Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 07:58 AM EDT

PDB ID	:	6XIZ
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 (i) 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 (i)) were used in the production of this report:

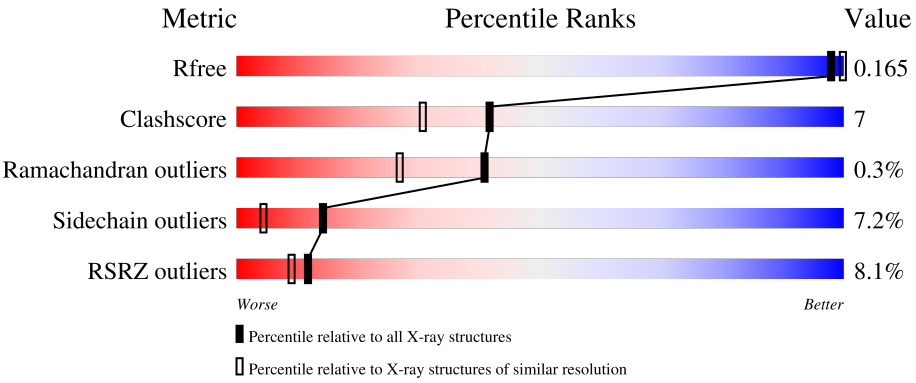
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	8% 79% 17%
1	B	477	8% 77% 17%

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 (i)

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			

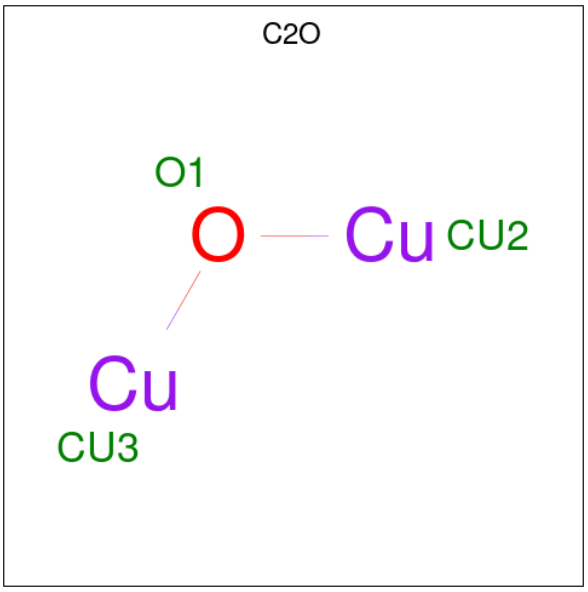
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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 (three-letter code: C2O) (formula: Cu_2O) (labeled as "Ligand of Interest" by depositor).

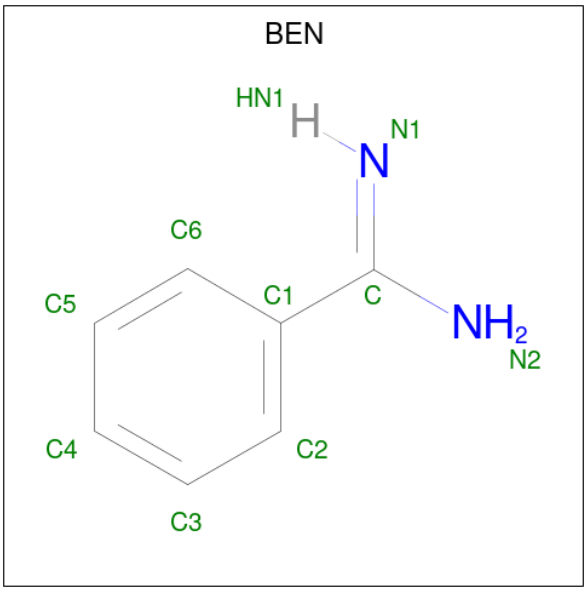


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu O 3 2 1	0	0
3	B	1	Total Cu O 3 2 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).



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

- Molecule 6 is water.

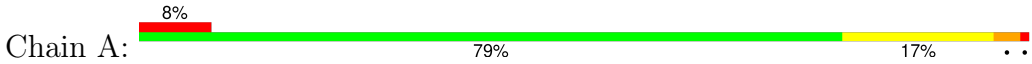
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	315	Total O 317 317	0	13
6	B	294	Total O 297 297	0	15

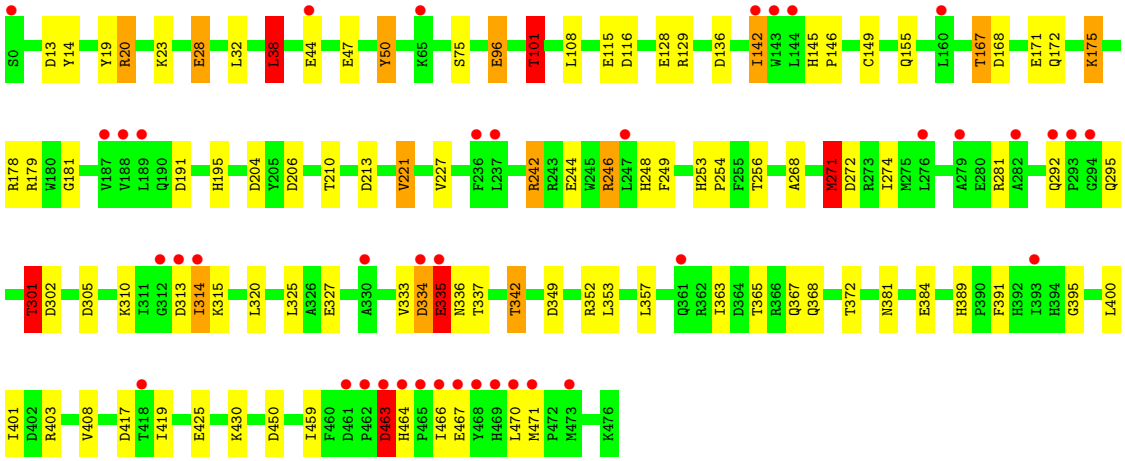
3 Residue-property plots (i)

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

• Molecule 1: Copper oxidase

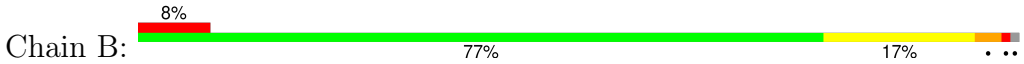
Chain A:

