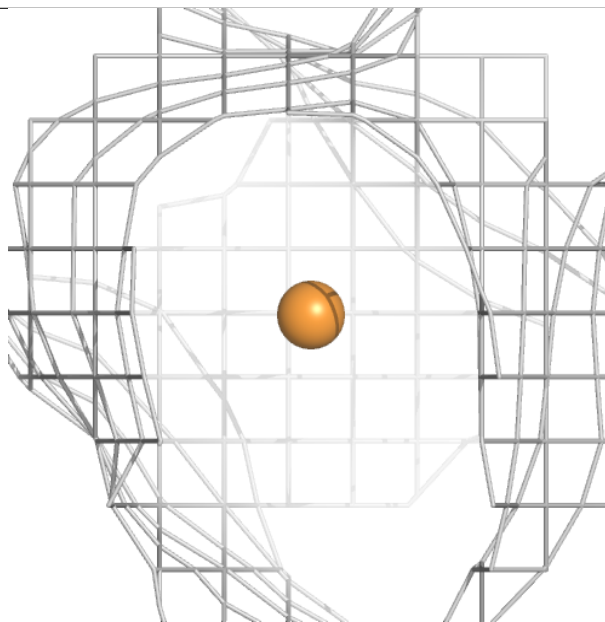
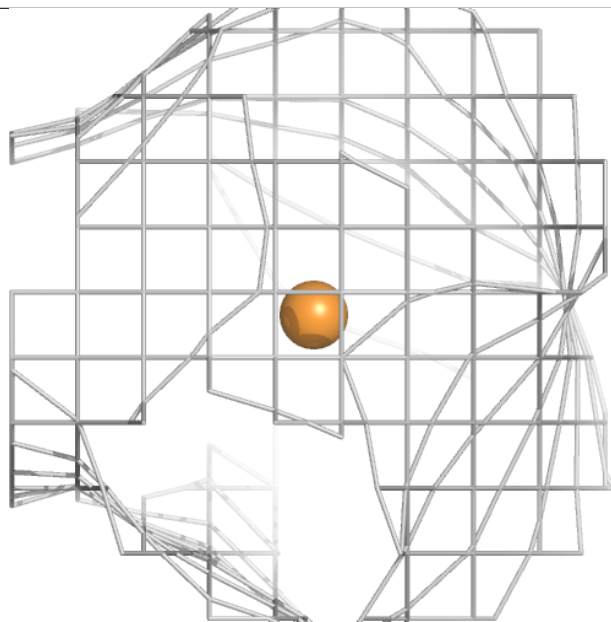
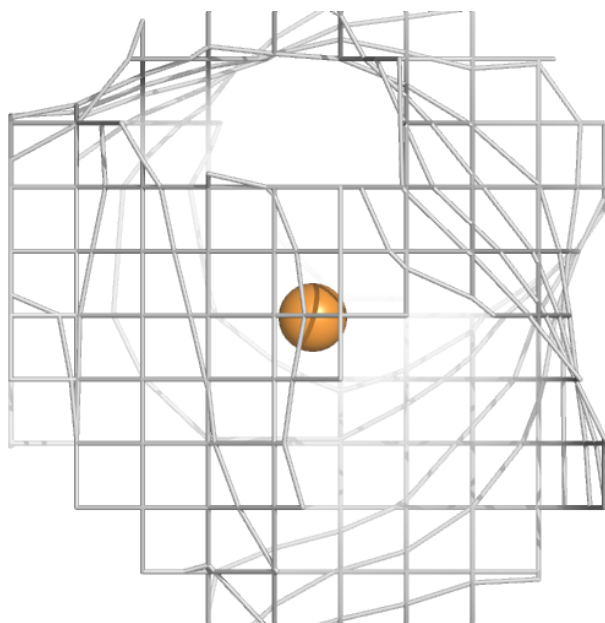
Electron density around CU C 601:

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



