wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 03:01 am GMT

PDB ID	:	5O3K
Title	:	Crystal Structure of mutant M54L/M64L/M96L of Two-Domain Laccase from Streptomyces griseoflavus with 1 mM copper sulfate on growth medium
Authors	:	Gabdulkhakov, A.G.; Tishchenko, T.V.
Deposited on	:	2017-05-24
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

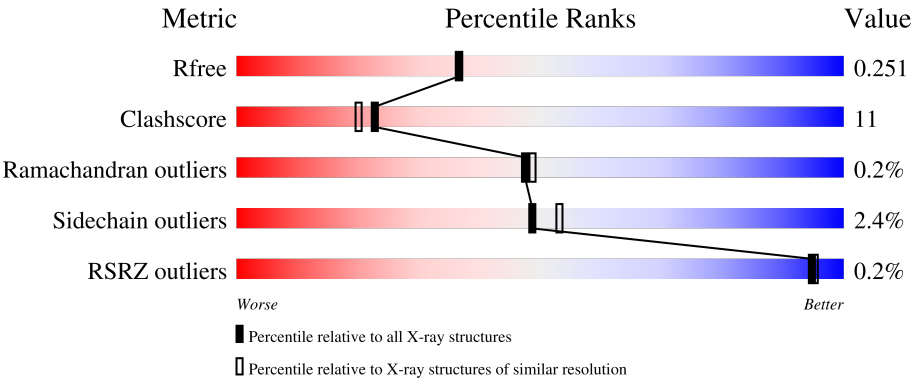
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	322	63% 24% 13%
1	B	322	% 61% 24% · 14%
1	C	322	65% 20% · 14%
1	D	322	66% 21% 13%
1	E	322	66% 20% 14%

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Mol	Chain	Length	Quality of chain
1	F	322	61% 25% 14%
1	G	322	70% 18% 13%
1	H	322	64% 21% 14%
1	I	322	56% 29% 15%
1	J	322	62% 24% 13%
1	K	322	66% 19% 14%
1	L	322	66% 19% 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25889 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 Two-domain laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2158	1347	395	407	9			
1	B	278	Total	C	N	O	S	0	1	0
			2139	1336	391	403	9			
1	C	277	Total	C	N	O	S	0	0	0
			2125	1328	388	400	9			
1	D	281	Total	C	N	O	S	0	1	0
			2164	1350	396	408	10			
1	E	278	Total	C	N	O	S	0	1	0
			2139	1336	391	403	9			
1	F	276	Total	C	N	O	S	0	1	0
			2125	1327	388	401	9			
1	G	281	Total	C	N	O	S	0	1	0
			2164	1350	396	408	10			
1	H	278	Total	C	N	O	S	0	1	0
			2139	1336	391	403	9			
1	I	275	Total	C	N	O	S	0	1	0
			2117	1323	387	398	9			
1	J	281	Total	C	N	O	S	0	1	0
			2164	1350	396	408	10			
1	K	278	Total	C	N	O	S	0	1	0
			2139	1336	391	403	9			
1	L	276	Total	C	N	O	S	0	0	0
			2118	1323	387	399	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
A	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
A	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
B	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
B	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81

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Chain	Residue	Modelled	Actual	Comment	Reference
B	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
C	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
C	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
C	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
D	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
D	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
D	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
E	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
E	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
E	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
F	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
F	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
F	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
G	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
G	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
G	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
H	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
H	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
H	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
I	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
I	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
I	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
J	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
J	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
J	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
K	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
K	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
K	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81
L	54	LEU	MET	engineered mutation	UNP A0A0M4FJ81
L	64	LEU	MET	engineered mutation	UNP A0A0M4FJ81
L	96	LEU	MET	engineered mutation	UNP A0A0M4FJ81

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cu 3 3	0	0
2	B	3	Total Cu 3 3	0	0
2	C	3	Total Cu 3 3	0	0
2	D	3	Total Cu 3 3	0	0