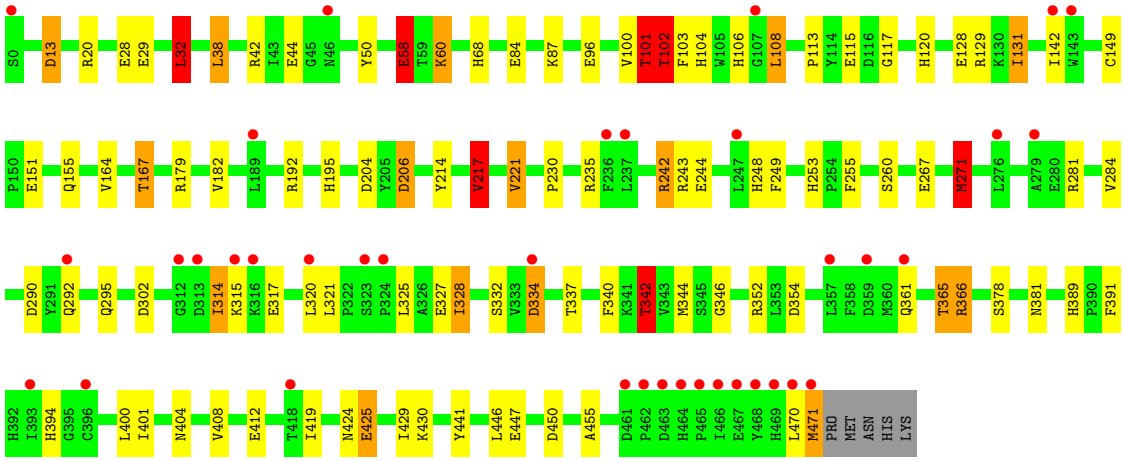




• Molecule 1: Copper oxidase

Chain B:





4 Data and refinement statistics (i)

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 29.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.65-1.80) 100.0 (29.63-1.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.114 , 0.161 0.124 , 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)	0.37 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, C2O, 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	1.41	23/3962 (0.6%)	1.28	31/5396 (0.6%)
1	B	1.46	23/3932 (0.6%)	1.28	33/5356 (0.6%)
All	All	1.43	46/7894 (0.6%)	1.28	64/10752 (0.6%)

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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CD-OE2	15.97	1.43	1.25
1	B	244	GLU	CD-OE1	8.61	1.35	1.25
1	A	96	GLU	CD-OE2	8.16	1.34	1.25
1	B	260	SER	CB-OG	8.02	1.52	1.42
1	B	327	GLU	CD-OE1	7.85	1.34	1.25
1	A	96	GLU	CD-OE1	7.40	1.33	1.25
1	B	102	THR	CB-CG2	-7.22	1.28	1.52
1	B	96	GLU	CB-CG	6.72	1.65	1.52
1	A	115	GLU	CD-OE2	6.60	1.32	1.25
1	A	342	THR	CB-CG2	-6.54	1.30	1.52
1	B	58[A]	GLU	CG-CD	6.54	1.61	1.51
1	B	58[B]	GLU	CG-CD	6.54	1.61	1.51
1	A	50	TYR	CE1-CZ	-6.53	1.30	1.38
1	B	128	GLU	CD-OE2	-6.36	1.18	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	TYR	CG-CD2	-6.32	1.30	1.39
1	A	242	ARG	CG-CD	-6.17	1.36	1.51
1	A	50	TYR	CG-CD2	-6.16	1.31	1.39
1	B	346	GLY	C-O	6.07	1.33	1.23
1	B	412	GLU	CD-OE1	6.04	1.32	1.25
1	A	246	ARG	CZ-NH2	5.96	1.40	1.33
1	A	101	THR	CB-CG2	-5.90	1.32	1.52
1	B	29	GLU	CD-OE1	5.84	1.32	1.25
1	A	13	ASP	C-O	5.84	1.34	1.23
1	A	301	THR	CB-CG2	-5.80	1.33	1.52
1	B	424	ASN	CB-CG	-5.64	1.38	1.51
1	B	214	TYR	CE1-CZ	-5.59	1.31	1.38
1	A	14	TYR	CD1-CE1	5.54	1.47	1.39
1	A	28	GLU	CG-CD	5.53	1.60	1.51
1	B	267	GLU	CD-OE2	5.53	1.31	1.25
1	B	378	SER	CB-OG	-5.38	1.35	1.42
1	A	75	SER	CB-OG	5.36	1.49	1.42
1	A	425	GLU	CG-CD	5.34	1.59	1.51
1	B	284	VAL	CB-CG1	-5.34	1.41	1.52
1	B	101	THR	CB-CG2	-5.33	1.34	1.52
1	B	334	ASP	CB-CG	5.33	1.62	1.51
1	B	214	TYR	CD1-CE1	5.29	1.47	1.39
1	B	115	GLU	CD-OE2	5.28	1.31	1.25
1	A	244	GLU	CD-OE1	5.21	1.31	1.25
1	A	244	GLU	CG-CD	5.18	1.59	1.51
1	A	463	ASP	CB-CG	5.15	1.62	1.51
1	A	28	GLU	CD-OE2	5.14	1.31	1.25
1	B	425	GLU	CD-OE1	5.13	1.31	1.25
1	A	327	GLU	CD-OE2	5.06	1.31	1.25
1	A	384	GLU	CG-CD	5.05	1.59	1.51
1	A	210	THR	N-CA	-5.05	1.36	1.46
1	B	115	GLU	CD-OE1	5.05	1.31	1.25

