



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:05 PM UTC

PDB ID : 8U8T / pdb_00008u8t
Title : Y229F/V290N Streptomyces coelicolor Laccase
Authors : Wang, J.-X.; Lu, Y.
Deposited on : 2023-09-18
Resolution : 2.90 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

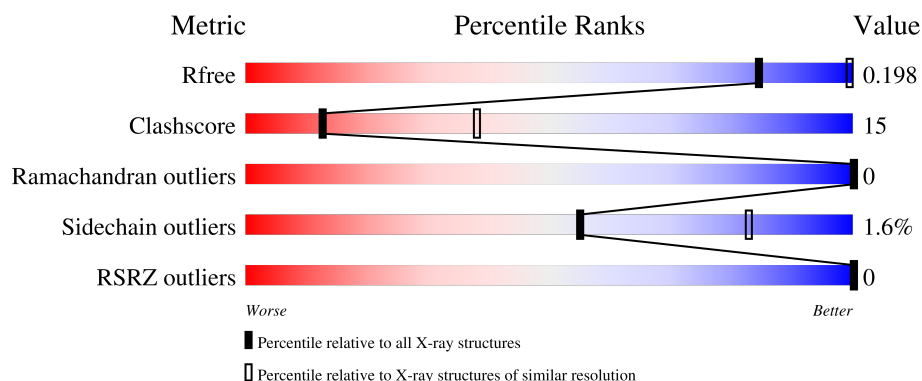
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	351	
1	B	351	
1	C	351	

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	407	-	X	-	-
4	GLY	A	416	-	X	-	-
4	GLY	C	407	-	X	-	-
4	GLY	C	408	-	-	X	-
4	GLY	C	409	-	X	-	-
4	GLY	C	410	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7164 atoms, of which 350 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	H	N	O	S	0	0	0
			2155	1343	5	393	403	11			
1	B	278	Total	C	H	N	O	S	0	0	0
			2158	1343	8	393	403	11			
1	C	278	Total	C	H	N	O	S	0	0	0
			2229	1343	79	393	403	11			

There are 30 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	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	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
C	290	ASN	VAL	engineered mutation	UNP Q9XAL8
C	344	LEU	-	expression tag	UNP Q9XAL8

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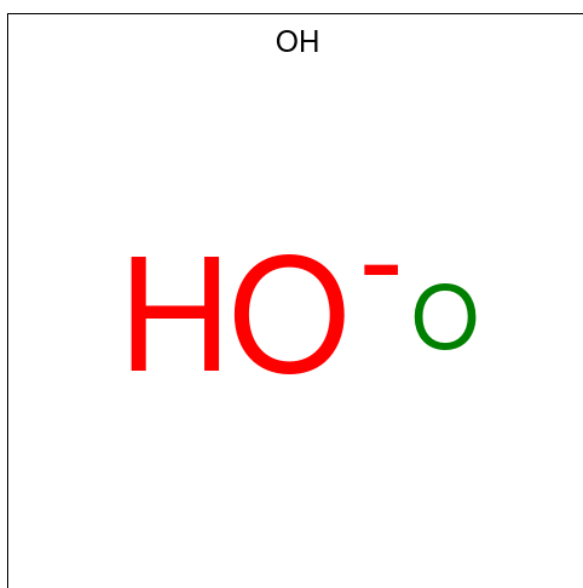
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Chain	Residue	Modelled	Actual	Comment	Reference
C	345	GLU	-	expression tag	UNP Q9XAL8
C	346	HIS	-	expression tag	UNP Q9XAL8
C	347	HIS	-	expression tag	UNP Q9XAL8
C	348	HIS	-	expression tag	UNP Q9XAL8
C	349	HIS	-	expression tag	UNP Q9XAL8
C	350	HIS	-	expression tag	UNP Q9XAL8
C	351	HIS	-	expression tag	UNP Q9XAL8

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

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

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



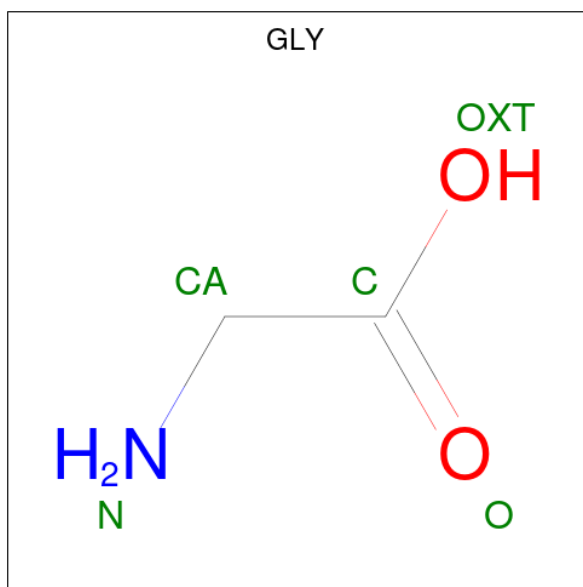
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



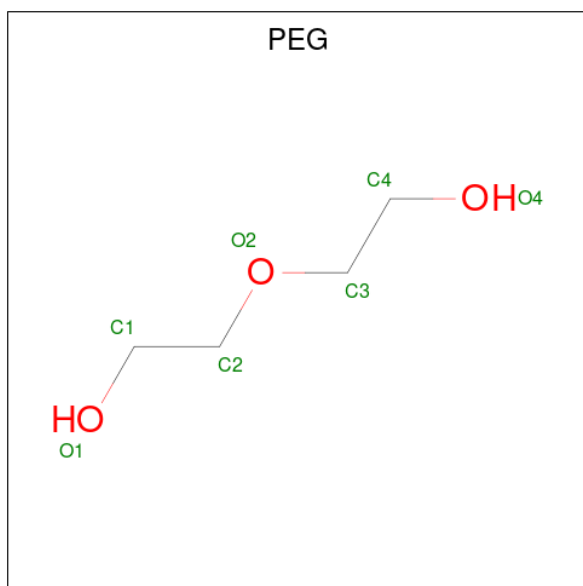
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N O 10 2 5 1 2	0	0
4	A	1	Total C H N O 10 2 5 1 2	0	0
4	A	1	Total C H N O 10 2 5 1 2	0	0
4	A	1	Total C H N O 10 2 5 1 2	0	0
4	A	1	Total C H N O 10 2 5 1 2	0	0
4	A	1	Total C H N O 10 2 5 1 2	0	0
4	B	1	Total C H N O 10 2 5 1 2	0	0
4	B	1	Total C H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

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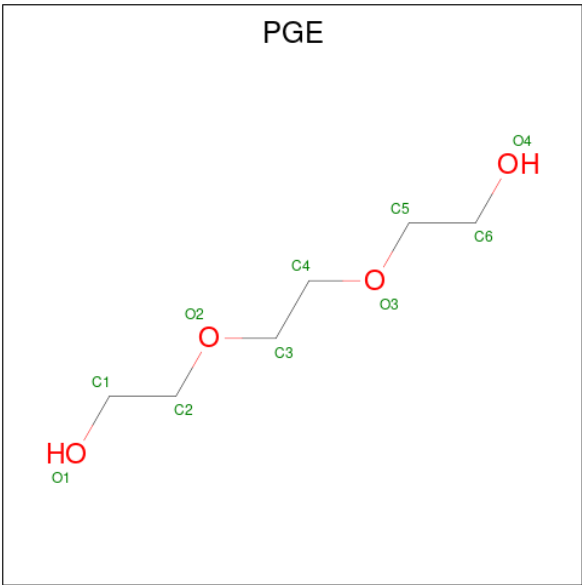
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



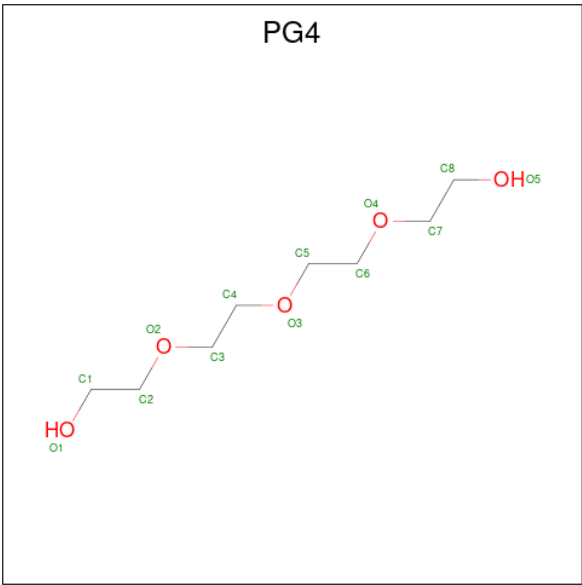
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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 (CCD ID: PG4) (formula: C₈H₁₈O₅).



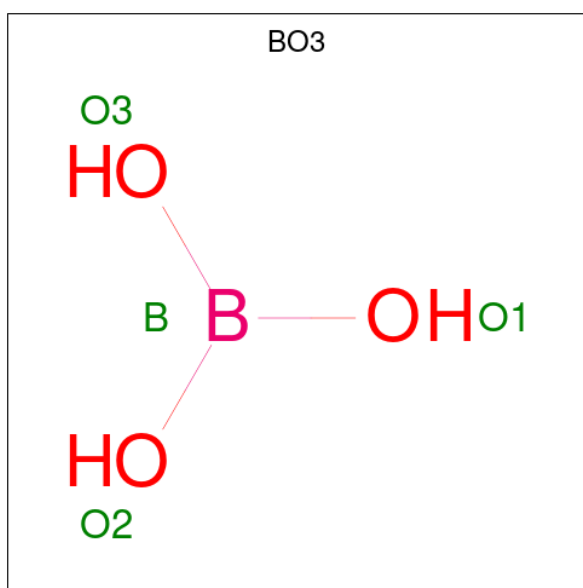
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			31	8	18	5		

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

- Molecule 8 is BORIC ACID (CCD ID: BO3) (formula: BH_3O_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	B	H	O	0	0
			7	1	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	46	Total	O	0	0
			46	46		
9	B	41	Total	O	0	0
			41	41		
9	C	54	Total	O	0	0
			54	54		

ALA	V222	T94
LYS	M223	T95
SER	I224	D96
GLY		T97
GLU	T232	R98
SER		A99
GLY	A241	
GLU	G246	G105
PRO	I247	L106
THR	L248	D107
GLY	T249	Y108
GLY	G250	I110
ALA	D251	S111
ALA	D252	S112
HIS	D253	D113
GLU	P254	G114
HIS	S255	T115
GLU	R256	A116
HIS		M117
LEU	N260	N118
GLU	K261	
HIS	I262	D121
HIS	T263	
HIS	G264	P124
HIS		
HIS	D267	R128
HIS	S268	T129
HIS	F269	
	A281	H135
	M285	D142
	Y286	
	H287	Y152
	C288	M153
		H154
		Y155
	S292	
		V159
	M296	
	G297	M171
	M298	G172
	V299	L173
	G300	Y174
		G175
	V304	
	K305	I193
		V194
	I311	M202
		R203
GLU	Y314	K204
PRO		P205
HIS		H206
GLU		T207
HIS		G208
GLY		P209
GLY		D210
ALA		
THR		T211

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.99Å 176.99Å 176.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.15 – 2.90 79.15 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (79.15-2.90) 92.9 (79.15-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.166 , 0.198 0.166 , 0.198	Depositor DCC
R_{free} test set	4051 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.457 for -h,-l,-k 0.457 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7164	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: PGE, PEG, BO3, CU, PG4, 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	0.37	0/2212	0.58	0/3001
1	B	0.37	0/2212	0.59	0/3001
1	C	0.37	0/2212	0.58	0/3001
All	All	0.37	0/6636	0.58	0/9003

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	2150	5	2032	72	0
1	B	2150	8	2032	70	0
1	C	2150	79	2032	65	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	30	30	12	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	20	8	4	0
4	C	25	25	10	6	0
5	A	7	10	10	0	0
5	B	7	10	10	1	0
5	C	7	10	10	0	0
6	A	10	14	14	1	0
6	B	10	14	14	3	0
6	C	10	14	14	0	0
7	A	26	36	36	5	0
7	B	26	36	36	3	0
7	C	26	36	36	2	0
8	A	4	3	3	0	0
9	A	46	0	0	2	0
9	B	41	0	0	4	0
9	C	54	0	0	0	0
All	All	6814	350	6309	197	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 15.

