



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:00 PM UTC

PDB ID : 5O4Q / pdb_00005o4q
Title : Crystal Structure of mutant M54L/M64L/M96L of Two-Domain Laccase from Streptomyces griseoflavus with 0.25 mM copper sulfate on growth medium
Authors : Gabdulkhakov, A.G.; Tishchenko, T.V.
Deposited on : 2017-05-30
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

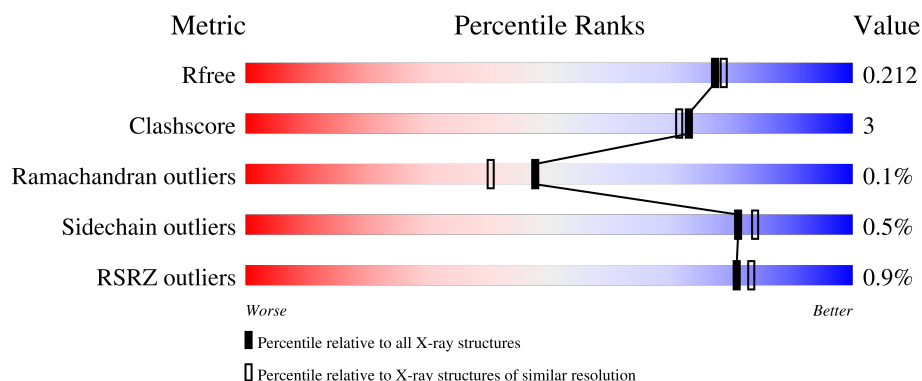
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	% 80% 7% 13%
1	B	322	% 77% 9% 14%
1	C	322	% 77% 8% 15%
1	D	322	% 80% 6% 14%
1	E	322	% 79% 7% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	322	
1	G	322	
1	H	322	
1	I	322	
1	J	322	
1	K	322	
1	L	322	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AZI	B	403	-	X	-	-
4	AZI	E	403	-	X	-	-
4	AZI	H	403	-	X	-	-
4	AZI	J	403	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26408 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	2	0
			2171	1355	397	409	10			
1	B	278	Total	C	N	O	S	0	1	0
			2139	1336	391	403	9			
1	C	275	Total	C	N	O	S	0	3	0
			2133	1333	389	402	9			
1	D	278	Total	C	N	O	S	0	0	0
			2130	1331	389	401	9			
1	E	278	Total	C	N	O	S	0	2	0
			2144	1341	391	403	9			
1	F	275	Total	C	N	O	S	0	0	0
			2110	1319	386	396	9			
1	G	278	Total	C	N	O	S	0	0	0
			2130	1331	389	401	9			
1	H	278	Total	C	N	O	S	0	1	0
			2133	1333	389	401	10			
1	I	275	Total	C	N	O	S	0	0	0
			2110	1319	386	396	9			
1	J	280	Total	C	N	O	S	0	0	0
			2148	1341	392	406	9			
1	K	278	Total	C	N	O	S	0	1	0
			2133	1333	389	401	10			
1	L	275	Total	C	N	O	S	0	0	0
			2110	1319	386	396	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

Continued on next page...

Continued from previous page...

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 (CCD ID: CU) (formula: Cu).

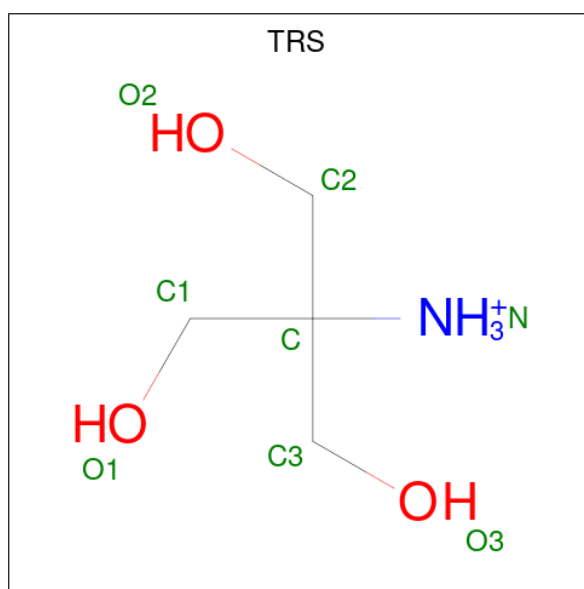
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0

Continued on next page...