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	271	MET	CG-SD-CE	-10.24	83.81	100.20
1	B	344	MET	CG-SD-CE	-10.04	84.14	100.20
1	A	352	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	352	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	B	352	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	B	281	ARG	NE-CZ-NH2	-8.25	116.18	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	221	VAL	CG1-CB-CG2	8.17	123.97	110.90
1	B	101	THR	CB-CA-C	-8.09	89.76	111.60
1	B	271	MET	CA-CB-CG	8.06	127.00	113.30
1	B	235	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	13[A]	ASP	CB-CG-OD1	-7.65	111.41	118.30
1	B	13[B]	ASP	CB-CG-OD1	-7.65	111.41	118.30
1	A	450	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	221	VAL	CG1-CB-CG2	7.54	122.96	110.90
1	A	221	VAL	N-CA-CB	-7.42	95.17	111.50
1	B	32	LEU	CB-CG-CD2	7.36	123.51	111.00
1	A	301	THR	CB-CA-C	-7.24	92.06	111.60
1	A	20[A]	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	20[B]	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	221	VAL	N-CA-CB	-6.92	96.27	111.50
1	B	42	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	102	THR	N-CA-CB	-6.84	97.29	110.30
1	B	328	ILE	CG1-CB-CG2	-6.75	96.55	111.40
1	A	352	ARG	CG-CD-NE	-6.64	97.85	111.80
1	A	246	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	B	167	THR	CB-CA-C	-6.42	94.26	111.60
1	B	192	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	243	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	242	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	206	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	168	ASP	CB-CG-OD2	6.27	123.95	118.30
1	A	271	MET	CG-SD-CE	-6.24	90.22	100.20
1	A	403	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	191	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	A	463	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	136	ASP	CB-CG-OD1	6.06	123.76	118.30
1	A	23	LYS	CB-CA-C	-5.90	98.59	110.40
1	B	342	THR	CB-CA-C	-5.89	95.70	111.60
1	B	217	VAL	CG1-CB-CG2	5.84	120.25	110.90
1	B	96	GLU	CA-CB-CG	5.81	126.19	113.40
1	B	334	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	58[A]	GLU	CA-CB-CG	5.72	125.98	113.40
1	B	58[B]	GLU	CA-CB-CG	5.72	125.98	113.40
1	B	42	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	310	LYS	CD-CE-NZ	5.69	124.78	111.70
1	A	101	THR	CB-CA-C	-5.65	96.33	111.60
1	B	167	THR	N-CA-CB	5.53	120.81	110.30
1	A	272	ASP	CB-CG-OD1	5.52	123.27	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	32	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	281	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	366	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	471	MET	CG-SD-CE	5.44	108.91	100.20
1	A	403	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	38	LEU	CB-CG-CD2	5.41	120.19	111.00
1	A	417	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	450	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	305	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	217	VAL	CA-CB-CG2	5.30	118.86	110.90
1	A	175	LYS	CA-CB-CG	5.28	125.02	113.40
1	A	342	THR	CB-CA-C	-5.25	97.43	111.60
1	A	305	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	206	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	368	GLN	CB-CA-C	-5.02	100.35	110.40
1	B	108	LEU	CA-CB-CG	5.01	126.83	115.30

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 (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	3851	0	3711	46	0
1	B	3823	0	3669	55	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	105	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 (105) 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	1.47	0.94
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: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:271:MET:HE1	1:A:274:ILE:CD1	2.27	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:A:271:MET:HE3	1:A:274:ILE:HB	1.82	0.59
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:PHE:CE2	1:B:271:MET:HE3	2.43	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: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
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:A:271:MET:HE1	1:A:274:ILE:HB	1.95	0.47
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:HE3	1:B:271:MET:HB2	1.76	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419[A]:ILE:HD12	1:B:419[A]:ILE:HA	1.80	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:B:230:PRO:HB3	1:B:314:ILE:HG23	2.01	0.42
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%)	47 33
1	B	474/477 (99%)	450 (95%)	22 (5%)	2 (0%)	34 21
All	All	951/954 (100%)	904 (95%)	44 (5%)	3 (0%)	41 27

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%)	388 (92%)	32 (8%)	13 4
1	B	417/418 (100%)	387 (93%)	30 (7%)	14 4
All	All	837/836 (100%)	775 (93%)	62 (7%)	14 4

All (62) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	A	171	GLU
1	A	175	LYS
1	A	179	ARG
1	A	221	VAL
1	A	271	MET
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	365	THR
1	A	463	ASP
1	A	464	HIS
1	A	466	ILE
1	A	467	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	129	ARG
1	B	131	ILE
1	B	149	CYS
1	B	167	THR
1	B	217	VAL
1	B	221	VAL
1	B	271	MET
1	B	314	ILE
1	B	317	GLU
1	B	320	LEU
1	B	325	LEU
1	B	328	ILE
1	B	332	SER
1	B	342	THR
1	B	365	THR
1	B	366	ARG
1	B	471	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	195	HIS
1	A	222	ASN
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	68	HIS
1	B	195	HIS
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 monosaccharides 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	$\#\|Z\| > 2$
3	C2O	A	502	1	0,2,2	-	-	-		
3	C2O	B	502	1	0,2,2	-	-	-		
5	BEN	B	504	-	9,9,9	3.08	8 (88%)	7,11,11	2.14	2 (28%)

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

Continued on next page...

Continued from previous page...

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(^{o})	Ideal(^{o})
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.

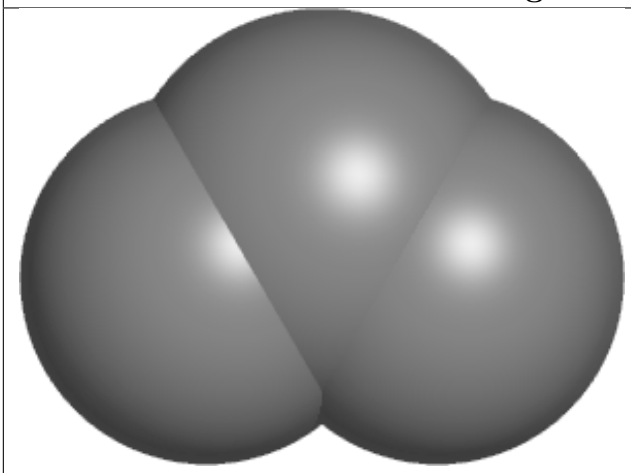
There are no ring outliers.

