



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:17 AM UTC

PDB ID : 6XIZ / pdb_00006xiz
Title : Crystal structure of multi-copper oxidase from *Pediococcus acidilactici*
Authors : Pardo, I.; Soares, A.S.; Collins, R.; Partowmah, S.H.; Coler, E.A.
Deposited on : 2020-06-22
Resolution : 1.80 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

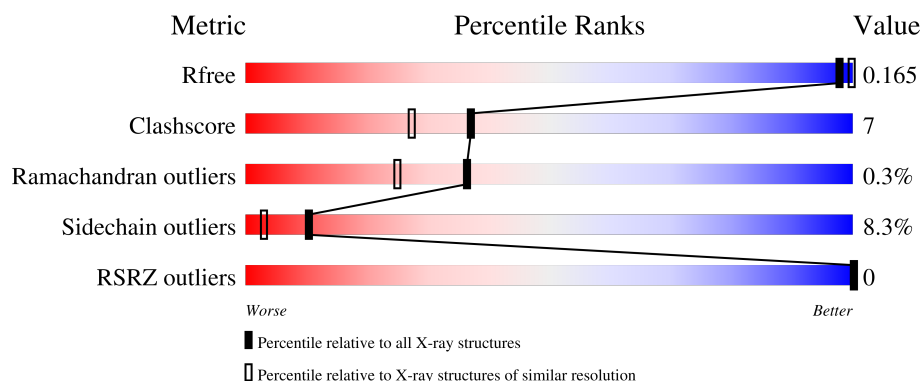
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	477	 73% 21% 5% .
1	B	477	 70% 24% . .

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
5	BEN	B	504	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8309 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 oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	2	0
			3851	2449	667	717	18			
1	B	472	Total	C	N	O	S	0	4	0
			3823	2430	658	718	17			

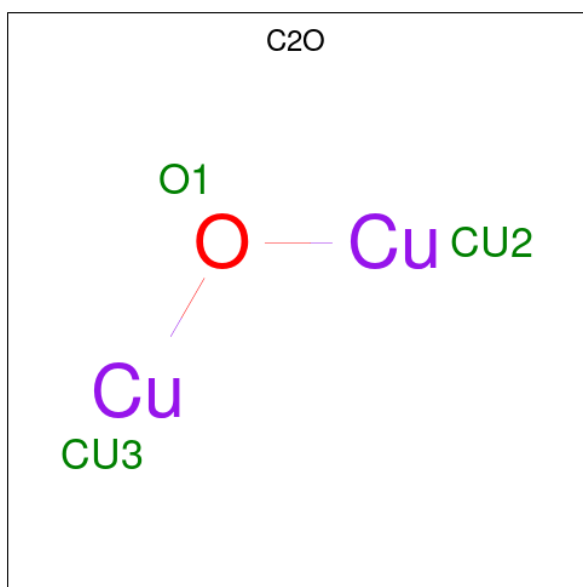
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A1A5VCP7
A	270	LYS	GLU	conflict	UNP A0A1A5VCP7
B	0	SER	-	expression tag	UNP A0A1A5VCP7
B	270	LYS	GLU	conflict	UNP A0A1A5VCP7

- 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	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

- Molecule 3 is CU-O-CU LINKAGE (CCD ID: C2O) (formula: Cu₂O) (labeled as "Ligand of Interest" by depositor).

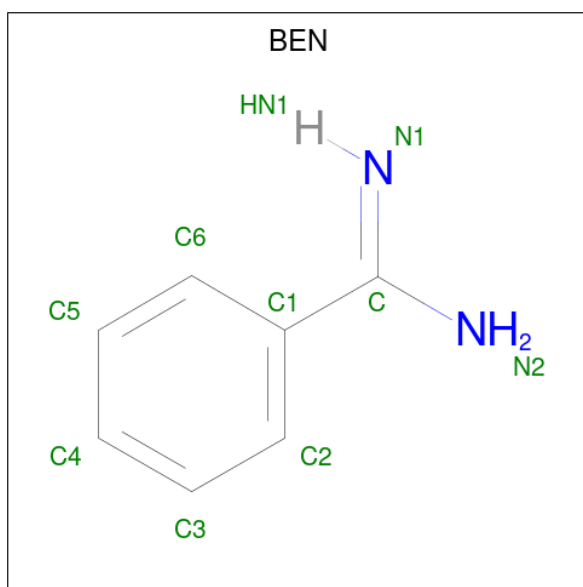


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Cu	O	0	0
			3	2	1		
3	B	1	Total	Cu	O	0	0
			3	2	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			9	7	2		

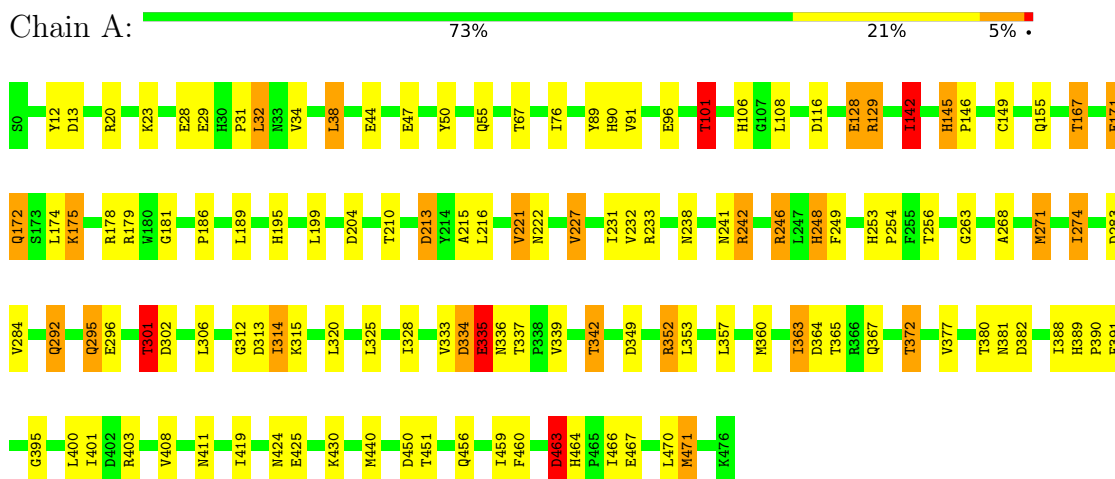
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	315	Total	O	0	13
			317	317		
6	B	294	Total	O	0	15
			297	297		