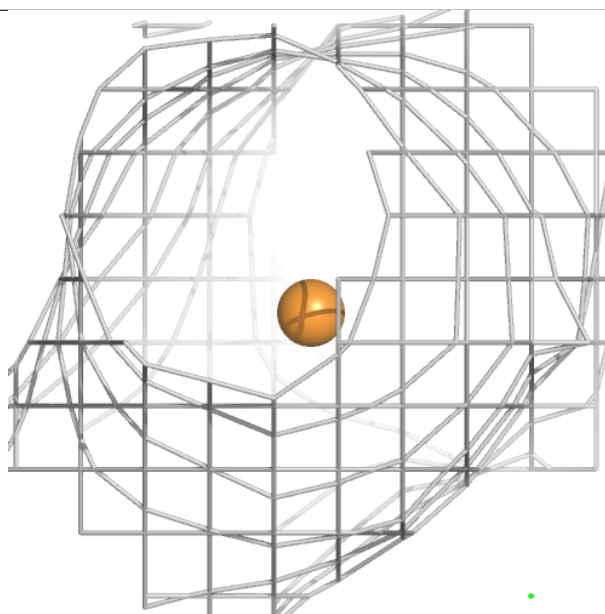
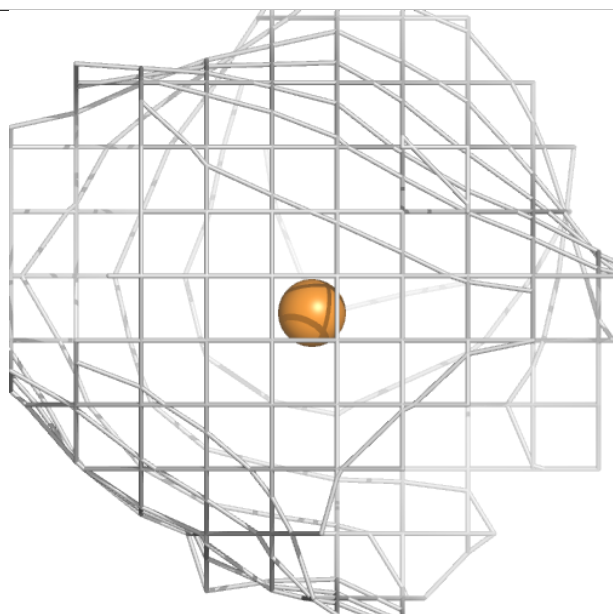
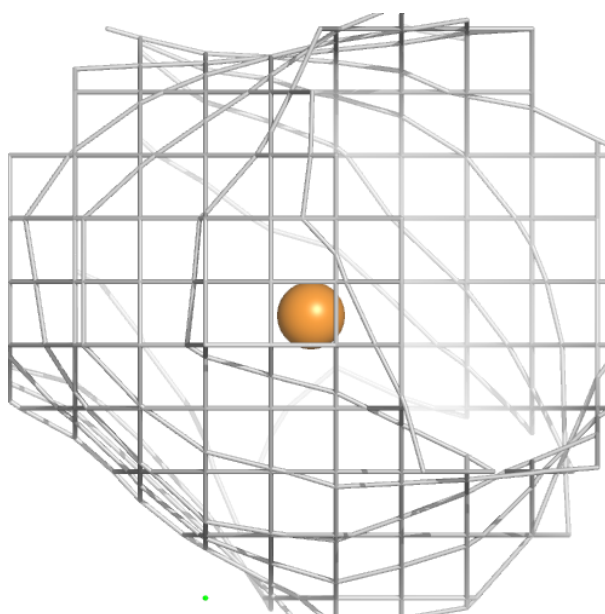
Electron density around CU A 602:

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