1 monomer is involved in 4 short contacts:

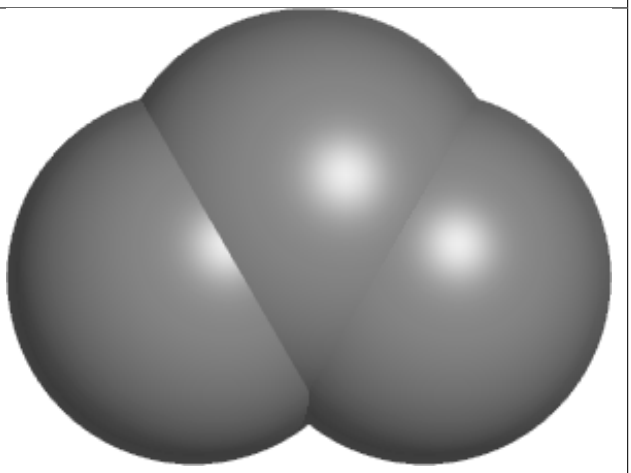
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	BEN	4	0

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 then 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.

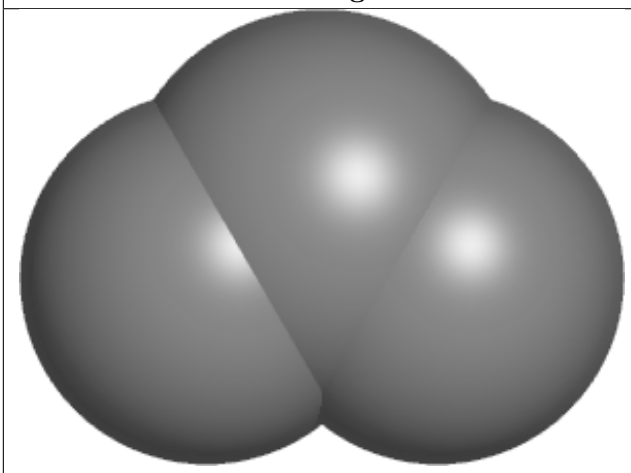
Ligand C2O A 502



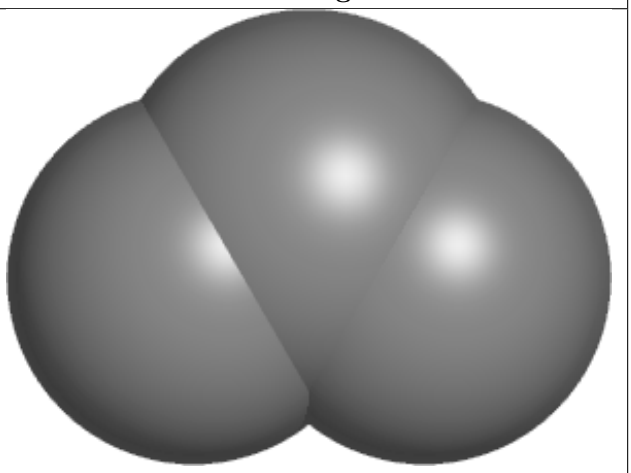
Bond lengths



Bond angles

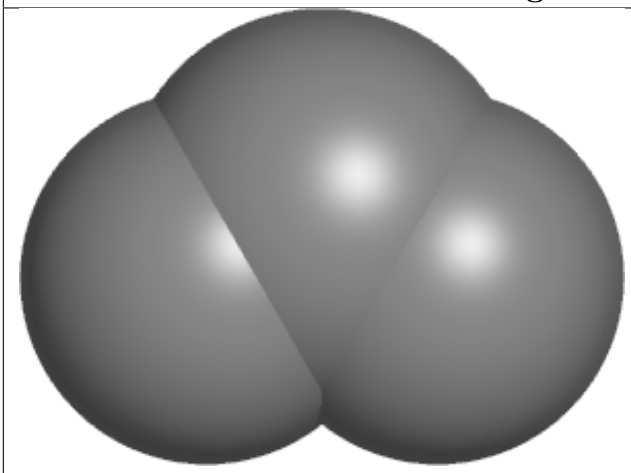


Torsions

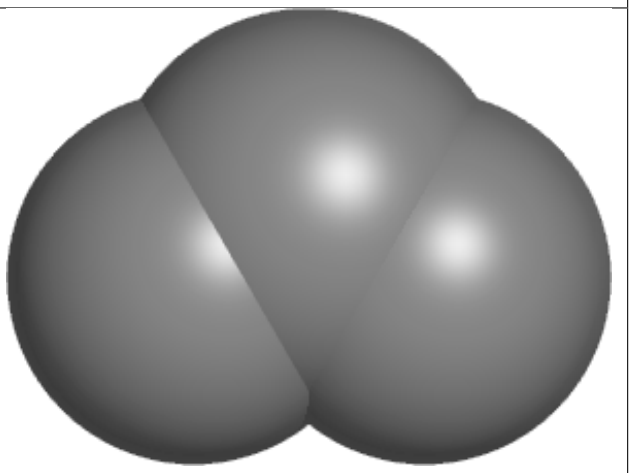


Rings

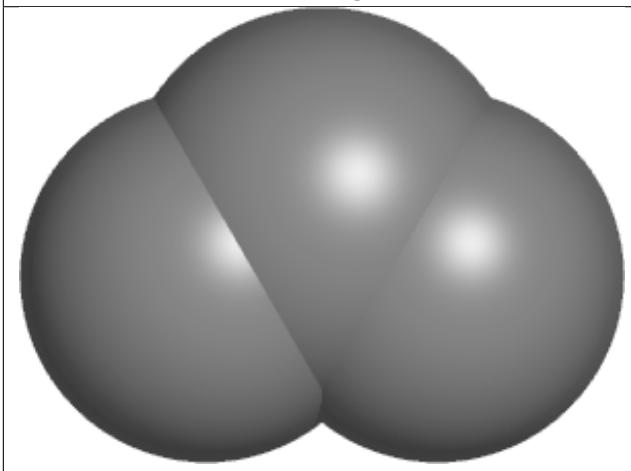
Ligand C2O B 502



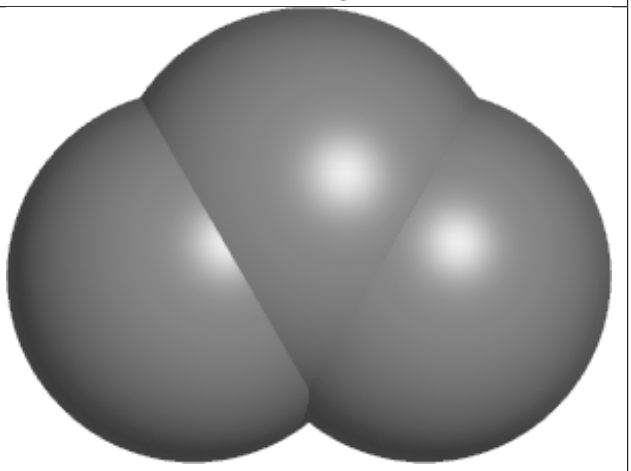
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.03	40 (8%)	11	8	28, 42, 78, 120	0
1	B	472/477 (98%)	0.06	37 (7%)	13	10	30, 42, 75, 129	0
All	All	949/954 (99%)	0.05	77 (8%)	12	9	28, 42, 77, 129	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	471	MET	10.8
1	B	469	HIS	6.8
1	B	465	PRO	6.4
1	A	463	ASP	6.3
1	A	464	HIS	6.1
1	B	463	ASP	5.7
1	B	466	ILE	5.3
1	B	320	LEU	5.3
1	A	237	LEU	5.0
1	B	462	PRO	4.6
1	B	464	HIS	4.5
1	B	237	LEU	4.0
1	A	466	ILE	3.9
1	B	467	GLU	3.9
1	B	46	ASN	3.8
1	A	313	ASP	3.7
1	A	189	LEU	3.7
1	B	470	LEU	3.6
1	B	143	TRP	3.5
1	B	313	ASP	3.5
1	A	143	TRP	3.4
1	A	465	PRO	3.4
1	B	461	ASP	3.3
1	A	188	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	279	ALA	3.2
1	A	187	VAL	3.1
1	B	468	TYR	3.1
1	B	189	LEU	3.0
1	A	330	ALA	3.0
1	A	0	SER	3.0