Continued from previous page...

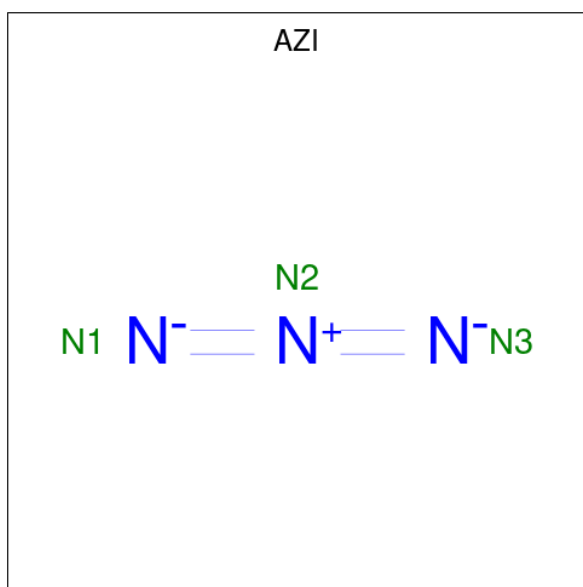
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Cu	0	0
			2	2		
2	F	2	Total	Cu	0	0
			2	2		
2	G	2	Total	Cu	0	0
			2	2		
2	H	2	Total	Cu	0	0
			2	2		
2	I	2	Total	Cu	0	0
			2	2		
2	J	2	Total	Cu	0	0
			2	2		
2	K	2	Total	Cu	0	0
			2	2		
2	L	2	Total	Cu	0	0
			2	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



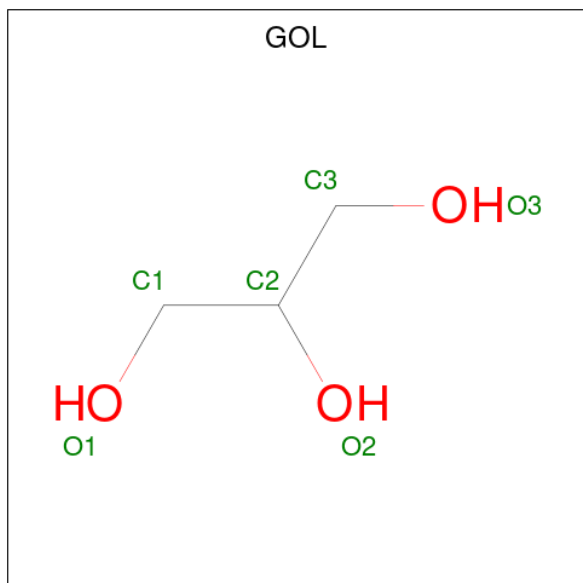
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	J	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is AZIDE ION (CCD ID: AZI) (formula: N_3).



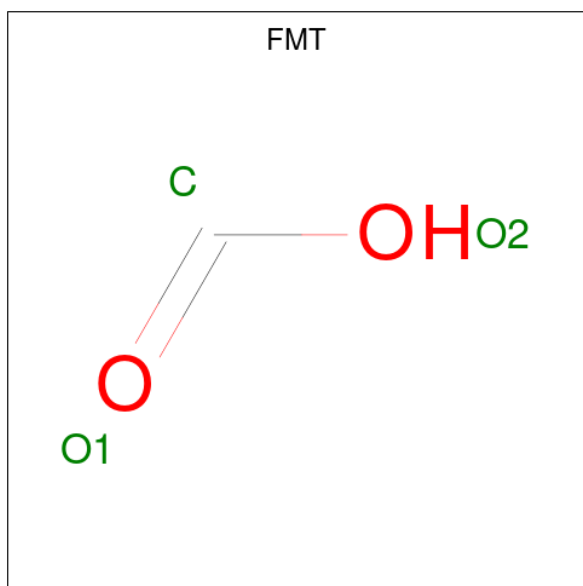
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total N 3 3	0	0
4	E	1	Total N 3 3	0	0
4	H	1	Total N 3 3	0	0
4	J	1	Total N 3 3	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