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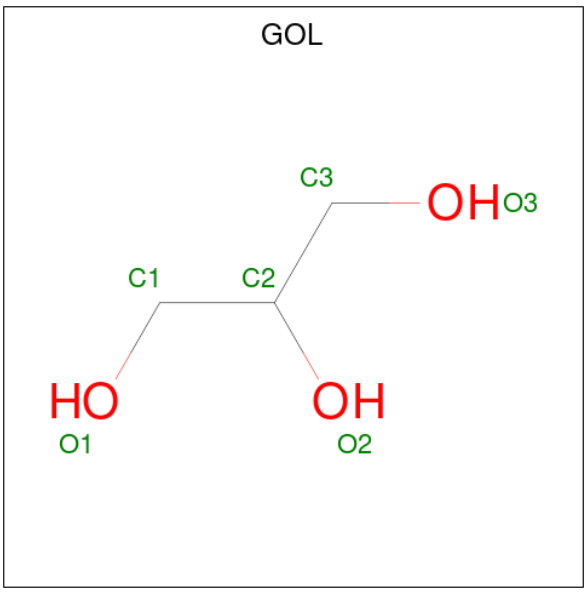
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	3	Total Cu 3 3	0	0
2	F	4	Total Cu 4 4	0	0
2	G	4	Total Cu 4 4	0	0
2	H	4	Total Cu 4 4	0	0
2	I	3	Total Cu 3 3	0	0
2	J	3	Total Cu 3 3	0	0
2	K	3	Total Cu 3 3	0	0
2	L	4	Total Cu 4 4	0	0

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

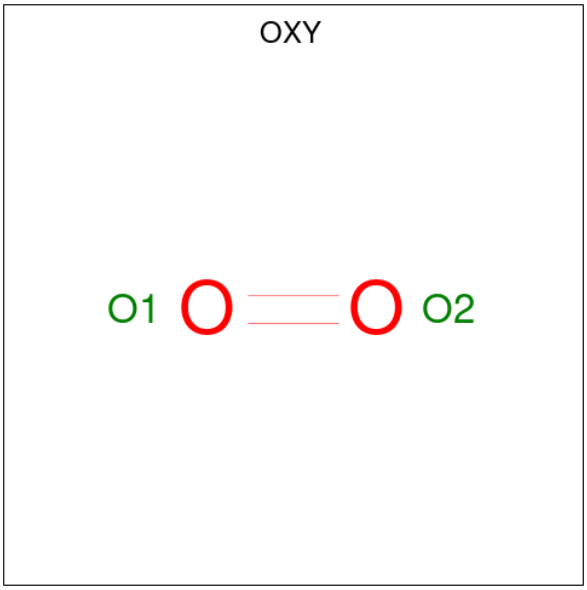
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	14	Total O 14 14	0	0
6	B	12	Total O 12 12	0	0
6	C	10	Total O 10 10	0	0
6	D	10	Total O 10 10	0	0
6	E	9	Total O 9 9	0	0
6	F	15	Total O 15 15	0	0

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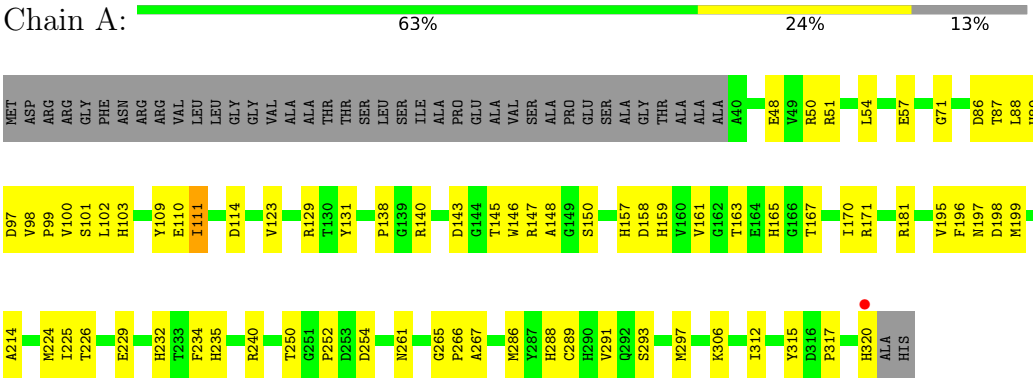
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	10	Total O 10 10	0	0
6	H	7	Total O 7 7	0	0
6	I	15	Total O 15 15	0	0
6	J	15	Total O 15 15	0	0
6	K	7	Total O 7 7	0	0
6	L	13	Total O 13 13	0	0

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.