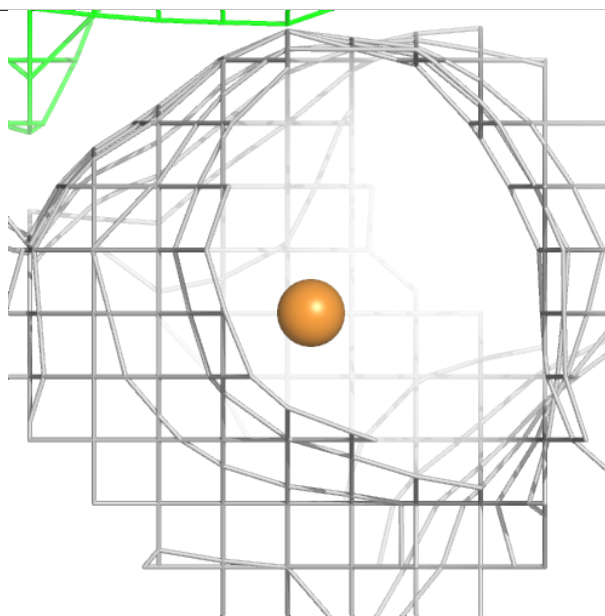
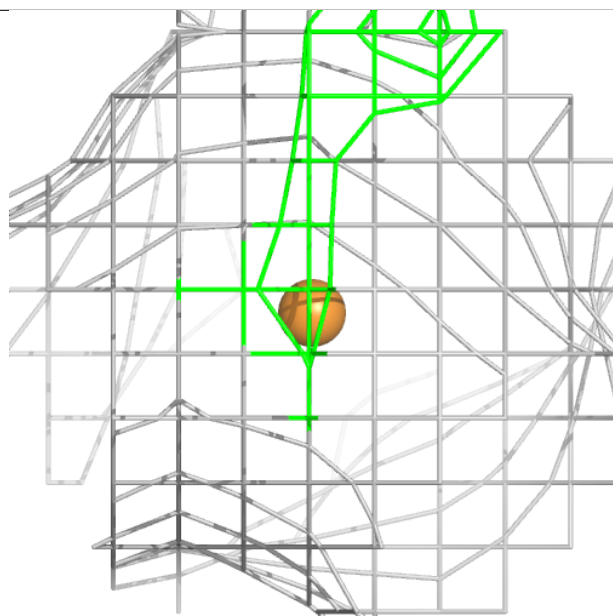
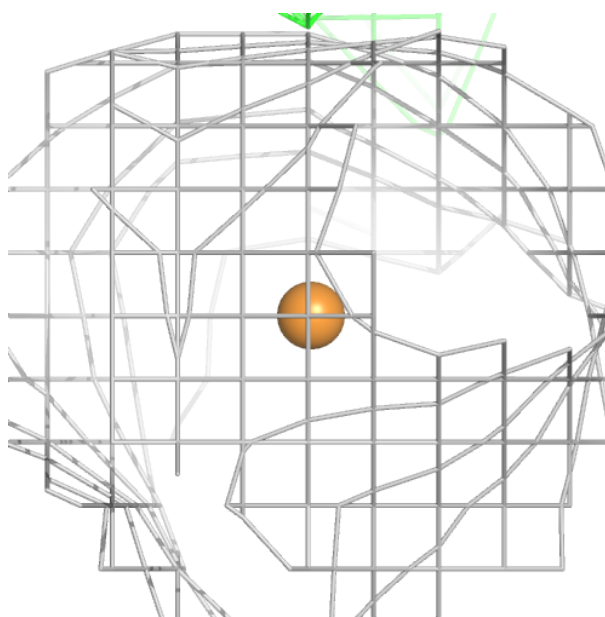
Electron density around CU B 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



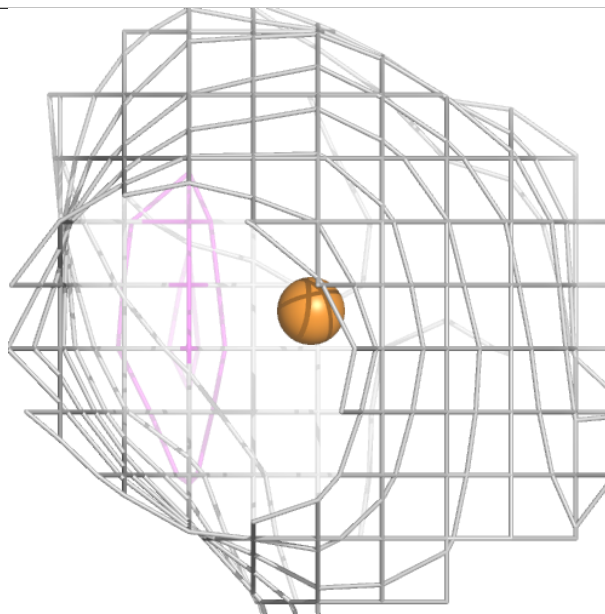