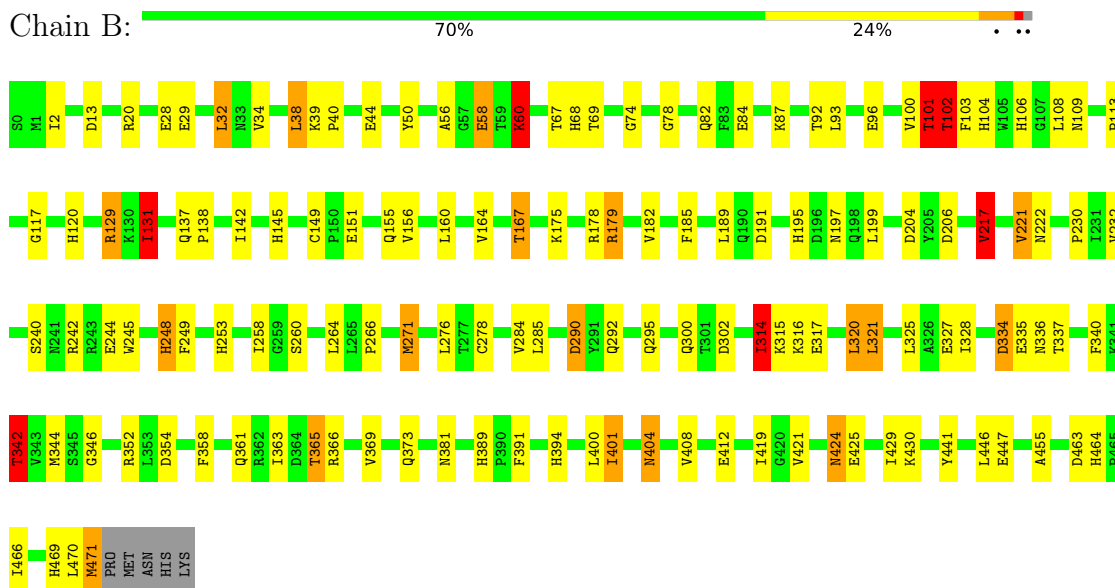
3 Residue-property plots

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

• Molecule 1: Copper oxidase



• Molecule 1: Copper oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.06Å 147.30Å 65.46Å 90.00° 98.55° 90.00°	Depositor
Resolution (Å)	73.65 – 1.80 73.65 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.65-1.80) 100.0 (73.65-1.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.114 , 0.161 0.125 , 0.165	Depositor DCC
R_{free} test set	4742 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.3	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	0.99	EDS
Total number of atoms	8309	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: C2O, CL, CU, BEN