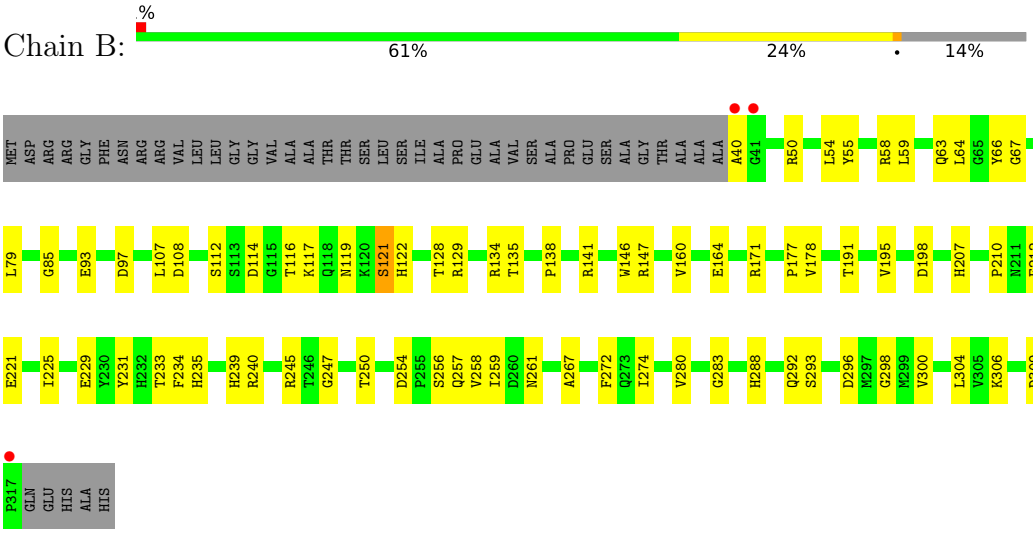
• Molecule 1: Two-domain laccase

Chain A:



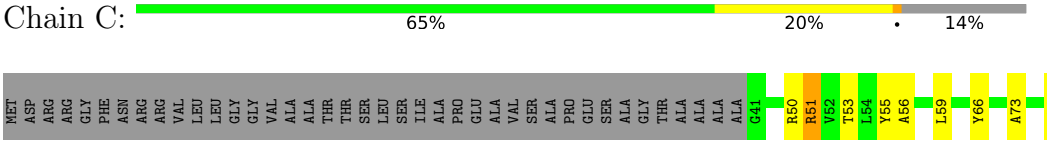
• Molecule 1: Two-domain laccase

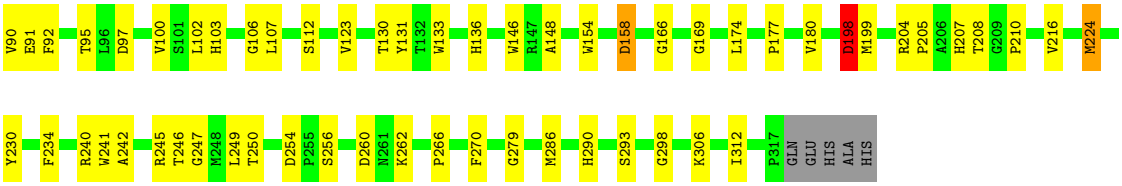
Chain B:



• Molecule 1: Two-domain laccase

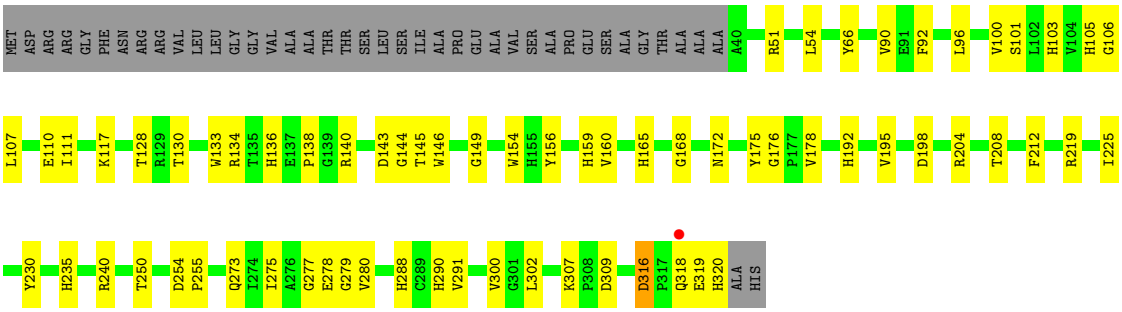
Chain C:





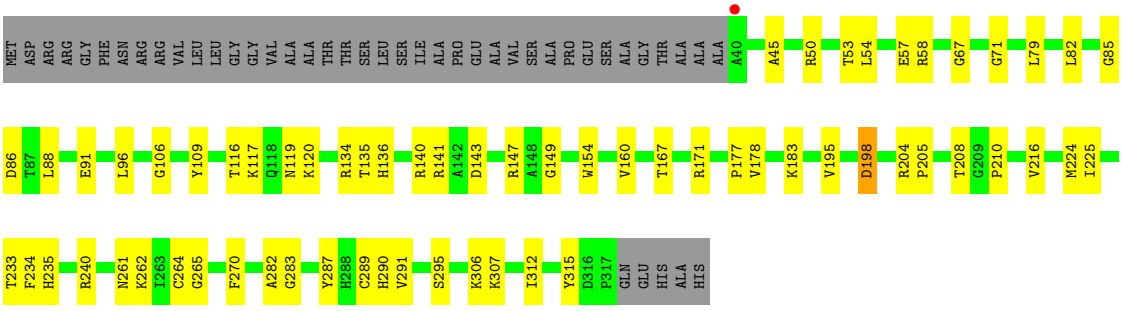
• Molecule 1: Two-domain laccase

Chain D:



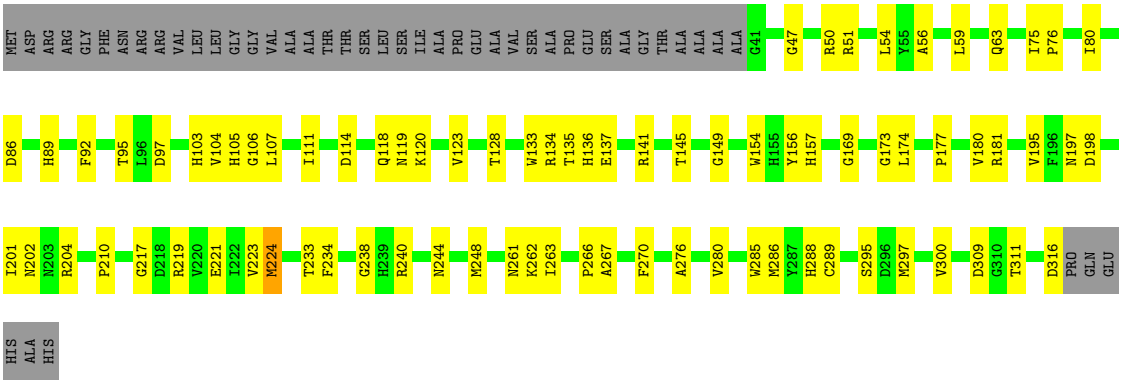
• Molecule 1: Two-domain laccase

Chain E:



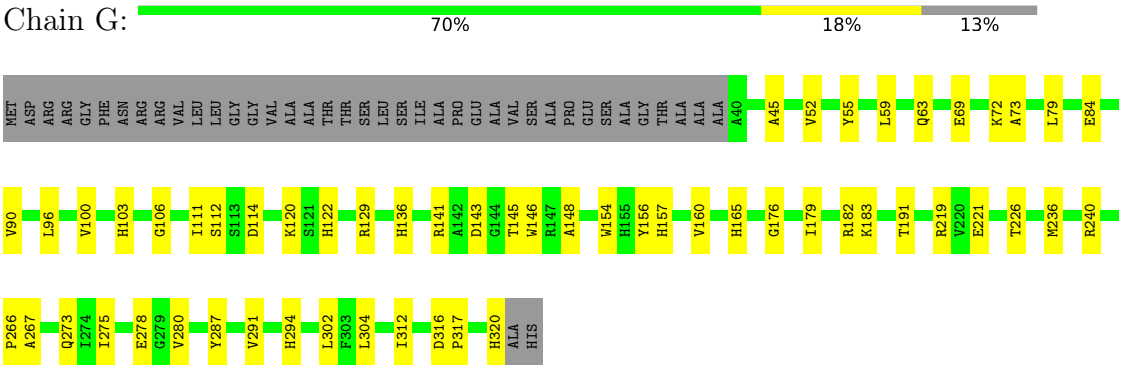
• Molecule 1: Two-domain laccase

Chain F:



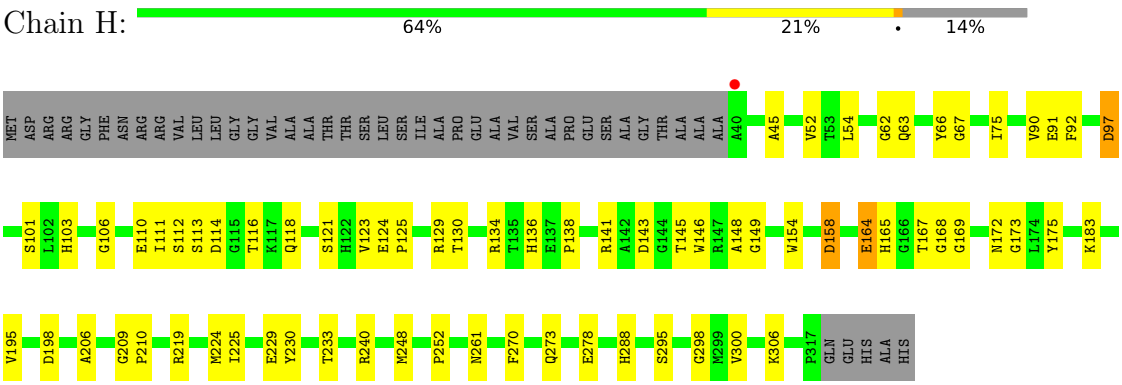
• Molecule 1: Two-domain laccase

Chain G:



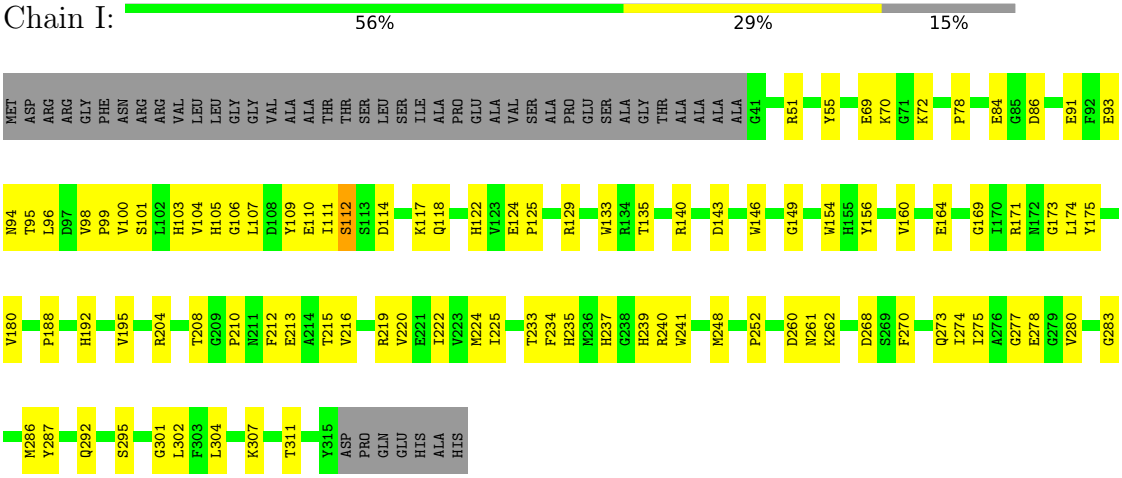
• Molecule 1: Two-domain laccase

Chain H:



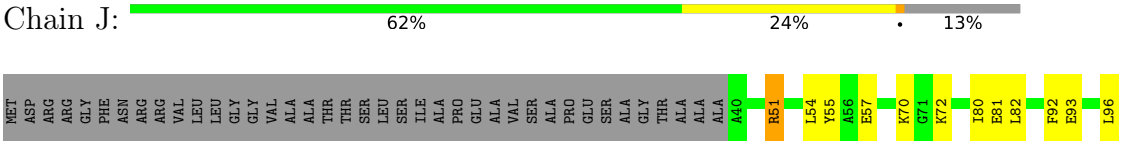
• Molecule 1: Two-domain laccase

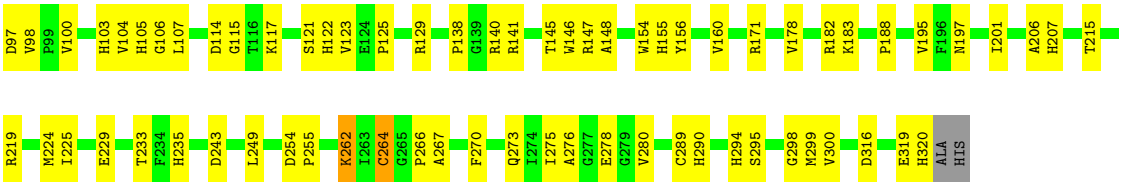
Chain I:



• Molecule 1: Two-domain laccase

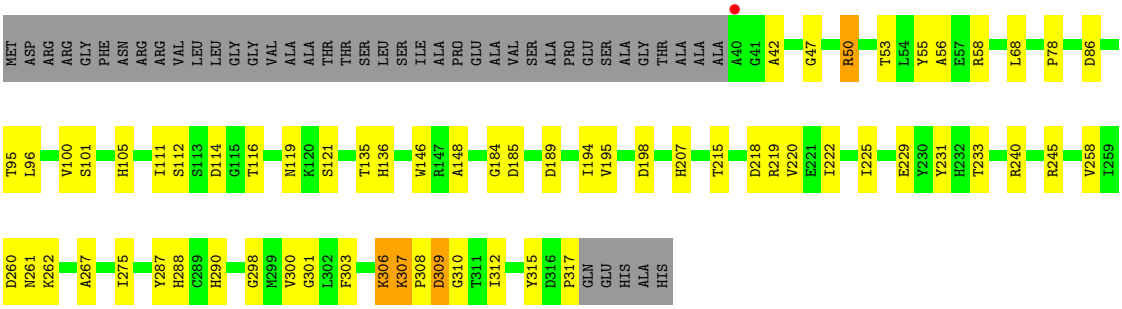
Chain J:





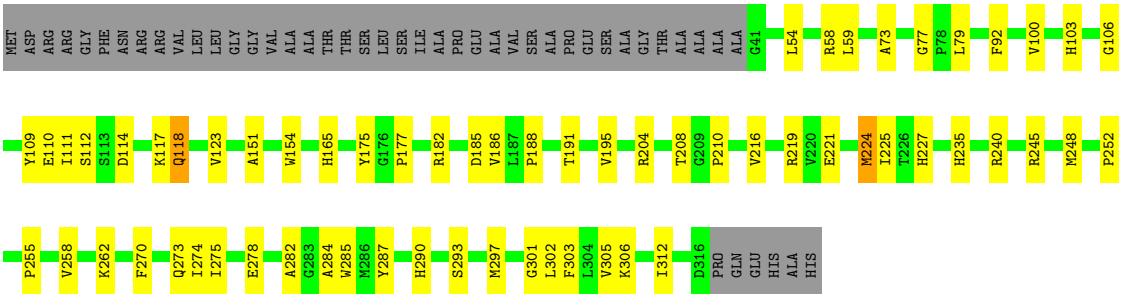
• Molecule 1: Two-domain laccase

Chain K:



• Molecule 1: Two-domain laccase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.03Å 94.96Å 116.46Å 89.88° 90.07° 91.70°	Depositor
Resolution (Å)	49.59 – 2.10 49.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.59-2.10) 91.2 (49.59-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.196 , 0.262 0.182 , 0.251	Depositor DCC
R_{free} test set	8929 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 20.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.176 for h,-k,-l 0.177 for -h,k,-l 0.417 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25889	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, O, GOL, OXY

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	0.54	2/2221 (0.1%)	0.65	0/3020
1	B	0.44	0/2201	0.65	0/2993
1	C	0.52	0/2187	0.66	2/2974 (0.1%)
1	D	0.44	0/2227	0.64	0/3028
1	E	0.49	1/2201 (0.0%)	0.65	0/2993
1	F	0.42	0/2186	0.63	0/2972
1	G	0.43	0/2227	0.62	0/3028
1	H	0.46	0/2201	0.63	0/2993
1	I	0.44	0/2178	0.62	1/2961 (0.0%)
1	J	0.50	0/2227	0.66	0/3028
1	K	0.47	0/2201	0.64	0/2993
1	L	0.47	0/2179	0.65	0/2962
All	All	0.47	3/26436 (0.0%)	0.64	3/35945 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	198	ASP	C-O	-6.82	1.10	1.23
1	A	196	PHE	CG-CD2	-5.92	1.29	1.38
1	A	197	ASN	C-O	-5.69	1.12	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	198	ASP	CB-CG-OD1	6.26	123.93	118.30
1	I	268	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	198	ASP	CB-CG-OD2	-5.13	113.68	118.30

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	2158	0	2029	62	0
1	B	2139	0	2014	58	0
1	C	2125	0	2002	46	0
1	D	2164	0	2032	50	0
1	E	2139	0	2015	53	0
1	F	2125	0	2001	54	0
1	G	2164	0	2032	41	0
1	H	2139	0	2014	53	0
1	I	2117	0	1997	64	0
1	J	2164	0	2032	63	0
1	K	2139	0	2014	50	0
1	L	2118	0	1995	48	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	1	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	4	0	0	0	0
3	A	1	0	0	1	0
4	B	6	0	8	1	0
4	C	6	0	8	0	0
4	K	6	0	8	1	0
5	D	2	0	0	0	0
6	A	14	0	0	3	0
6	B	12	0	0	5	0
6	C	10	0	0	0	0
6	D	10	0	0	4	0
6	E	9	0	0	2	0
6	F	15	0	0	2	0
6	G	10	0	0	0	0
6	H	7	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	15	0	0	0	0
6	J	15	0	0	2	0
6	K	7	0	0	0	0
6	L	13	0	0	5	0
All	All	25889	0	24201	572	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 11.