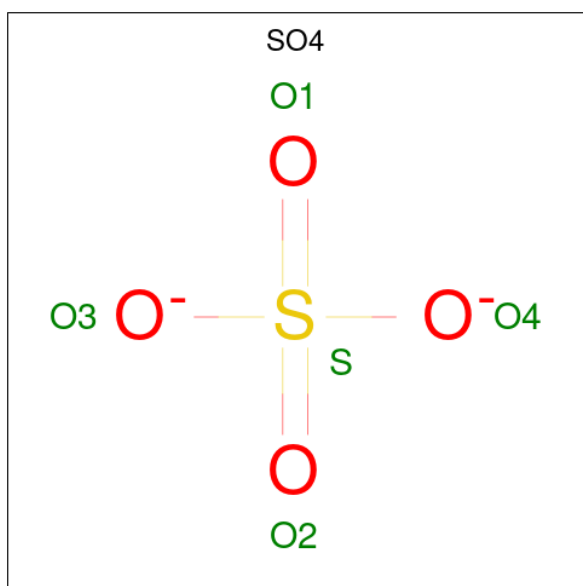
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	K	1	Total	O	S	0	0
			5	4	1		

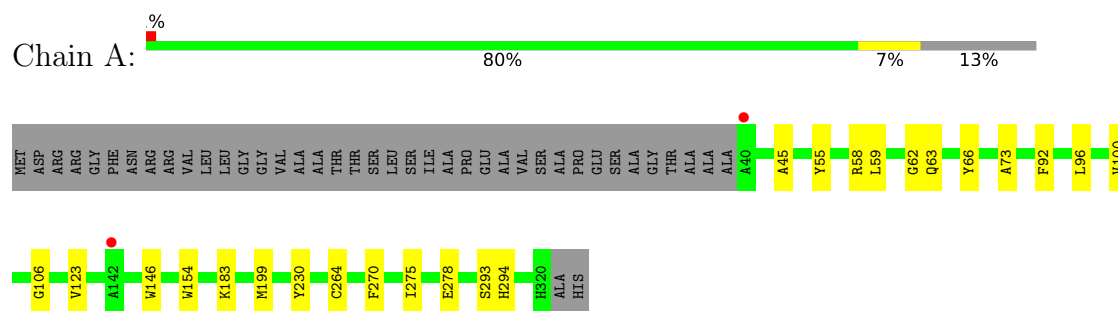
- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	74	Total	O		0	0
			74	74			
8	B	68	Total	O		0	0
			68	68			
8	C	59	Total	O		0	0
			59	59			
8	D	56	Total	O		0	0
			56	56			
8	E	76	Total	O		0	0
			76	76			
8	F	73	Total	O		0	0
			73	73			
8	G	61	Total	O		0	0
			61	61			
8	H	55	Total	O		0	0
			55	55			
8	I	46	Total	O		0	0
			46	46			
8	J	66	Total	O		0	0
			66	66			
8	K	71	Total	O		0	0
			71	71			
8	L	46	Total	O		0	0
			46	46			

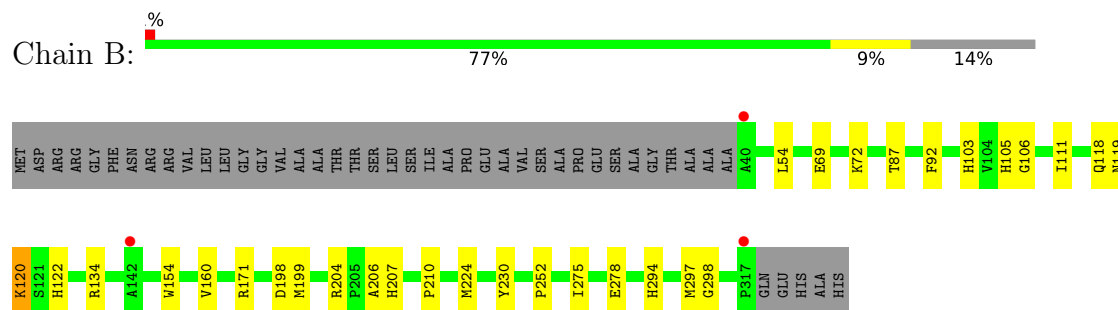
3 Residue-property plots [i](#)

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.