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	1.80	63/3962 (1.6%)	1.40	22/5396 (0.4%)
1	B	1.83	63/3932 (1.6%)	1.41	30/5356 (0.6%)
All	All	1.81	126/7894 (1.6%)	1.40	52/10752 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CD-OE2	9.40	1.43	1.25
1	A	390	PRO	C-O	-8.82	1.17	1.24
1	A	13	ASP	C-O	8.76	1.34	1.24
1	A	210	THR	N-CA	-8.07	1.36	1.46
1	A	232	VAL	CA-C	7.76	1.61	1.52
1	A	90	HIS	CA-CB	7.46	1.64	1.53
1	A	142	ILE	CA-C	-7.41	1.43	1.52
1	B	160	LEU	N-CA	7.36	1.55	1.46
1	B	102	THR	CB-CG2	-7.28	1.28	1.52
1	B	221	VAL	N-CA	7.04	1.54	1.46
1	A	382	ASP	N-CA	7.02	1.54	1.46
1	A	364	ASP	C-O	-6.96	1.15	1.24
1	A	215	ALA	N-CA	-6.93	1.37	1.46
1	A	222	ASN	C-O	6.76	1.26	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	ARG	C-O	6.74	1.31	1.24
1	A	186	PRO	CA-CB	-6.73	1.45	1.53
1	B	138	PRO	N-CA	-6.72	1.39	1.47
1	B	175	LYS	C-O	-6.70	1.15	1.23
1	B	56	ALA	N-CA	6.66	1.53	1.45
1	A	274	ILE	N-CA	-6.66	1.38	1.46
1	A	342	THR	CB-CG2	-6.61	1.30	1.52
1	B	74	GLY	N-CA	6.60	1.51	1.45
1	A	222	ASN	CA-CB	6.58	1.58	1.52
1	B	412	GLU	CA-C	6.51	1.61	1.52
1	A	312	GLY	N-CA	6.49	1.52	1.45
1	B	96	GLU	CA-CB	6.41	1.64	1.53
1	B	421	VAL	CA-C	6.35	1.60	1.52
1	A	231	ILE	CA-CB	-6.30	1.46	1.53
1	B	131	ILE	CB-CG1	-6.28	1.40	1.53
1	A	296	GLU	C-O	-6.28	1.16	1.24
1	B	346	GLY	C-O	6.27	1.33	1.23
1	B	129	ARG	N-CA	6.26	1.53	1.46
1	A	363	ILE	C-O	-6.22	1.17	1.24
1	A	91	VAL	CA-CB	6.20	1.62	1.54
1	B	189	LEU	CA-C	-6.20	1.45	1.52
1	A	450	ASP	C-O	-6.17	1.16	1.24
1	B	248	HIS	CA-C	-6.15	1.44	1.52
1	A	263	GLY	N-CA	6.13	1.50	1.45
1	B	278	CYS	N-CA	6.10	1.53	1.46
1	A	233	ARG	CA-C	-6.04	1.45	1.52
1	B	222	ASN	C-O	6.03	1.26	1.23
1	B	369	VAL	CA-CB	6.03	1.60	1.54
1	B	240	SER	CA-C	-6.00	1.44	1.53
1	B	34	VAL	C-O	-6.00	1.16	1.24
1	A	306	LEU	CA-C	5.99	1.57	1.52
1	A	227	VAL	CA-CB	-5.98	1.47	1.54
1	A	128	GLU	C-O	-5.98	1.16	1.23
1	A	101	THR	CB-CG2	-5.96	1.32	1.52
1	A	32	LEU	N-CA	5.90	1.53	1.46
1	B	217	VAL	C-O	-5.88	1.17	1.24
1	A	451	THR	C-O	-5.88	1.16	1.24
1	B	363	ILE	C-O	-5.88	1.17	1.24
1	A	301	THR	CB-CG2	-5.87	1.33	1.52
1	A	372	THR	C-O	-5.87	1.16	1.24
1	A	199	LEU	CA-C	-5.86	1.45	1.52
1	A	142	ILE	CB-CG1	-5.83	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	TYR	N-CA	-5.79	1.38	1.45
1	A	390	PRO	CA-C	5.79	1.57	1.52
1	B	191	ASP	C-O	-5.75	1.17	1.23
1	A	174	LEU	C-O	5.75	1.31	1.23
1	B	109	ASN	N-CA	5.74	1.53	1.46
1	A	90	HIS	CA-C	-5.74	1.45	1.52
1	B	156	VAL	CA-CB	5.71	1.61	1.54
1	B	266	PRO	N-CA	5.71	1.55	1.47
1	A	411	ASN	C-O	-5.71	1.16	1.24
1	B	199	LEU	C-O	-5.69	1.16	1.23
1	A	89	TYR	CA-C	-5.68	1.45	1.52
1	B	69	THR	CA-C	5.67	1.59	1.52
1	A	246	ARG	CZ-NH2	5.65	1.40	1.33
1	B	352	ARG	CD-NE	-5.64	1.38	1.46
1	B	463	ASP	CA-C	5.62	1.60	1.52
1	B	245	TRP	C-O	5.61	1.30	1.24
1	B	424	ASN	CB-CG	-5.59	1.38	1.52
1	B	404	ASN	CG-ND2	-5.59	1.21	1.33
1	A	425	GLU	N-CA	-5.59	1.39	1.45
1	A	172	GLN	C-O	-5.55	1.17	1.24
1	A	145	HIS	CA-CB	5.54	1.61	1.54
1	B	221	VAL	C-O	5.51	1.31	1.24
1	A	380	THR	C-O	-5.51	1.16	1.24
1	B	264	LEU	N-CA	-5.51	1.39	1.46
1	B	401	ILE	C-O	-5.51	1.17	1.24
1	B	290	ASP	C-O	-5.50	1.16	1.24
1	B	93	LEU	N-CA	-5.50	1.39	1.46
1	B	29	GLU	CA-C	-5.49	1.45	1.52
1	B	258	ILE	CA-CB	-5.48	1.48	1.54
1	B	466	ILE	N-CA	5.47	1.53	1.46
1	A	241	ASN	N-CA	-5.44	1.39	1.46
1	A	306	LEU	C-O	-5.44	1.16	1.23
1	A	29	GLU	N-CA	-5.43	1.39	1.46
1	A	463	ASP	N-CA	5.42	1.53	1.46
1	A	388	ILE	C-O	-5.40	1.18	1.24
1	B	101	THR	CB-CG2	-5.39	1.34	1.52
1	A	55	GLN	N-CA	5.31	1.52	1.45
1	B	39	LYS	C-O	5.31	1.31	1.24
1	A	242	ARG	CG-CD	-5.31	1.36	1.52
1	A	76	ILE	C-O	-5.30	1.17	1.23
1	B	336	ASN	N-CA	5.30	1.52	1.46
1	A	248	HIS	CA-C	5.28	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLN	CA-CB	-5.28	1.45	1.53
1	A	377	VAL	CA-CB	5.27	1.60	1.54
1	B	260	SER	CB-OG	5.26	1.52	1.42
1	A	34	VAL	CA-C	-5.24	1.48	1.52
1	B	185	PHE	CA-CB	5.24	1.62	1.54
1	A	460	PHE	N-CA	5.22	1.52	1.45
1	B	145	HIS	C-N	-5.22	1.27	1.33
1	A	67	THR	N-CA	5.21	1.52	1.46
1	A	175	LYS	N-CA	5.21	1.53	1.46
1	A	216	LEU	CA-C	-5.21	1.46	1.52
1	B	276	LEU	N-CA	5.20	1.52	1.46
1	A	215	ALA	CA-CB	-5.20	1.46	1.53
1	B	321	LEU	N-CA	5.18	1.53	1.46
1	B	92	THR	C-O	-5.17	1.17	1.24
1	B	232	VAL	N-CA	-5.16	1.40	1.46
1	B	344	MET	SD-CE	-5.15	1.66	1.79
1	B	2	ILE	N-CA	5.15	1.52	1.46
1	B	67	THR	CA-C	5.15	1.59	1.52
1	B	244	GLU	CD-OE1	5.14	1.35	1.25
1	A	31	PRO	CA-C	5.14	1.59	1.52
1	B	316	LYS	C-O	-5.10	1.17	1.23
1	B	469	HIS	CA-C	5.09	1.57	1.52
1	A	171	GLU	N-CA	-5.09	1.40	1.46
1	B	145	HIS	C-O	-5.07	1.17	1.24
1	A	189	LEU	N-CA	-5.07	1.40	1.46
1	B	285	LEU	C-O	5.03	1.30	1.24
1	B	300	GLN	CA-C	-5.01	1.46	1.52
1	B	373	GLN	CA-C	5.00	1.58	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	THR	CB-CA-C	-10.38	89.76	110.42
1	A	301	THR	CB-CA-C	-10.21	92.06	109.72
1	B	167	THR	CB-CA-C	-9.05	94.26	110.36
1	B	102	THR	N-CA-CB	-8.27	97.29	111.69
1	B	221	VAL	N-CA-CB	-7.89	96.27	110.95
1	B	271	MET	CG-SD-CE	-7.77	83.81	100.90
1	A	221	VAL	N-CA-CB	-7.64	95.17	111.37
1	B	344	MET	CG-SD-CE	-7.62	84.14	100.90
1	B	314	ILE	N-CA-CB	-7.19	102.88	110.72
1	A	101	THR	CB-CA-C	-7.04	96.33	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	VAL	CB-CA-C	6.97	120.88	111.19
1	B	342	THR	CB-CA-C	-6.89	95.70	109.35
1	B	167	THR	N-CA-CB	6.78	120.81	110.70
1	B	137	GLN	CA-C-N	-6.64	113.87	120.98
1	B	137	GLN	C-N-CA	-6.64	113.87	120.98
1	B	334	ASP	CB-CA-C	6.61	120.34	109.70
1	A	129	ARG	N-CA-C	-6.52	99.39	109.24
1	B	271	MET	CA-CB-CG	6.45	127.00	114.10
1	A	352	ARG	CG-CD-NE	-6.43	97.85	112.00
1	B	320	LEU	N-CA-C	6.29	120.80	111.04
1	A	283	ASP	N-CA-C	-6.10	98.57	108.52
1	B	96	GLU	CA-CB-CG	6.04	126.19	114.10
1	A	342	THR	CB-CA-C	-6.02	97.43	109.35
1	B	221	VAL	CG1-CB-CG2	5.99	123.97	110.80
1	B	221	VAL	CB-CA-C	5.87	120.43	111.68
1	A	175	LYS	CB-CA-C	5.85	119.05	111.50
1	A	292	GLN	CA-CB-CG	-5.83	102.44	114.10
1	B	131	ILE	N-CA-CB	-5.68	102.13	111.45
1	A	142	ILE	N-CA-CB	-5.57	102.03	111.23
1	B	314	ILE	CB-CA-C	5.56	117.80	110.91
1	A	221	VAL	CG1-CB-CG2	5.53	122.96	110.80
1	A	142	ILE	CA-CB-CG2	5.50	119.85	110.50
1	B	78	GLY	CA-C-N	5.49	125.47	120.03
1	B	78	GLY	C-N-CA	5.49	125.47	120.03
1	A	213	ASP	N-CA-C	5.49	118.19	111.82
1	A	221	VAL	CB-CA-C	5.47	119.58	111.31
1	A	175	LYS	CA-CB-CG	5.46	125.02	114.10
1	A	23	LYS	CB-CA-C	-5.45	98.59	109.33
1	A	263	GLY	N-CA-C	5.44	118.41	110.63
1	A	328	ILE	CB-CA-C	-5.44	104.60	110.85
1	A	301	THR	CA-CB-OG1	5.40	117.70	109.60
1	A	295	GLN	N-CA-C	5.40	117.69	110.35
1	A	339	VAL	N-CA-CB	-5.32	104.92	110.72
1	B	60	LYS	CA-C-N	-5.26	117.77	123.08
1	B	60	LYS	C-N-CA	-5.26	117.77	123.08
1	B	40	PRO	CB-CA-C	-5.21	104.73	111.46
1	B	358	PHE	N-CA-C	5.15	117.56	110.35
1	B	321	LEU	CA-C-N	-5.11	115.33	120.85
1	B	321	LEU	C-N-CA	-5.11	115.33	120.85
1	B	197	ASN	N-CA-C	5.09	119.33	113.38
1	A	101	THR	N-CA-CB	5.08	119.24	111.22
1	B	316	LYS	CB-CA-C	-5.07	100.67	109.64

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ARG	Sidechain
1	A	335	GLU	Peptide
1	A	463	ASP	Peptide
1	B	242	ARG	Sidechain