All (197) 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:63:MET:HE2	1:C:95:MET:SD	1.97	1.04
1:B:247:ILE:HD11	1:B:272:GLN:HB2	1.50	0.94
1:B:49:ARG:HD3	7:B:412:PG4:H52	1.62	0.82
1:B:305:LYS:HG2	1:B:311:ILE:CD1	2.10	0.81
1:B:305:LYS:HG2	1:B:311:ILE:HD11	1.63	0.81
1:A:308:ASP:HB2	1:A:310:THR:OG1	1.81	0.81
1:B:249:THR:HG23	1:B:253:ASP:OD2	1.83	0.78
1:C:121:ASP:HB3	1:C:159:VAL:HG11	1.67	0.77
1:C:53:MET:HE3	1:C:89:ILE:HG21	1.65	0.76
1:A:256:ARG:HD2	4:C:408:GLY:OXT	1.88	0.74
1:A:121:ASP:HB3	1:A:159:VAL:HG11	1.69	0.73
1:C:249:THR:HG23	1:C:253:ASP:OD2	1.91	0.70
1:A:210:ASP:H	7:A:414:PG4:H82	1.57	0.70
1:B:53:MET:HE3	1:B:89:ILE:HG21	1.73	0.69
1:C:292:SER:HB2	1:C:296:MET:HE3	1.72	0.69
1:B:146:ARG:HD2	6:B:411:PGE:H3	1.73	0.69
1:A:247:ILE:HD11	1:A:272:GLN:HB2	1.73	0.69
1:C:292:SER:HB2	1:C:296:MET:CE	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:H	7:A:413:PG4:H31	1.59	0.67
1:A:249:THR:HG23	1:A:253:ASP:OD2	1.94	0.67
1:A:264:GLY:O	1:A:267:ASP:HB2	1.94	0.67
1:A:198:MET:HA	1:A:198:MET:HE3	1.76	0.66
1:A:235:MET:HE1	1:A:273:ILE:CD1	2.26	0.66
1:B:145:TRP:CH2	1:C:251:PRO:HG3	2.32	0.64
1:B:235:MET:HE1	1:B:271:PHE:HZ	1.62	0.64
4:B:407:GLY:OXT	1:C:256:ARG:HD3	1.97	0.64
1:B:62:GLN:HE22	5:B:410:PEG:H22	1.62	0.63
1:A:274:ILE:HB	1:A:277:GLU:HB2	1.81	0.62
1:C:203:ARG:HD3	1:C:209:PRO:HD3	1.81	0.61
1:B:53:MET:HE3	1:B:89:ILE:CG2	2.31	0.61
1:A:193:ILE:HD12	1:A:221:ILE:HG23	1.83	0.61
1:C:241:ALA:O	1:C:246:GLY:HA2	1.99	0.61
1:B:305:LYS:CG	1:B:311:ILE:HD11	2.31	0.60
1:B:63:MET:HE2	1:B:95:MET:SD	2.42	0.60
4:A:408:GLY:OXT	1:B:256:ARG:HD3	2.02	0.60
1:A:198:MET:HE1	1:A:293:HIS:CG	2.37	0.59
1:A:49:ARG:HB3	7:A:413:PG4:H61	1.85	0.59
1:B:247:ILE:CD1	1:B:272:GLN:HB2	2.30	0.59
1:A:145:TRP:CH2	1:B:251:PRO:HG3	2.38	0.59
1:B:305:LYS:HG2	1:B:311:ILE:HD12	1.84	0.58
1:B:241:ALA:O	1:B:246:GLY:HA2	2.04	0.58
1:A:235:MET:HE1	1:A:273:ILE:HD11	1.86	0.58
1:B:72:ALA:H	4:B:409:GLY:N	2.00	0.58
1:A:241:ALA:O	1:A:246:GLY:HA2	2.04	0.57
1:B:121:ASP:HB3	1:B:159:VAL:HG11	1.86	0.57
1:C:253:ASP:OD1	1:C:255:SER:OG	2.18	0.57
1:B:242:ASP:OD1	1:C:256:ARG:NH2	2.37	0.57
1:A:203:ARG:HD3	1:A:209:PRO:HD3	1.87	0.56
1:A:269:PHE:HB2	9:A:535:HOH:O	2.04	0.56
1:C:152:TYR:O	4:C:408:GLY:HA2	2.05	0.56
1:B:232:THR:O	1:B:288:CYS:HA	2.06	0.56
1:C:128:ARG:HG2	1:C:129:THR:N	2.21	0.55
1:C:206:HIS:CD2	1:C:297:GLY:HA2	2.42	0.54
1:A:78:LEU:HD12	1:A:176:PRO:HG2	1.89	0.54
1:C:205:PRO:O	1:C:207:THR:HG23	2.07	0.54
1:B:57:LYS:HE3	1:B:96:ASP:OD1	2.08	0.54
1:B:71:LYS:NZ	9:B:501:HOH:O	2.40	0.54
1:C:264:GLY:O	1:C:267:ASP:HB2	2.07	0.54
1:C:105:GLY:HA3	1:C:153:TRP:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HD2	6:A:412:PGE:H42	1.90	0.54
1:A:108:TYR:HE2	1:A:113:ASP:CB	2.21	0.53
1:A:139:ARG:HD2	1:A:143:GLY:O	2.08	0.53
1:B:193:ILE:HD12	1:B:221:ILE:HG23	1.91	0.53
1:B:235:MET:HE1	1:B:271:PHE:CZ	2.42	0.53
1:A:105:GLY:HA3	1:A:153:TRP:CD2	2.44	0.52
1:A:194:VAL:HA	1:A:224:ILE:O	2.10	0.52
1:A:198:MET:HE2	1:A:296:MET:HE2	1.90	0.52
1:B:264:GLY:O	1:B:267:ASP:HB2	2.09	0.52
1:B:205:PRO:O	1:B:207:THR:HG23	2.10	0.52
1:C:223:MET:HB3	1:C:269:PHE:CE1	2.45	0.52
1:C:62:GLN:HG2	1:C:171:ASN:O	2.09	0.52
1:A:49:ARG:HB3	7:A:413:PG4:H72	1.92	0.51
1:C:193:ILE:HD12	1:C:221:ILE:HG23	1.91	0.51
1:A:286:TYR:CE1	1:A:300:GLY:HA3	2.44	0.51
1:C:95:MET:O	1:C:124:PRO:HB3	2.10	0.51
1:B:274:ILE:HB	1:B:277:GLU:HB2	1.93	0.51
1:C:49:ARG:NH1	1:C:85:ASP:OD2	2.44	0.51
1:A:38:THR:O	1:A:38:THR:OG1	2.27	0.50
1:A:313:GLY:O	1:A:314:TYR:C	2.54	0.50
1:B:147:PRO:HB3	1:C:248:LEU:CD1	2.42	0.50
1:B:194:VAL:HG22	1:B:224:ILE:HB	1.92	0.50
1:A:256:ARG:HG2	1:A:258:ILE:CG2	2.42	0.49
1:B:105:GLY:HA3	1:B:153:TRP:CD2	2.47	0.49
1:A:108:TYR:HE2	1:A:113:ASP:HB2	1.76	0.49
1:C:155:TYR:CZ	1:C:175:GLY:HA3	2.48	0.48
1:B:194:VAL:HA	1:B:224:ILE:O	2.14	0.48
1:B:285:MET:HG3	9:B:508:HOH:O	2.14	0.48
1:B:146:ARG:HH11	6:B:411:PGE:H3	1.79	0.48
1:C:93:ASN:OD1	1:C:95:MET:HB2	2.13	0.47
1:A:157:ASP:OD2	1:A:160:VAL:HB	2.14	0.47
1:A:204:LYS:O	1:A:207:THR:HG23	2.14	0.47
1:A:180:ARG:HD3	4:A:407:GLY:OXT	2.14	0.47
1:B:286:TYR:CE1	1:B:300:GLY:HA3	2.49	0.47
1:C:99:ALA:HA	1:C:159:VAL:CG2	2.45	0.47
1:A:256:ARG:CD	4:C:408:GLY:OXT	2.59	0.47
1:B:80:GLU:H	7:B:412:PG4:H31	1.79	0.47
1:B:206:HIS:CD2	1:B:297:GLY:HA2	2.50	0.47
1:B:210:ASP:OD2	7:B:413:PG4:H51	2.15	0.47
1:C:53:MET:HE3	1:C:89:ILE:CG2	2.39	0.47
1:B:53:MET:HE1	1:B:89:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASP:OD1	1:B:255:SER:OG	2.13	0.46
1:C:99:ALA:HA	1:C:159:VAL:HG22	1.97	0.46
1:B:62:GLN:HB3	1:B:171:ASN:O	2.15	0.46
9:B:521:HOH:O	1:C:285:MET:HG3	2.16	0.46
1:A:117:MET:HE3	1:A:117:MET:HB2	1.80	0.46
1:A:288:CYS:O	1:A:294:SER:HB3	2.16	0.46
1:A:109:GLU:HG3	1:A:133:ARG:HH21	1.81	0.46
1:A:256:ARG:HG2	1:A:258:ILE:HG23	1.98	0.46
1:A:223:MET:HB3	1:A:269:PHE:CE1	2.51	0.46
1:A:105:GLY:HA3	1:A:153:TRP:CE3	2.51	0.45
4:B:407:GLY:OXT	1:C:256:ARG:CD	2.63	0.45
1:C:117:MET:HE2	1:C:117:MET:HB3	1.85	0.45
1:C:210:ASP:H	7:C:414:PG4:H71	1.80	0.45
1:C:194:VAL:HA	1:C:224:ILE:O	2.16	0.45
1:A:262:ILE:H	4:A:406:GLY:N	2.14	0.45
1:B:86:THR:HG23	1:B:133:ARG:HG2	1.98	0.45
1:A:108:TYR:CE2	1:A:113:ASP:CB	3.00	0.45
1:C:262:ILE:H	4:C:406:GLY:N	2.15	0.45
1:B:204:LYS:O	1:B:207:THR:HG23	2.17	0.45
1:A:232:THR:O	1:A:288:CYS:HA	2.17	0.45
1:A:95:MET:O	1:A:124:PRO:HB3	2.17	0.44
1:B:108:TYR:HE1	1:B:113:ASP:CB	2.31	0.44
1:C:98:ARG:HE	1:C:121:ASP:CG	2.25	0.44
1:C:232:THR:O	1:C:288:CYS:HA	2.17	0.44
1:A:140:ARG:HD2	1:A:144:THR:OG1	2.16	0.44
1:B:119:LYS:HB2	1:B:119:LYS:HE2	1.88	0.44
1:C:65:TYR:CZ	1:C:173:LEU:HD22	2.53	0.44
1:A:285:MET:HE1	1:C:115:THR:HG21	1.98	0.44
1:B:54:TYR:O	1:B:65:TYR:HA	2.17	0.44
1:C:72:ALA:H	4:C:410:GLY:N	2.16	0.44
1:C:108:TYR:HE1	1:C:113:ASP:CB	2.30	0.44
1:C:305:LYS:HE2	1:C:305:LYS:HB2	1.81	0.44
1:C:107:ASP:OD2	1:C:135:HIS:ND1	2.34	0.44
1:B:281:ALA:HB1	1:B:304:VAL:O	2.18	0.44
1:C:50:HIS:H	7:C:413:PG4:H81	1.83	0.43
1:A:238:HIS:HA	9:A:515:HOH:O	2.19	0.43
1:B:108:TYR:CE1	1:B:113:ASP:CB	3.02	0.43
1:B:147:PRO:HB3	1:C:248:LEU:HD11	2.00	0.43
1:C:281:ALA:HB1	1:C:304:VAL:O	2.18	0.43
1:C:57:LYS:NZ	1:C:96:ASP:OD1	2.46	0.43
1:A:72:ALA:H	4:A:410:GLY:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:416:GLY:N	1:B:262:ILE:H	2.16	0.43
1:C:53:MET:CE	1:C:89:ILE:HG21	2.43	0.43
1:C:110:ILE:HD11	1:C:118:ASN:ND2	2.34	0.43
1:C:288:CYS:HB2	1:C:298:MET:HE2	2.00	0.43
1:A:108:TYR:CE2	1:A:113:ASP:HB2	2.53	0.43
1:A:281:ALA:HB1	1:A:304:VAL:O	2.19	0.43
1:A:235:MET:CE	1:A:273:ILE:CD1	2.95	0.43
1:C:105:GLY:HA3	1:C:153:TRP:CE3	2.54	0.43
4:A:408:GLY:OXT	1:B:256:ARG:CD	2.66	0.42
1:B:129:THR:O	1:B:129:THR:HG22	2.19	0.42
1:B:235:MET:HE2	1:B:235:MET:HB2	1.73	0.42
1:A:60:ASP:OD1	1:A:60:ASP:C	2.62	0.42
1:A:290:ASN:HB3	1:A:293:HIS:HB2	2.00	0.42
1:C:62:GLN:HE21	1:C:202:ASN:HD22	1.66	0.42
1:C:108:TYR:CE1	1:C:113:ASP:CB	3.03	0.42
1:A:145:TRP:CG	1:B:250:GLY:HA2	2.54	0.42
4:A:416:GLY:OXT	1:B:256:ARG:NH1	2.52	0.42
1:B:95:MET:O	1:B:124:PRO:HB3	2.18	0.42
1:B:155:TYR:CZ	1:B:175:GLY:HA3	2.54	0.42
1:A:249:THR:HG23	1:A:249:THR:H	1.58	0.42
1:B:69:LYS:NZ	9:B:506:HOH:O	2.52	0.42
1:B:145:TRP:CG	1:C:250:GLY:HA2	2.55	0.42
1:C:121:ASP:OD1	1:C:121:ASP:N	2.53	0.42
1:A:285:MET:HE3	1:A:285:MET:HB2	1.66	0.42
1:C:96:ASP:OD1	1:C:96:ASP:N	2.51	0.42
1:C:305:LYS:HG3	1:C:311:ILE:HD11	2.01	0.42
1:A:98:ARG:HE	1:A:121:ASP:CG	2.27	0.41
1:C:53:MET:HE1	1:C:89:ILE:HD13	2.02	0.41
1:A:200:ILE:O	1:A:203:ARG:HG3	2.20	0.41
1:B:53:MET:HE2	1:B:53:MET:HB2	1.74	0.41
1:B:67:PHE:CE2	1:B:77:PRO:HB2	2.56	0.41
1:B:200:ILE:O	1:B:203:ARG:HG3	2.21	0.41
1:C:286:TYR:CE2	1:C:300:GLY:HA3	2.55	0.41
1:A:155:TYR:CZ	1:A:175:GLY:HA3	2.56	0.41
1:A:305:LYS:HG2	1:A:311:ILE:HD11	2.03	0.41
1:B:142:ASP:HB2	1:C:39:ALA:HB2	2.02	0.41
1:A:230:TYR:CD1	1:A:230:TYR:N	2.89	0.41
1:A:49:ARG:HD3	7:A:413:PG4:H52	2.01	0.41
1:B:146:ARG:HH11	6:B:411:PGE:C3	2.34	0.41
1:A:38:THR:HG23	1:C:142:ASP:HA	2.03	0.41
1:A:99:ALA:HA	1:A:159:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:THR:HB	1:C:260:ASN:HD21	1.86	0.41
1:A:63:MET:HE2	1:A:95:MET:SD	2.61	0.41
1:A:87:LEU:HD23	1:A:89:ILE:HD11	2.03	0.41
1:B:206:HIS:NE2	1:B:297:GLY:HA2	2.36	0.41
1:C:62:GLN:NE2	1:C:202:ASN:HD22	2.18	0.41
1:B:180:ARG:HD3	4:B:406:GLY:OXT	2.21	0.41
1:A:214:THR:O	1:A:215:VAL:C	2.62	0.40
1:A:256:ARG:CG	4:C:408:GLY:OXT	2.69	0.40
1:A:67:PHE:CE2	1:A:77:PRO:HB2	2.57	0.40
1:B:311:ILE:CG2	1:B:314:TYR:HB2	2.51	0.40
1:A:49:ARG:HB2	1:A:87:LEU:HD12	2.02	0.40
1:B:230:TYR:CD1	1:B:230:TYR:N	2.89	0.40
1:C:194:VAL:HG22	1:C:224:ILE:HB	2.03	0.40
1:B:190:THR:HG23	1:B:220:GLU:HG2	2.04	0.40
1:C:54:TYR:O	1:C:65:TYR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	276/351 (79%)	259 (94%)	17 (6%)	0	100	100
1	B	276/351 (79%)	261 (95%)	15 (5%)	0	100	100
1	C	276/351 (79%)	263 (95%)	13 (5%)	0	100	100
All	All	828/1053 (79%)	783 (95%)	45 (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%)	218 (98%)	5 (2%)	45	77
1	B	223/270 (83%)	219 (98%)	4 (2%)	51	80
1	C	223/270 (83%)	221 (99%)	2 (1%)	70	90
All	All	669/810 (83%)	658 (98%)	11 (2%)	55	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	78	LEU
1	A	111	SER
1	A	249	THR
1	A	310	THR
1	B	38	THR
1	B	111	SER
1	B	113	ASP
1	B	214	THR
1	C	111	SER
1	C	113	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	A	226	HIS
1	B	62	GLN
1	B	82	ASN
1	B	118	ASN
1	B	164	HIS
1	B	291	GLN
1	C	62	GLN
1	C	82	ASN
1	C	171	ASN