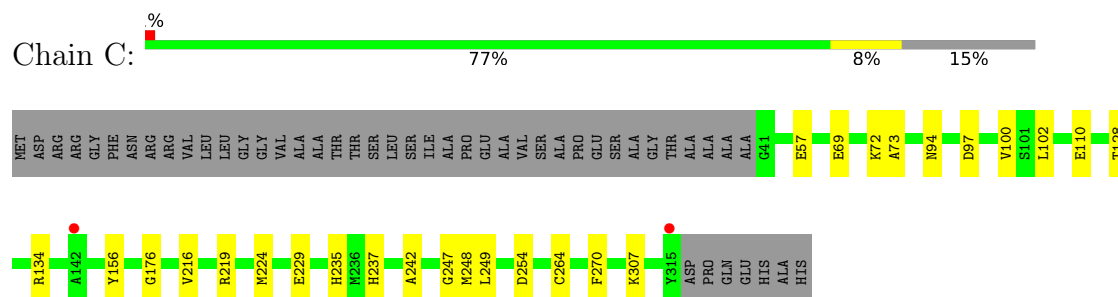
- Molecule 1: Two-domain laccase



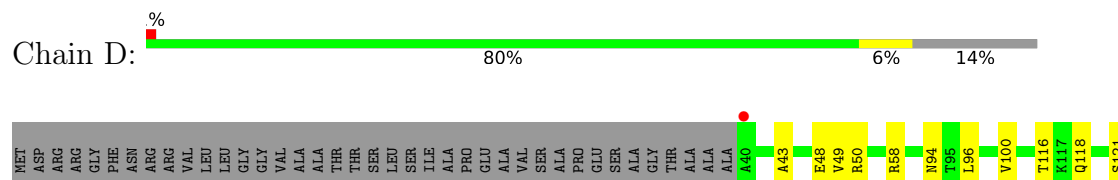
- Molecule 1: Two-domain laccase



- Molecule 1: Two-domain laccase

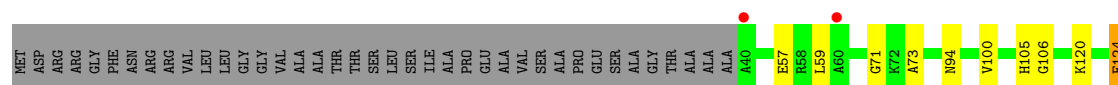
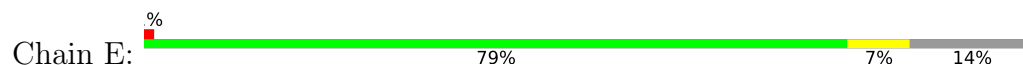


- Molecule 1: Two-domain laccase

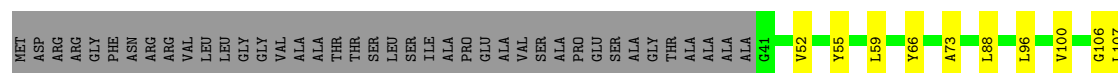
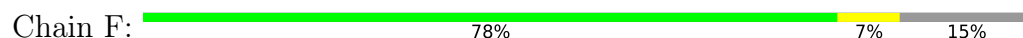




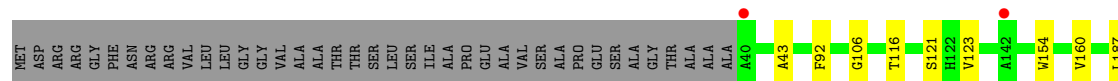
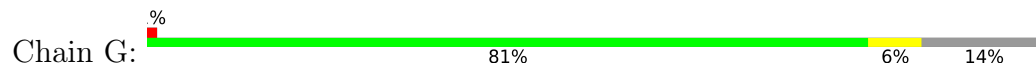
- Molecule 1: Two-domain laccase



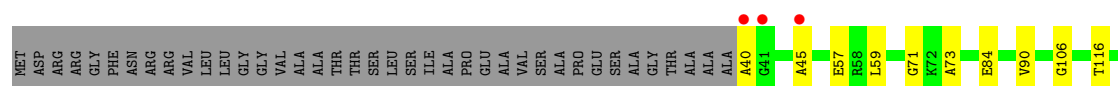
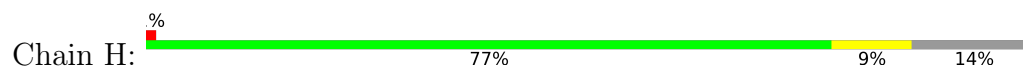
- Molecule 1: Two-domain laccase