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	3851	0	3711	49	0
1	B	3823	0	3669	54	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	9	0	7	4	0
6	A	317	0	0	12	1
6	B	297	0	0	13	1
All	All	8309	0	7387	107	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (107) 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:A:142:ILE:HG21	6:A:881:HOH:O	1.22	1.33
1:A:357:LEU:HG	6:A:827:HOH:O	1.15	1.29
1:B:131:ILE:HG21	6:B:839:HOH:O	1.38	1.20
1:A:167:THR:HB	6:A:601:HOH:O	1.52	1.06
1:A:167:THR:CB	6:A:601:HOH:O	2.06	1.01
1:A:271:MET:HE1	1:A:274:ILE:HD12	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG21	6:A:782:HOH:O	1.72	0.87
1:A:178:ARG:NH2	6:A:603:HOH:O	2.15	0.79
1:B:58[B]:GLU:O	1:B:58[B]:GLU:HG3	1.81	0.78
1:A:271:MET:HE3	1:A:274:ILE:HB	1.65	0.78
1:A:248:HIS:HE1	1:A:302:ASP:O	1.70	0.74
1:A:167:THR:OG1	6:A:601:HOH:O	2.07	0.71
1:B:248:HIS:HD2	1:B:249:PHE:O	1.77	0.68
1:A:181:GLY:O	6:A:602:HOH:O	2.13	0.66
1:A:271:MET:CE	1:A:274:ILE:HB	2.27	0.65
1:B:195:HIS:HE1	1:B:204:ASP:OD2	1.80	0.64
1:A:20[B]:ARG:HD3	1:A:213:ASP:OD1	1.97	0.64
1:B:292:GLN:H	1:B:295:GLN:HE21	1.44	0.64
1:A:248:HIS:CE1	1:A:302:ASP:O	2.51	0.63
1:A:292:GLN:H	1:A:295:GLN:HE21	1.45	0.63
1:B:102:THR:HG23	1:B:117:GLY:O	1.99	0.62
1:A:38:LEU:HD13	1:A:50:TYR:CD1	2.36	0.60
1:A:195:HIS:HE1	1:A:204:ASP:OD2	1.85	0.60
1:B:32:LEU:HD21	1:B:217:VAL:HG22	1.83	0.60
1:B:60:LYS:CD	6:B:893:HOH:O	2.49	0.59
1:B:100:VAL:HG23	6:B:758:HOH:O	2.04	0.58
1:A:401:ILE:HD11	1:A:430:LYS:HG3	1.85	0.57
1:B:68:HIS:HB3	6:B:846:HOH:O	2.04	0.57
1:B:102:THR:CG2	1:B:117:GLY:O	2.54	0.55
1:B:142:ILE:HG13	1:B:164:VAL:HB	1.89	0.54
1:B:58[A]:GLU:HG3	1:B:68:HIS:CE1	2.43	0.53
1:B:381:ASN:HD21	1:B:389:HIS:HE2	1.57	0.53
1:A:101:THR:HG23	1:A:155:GLN:OE1	2.08	0.53
1:A:248:HIS:HD2	1:A:249:PHE:O	1.90	0.53
1:B:361:GLN:NE2	1:B:471:MET:HA	2.24	0.53
1:B:419[A]:ILE:O	1:B:419[A]:ILE:HG23	2.09	0.53
1:B:340:PHE:CE1	1:B:365:THR:HG21	2.45	0.52
1:B:400:LEU:HB3	1:B:408:VAL:HG11	1.92	0.51
1:A:381:ASN:HD21	1:A:389:HIS:HE2	1.58	0.51
1:A:101:THR:CG2	1:A:155:GLN:OE1	2.59	0.51
1:A:246:ARG:H	1:A:301:THR:HG22	1.75	0.51
5:B:504:BEN:C6	6:B:704[B]:HOH:O	2.59	0.50
1:A:271:MET:HE1	1:A:274:ILE:CD1	2.28	0.50
1:A:357:LEU:HD12	1:A:357:LEU:N	2.26	0.50
1:B:131:ILE:HG12	6:B:839:HOH:O	2.13	0.49
1:B:103:PHE:O	1:B:117:GLY:HA3	2.13	0.49
1:B:419[A]:ILE:O	1:B:419[A]:ILE:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:HIS:HE1	1:B:302:ASP:O	1.96	0.49
1:B:253:HIS:HE1	1:B:290:ASP:OD1	1.95	0.49
1:A:400:LEU:HB3	1:A:408:VAL:HG11	1.95	0.49
1:A:401:ILE:HD11	1:A:430:LYS:CG	2.43	0.49
1:A:227:VAL:HG12	1:A:314:ILE:HD11	1.93	0.49
1:A:116:ASP:HB3	6:A:636:HOH:O	2.13	0.48
1:B:334:ASP:O	1:B:337:THR:HG22	2.13	0.48
1:B:292:GLN:N	1:B:295:GLN:HE21	2.11	0.48
1:B:101:THR:CG2	1:B:155:GLN:OE1	2.63	0.46
1:B:314:ILE:HD13	1:B:314:ILE:HA	1.75	0.46
1:A:145:HIS:HB2	1:A:146:PRO:HD2	1.95	0.46
1:B:101:THR:HG23	1:B:155:GLN:OE1	2.15	0.46
1:B:248:HIS:CD2	1:B:249:PHE:O	2.64	0.46
1:A:334:ASP:OD2	1:A:334:ASP:N	2.46	0.46
1:A:333:VAL:HG22	1:A:372:THR:HG22	1.98	0.45
1:A:419[A]:ILE:O	1:A:419[A]:ILE:CG2	2.64	0.45
1:B:84:GLU:OE2	1:B:87:LYS:HE3	2.16	0.45
1:B:391:PHE:HB3	1:B:419[A]:ILE:HG22	1.99	0.45
1:B:271:MET:HB2	1:B:271:MET:HE3	1.53	0.45
1:B:230:PRO:HG2	6:B:794:HOH:O	2.17	0.44
1:A:395:GLY:HA2	6:A:739:HOH:O	2.18	0.44
1:A:440:MET:HE1	1:A:456:GLN:OE1	2.18	0.44
1:B:419[A]:ILE:HD12	1:B:419[A]:ILE:HA	1.80	0.44
1:A:471:MET:HA	1:A:471:MET:HE2	2.00	0.44
1:A:106:HIS:CD2	1:A:106:HIS:C	2.96	0.44
1:B:400:LEU:HG	1:B:429:ILE:HG22	2.00	0.44
1:A:391:PHE:HB3	1:A:419[A]:ILE:HG22	1.99	0.43
1:A:334:ASP:O	1:A:336:ASN:N	2.48	0.43
1:A:363:ILE:HD11	1:A:470:LEU:HD11	1.99	0.43
1:B:32:LEU:CD2	1:B:217:VAL:HG22	2.47	0.43
1:B:38:LEU:HD13	1:B:50:TYR:CD1	2.53	0.43
1:B:342:THR:HG23	1:B:354:ASP:OD2	2.18	0.43
1:B:401:ILE:HD11	1:B:430:LYS:HG2	1.99	0.43
5:B:504:BEN:C5	6:B:704[B]:HOH:O	2.66	0.43
1:B:179:ARG:HB2	1:B:182:VAL:HB	2.00	0.42
1:B:446:LEU:HG	6:B:618:HOH:O	2.18	0.42
1:B:230:PRO:HD2	6:B:794:HOH:O	2.19	0.42
1:B:404:ASN:HD21	1:B:425:GLU:HA	1.84	0.42
1:B:342:THR:CG2	1:B:354:ASP:OD2	2.67	0.42
1:A:238:ASN:OD1	1:A:238:ASN:C	2.62	0.42
1:B:230:PRO:HB3	1:B:314:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASP:N	1:A:349:ASP:OD1	2.45	0.42
1:B:230:PRO:HG3	1:B:315:LYS:O	2.19	0.42
1:A:253:HIS:CD2	1:A:254:PRO:O	2.73	0.42
1:B:441:TYR:CZ	1:B:455:ALA:HB3	2.55	0.42
5:B:504:BEN:H4	6:B:693[A]:HOH:O	2.19	0.41
1:B:104:HIS:CE1	1:B:394:HIS:CE1	3.08	0.41
1:B:106:HIS:O	1:B:142:ILE:HB	2.19	0.41
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.83	0.41
1:B:58[B]:GLU:O	1:B:58[B]:GLU:CG	2.59	0.41
1:A:178:ARG:NE	6:A:619:HOH:O	2.54	0.41
1:A:335:GLU:HB3	6:A:846:HOH:O	2.20	0.41
1:B:151:GLU:O	1:B:155:GLN:HG3	2.21	0.41
1:B:60:LYS:HD3	6:B:893:HOH:O	2.20	0.41
1:B:113:PRO:HB2	1:B:120:HIS:HB2	2.02	0.41
1:B:206:ASP:O	1:B:447:GLU:HG2	2.21	0.40
5:B:504:BEN:H6	6:B:704[B]:HOH:O	2.20	0.40
1:A:167:THR:HG21	1:A:172:GLN:NE2	2.36	0.40
1:A:367:GLN:O	1:A:459:ILE:HA	2.22	0.40
1:A:256:THR:CG2	1:A:268:ALA:HB1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:872:HOH:O	6:B:846:HOH:O[2_1056]	1.96	0.24