1	B	393	ILE	2.9
1	A	393	ILE	2.8
1	B	0	SER	2.8
1	B	142	ILE	2.8
1	A	293	PRO	2.8
1	A	312	GLY	2.8
1	A	314	ILE	2.8
1	B	276	LEU	2.8
1	A	461	ASP	2.7
1	A	471	MET	2.7
1	B	361	GLN	2.7
1	B	418	THR	2.7
1	A	292	GLN	2.7
1	A	279	ALA	2.6
1	B	323	SER	2.6
1	B	312	GLY	2.6
1	B	247	LEU	2.6
1	A	236	PHE	2.5
1	B	334	ASP	2.5
1	B	357	LEU	2.5
1	B	359	ASP	2.5
1	B	324	PRO	2.5
1	A	247	LEU	2.5
1	A	294	GLY	2.5
1	A	467	GLU	2.5
1	A	469	HIS	2.5
1	A	144	LEU	2.3
1	A	276	LEU	2.3
1	B	315	LYS	2.3
1	A	361	GLN	2.3
1	A	462	PRO	2.3
1	B	316	LYS	2.3
1	B	396	CYS	2.3
1	A	473	MET	2.2
1	A	282	ALA	2.2
1	B	292	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	2.2
1	A	65	LYS	2.2
1	A	44	GLU	2.2
1	B	107	GLY	2.2
1	A	160	LEU	2.1
1	A	468	TYR	2.1
1	B	236	PHE	2.1
1	A	418	THR	2.1
1	A	334	ASP	2.1
1	A	470	LEU	2.1
1	A	335	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

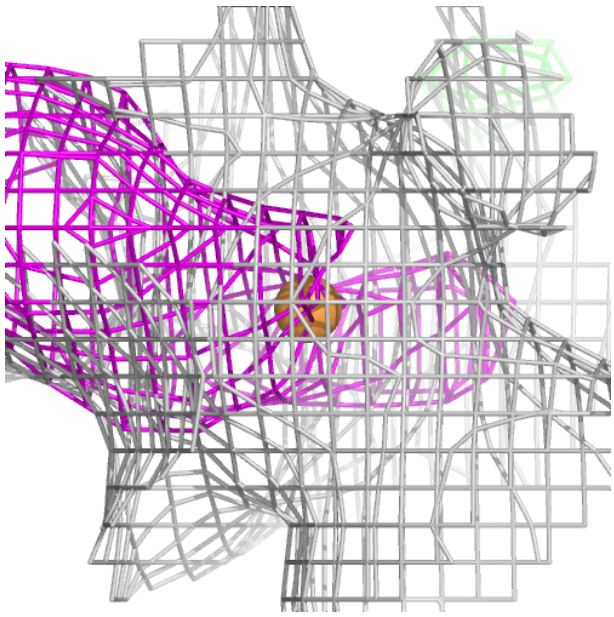
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	504	1/1	0.87	0.16	79,79,79,79	0
4	CL	B	505	1/1	0.90	0.17	85,85,85,85	0
5	BEN	B	504	9/9	0.96	0.12	34,43,56,60	0
2	CU	A	503	1/1	0.99	0.05	60,60,60,60	0
2	CU	B	503	1/1	0.99	0.05	64,64,64,64	0
3	C2O	B	502	3/3	0.99	0.07	28,28,42,60	0
2	CU	A	501	1/1	1.00	0.07	37,37,37,37	0
3	C2O	A	502	3/3	1.00	0.08	26,26,42,58	0
2	CU	B	501	1/1	1.00	0.06	38,38,38,38	0

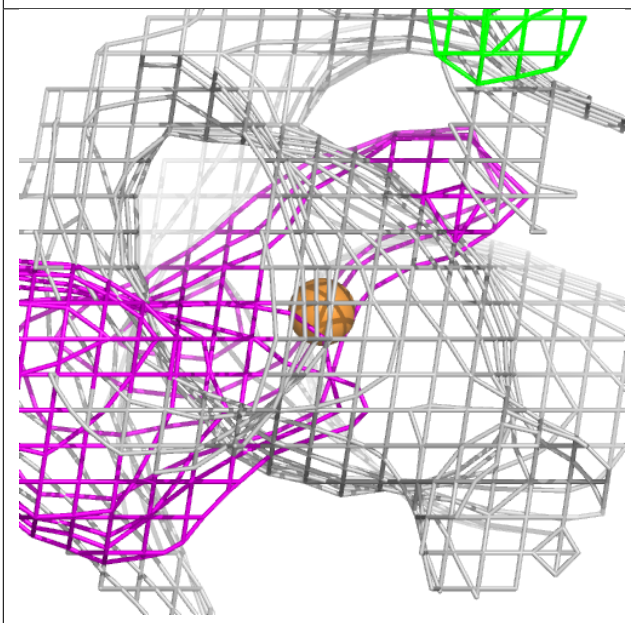
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