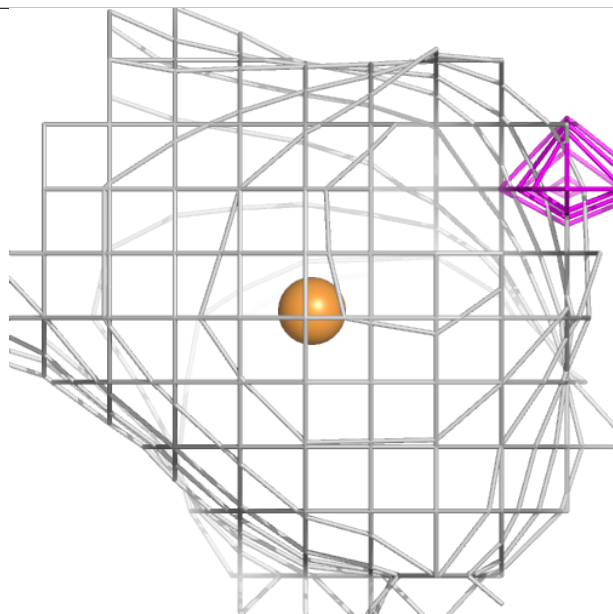
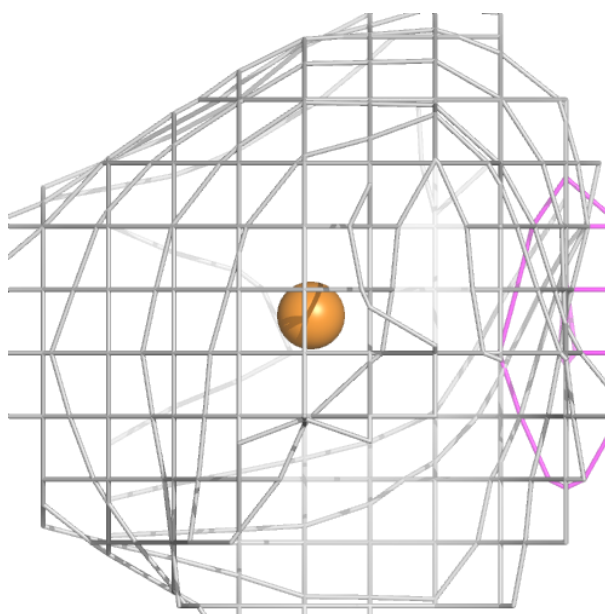
Electron density around CU A 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



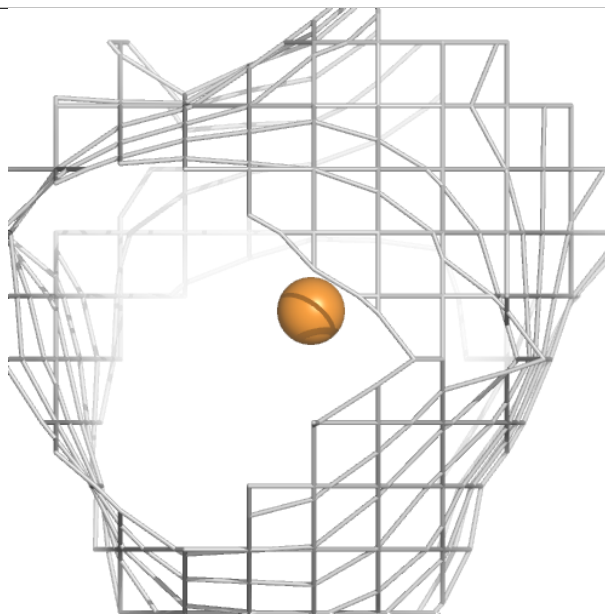