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	477/477 (100%)	454 (95%)	22 (5%)	1 (0%)	43 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/477 (99%)	450 (95%)	22 (5%)	2 (0%)	30	19
All	All	951/954 (100%)	904 (95%)	44 (5%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	LEU
1	B	470	LEU
1	B	321	LEU

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	420/418 (100%)	383 (91%)	37 (9%)	9	2
1	B	417/418 (100%)	383 (92%)	34 (8%)	10	3
All	All	837/836 (100%)	766 (92%)	71 (8%)	10	3

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	32	LEU
1	A	38	LEU
1	A	44	GLU
1	A	47	GLU
1	A	96	GLU
1	A	101	THR
1	A	108	LEU
1	A	128	GLU
1	A	129	ARG
1	A	142	ILE
1	A	149	CYS
1	A	167	THR

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Mol	Chain	Res	Type
1	A	171	GLU
1	A	175	LYS
1	A	179	ARG
1	A	221	VAL
1	A	271	MET
1	A	284	VAL
1	A	301	THR
1	A	313	ASP
1	A	314	ILE
1	A	315	LYS
1	A	325	LEU
1	A	334	ASP
1	A	335	GLU
1	A	337	THR
1	A	342	THR
1	A	352	ARG
1	A	360	MET
1	A	365	THR
1	A	424	ASN
1	A	463	ASP
1	A	464	HIS
1	A	466	ILE
1	A	467	GLU
1	A	471	MET
1	B	13[A]	ASP
1	B	13[B]	ASP
1	B	20	ARG
1	B	28	GLU
1	B	32	LEU
1	B	38	LEU
1	B	44	GLU
1	B	58[A]	GLU
1	B	58[B]	GLU
1	B	60	LYS
1	B	101	THR
1	B	102	THR
1	B	108	LEU
1	B	129	ARG
1	B	131	ILE
1	B	149	CYS
1	B	167	THR
1	B	178	ARG

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Mol	Chain	Res	Type
1	B	179	ARG
1	B	217	VAL
1	B	221	VAL
1	B	284	VAL
1	B	314	ILE
1	B	317	GLU
1	B	320	LEU
1	B	325	LEU
1	B	328	ILE
1	B	335	GLU
1	B	342	THR
1	B	365	THR
1	B	366	ARG
1	B	424	ASN
1	B	464	HIS
1	B	471	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	172	GLN
1	A	195	HIS
1	A	248	HIS
1	A	253	HIS
1	A	295	GLN
1	A	318	ASN
1	A	381	ASN
1	A	404	ASN
1	B	55	GLN
1	B	68	HIS
1	B	172	GLN
1	B	195	HIS
1	B	222	ASN
1	B	248	HIS
1	B	253	HIS
1	B	295	GLN
1	B	361	GLN
1	B	381	ASN
1	B	404	ASN

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
5	BEN	B	504	-	9,9,9	3.08	8 (88%)	7,11,11	2.14	2 (28%)
3	C2O	A	502	1	0,2,2	-	-	-		
3	C2O	B	502	1	0,2,2	-	-	-		

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
5	BEN	B	504	-	-	0/4/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	BEN	C4-C3	-4.52	1.28	1.38
5	B	504	BEN	C6-C1	-4.14	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	BEN	C-N2	-3.24	1.25	1.33
5	B	504	BEN	C1-C	-3.08	1.41	1.47
5	B	504	BEN	C5-C6	2.81	1.43	1.38
5	B	504	BEN	C5-C4	-2.70	1.32	1.38
5	B	504	BEN	C2-C1	-2.67	1.35	1.39
5	B	504	BEN	C3-C2	2.20	1.42	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	504	BEN	C4-C3-C2	-3.52	115.90	120.24
5	B	504	BEN	C5-C4-C3	3.43	124.57	119.87

There are no chirality outliers.