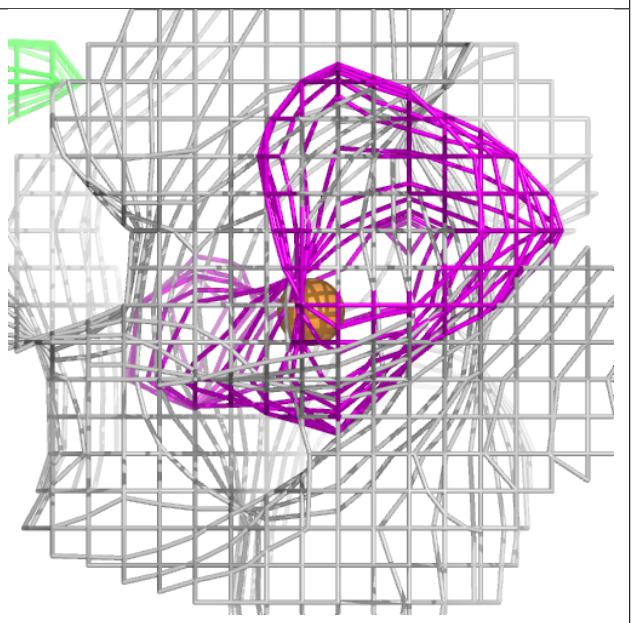
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

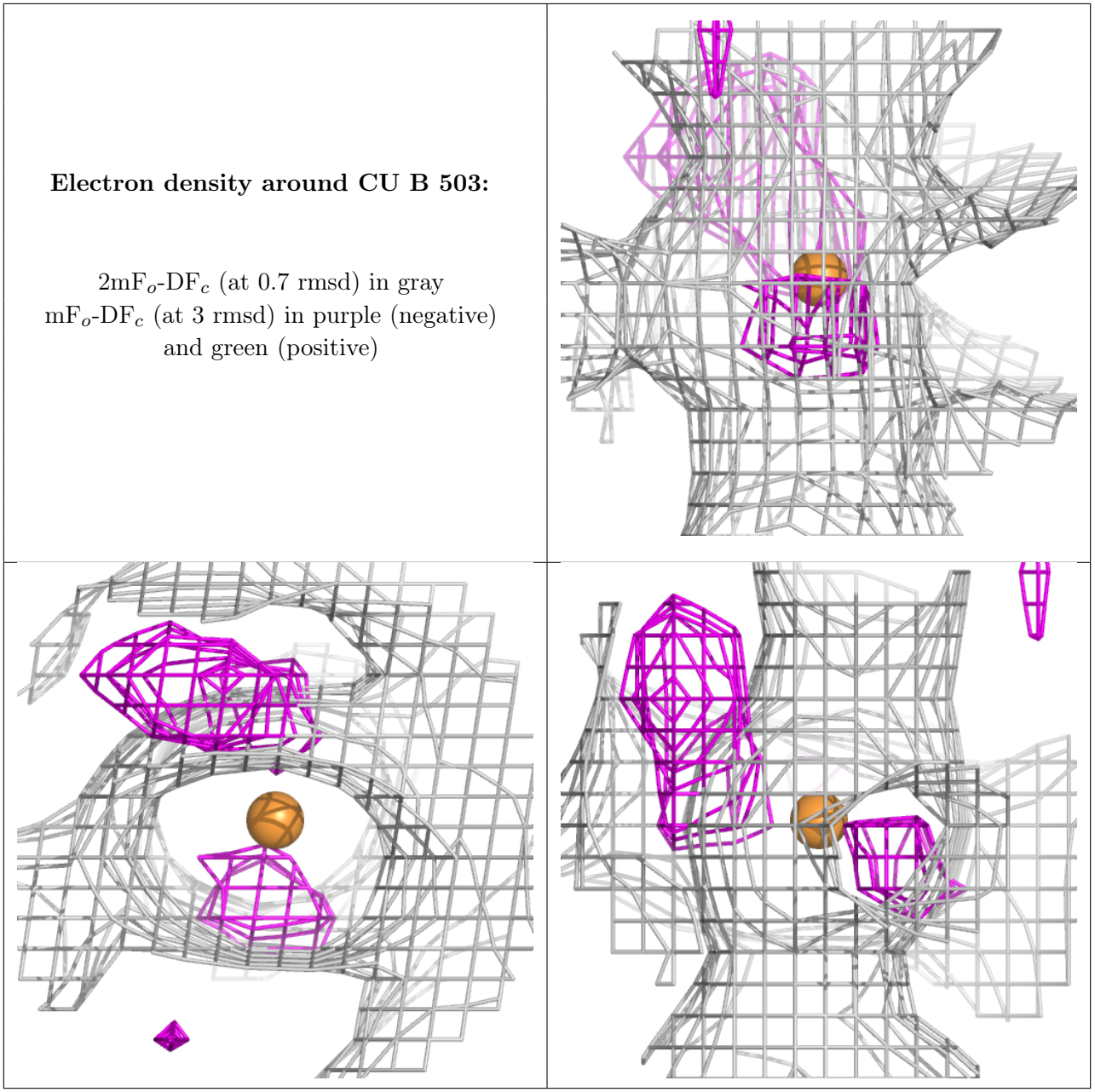






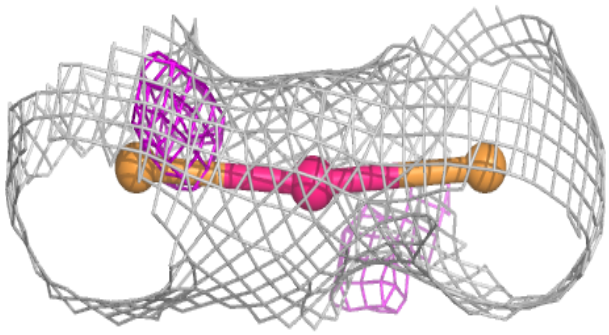
Electron density around CU B 503:

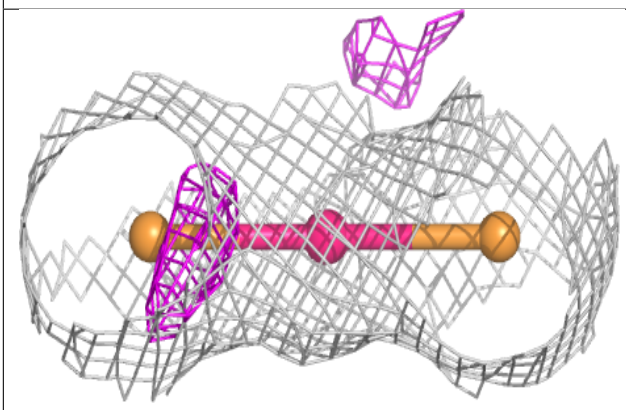
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

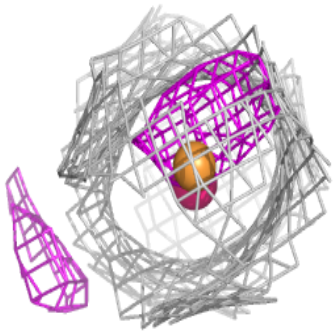


Electron density around C2O B 502:

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

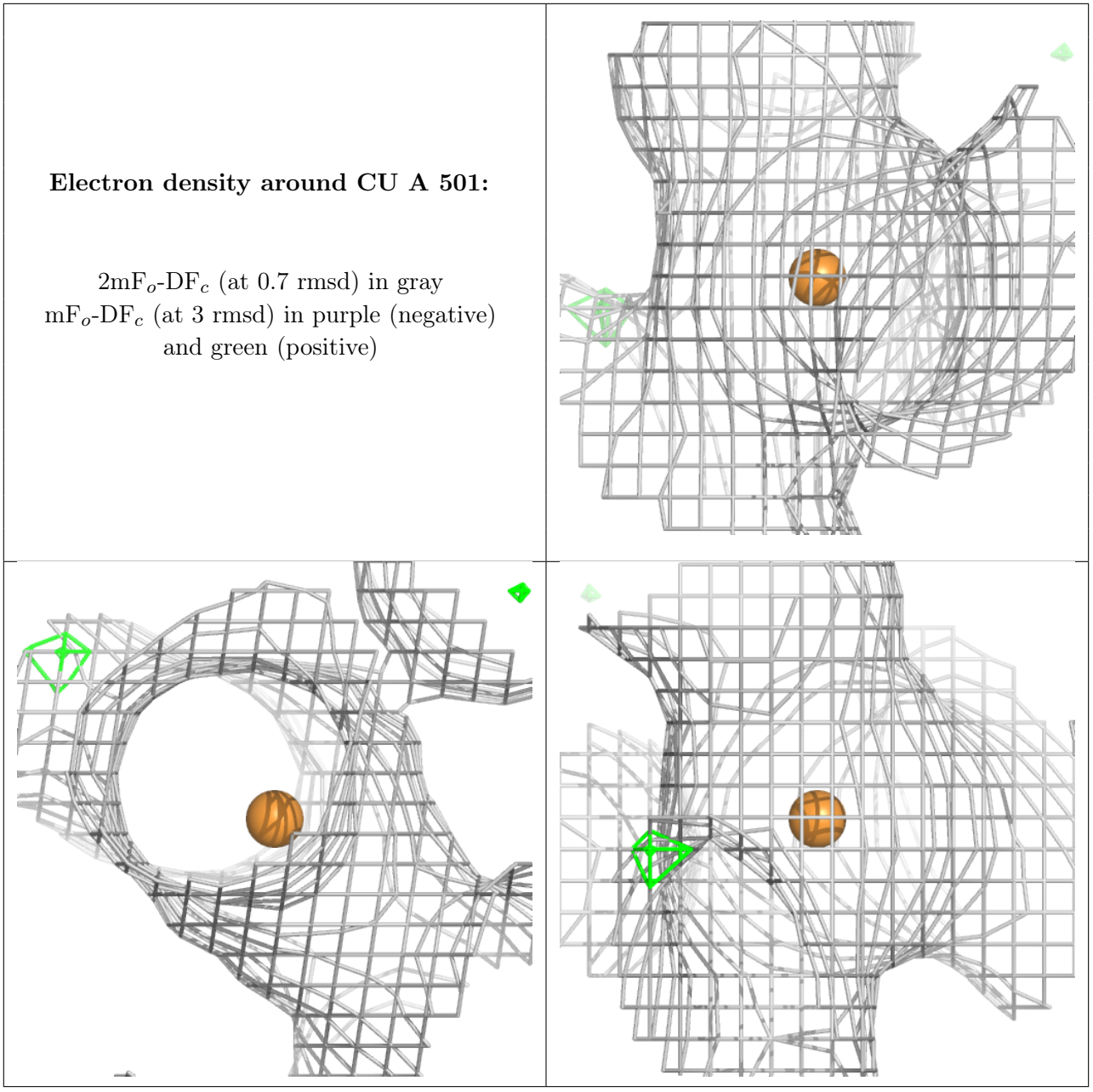