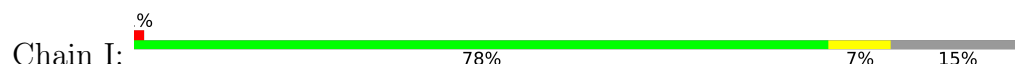
- Molecule 1: Two-domain laccase

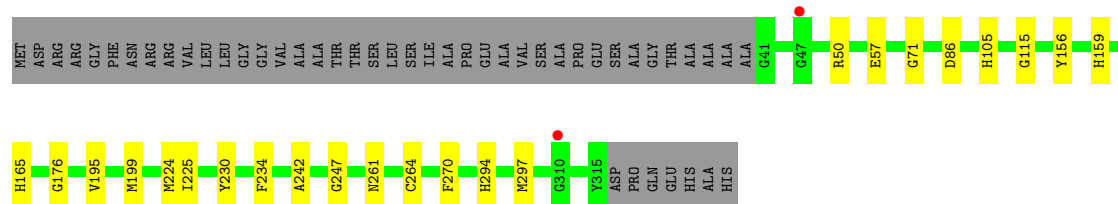


- Molecule 1: Two-domain laccase

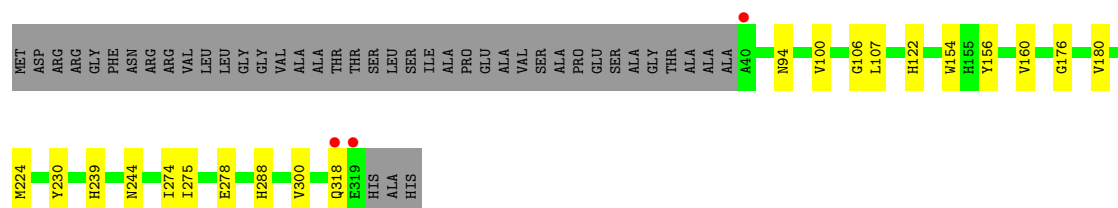
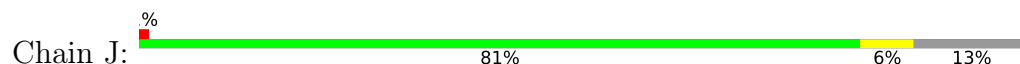


- Molecule 1: Two-domain laccase

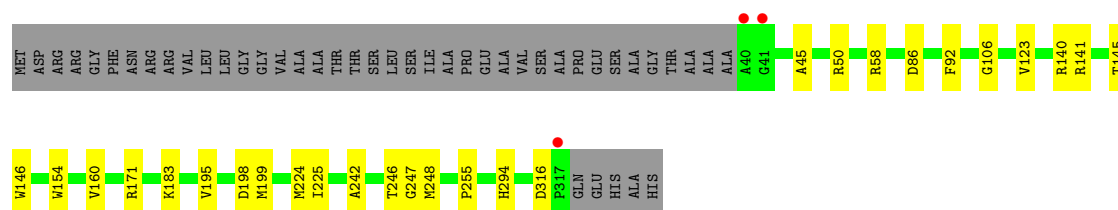
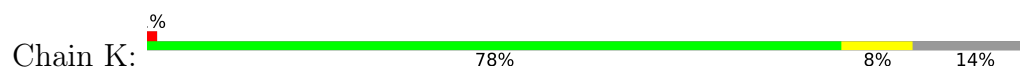




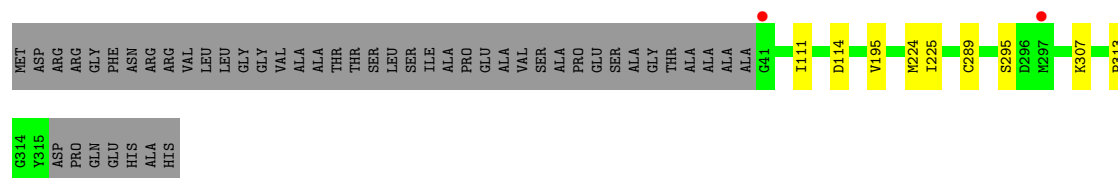
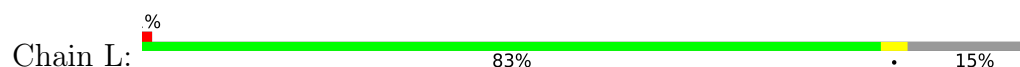
• Molecule 1: Two-domain laccase