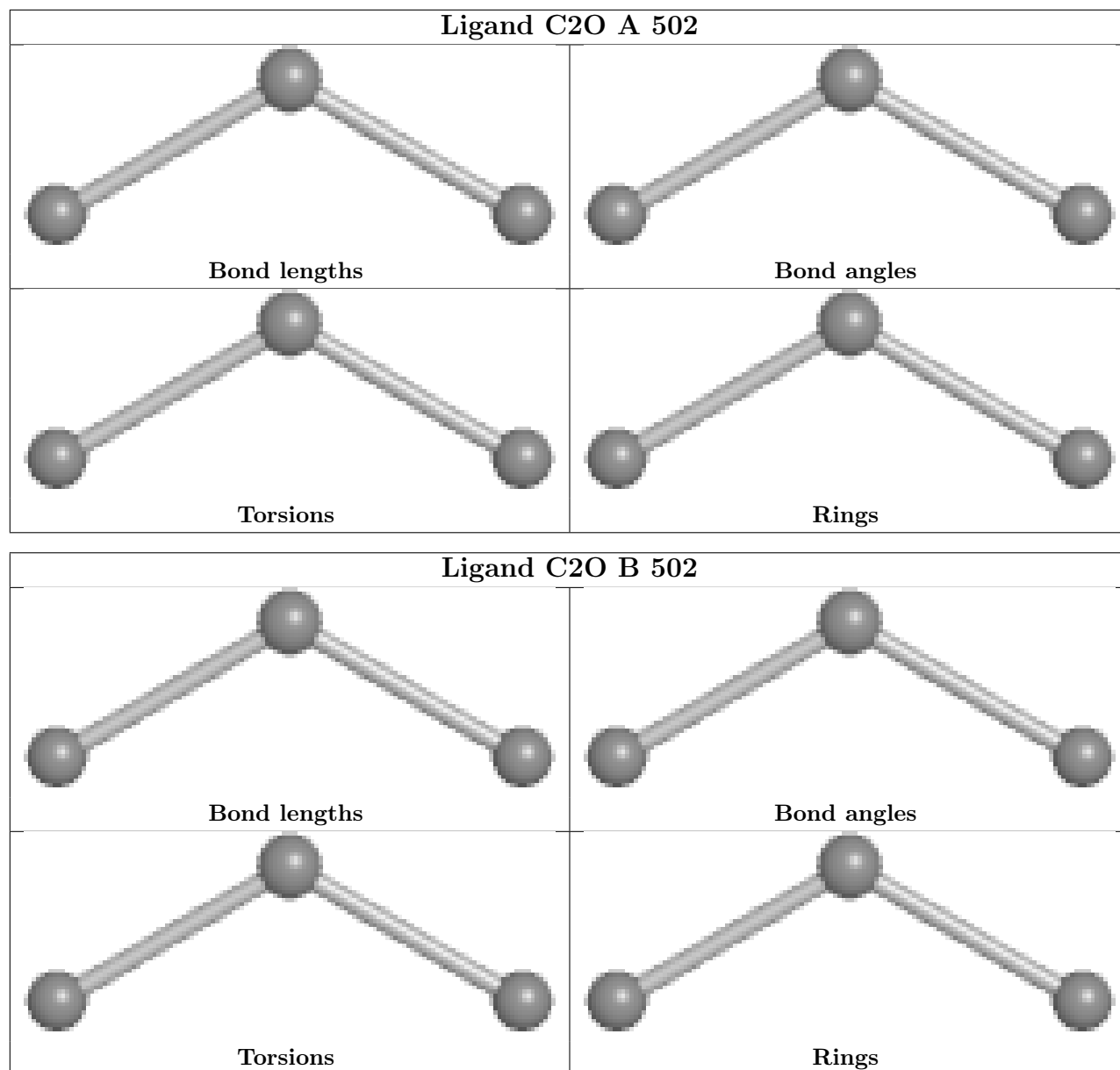
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	BEN	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [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	477/477 (100%)	-0.70	0 100 100	19, 42, 78, 120	2 (0%)
1	B	472/477 (98%)	-0.71	0 100 100	18, 42, 75, 129	4 (0%)
All	All	949/954 (99%)	-0.71	0 100 100	18, 42, 77, 129	6 (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	CL	A	504	1/1	0.98	0.08	79,79,79,79	0
4	CL	B	505	1/1	0.98	0.12	85,85,85,85	0
5	BEN	B	504	9/9	0.98	0.06	34,43,56,60	0
2	CU	A	503	1/1	0.99	0.09	60,60,60,60	0
2	CU	B	503	1/1	0.99	0.09	64,64,64,64	0
3	C2O	B	502	3/3	0.99	0.04	28,28,42,60	0
2	CU	A	501	1/1	1.00	0.01	37,37,37,37	0

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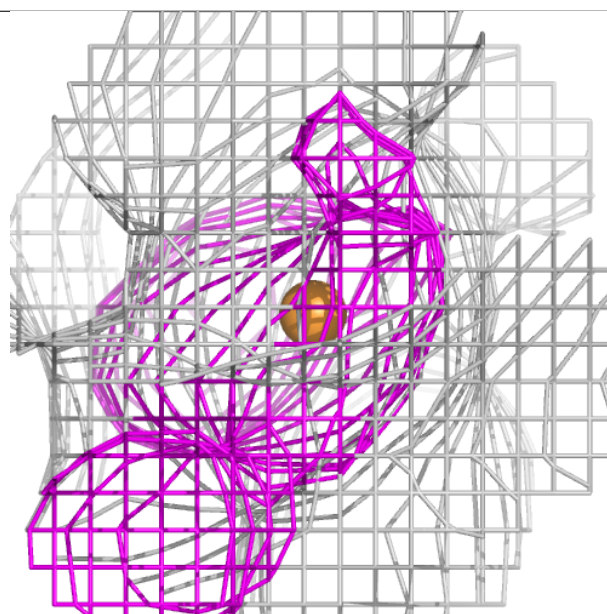
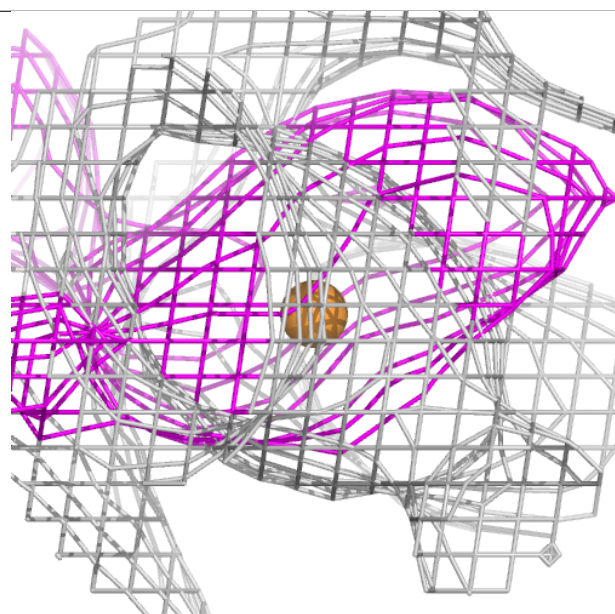
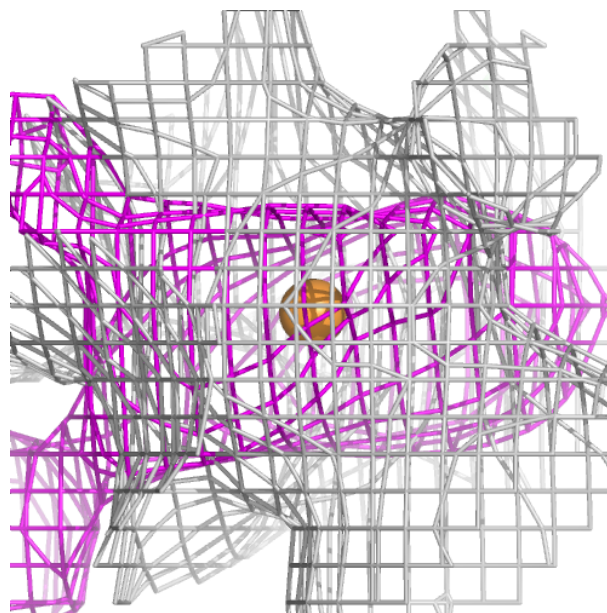
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C2O	A	502	3/3	1.00	0.04	26,26,42,58	0
2	CU	B	501	1/1	1.00	0.01	38,38,38,38	0

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.