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Mol	Chain	Res	Type
1	C	196	ASN
1	C	226	HIS
1	C	291	GLN
1	C	293	HIS

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 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	$\# Z > 2$
6	PGE	A	412	-	9,9,9	0.41	0	8,8,8	0.36	0
5	PEG	A	411	-	6,6,6	0.24	0	5,5,5	0.13	0
7	PG4	B	412	-	12,12,12	0.23	0	11,11,11	0.54	0
7	PG4	C	413	-	12,12,12	0.24	0	11,11,11	0.70	0
5	PEG	C	411	-	6,6,6	0.28	0	5,5,5	0.11	0
4	GLY	B	408	-	4,4,4	1.01	0	3,4,4	1.57	1 (33%)
7	PG4	C	414	-	12,12,12	0.22	0	11,11,11	0.70	1 (9%)
4	GLY	A	406	-	4,4,4	1.18	1 (25%)	3,4,4	1.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLY	C	410	-	4,4,4	1.04	1 (25%)	3,4,4	1.82	2 (66%)
4	GLY	B	407	-	4,4,4	1.01	0	3,4,4	2.10	2 (66%)
4	GLY	C	409	-	4,4,4	1.08	1 (25%)	3,4,4	1.97	2 (66%)
7	PG4	A	413	-	12,12,12	0.25	0	11,11,11	0.70	0
6	PGE	C	412	-	9,9,9	0.38	0	8,8,8	0.36	0
4	GLY	C	407	-	4,4,4	0.90	0	3,4,4	1.90	2 (66%)
7	PG4	A	414	-	12,12,12	0.28	0	11,11,11	0.74	0
4	GLY	C	408	-	4,4,4	1.21	1 (25%)	3,4,4	1.79	1 (33%)
4	GLY	B	409	-	4,4,4	1.10	1 (25%)	3,4,4	1.60	0
6	PGE	B	411	-	9,9,9	0.48	0	8,8,8	0.52	0
4	GLY	A	409	-	4,4,4	1.05	0	3,4,4	1.77	1 (33%)
4	GLY	C	406	-	4,4,4	1.17	1 (25%)	3,4,4	1.37	0
4	GLY	A	407	-	4,4,4	1.17	1 (25%)	3,4,4	1.84	2 (66%)
8	BO3	A	415	-	3,3,3	0.59	0	3,3,3	1.24	0
4	GLY	A	410	-	4,4,4	1.11	1 (25%)	3,4,4	1.56	0
4	GLY	B	406	-	4,4,4	1.01	0	3,4,4	1.86	2 (66%)
4	GLY	A	416	-	4,4,4	1.07	1 (25%)	3,4,4	1.70	1 (33%)
4	GLY	A	408	-	4,4,4	1.05	0	3,4,4	1.75	2 (66%)
5	PEG	B	410	-	6,6,6	0.24	0	5,5,5	0.11	0
7	PG4	B	413	-	12,12,12	0.23	0	11,11,11	0.78	1 (9%)

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
6	PGE	A	412	-	-	4/7/7/7	-
5	PEG	A	411	-	-	3/4/4/4	-
7	PG4	B	412	-	-	2/10/10/10	-
7	PG4	C	413	-	-	5/10/10/10	-
5	PEG	C	411	-	-	3/4/4/4	-
4	GLY	B	408	-	-	2/2/2/2	-
7	PG4	C	414	-	-	6/10/10/10	-
4	GLY	A	406	-	-	0/2/2/2	-
4	GLY	C	410	-	-	2/2/2/2	-
4	GLY	B	407	-	-	1/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLY	C	409	-	-	1/2/2/2	-
7	PG4	A	413	-	-	6/10/10/10	-
6	PGE	C	412	-	-	3/7/7/7	-
4	GLY	C	407	-	-	2/2/2/2	-
7	PG4	A	414	-	-	9/10/10/10	-
4	GLY	C	408	-	-	1/2/2/2	-
4	GLY	B	409	-	-	2/2/2/2	-
6	PGE	B	411	-	-	4/7/7/7	-
4	GLY	A	409	-	-	2/2/2/2	-
4	GLY	C	406	-	-	2/2/2/2	-
4	GLY	A	407	-	-	2/2/2/2	-
4	GLY	A	410	-	-	2/2/2/2	-
4	GLY	B	406	-	-	0/2/2/2	-
4	GLY	A	416	-	-	2/2/2/2	-
4	GLY	A	408	-	-	0/2/2/2	-
5	PEG	B	410	-	-	3/4/4/4	-
7	PG4	B	413	-	-	6/10/10/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	408	GLY	OXT-C	-2.31	1.23	1.30
4	A	406	GLY	OXT-C	-2.18	1.23	1.30
4	C	406	GLY	OXT-C	-2.17	1.23	1.30
4	A	407	GLY	OXT-C	-2.14	1.23	1.30
4	A	410	GLY	OXT-C	-2.07	1.24	1.30
4	C	409	GLY	OXT-C	-2.07	1.24	1.30
4	B	409	GLY	OXT-C	-2.06	1.24	1.30
4	A	416	GLY	OXT-C	-2.04	1.24	1.30
4	C	410	GLY	OXT-C	-2.01	1.24	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	407	GLY	OXT-C-CA	2.55	123.53	113.38
4	B	407	GLY	OXT-C-O	-2.50	116.91	123.33
4	B	406	GLY	OXT-C-O	-2.50	116.91	123.33
4	A	407	GLY	OXT-C-O	-2.47	116.98	123.33
4	C	408	GLY	OXT-C-O	-2.47	116.99	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	409	GLY	OXT-C-CA	2.42	122.99	113.38
4	C	407	GLY	OXT-C-O	-2.35	117.28	123.33
4	C	409	GLY	OXT-C-O	-2.33	117.34	123.33
4	A	409	GLY	OXT-C-CA	2.30	122.54	113.38
4	C	407	GLY	OXT-C-CA	2.26	122.36	113.38
4	C	410	GLY	OXT-C-CA	2.25	122.31	113.38
4	A	408	GLY	OXT-C-CA	2.19	122.09	113.38
4	A	416	GLY	OXT-C-O	-2.18	117.72	123.33
4	C	410	GLY	OXT-C-O	-2.11	117.90	123.33
7	B	413	PG4	C5-O3-C4	-2.10	104.06	113.26
4	B	408	GLY	OXT-C-CA	2.03	121.46	113.38
4	B	406	GLY	OXT-C-CA	2.02	121.41	113.38
7	C	414	PG4	C5-O3-C4	-2.02	104.42	113.26
4	A	408	GLY	OXT-C-O	-2.01	118.15	123.33
4	A	407	GLY	OXT-C-CA	2.01	121.36	113.38