• Molecule 1: Two-domain laccase



• Molecule 1: Two-domain laccase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.84Å 94.85Å 116.61Å 90.04° 90.29° 91.49°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-1.90) 95.7 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.187 , 0.213 0.189 , 0.212	Depositor DCC
R_{free} test set	12501 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l 0.155 for -h,k,-l 0.115 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26408	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: SO4, CU, GOL, AZI, FMT, TRS

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	0.44	0/2234	0.61	0/3038
1	B	0.43	0/2201	0.59	0/2993
1	C	0.41	0/2194	0.60	0/2983
1	D	0.43	0/2192	0.61	0/2981
1	E	0.47	0/2206	0.62	1/3001 (0.0%)
1	F	0.45	0/2171	0.61	0/2951
1	G	0.42	0/2192	0.59	0/2981
1	H	0.43	0/2198	0.60	0/2989
1	I	0.42	0/2171	0.57	0/2951
1	J	0.46	1/2210 (0.0%)	0.60	0/3005
1	K	0.42	0/2198	0.58	0/2989
1	L	0.41	0/2171	0.58	0/2951
All	All	0.43	1/26338 (0.0%)	0.60	1/35813 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	318	GLN	C-O	-5.14	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	233	THR	CB-CA-C	6.25	119.61	111.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2171	0	2040	17	0
1	B	2139	0	2014	19	0
1	C	2133	0	2010	18	0
1	D	2130	0	2007	13	0
1	E	2144	0	2023	13	0
1	F	2110	0	1991	13	0
1	G	2130	0	2007	12	0
1	H	2133	0	2012	23	0
1	I	2110	0	1991	15	0
1	J	2148	0	2021	12	0
1	K	2133	0	2012	14	0
1	L	2110	0	1991	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	8	0	12	4	0
3	J	8	0	12	1	0
4	B	3	0	0	1	0
4	E	3	0	0	1	0
4	H	3	0	0	0	0
4	J	3	0	0	0	0
5	B	6	0	8	1	0
6	D	3	0	1	0	0
7	K	5	0	0	1	0
8	A	74	0	0	2	0
8	B	68	0	0	0	0
8	C	59	0	0	0	0
8	D	56	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	76	0	0	0	0
8	F	73	0	0	0	0
8	G	61	0	0	0	0
8	H	55	0	0	1	0
8	I	46	0	0	0	0
8	J	66	0	0	0	0
8	K	71	0	0	0	0
8	L	46	0	0	0	0
All	All	26408	0	24152	161	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 3.