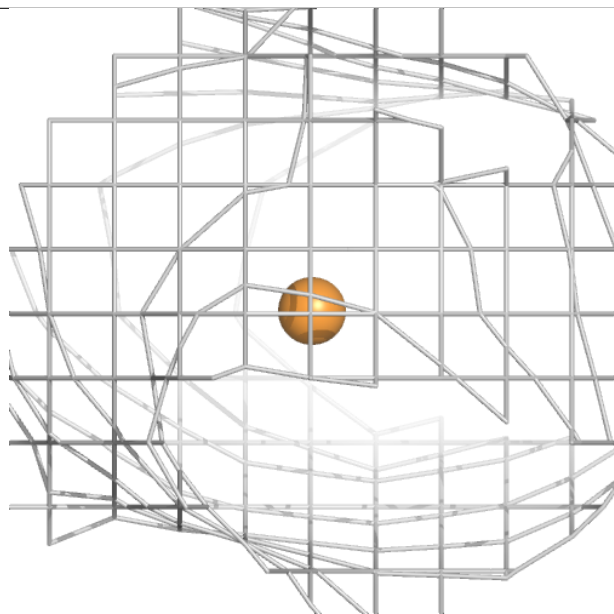
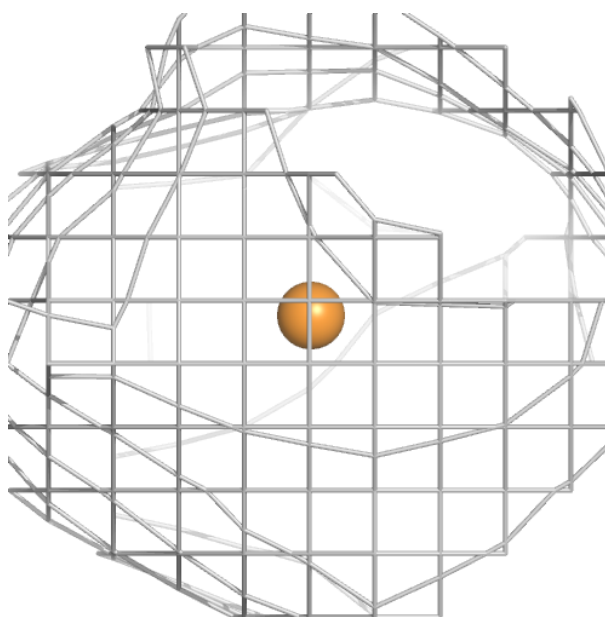
Electron density around CU D 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



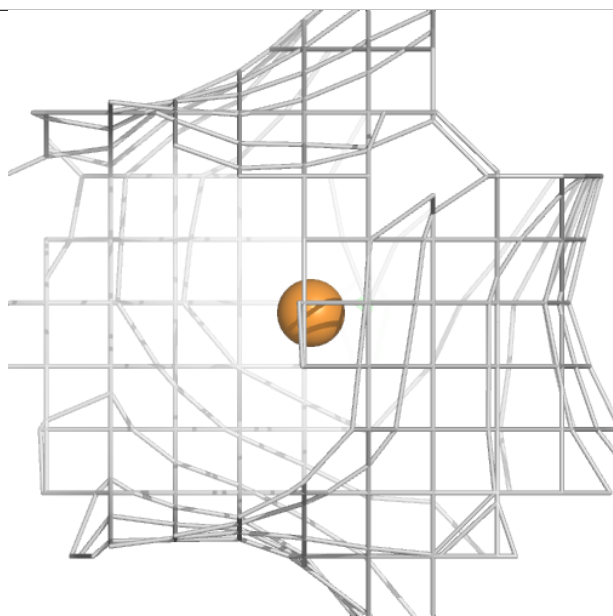