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	409	GLY	O-C-CA-N
4	A	410	GLY	O-C-CA-N
4	A	410	GLY	OXT-C-CA-N
4	B	408	GLY	O-C-CA-N
4	B	409	GLY	O-C-CA-N
4	B	409	GLY	OXT-C-CA-N
4	C	407	GLY	O-C-CA-N
4	C	410	GLY	O-C-CA-N
4	C	410	GLY	OXT-C-CA-N
4	A	407	GLY	O-C-CA-N
6	A	412	PGE	O2-C3-C4-O3
7	C	413	PG4	O2-C3-C4-O3
4	A	409	GLY	OXT-C-CA-N
4	C	407	GLY	OXT-C-CA-N
6	B	411	PGE	O2-C3-C4-O3
6	C	412	PGE	O1-C1-C2-O2
7	C	413	PG4	O1-C1-C2-O2
7	B	413	PG4	O3-C5-C6-O4
7	B	413	PG4	O2-C3-C4-O3
7	C	414	PG4	O2-C3-C4-O3
4	A	407	GLY	OXT-C-CA-N
4	B	408	GLY	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
5	B	410	PEG	O1-C1-C2-O2
5	C	411	PEG	O2-C3-C4-O4
7	A	414	PG4	O2-C3-C4-O3
5	A	411	PEG	O2-C3-C4-O4
5	C	411	PEG	O1-C1-C2-O2
6	B	411	PGE	O3-C5-C6-O4
7	A	414	PG4	O4-C7-C8-O5
7	C	414	PG4	O4-C7-C8-O5
7	A	413	PG4	O3-C5-C6-O4
7	B	413	PG4	O1-C1-C2-O2
7	A	414	PG4	O1-C1-C2-O2
6	A	412	PGE	O3-C5-C6-O4
4	A	416	GLY	OXT-C-CA-N
7	A	413	PG4	O1-C1-C2-O2
7	B	413	PG4	C5-C6-O4-C7
7	A	413	PG4	C5-C6-O4-C7
6	A	412	PGE	C1-C2-O2-C3
4	C	406	GLY	O-C-CA-N
7	B	413	PG4	C6-C5-O3-C4
7	A	414	PG4	C1-C2-O2-C3
5	B	410	PEG	O2-C3-C4-O4
6	C	412	PGE	C4-C3-O2-C2
7	A	413	PG4	C3-C4-O3-C5
6	B	411	PGE	C4-C3-O2-C2
7	C	414	PG4	C3-C4-O3-C5
5	A	411	PEG	C1-C2-O2-C3
5	B	410	PEG	C1-C2-O2-C3
7	A	414	PG4	C5-C6-O4-C7
7	C	414	PG4	C1-C2-O2-C3
5	A	411	PEG	C4-C3-O2-C2
7	B	412	PG4	C4-C3-O2-C2
6	A	412	PGE	C3-C4-O3-C5
7	C	413	PG4	O4-C7-C8-O5
7	A	414	PG4	C4-C3-O2-C2
7	C	414	PG4	O3-C5-C6-O4
7	A	414	PG4	C8-C7-O4-C6
7	A	414	PG4	C3-C4-O3-C5
4	A	416	GLY	O-C-CA-N
7	A	414	PG4	O3-C5-C6-O4
4	C	406	GLY	OXT-C-CA-N
7	B	413	PG4	C3-C4-O3-C5
7	A	413	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	C	408	GLY	O-C-CA-N
7	C	414	PG4	C5-C6-O4-C7
6	B	411	PGE	C6-C5-O3-C4
6	C	412	PGE	O3-C5-C6-O4
5	C	411	PEG	C4-C3-O2-C2
7	C	413	PG4	C4-C3-O2-C2
4	B	407	GLY	OXT-C-CA-N
4	C	409	GLY	OXT-C-CA-N
7	A	413	PG4	C8-C7-O4-C6
7	B	412	PG4	O3-C5-C6-O4
7	C	413	PG4	O3-C5-C6-O4

There are no ring outliers.

20 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	412	PGE	1	0
7	B	412	PG4	2	0
7	C	413	PG4	1	0
7	C	414	PG4	1	0
4	A	406	GLY	1	0
4	C	410	GLY	1	0
4	B	407	GLY	2	0
7	A	413	PG4	4	0
7	A	414	PG4	1	0
4	C	408	GLY	4	0
4	B	409	GLY	1	0
6	B	411	PGE	3	0
4	C	406	GLY	1	0
4	A	407	GLY	1	0
4	A	410	GLY	1	0
4	B	406	GLY	1	0
4	A	416	GLY	2	0
4	A	408	GLY	2	0
5	B	410	PEG	1	0
7	B	413	PG4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.69	0 100 100	38, 53, 73, 90	0
1	B	278/351 (79%)	-1.65	0 100 100	38, 53, 71, 89	0
1	C	278/351 (79%)	-1.66	0 100 100	40, 53, 74, 102	0
All	All	834/1053 (79%)	-1.67	0 100 100	38, 53, 73, 102	0

There are no RSRZ outliers to report.

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
4	GLY	A	406	5/5	0.99	0.04	57,68,73,92	0
4	GLY	A	409	5/5	0.99	0.07	72,86,88,88	0
4	GLY	B	407	5/5	0.99	0.06	65,78,88,93	0
4	GLY	B	408	5/5	0.99	0.05	69,82,97,97	0
4	GLY	B	409	5/5	0.99	0.04	64,76,91,95	0

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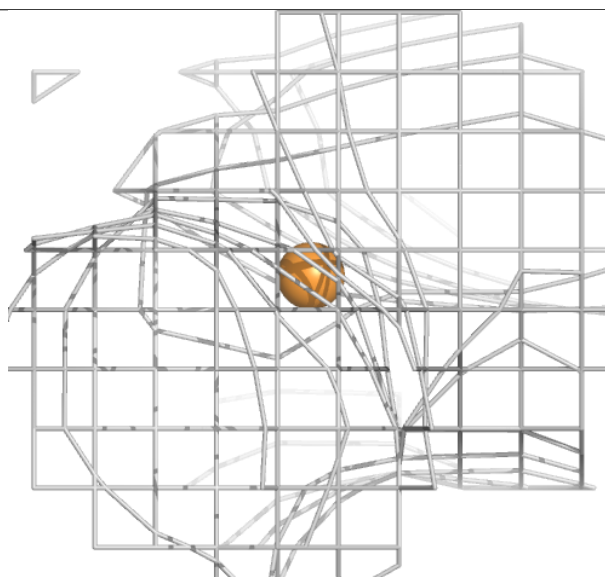
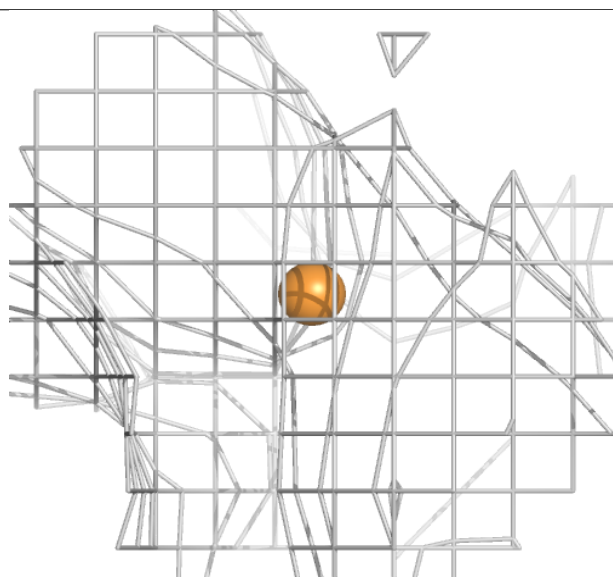
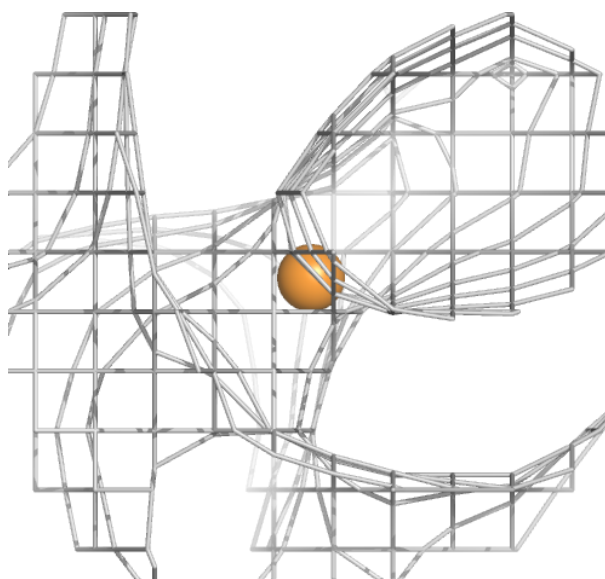
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GLY	C	406	5/5	0.99	0.05	58,70,81,86	0
4	GLY	C	409	5/5	0.99	0.06	68,85,86,87	0
5	PEG	A	411	7/7	0.99	0.05	80,100,121,121	0
5	PEG	B	410	7/7	0.99	0.06	75,101,121,121	0
5	PEG	C	411	7/7	0.99	0.05	74,106,134,134	0
6	PGE	A	412	10/10	0.99	0.06	74,99,113,121	0
6	PGE	B	411	10/10	0.99	0.05	70,89,113,116	0
6	PGE	C	412	10/10	0.99	0.05	65,93,112,113	0
7	PG4	A	413	13/13	0.99	0.05	59,93,115,121	0
7	PG4	A	414	13/13	0.99	0.04	77,100,120,127	0
7	PG4	B	412	13/13	0.99	0.05	70,93,114,118	0
7	PG4	B	413	13/13	0.99	0.06	81,107,129,129	0
7	PG4	C	413	13/13	0.99	0.06	65,97,116,123	0
7	PG4	C	414	13/13	0.99	0.06	82,105,122,136	0
4	GLY	A	410	5/5	1.00	0.03	64,77,85,86	0
4	GLY	A	416	5/5	1.00	0.05	52,63,75,84	0
4	GLY	B	406	5/5	1.00	0.03	57,68,73,77	0
2	CU	A	403	1/1	1.00	0.02	47,47,47,47	1
2	CU	A	404	1/1	1.00	0.01	55,55,55,55	1
2	CU	B	404	1/1	1.00	0.00	57,57,57,57	1
2	CU	B	403	1/1	1.00	0.02	47,47,47,47	1
4	GLY	C	407	5/5	1.00	0.03	53,68,82,82	0
4	GLY	C	408	5/5	1.00	0.04	70,84,91,91	0
2	CU	B	401	1/1	1.00	0.01	69,69,69,69	0
4	GLY	C	410	5/5	1.00	0.04	69,83,84,95	0
2	CU	B	402	1/1	1.00	0.01	77,77,77,77	1
2	CU	C	404	1/1	1.00	0.01	56,56,56,56	1
2	CU	C	401	1/1	1.00	0.01	66,66,66,66	0
2	CU	C	402	1/1	1.00	0.01	79,79,79,79	1
2	CU	C	403	1/1	1.00	0.03	48,48,48,48	1
3	OH	A	405	1/1	1.00	0.03	44,44,44,44	0
3	OH	B	405	1/1	1.00	0.04	43,43,43,43	0
3	OH	C	405	1/1	1.00	0.02	45,45,45,45	0
2	CU	A	401	1/1	1.00	0.01	65,65,65,65	0
4	GLY	A	407	5/5	1.00	0.04	52,66,80,80	0
4	GLY	A	408	5/5	1.00	0.05	68,82,87,90	0
2	CU	A	402	1/1	1.00	0.01	82,82,82,82	1
8	BO3	A	415	4/4	1.00	0.05	63,66,79,80	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.