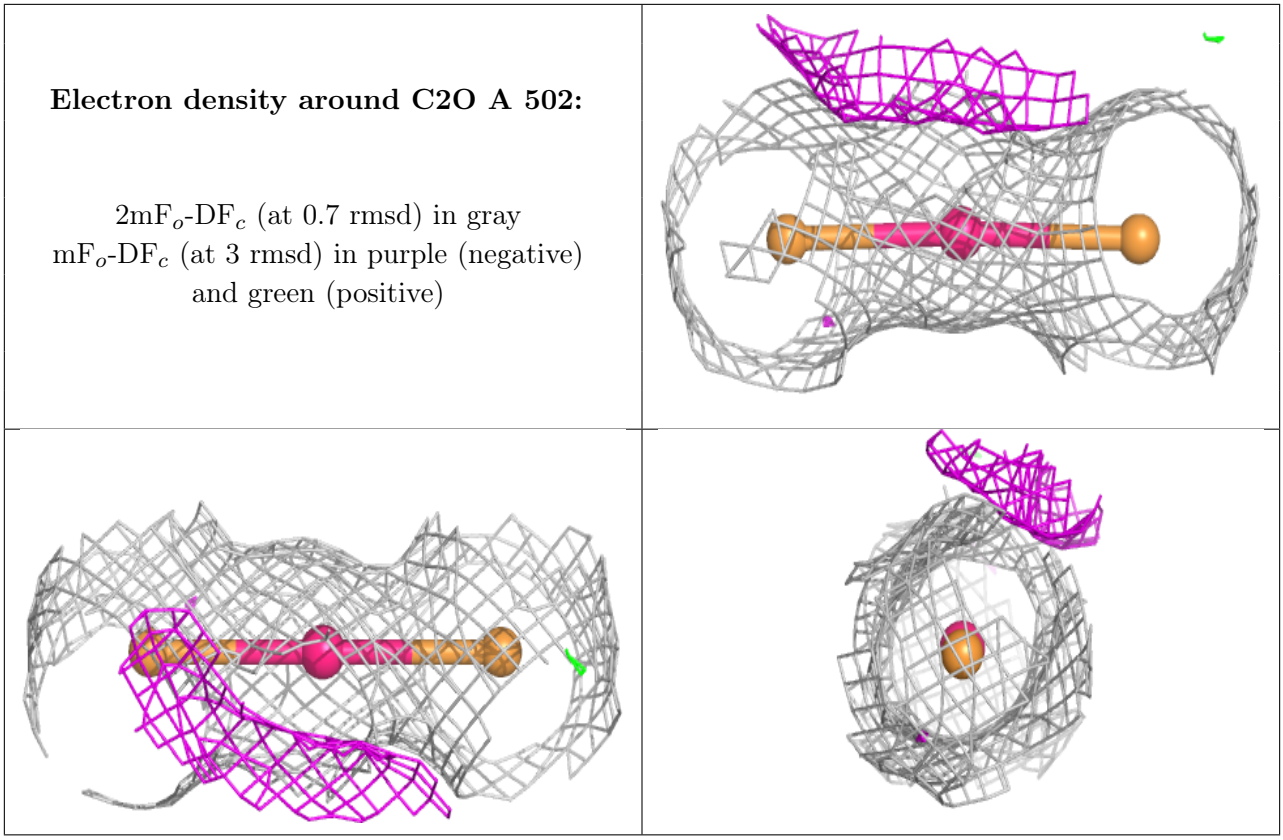
Electron density around CU A 501:

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



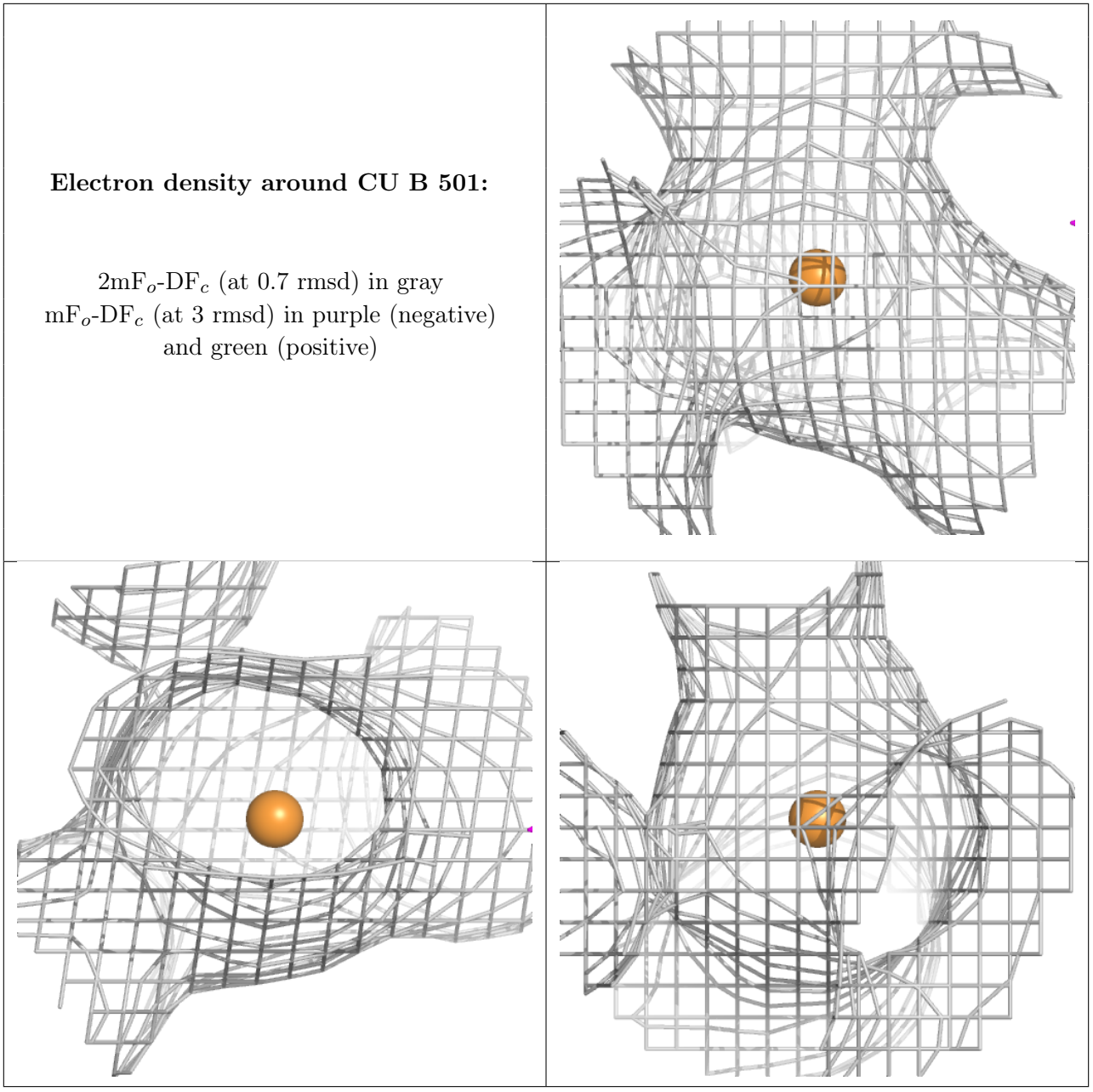
Electron density around C2O A 502:

$2mF_o$-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.