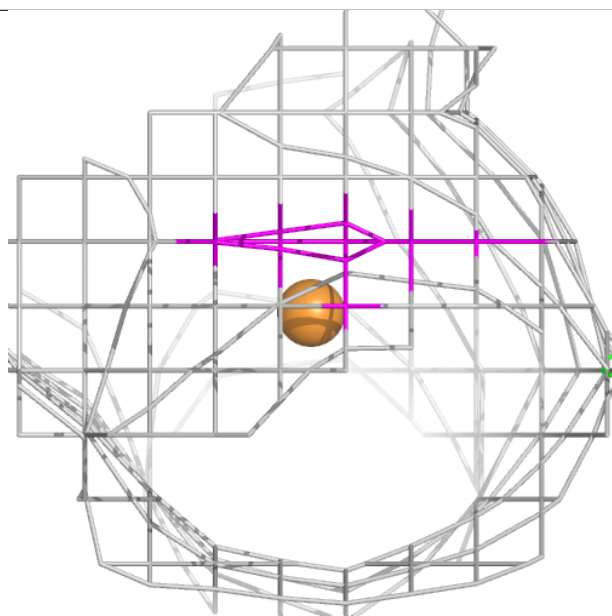
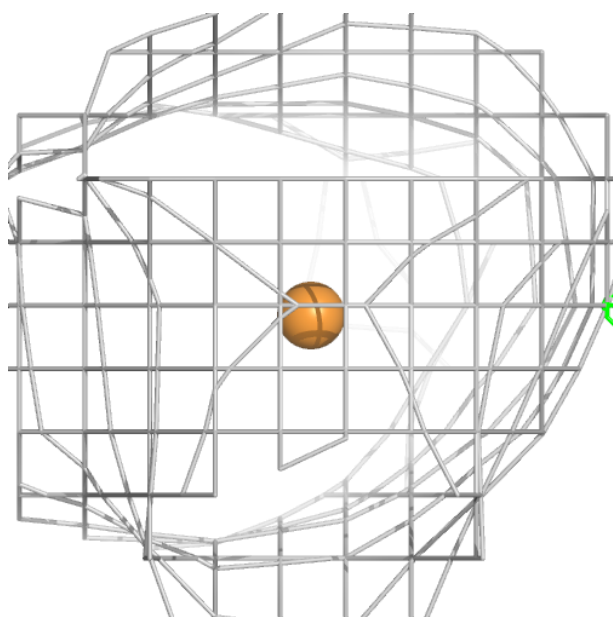
Electron density around CU D 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



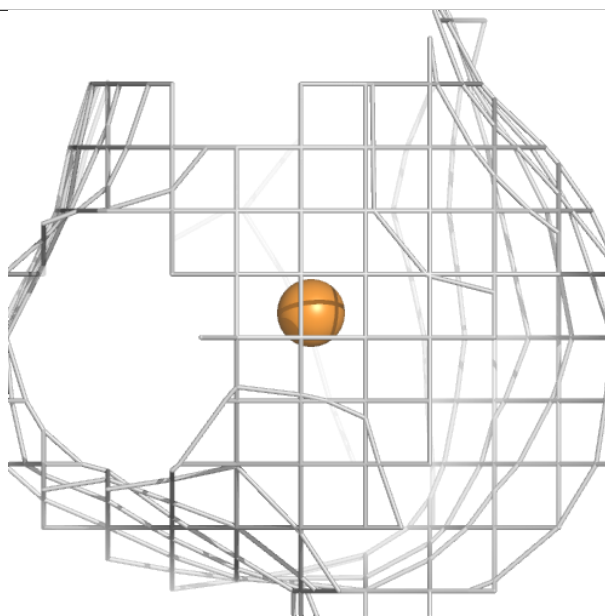
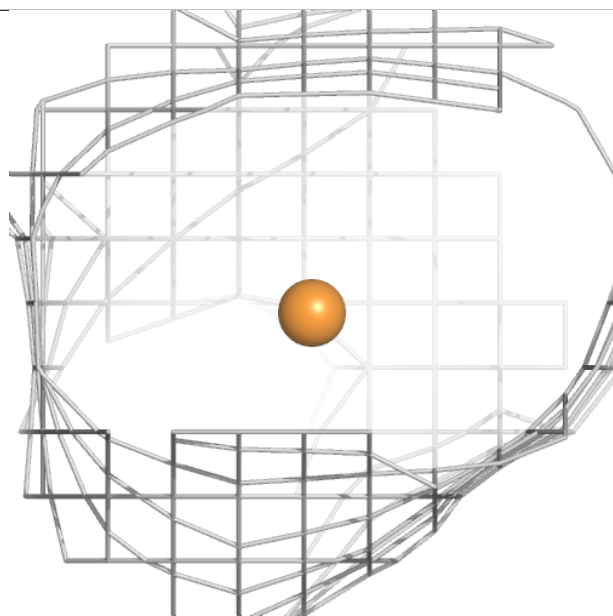