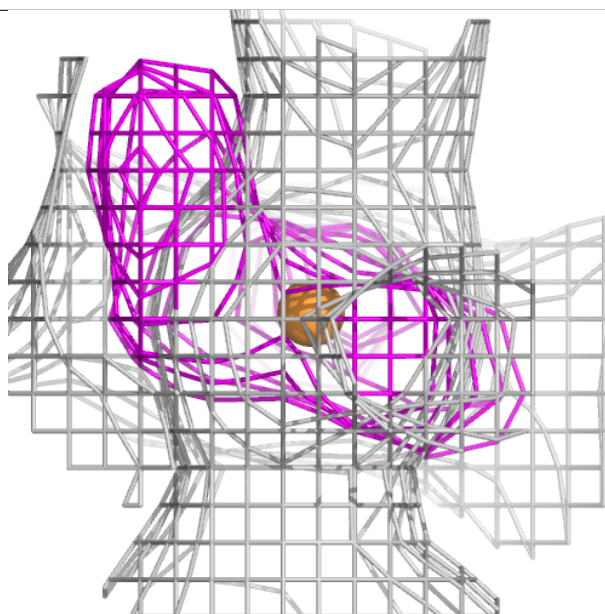
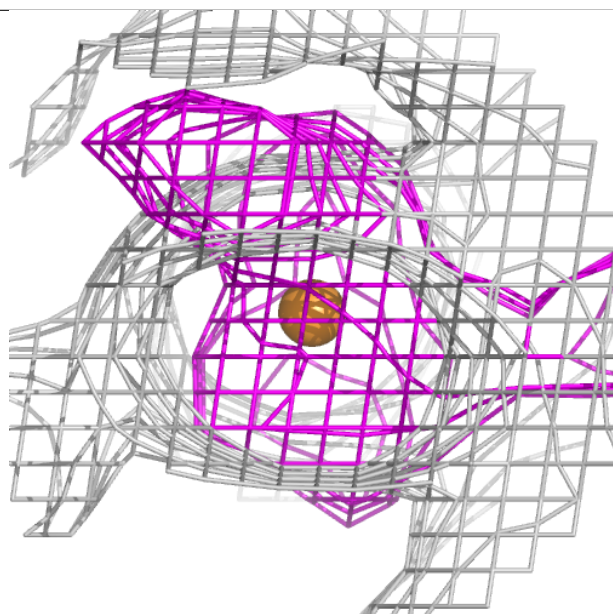
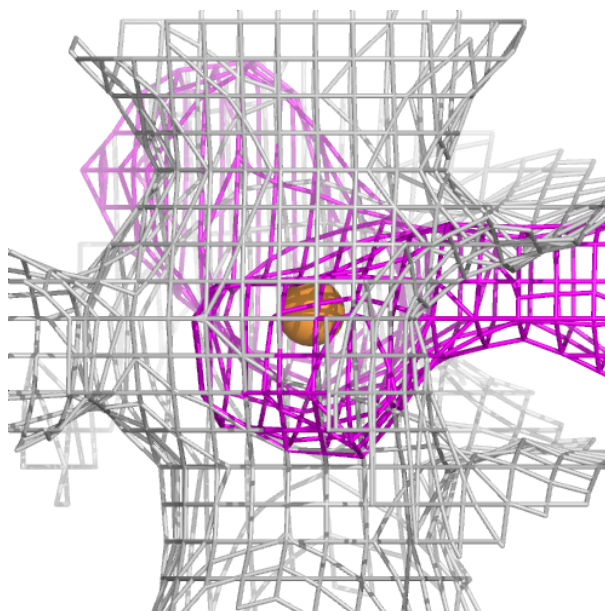
Electron density around CU A 503:

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



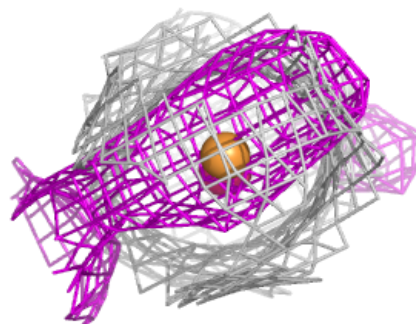
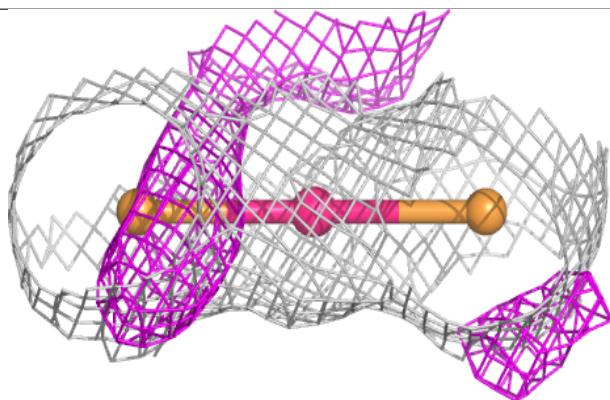
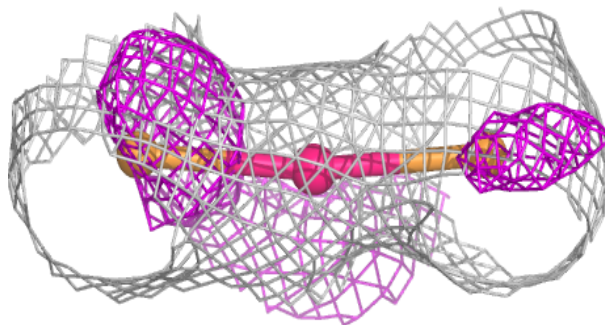
Electron density around CU B 503:

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



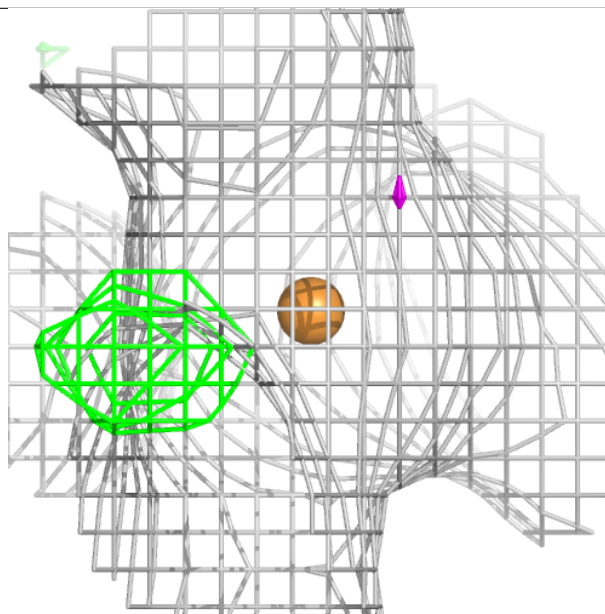
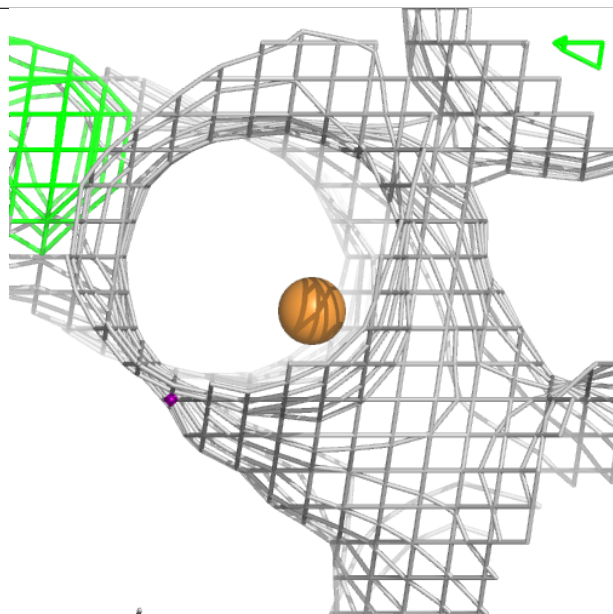
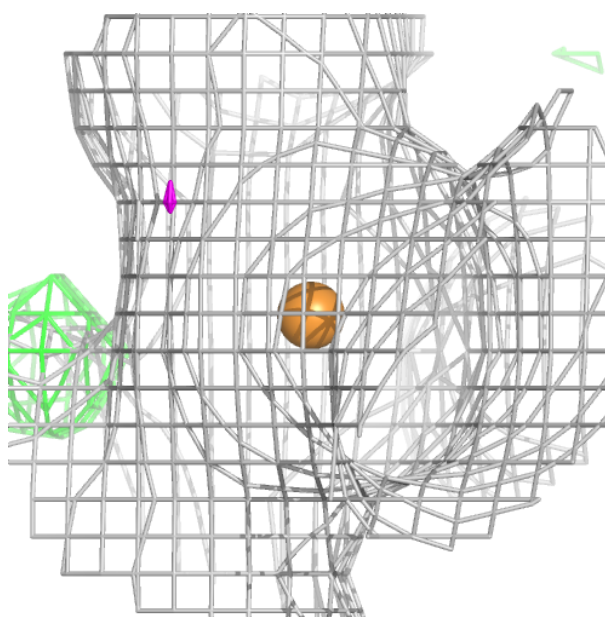
Electron density around C2O B 502:

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



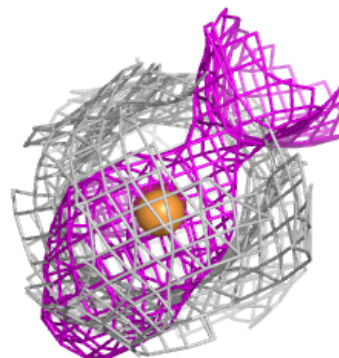
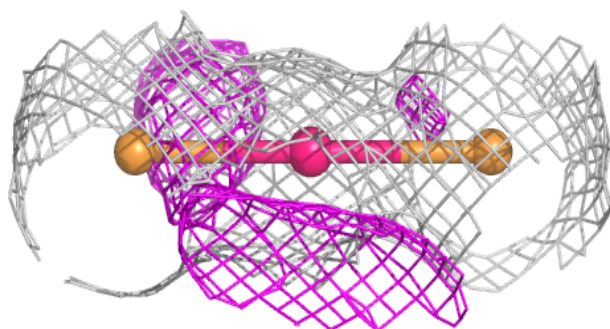
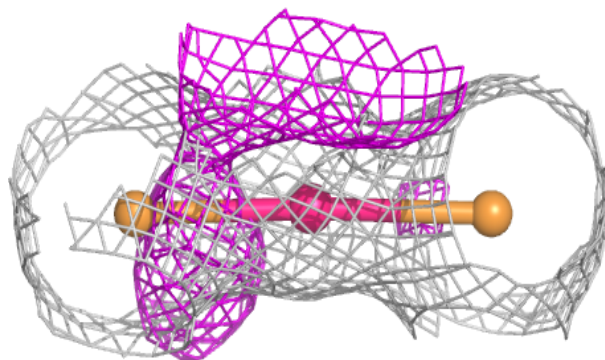
Electron density around CU A 501:

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



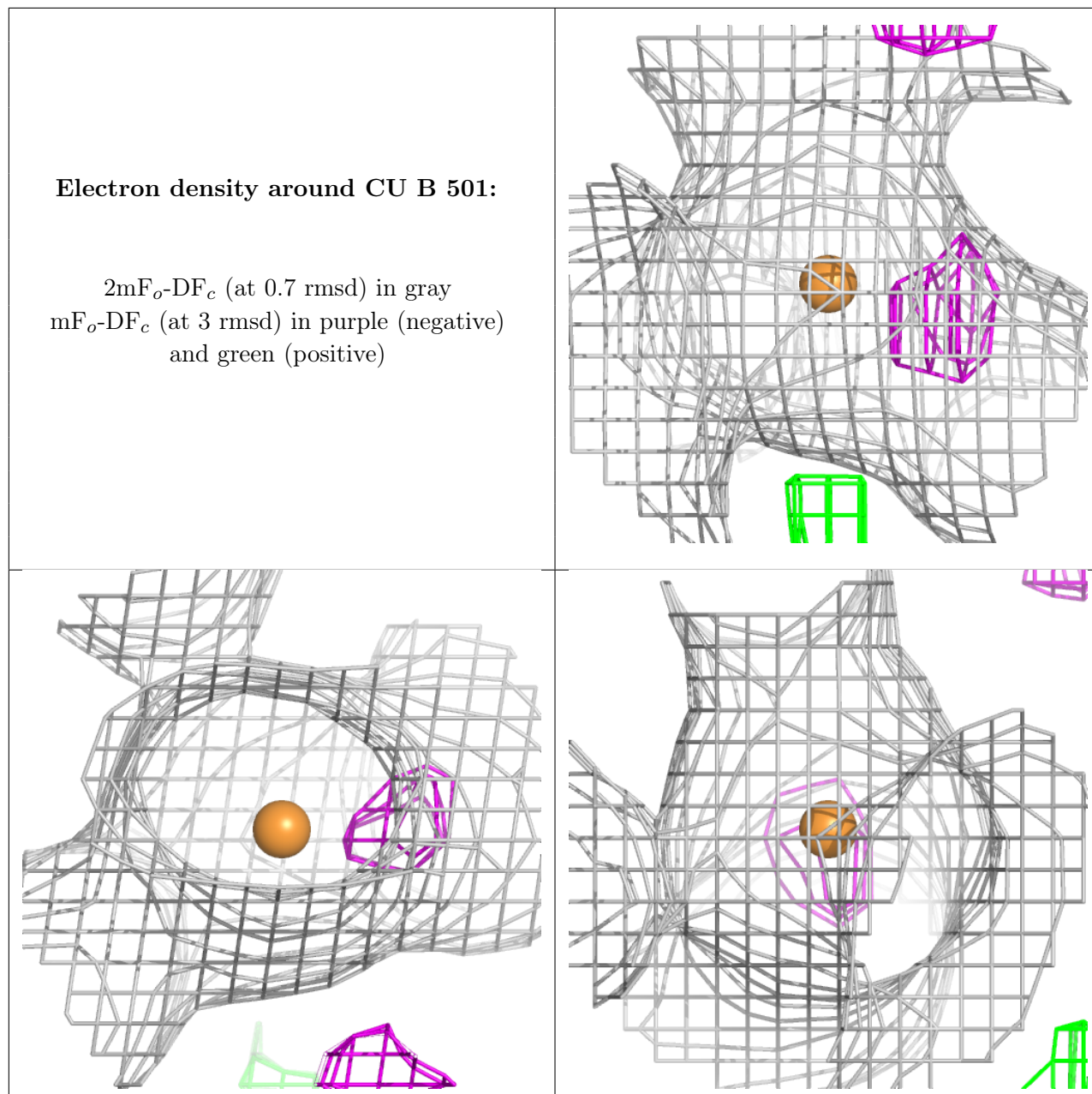
Electron density around C2O A 502:

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



Electron density around CU B 501:

$2mF_o-DF_c$ (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.