All (161) 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:H:45:ALA:HA	1:H:183:LYS:HG3	1.57	0.83
1:I:199:MET:HE3	1:I:230:TYR:CD2	2.19	0.78
1:I:199:MET:HE1	1:I:294:HIS:CE1	2.19	0.77
3:A:403:TRS:O2	3:A:403:TRS:O1	2.05	0.74
3:A:403:TRS:H22	8:H:549:HOH:O	1.88	0.72
1:A:293:SER:OG	1:C:229:GLU:OE1	2.06	0.72
1:C:224:MET:HE1	1:C:264:CYS:SG	2.31	0.70
1:D:116:THR:HG21	1:E:286:MET:HE1	1.77	0.67
3:A:403:TRS:H32	1:H:230:TYR:OH	1.96	0.65
1:A:230:TYR:OH	3:A:403:TRS:H12	1.98	0.64
1:H:84:GLU:OE1	1:H:183:LYS:NZ	2.27	0.63
1:A:58:ARG:HD2	8:A:501:HOH:O	1.99	0.62
1:C:224:MET:HE3	1:C:270:PHE:CE1	2.34	0.62
1:E:59:LEU:HD21	1:E:73:ALA:HB3	1.83	0.61
1:I:224:MET:HE1	1:I:264:CYS:SG	2.41	0.61
1:B:160:VAL:O	5:B:404:GOL:O3	2.15	0.61
1:G:286:MET:HE1	1:I:165:HIS:NE2	2.15	0.60
1:I:224:MET:HE3	1:I:270:PHE:CE1	2.35	0.60
1:A:96:LEU:HD12	1:A:100:VAL:HG21	1.84	0.60
1:B:120:LYS:HD3	1:B:122:HIS:HE1	1.68	0.58
1:K:242:ALA:O	1:K:247:GLY:HA2	2.05	0.57
1:J:107:LEU:HD21	1:J:180:VAL:HG21	1.87	0.56
1:E:315:TYR:O	1:E:317:PRO:HD3	2.06	0.55
1:A:199:MET:HE1	1:A:294:HIS:CD2	2.42	0.55
1:H:90:VAL:HG13	1:H:131:TYR:HB2	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:MET:HE1	1:K:294:HIS:CD2	2.42	0.54
1:K:316:ASP:OD1	1:K:316:ASP:N	2.39	0.54
1:F:199:MET:HE1	1:F:294:HIS:CD2	2.43	0.54
1:A:264[A]:CYS:SG	1:A:270:PHE:HE1	2.32	0.53
1:D:48:GLU:HG2	1:D:50:ARG:HG2	1.91	0.53
1:F:96:LEU:HD12	1:F:100:VAL:HG21	1.91	0.52
1:A:63:GLN:O	8:A:501:HOH:O	2.19	0.52
1:H:40:ALA:HB3	1:H:186:VAL:HG23	1.92	0.52
1:H:90:VAL:CG1	1:H:131:TYR:HB2	2.39	0.51
1:K:171:ARG:HD3	1:K:198:ASP:OD2	2.10	0.51
1:A:275:ILE:HB	1:A:278:GLU:HB2	1.93	0.51
1:D:94:ASN:CG	1:D:100:VAL:HG12	2.34	0.51
1:J:107:LEU:CD2	1:J:180:VAL:HG21	2.40	0.51
1:B:171:ARG:HD3	1:B:198:ASP:OD2	2.11	0.51
1:F:297:MET:HE2	1:F:297:MET:HA	1.92	0.51
1:J:239:HIS:CD2	1:J:274:ILE:HD12	2.46	0.51
1:L:307:LYS:HE3	1:L:313:PRO:HG3	1.92	0.51
1:G:116:THR:HG21	1:H:286:MET:CE	2.41	0.51
1:K:106:GLY:HA3	1:K:154:TRP:CD2	2.46	0.51
1:B:207:HIS:CD2	1:B:298:GLY:HA2	2.45	0.50
1:J:106:GLY:HA3	1:J:154:TRP:CD2	2.46	0.50
1:H:106:GLY:HA3	1:H:154:TRP:CD2	2.47	0.50
1:J:230:TYR:OH	3:J:404:TRS:H12	2.12	0.49
1:H:59:LEU:HD21	1:H:73:ALA:HB3	1.94	0.49
1:K:45:ALA:HB2	1:K:183:LYS:HD3	1.93	0.49
1:E:57:GLU:CD	1:E:71:GLY:H	2.21	0.49
1:B:199:MET:HE1	1:B:294:HIS:CD2	2.47	0.48
1:I:156:TYR:CZ	1:I:176:GLY:HA3	2.48	0.48
1:B:69:GLU:HB2	1:B:72:LYS:HD2	1.94	0.48
1:C:57:GLU:HG2	1:C:73:ALA:HB2	1.95	0.48
1:G:293:SER:O	1:G:297:MET:HG3	2.14	0.48
1:K:195:VAL:HA	1:K:225:ILE:O	2.14	0.48
1:B:120:LYS:HD3	1:B:122:HIS:CE1	2.47	0.48
1:C:219:ARG:HH22	1:C:248:MET:HE1	1.79	0.47
1:L:111:ILE:O	1:L:114:ASP:HB2	2.14	0.47