The worst 5 of 572 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:D:140:ARG:NH2	1:D:144:GLY:O	1.67	1.27
1:J:224:MET:HE2	1:J:270:PHE:CE1	1.89	1.08
1:E:289:CYS:HG	2:E:401:CU:CU	0.73	0.93
1:D:140:ARG:CZ	1:D:144:GLY:O	2.16	0.91
1:B:112:SER:O	1:B:129:ARG:NH2	2.05	0.90

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	279/322 (87%)	268 (96%)	10 (4%)	1 (0%)	34 32
1	B	277/322 (86%)	264 (95%)	13 (5%)	0	100 100
1	C	275/322 (85%)	264 (96%)	10 (4%)	1 (0%)	34 32
1	D	280/322 (87%)	267 (95%)	13 (5%)	0	100 100
1	E	277/322 (86%)	265 (96%)	11 (4%)	1 (0%)	34 32
1	F	275/322 (85%)	262 (95%)	13 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	280/322 (87%)	266 (95%)	14 (5%)	0	100 100
1	H	277/322 (86%)	266 (96%)	10 (4%)	1 (0%)	34 32
1	I	274/322 (85%)	265 (97%)	9 (3%)	0	100 100
1	J	280/322 (87%)	266 (95%)	14 (5%)	0	100 100
1	K	277/322 (86%)	264 (95%)	11 (4%)	2 (1%)	22 18
1	L	274/322 (85%)	258 (94%)	16 (6%)	0	100 100
All	All	3325/3864 (86%)	3175 (96%)	144 (4%)	6 (0%)	47 49

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	C	198	ASP
1	H	198	ASP
1	E	198	ASP
1	K	198	ASP

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	222/249 (89%)	215 (97%)	7 (3%)	39 41
1	B	220/249 (88%)	215 (98%)	5 (2%)	50 55
1	C	219/249 (88%)	213 (97%)	6 (3%)	44 48
1	D	223/249 (90%)	220 (99%)	3 (1%)	69 75
1	E	220/249 (88%)	217 (99%)	3 (1%)	67 73
1	F	219/249 (88%)	211 (96%)	8 (4%)	34 35
1	G	223/249 (90%)	220 (99%)	3 (1%)	69 75
1	H	220/249 (88%)	213 (97%)	7 (3%)	39 41
1	I	218/249 (88%)	213 (98%)	5 (2%)	50 55
1	J	223/249 (90%)	217 (97%)	6 (3%)	44 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	220/249 (88%)	214 (97%)	6 (3%)	44 48
1	L	218/249 (88%)	211 (97%)	7 (3%)	39 41
All	All	2645/2988 (88%)	2579 (98%)	66 (2%)	49 52

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	307	LYS
1	L	58	ARG
1	L	274	ILE
1	F	50	ARG
1	E	240	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	165	HIS
1	D	320	HIS
1	J	103	HIS
1	J	155	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 41 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	GOL	C	404	-	5,5,5	0.32	0	5,5,5	0.46	0
5	OXY	D	404	2	1,1,1	0.25	0	-		
4	GOL	K	404	-	5,5,5	0.49	0	5,5,5	1.16	1 (20%)
4	GOL	B	404	-	5,5,5	0.43	0	5,5,5	1.18	1 (20%)

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
4	GOL	C	404	-	-	1/4/4/4	-
4	GOL	K	404	-	-	2/4/4/4	-
4	GOL	B	404	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	404	GOL	O1-C1-C2	-2.16	99.85	110.20
4	B	404	GOL	O1-C1-C2	-2.00	100.60	110.20