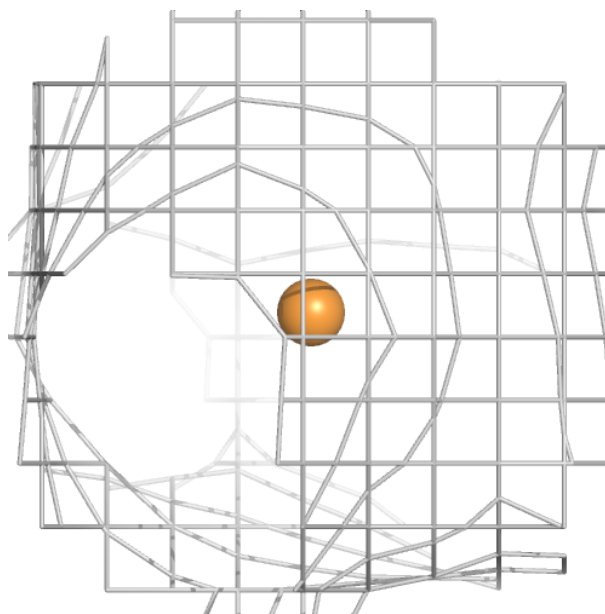
Electron density around CU E 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



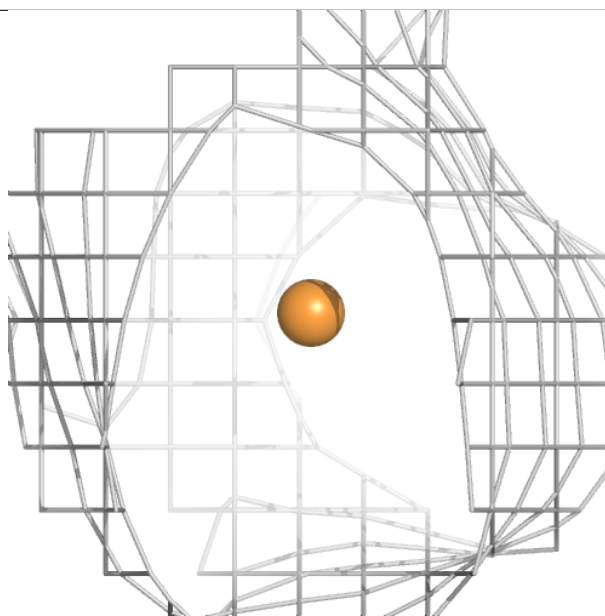
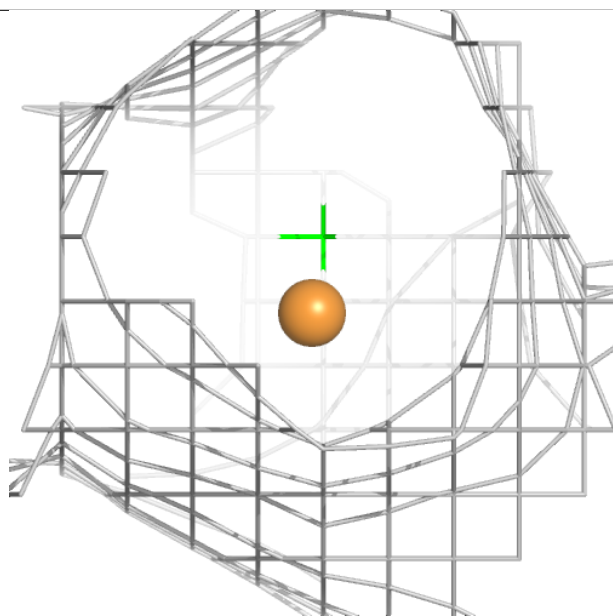