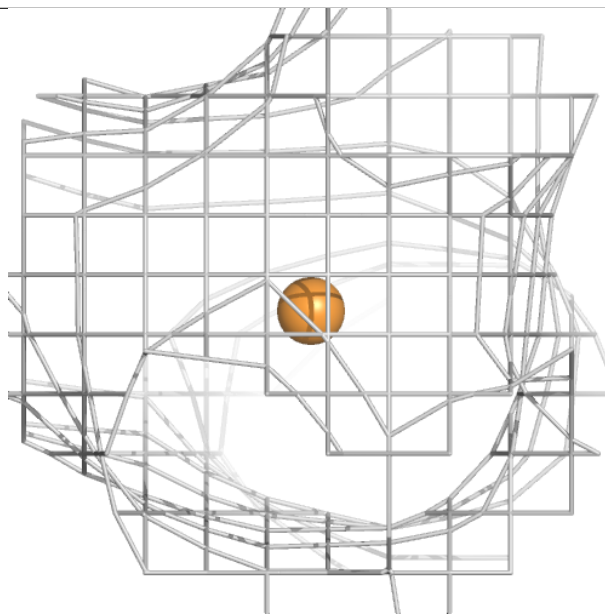
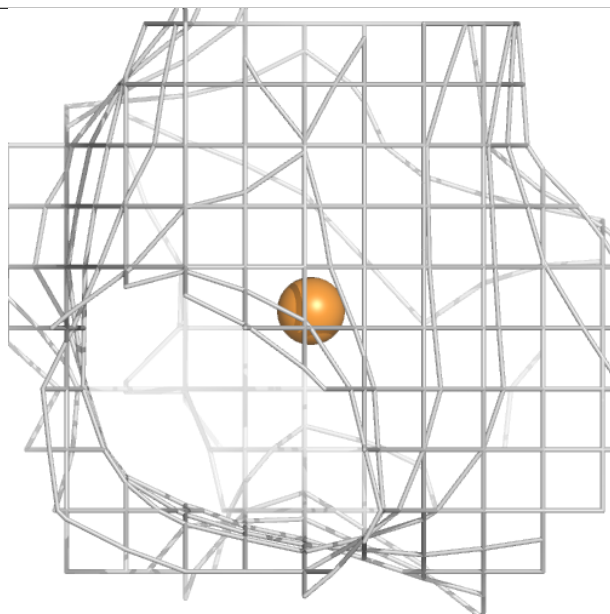
Electron density around CU A 403:

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



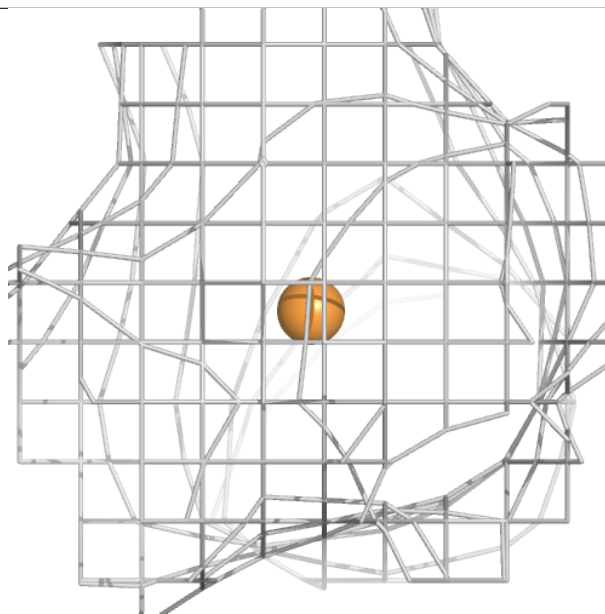
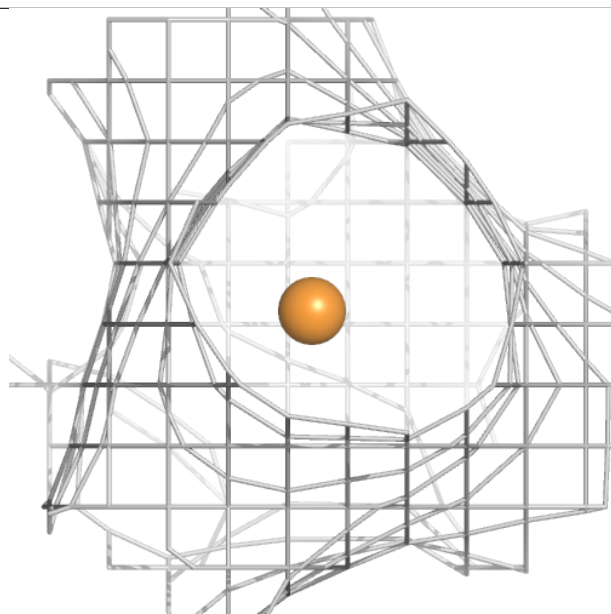
Electron density around CU A 404:

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and green (positive)



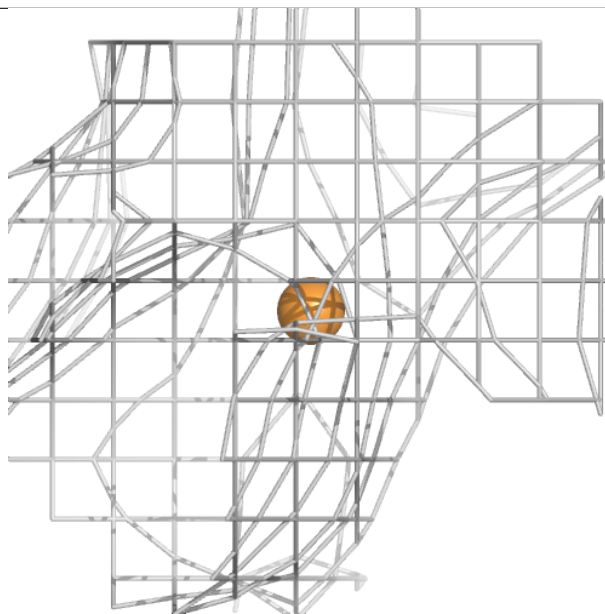
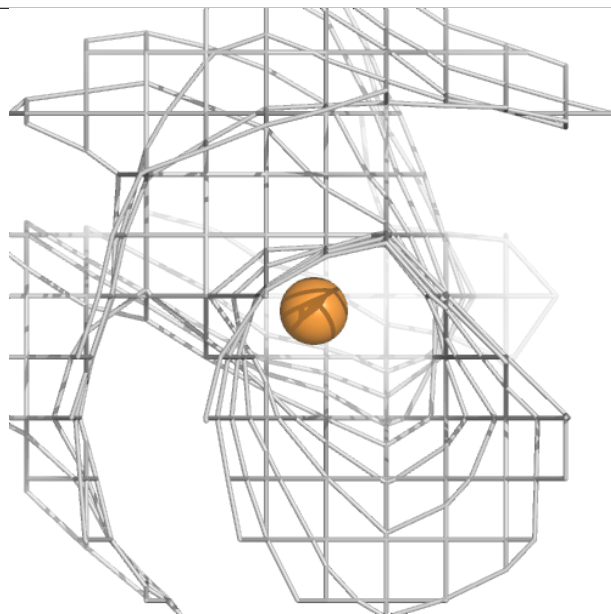
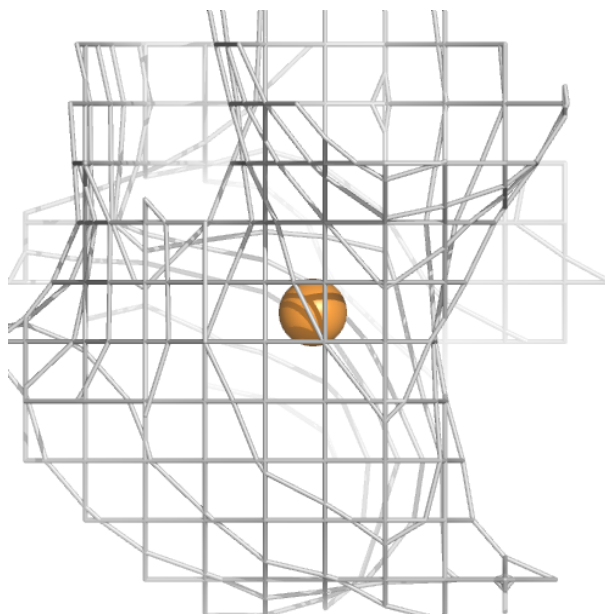
Electron density around CU B 404:

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



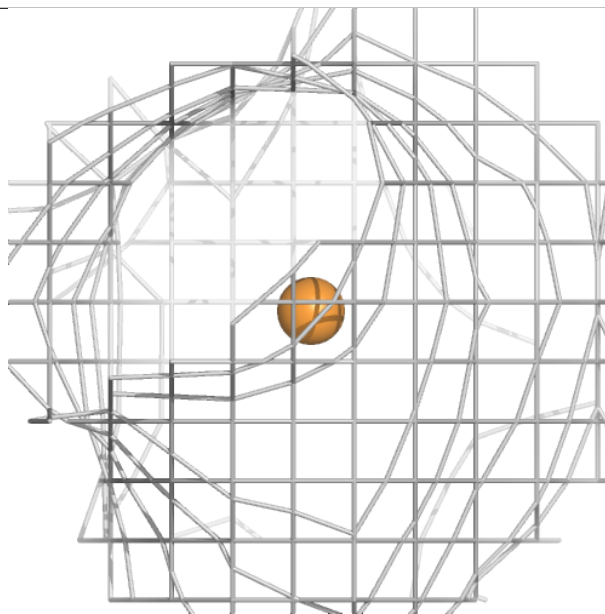
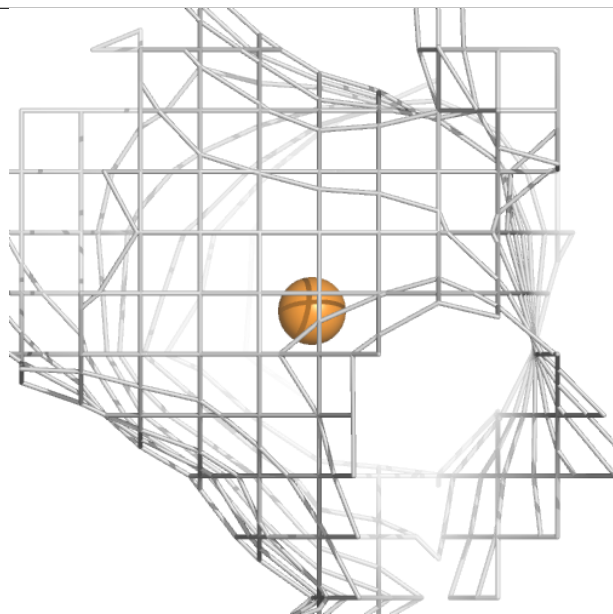
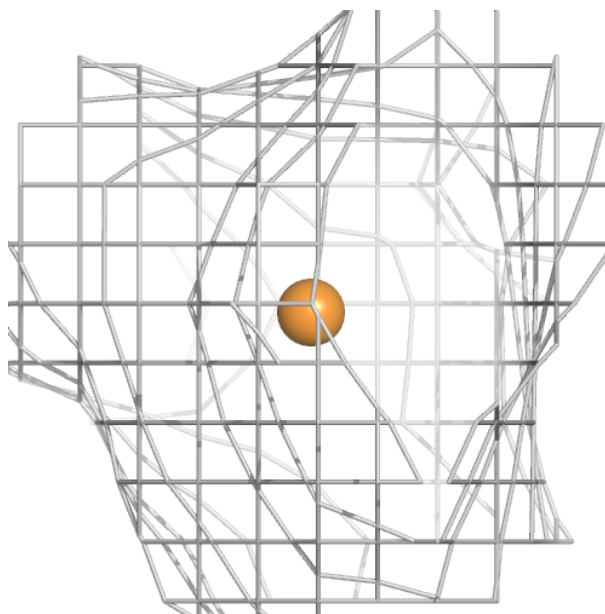
Electron density around CU B 403:

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



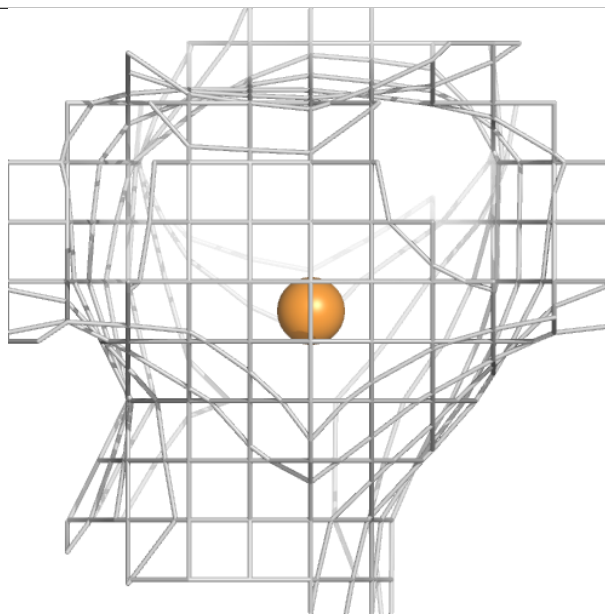
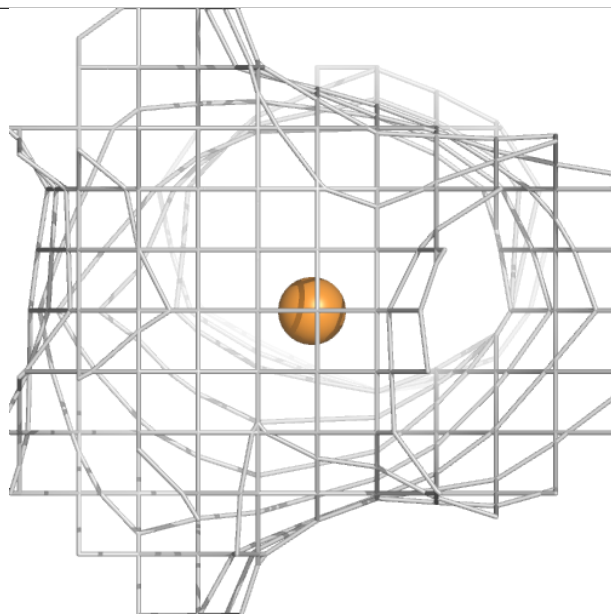
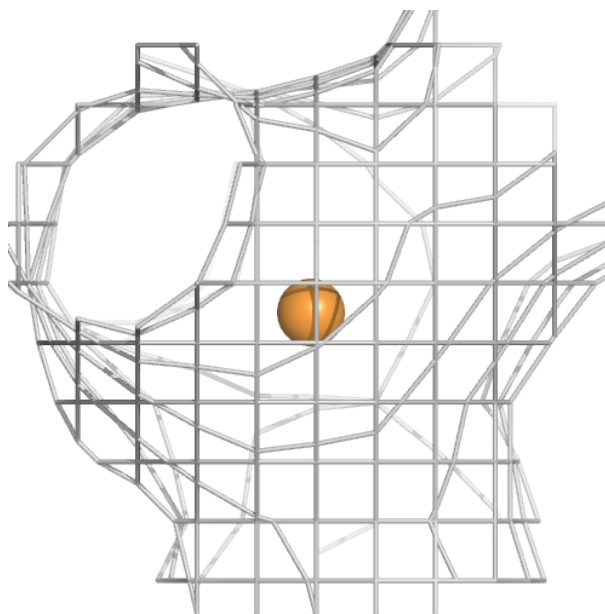
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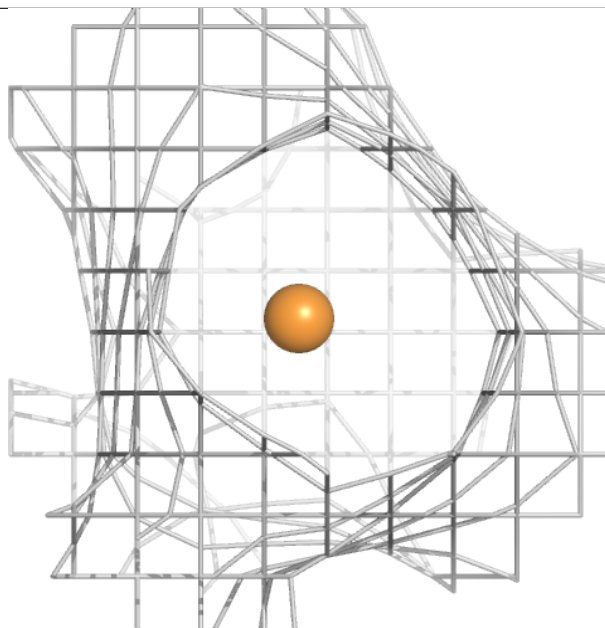
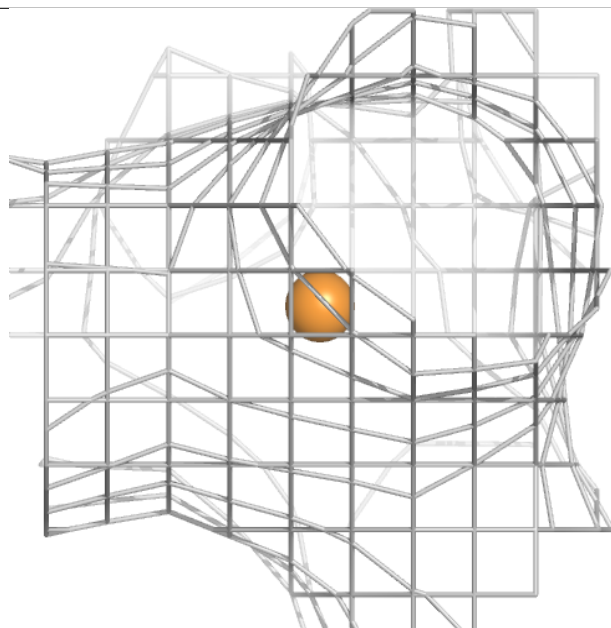
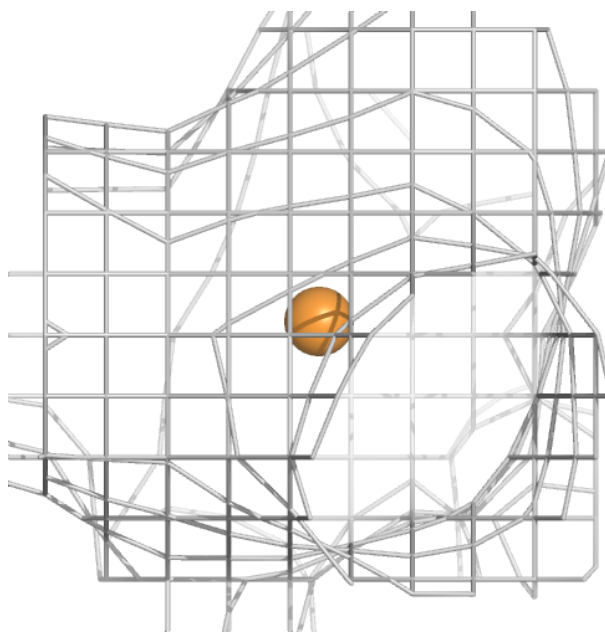
Electron density around CU B 402:

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and green (positive)



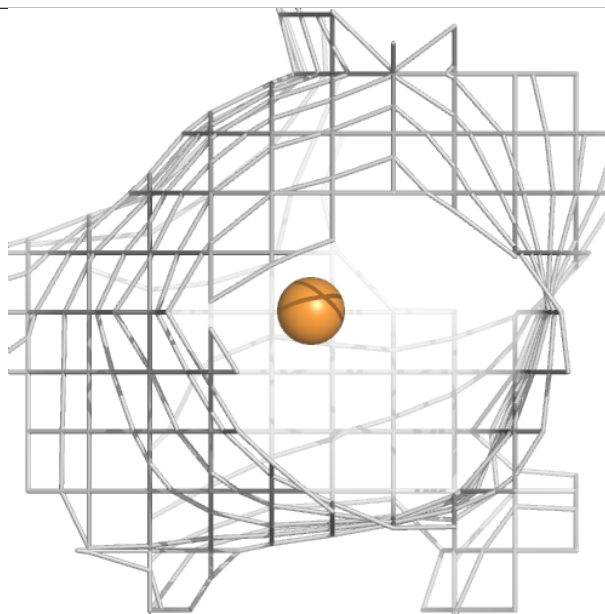
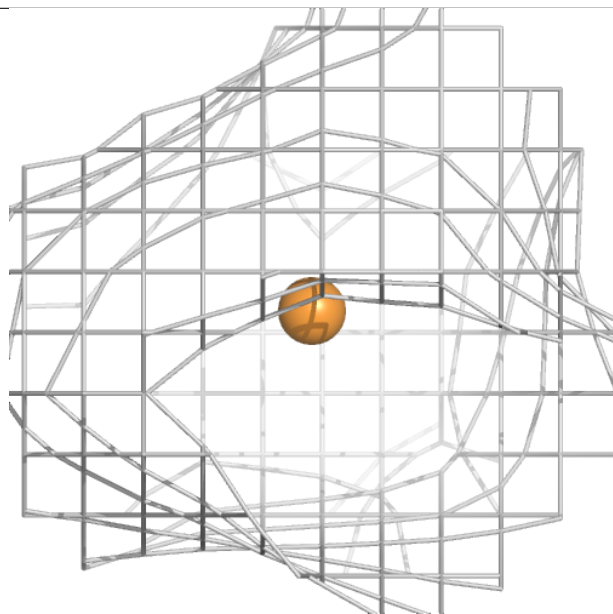
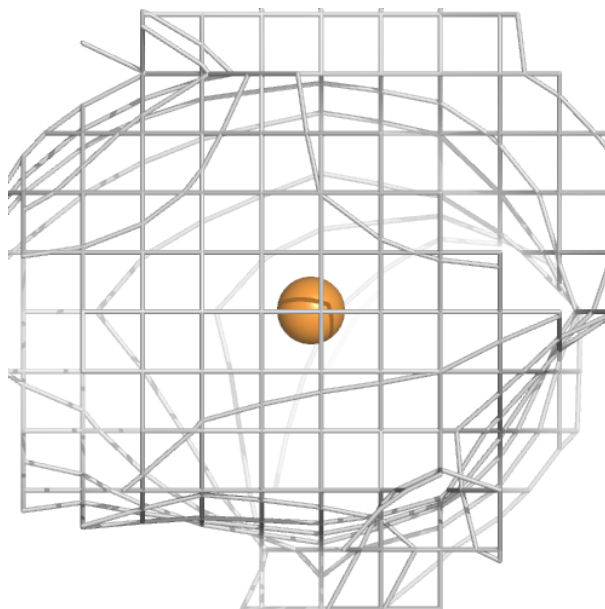
Electron density around CU C 404:

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



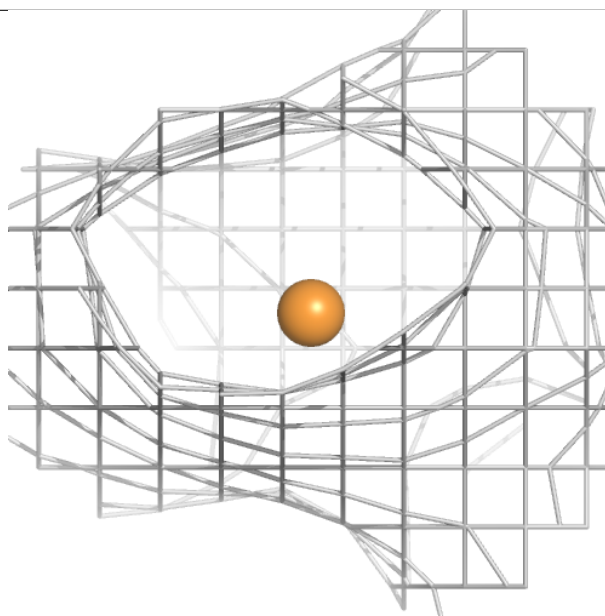
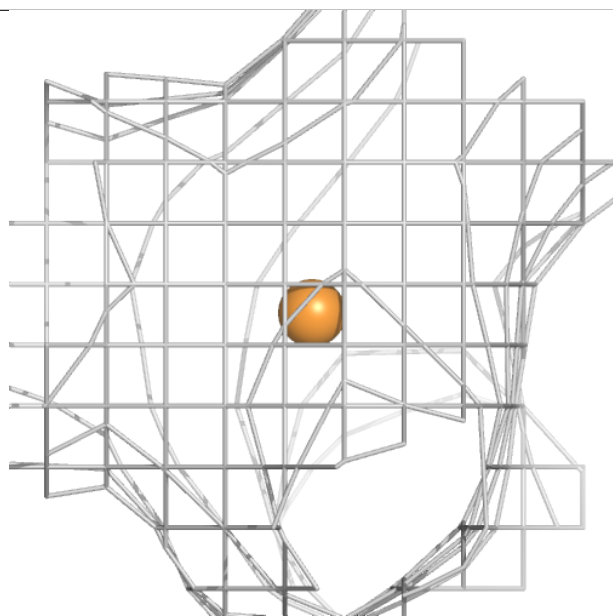
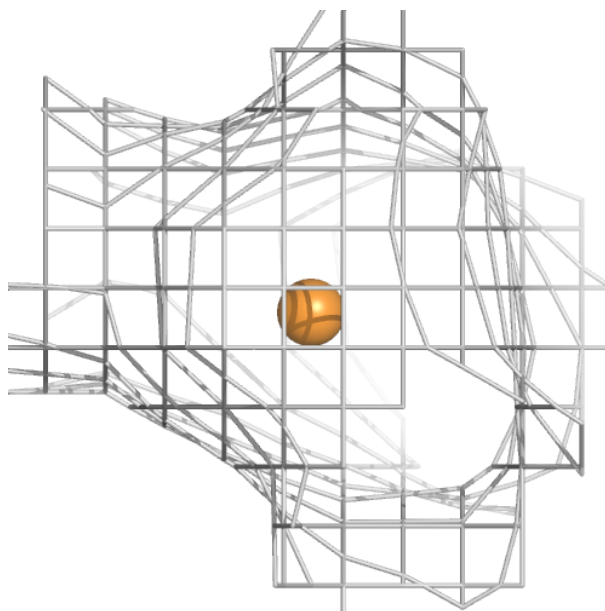
Electron density around CU C 401:

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



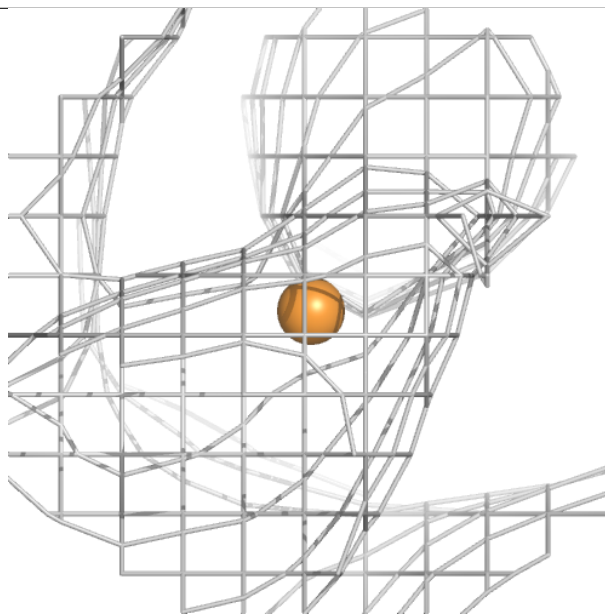
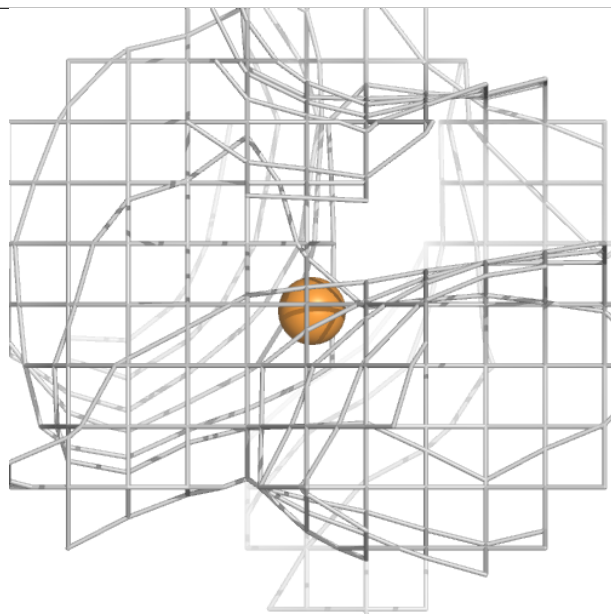
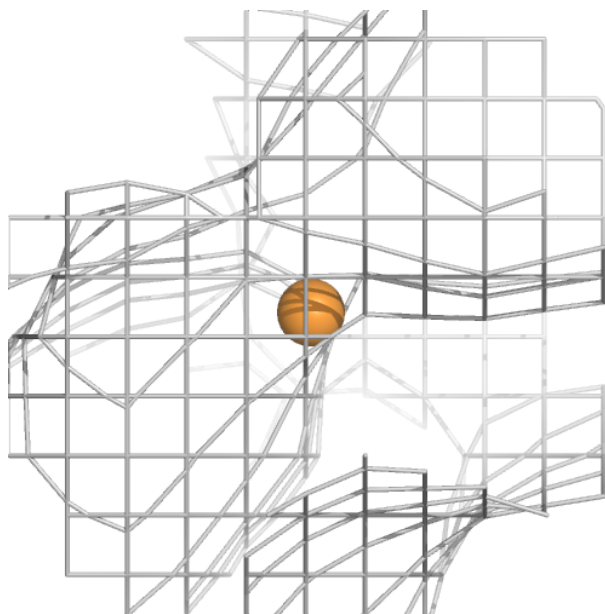
Electron density around CU C 402:

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and green (positive)



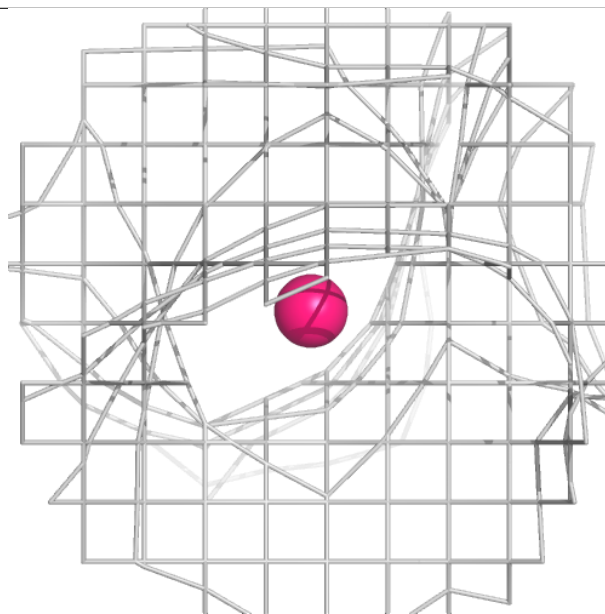
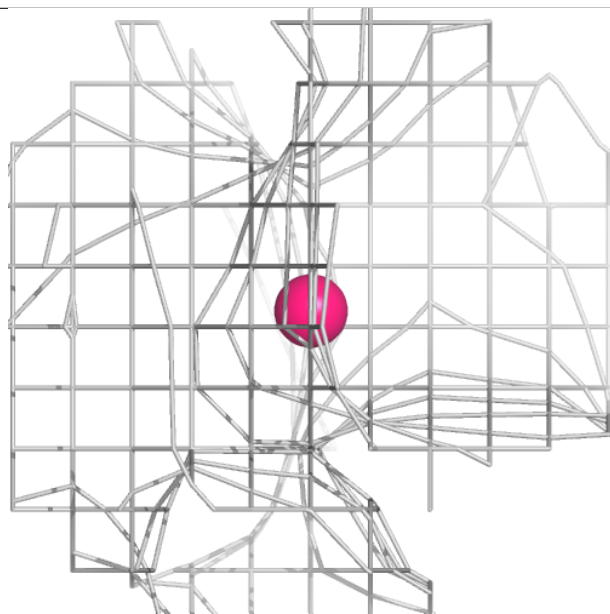
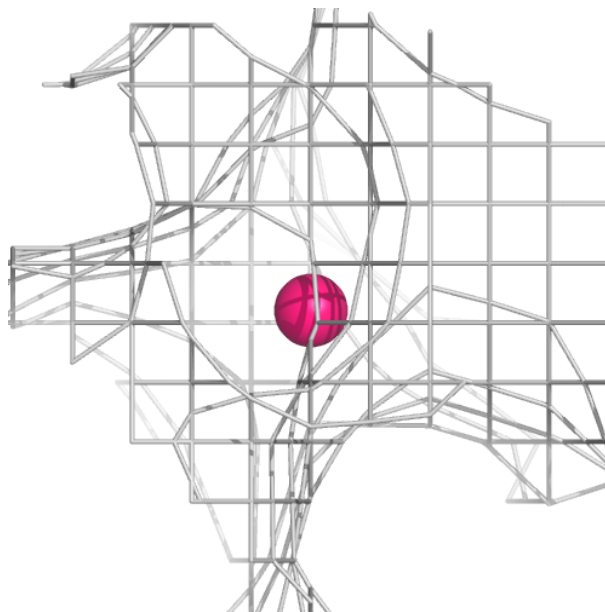
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and green (positive)



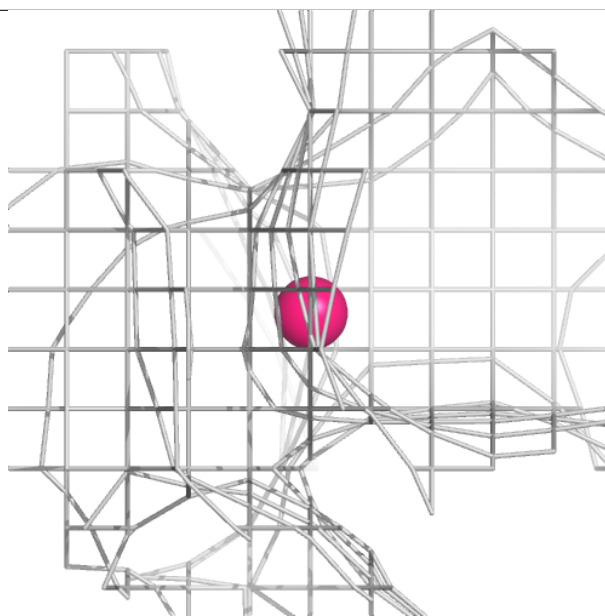
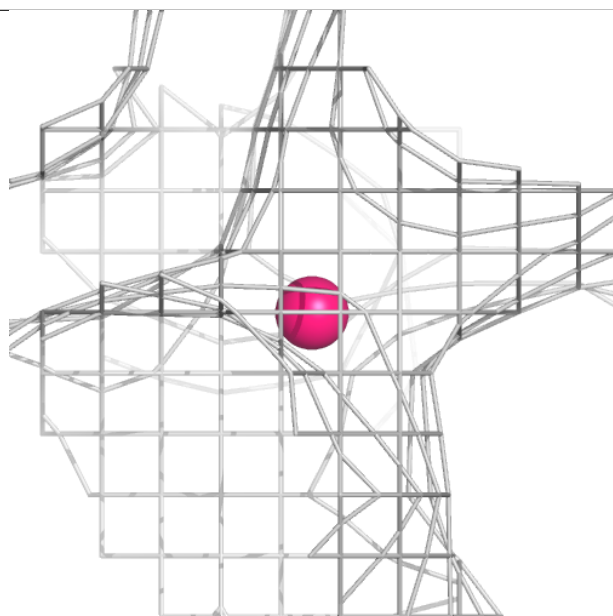
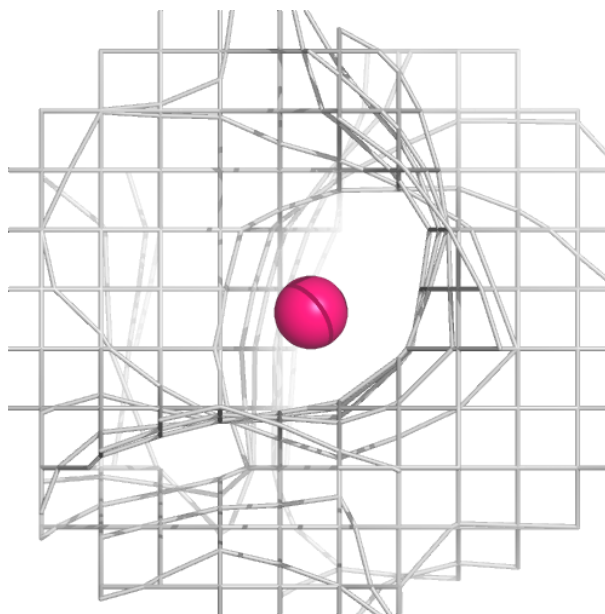
Electron density around OH A 405:

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



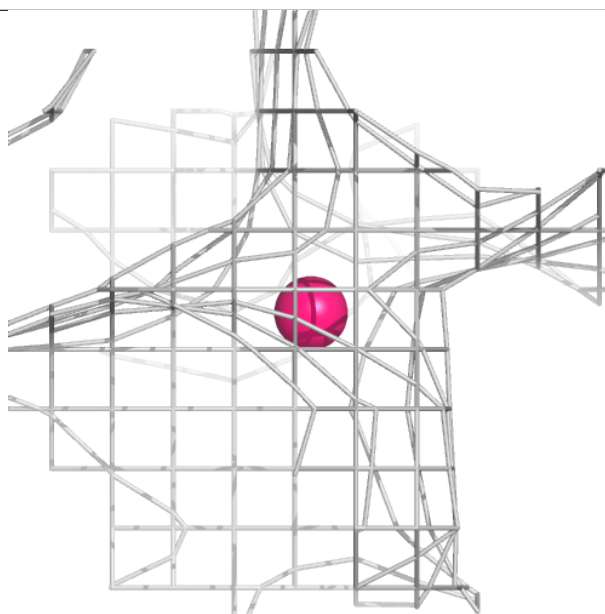
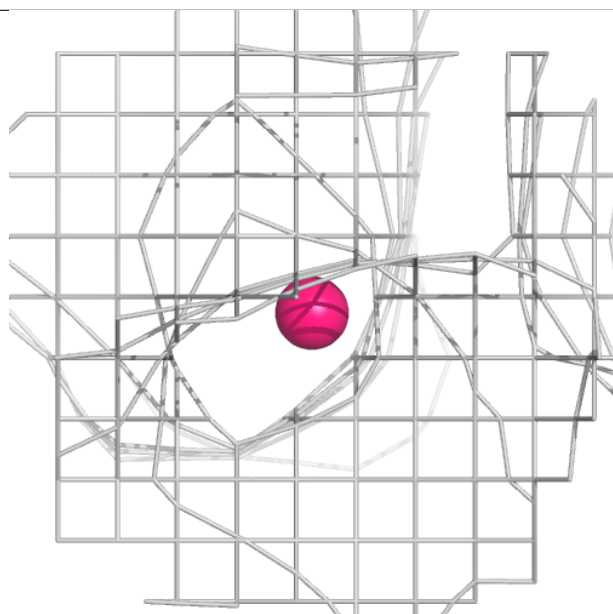
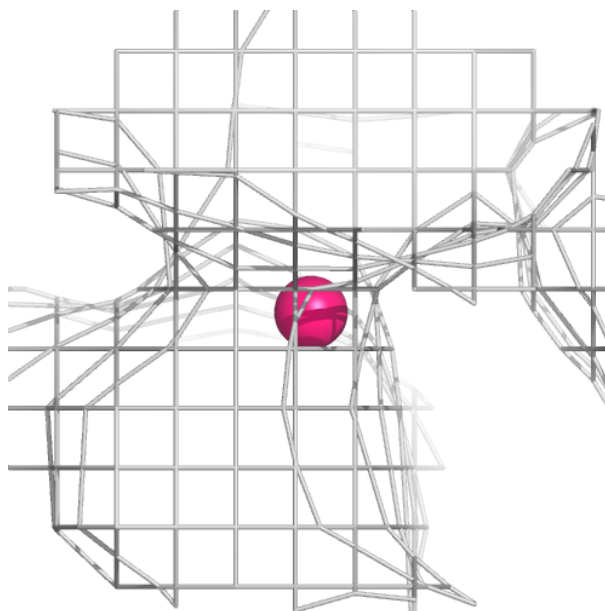
Electron density around OH B 405:

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and green (positive)



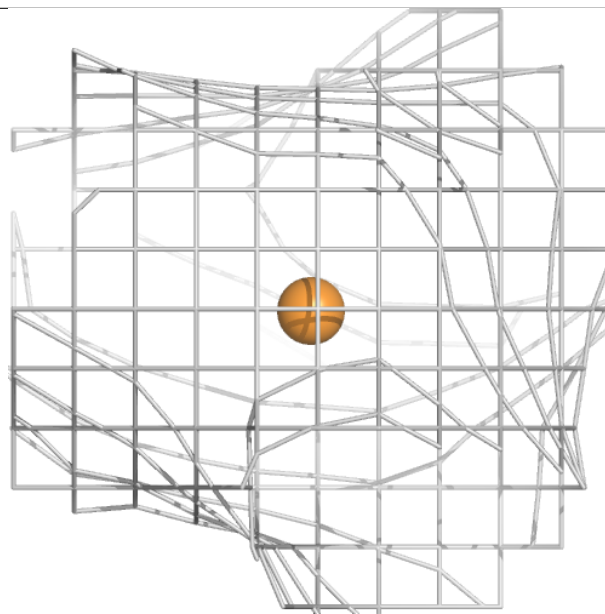
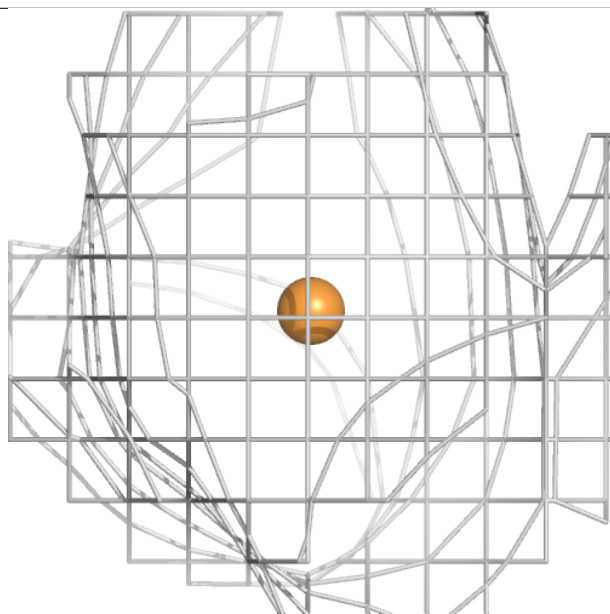
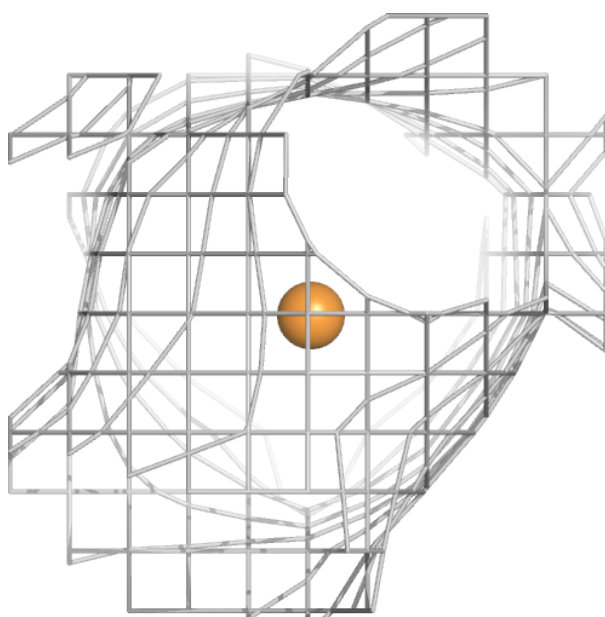
Electron density around OH C 405:

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



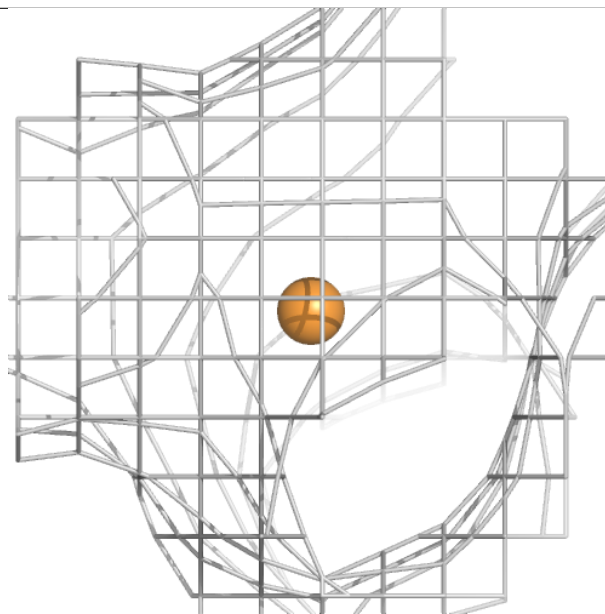
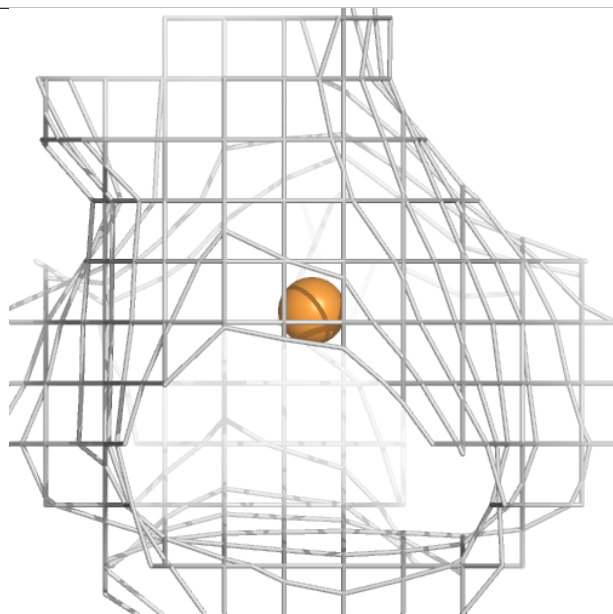
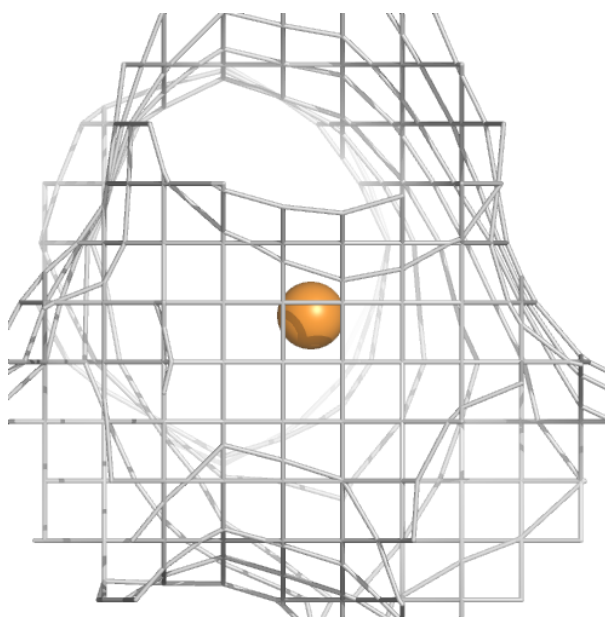
Electron density around CU A 401:

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



Electron density around CU A 402:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.