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	GOL	O1-C1-C2-C3
4	B	404	GOL	C1-C2-C3-O3
4	B	404	GOL	O2-C2-C3-O3
4	B	404	GOL	O1-C1-C2-O2
4	C	404	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	404	GOL	1	0
4	B	404	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	281/322 (87%)	-0.53	1 (0%) 92 93	12, 21, 36, 68	0
1	B	278/322 (86%)	-0.48	3 (1%) 80 84	14, 22, 36, 62	0
1	C	277/322 (86%)	-0.56	0 100 100	11, 20, 32, 40	0
1	D	281/322 (87%)	-0.54	1 (0%) 92 93	11, 20, 33, 74	0
1	E	278/322 (86%)	-0.50	1 (0%) 92 93	12, 21, 34, 62	0
1	F	276/322 (85%)	-0.54	0 100 100	9, 22, 35, 47	1 (0%)
1	G	281/322 (87%)	-0.52	0 100 100	12, 23, 38, 49	4 (1%)
1	H	278/322 (86%)	-0.46	1 (0%) 92 93	11, 23, 38, 52	3 (1%)
1	I	275/322 (85%)	-0.41	0 100 100	12, 24, 39, 50	2 (0%)
1	J	281/322 (87%)	-0.52	0 100 100	11, 21, 36, 58	4 (1%)
1	K	278/322 (86%)	-0.45	1 (0%) 92 93	13, 25, 36, 58	2 (0%)
1	L	276/322 (85%)	-0.58	0 100 100	12, 21, 31, 42	1 (0%)
All	All	3340/3864 (86%)	-0.51	8 (0%) 95 95	9, 22, 36, 74	17 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	ALA	4.3
1	B	41	GLY	4.2
1	H	40	ALA	3.1
1	K	40	ALA	2.8
1	B	317	PRO	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

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	GOL	K	404	6/6	0.97	0.09	13,16,19,21	0
4	GOL	B	404	6/6	0.98	0.10	17,19,25,28	0
4	GOL	C	404	6/6	0.98	0.08	8,14,18,23	0
2	CU	G	403	1/1	0.98	0.05	38,38,38,38	1
2	CU	B	402	1/1	0.99	0.07	34,34,34,34	0
2	CU	H	403	1/1	0.99	0.09	18,18,18,18	1
2	CU	K	402	1/1	0.99	0.07	36,36,36,36	0
2	CU	L	403	1/1	0.99	0.07	31,31,31,31	0
2	CU	L	404	1/1	0.99	0.04	29,29,29,29	1
2	CU	B	403	1/1	0.99	0.10	26,26,26,26	0
2	CU	D	402	1/1	0.99	0.06	30,30,30,30	0
2	CU	F	404	1/1	0.99	0.07	26,26,26,26	1
2	CU	E	401	1/1	1.00	0.09	24,24,24,24	0
2	CU	E	402	1/1	1.00	0.09	25,25,25,25	0
2	CU	E	403	1/1	1.00	0.11	27,27,27,27	0
2	CU	F	401	1/1	1.00	0.10	31,31,31,31	0
2	CU	F	402	1/1	1.00	0.07	19,19,19,19	0
2	CU	F	403	1/1	1.00	0.09	23,23,23,23	0
2	CU	B	401	1/1	1.00	0.10	18,18,18,18	0
2	CU	G	401	1/1	1.00	0.07	18,18,18,18	0
2	CU	G	402	1/1	1.00	0.09	25,25,25,25	0
2	CU	A	401	1/1	1.00	0.07	20,20,20,20	0
2	CU	G	404	1/1	1.00	0.09	27,27,27,27	0
2	CU	H	401	1/1	1.00	0.10	19,19,19,19	0
2	CU	H	402	1/1	1.00	0.07	30,30,30,30	0
2	CU	A	402	1/1	1.00	0.07	27,27,27,27	0
2	CU	H	404	1/1	1.00	0.07	30,30,30,30	0
2	CU	I	401	1/1	1.00	0.10	27,27,27,27	0
2	CU	I	402	1/1	1.00	0.09	23,23,23,23	0
2	CU	I	403	1/1	1.00	0.07	24,24,24,24	1
2	CU	J	401	1/1	1.00	0.09	19,19,19,19	0
2	CU	J	402	1/1	1.00	0.10	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	J	403	1/1	1.00	0.08	29,29,29,29	0
2	CU	K	401	1/1	1.00	0.10	26,26,26,26	0
2	CU	C	401	1/1	1.00	0.10	20,20,20,20	0
2	CU	K	403	1/1	1.00	0.09	27,27,27,27	0
2	CU	L	401	1/1	1.00	0.10	24,24,24,24	0
2	CU	L	402	1/1	1.00	0.09	20,20,20,20	0
2	CU	C	402	1/1	1.00	0.07	20,20,20,20	0
2	CU	C	403	1/1	1.00	0.07	27,27,27,27	0
3	O	A	403	1/1	1.00	0.08	15,15,15,15	0
2	CU	D	401	1/1	1.00	0.08	15,15,15,15	0
2	CU	A	404	1/1	1.00	0.07	28,28,28,28	0
2	CU	D	403	1/1	1.00	0.08	22,22,22,22	0
5	OXY	D	404	2/2	1.00	0.08	15,15,15,16	0

6.5 Other polymers (i)

There are no such residues in this entry.