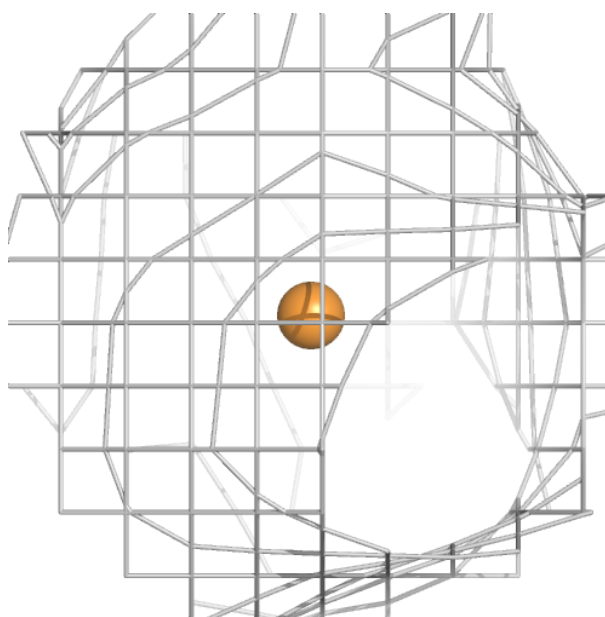
Electron density around CU C 602:

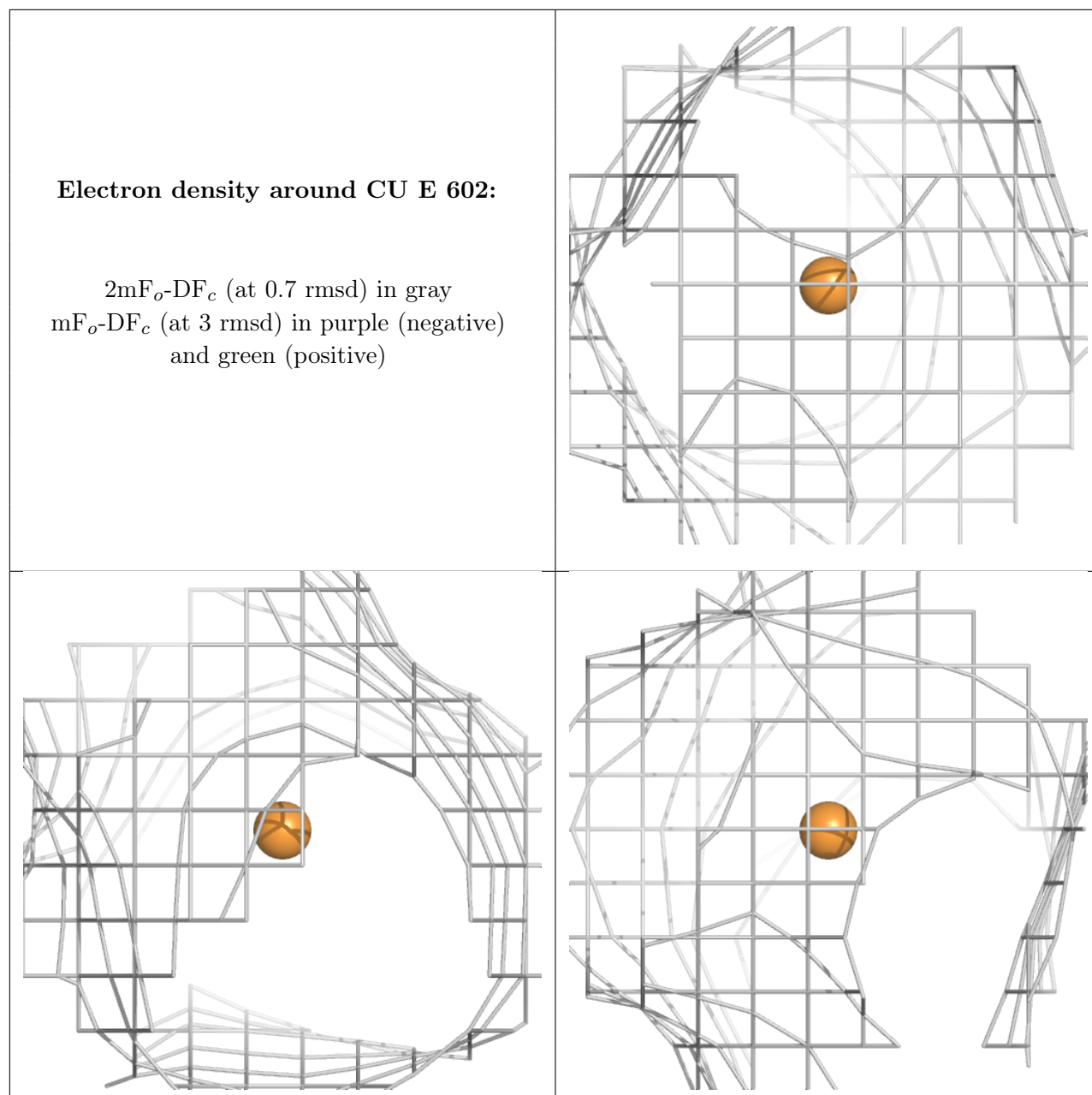
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



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.