1:J:156:TYR:CZ	1:J:176:GLY:HA3	2.50	0.47
1:A:264[A]:CYS:SG	1:A:270:PHE:CE1	3.07	0.47
1:D:275:ILE:HB	1:D:278:GLU:HB2	1.97	0.47
1:H:183:LYS:HE2	1:H:183:LYS:H	1.79	0.47
1:D:58:ARG:HH11	1:D:96:LEU:HD22	1.80	0.47
1:C:224:MET:HE3	1:C:270:PHE:HE1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:MET:HE1	1:E:272:PHE:CE1	2.49	0.46
1:F:55:TYR:O	1:F:66:TYR:HA	2.15	0.46
1:D:121:SER:O	1:D:131:TYR:OH	2.29	0.46
1:D:266:PRO:O	1:E:233:THR:HG21	2.15	0.46
1:K:50:ARG:NH2	1:K:86:ASP:OD2	2.47	0.46
1:A:199:MET:HE1	1:A:294:HIS:CG	2.51	0.45
1:H:195:VAL:HA	1:H:225:ILE:O	2.16	0.45
1:E:124:GLU:HG3	1:E:125:PRO:HD2	1.99	0.45
1:F:120:LYS:O	1:F:129:ARG:NH2	2.50	0.45
1:A:45:ALA:HA	1:A:183:LYS:HB2	1.99	0.45
1:A:146:TRP:CH2	1:B:252:PRO:HG3	2.52	0.45
1:H:116:THR:H	1:H:121:SER:HB3	1.82	0.45
1:L:195:VAL:HG22	1:L:225:ILE:HB	1.98	0.45
1:B:103:HIS:CE1	1:C:237:HIS:CE1	3.05	0.45
1:H:237:HIS:CE1	1:H:286:MET:HE3	2.51	0.45
1:F:233:THR:O	1:F:289:CYS:HA	2.17	0.45
1:G:266:PRO:O	1:H:233:THR:HG21	2.17	0.45
1:B:204:ARG:HD3	1:B:210:PRO:HD3	1.99	0.44
1:C:216:VAL:HG21	1:C:307:LYS:HD3	1.99	0.44
1:A:92:PHE:HD2	1:A:123:VAL:HG21	1.83	0.44
1:G:235:HIS:CE1	1:I:105:HIS:CE1	3.05	0.44
1:E:233:THR:CG2	1:E:290:HIS:HB3	2.48	0.44
1:K:92:PHE:HD2	1:K:123:VAL:HG21	1.83	0.44
1:E:106:GLY:HA3	1:E:154:TRP:CD2	2.52	0.44
1:A:55:TYR:O	1:A:66:TYR:HA	2.18	0.43
1:F:234:PHE:O	1:F:261:ASN:HA	2.17	0.43
1:J:107:LEU:HD21	1:J:180:VAL:CG2	2.47	0.43
1:B:275:ILE:HB	1:B:278:GLU:HB2	2.00	0.43
1:C:102:LEU:HD11	1:C:156:TYR:CD1	2.52	0.43
1:H:242:ALA:O	1:H:247:GLY:HA2	2.17	0.43
1:K:246:THR:HB	1:K:248:MET:HE3	2.00	0.43
1:C:229:GLU:HG2	1:I:297:MET:CE	2.48	0.43
1:D:48:GLU:HG3	1:D:49:VAL:N	2.34	0.43
1:E:94:ASN:CG	1:E:100[A]:VAL:HG12	2.43	0.43
1:C:156:TYR:CZ	1:C:176:GLY:HA3	2.54	0.43
1:D:118:GLN:OE1	1:D:118:GLN:N	2.43	0.43
1:G:289:CYS:O	1:G:295:SER:HB3	2.19	0.43
1:H:45:ALA:HA	1:H:183:LYS:CG	2.39	0.43
1:H:183:LYS:H	1:H:183:LYS:CD	2.31	0.43
1:I:57:GLU:CD	1:I:71:GLY:H	2.27	0.43
1:D:43:ALA:HB2	1:D:187:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:ALA:O	1:E:247:GLY:HA2	2.19	0.43
1:L:195:VAL:HA	1:L:225:ILE:O	2.19	0.43
1:B:54:LEU:O	1:B:92:PHE:HA	2.19	0.42
1:H:106:GLY:HA3	1:H:154:TRP:CE3	2.53	0.42
1:D:233:THR:O	1:D:289:CYS:HA	2.19	0.42
1:F:59:LEU:HD21	1:F:73:ALA:HB3	2.01	0.42
1:I:234:PHE:O	1:I:261:ASN:HA	2.19	0.42
1:G:242:ALA:O	1:G:247:GLY:HA2	2.19	0.42
1:H:205:PRO:HB2	1:H:208:THR:HG21	2.01	0.42
1:B:105:HIS:CE1	1:C:235:HIS:CE1	3.07	0.42
1:D:134:ARG:NH2	1:E:279:GLY:O	2.39	0.42
1:H:57:GLU:CD	1:H:71:GLY:H	2.27	0.42
1:J:275:ILE:HB	1:J:278:GLU:HB2	2.02	0.42
1:A:106:GLY:HA3	1:A:154:TRP:CD2	2.55	0.42
1:I:50:ARG:NH1	1:I:86:ASP:OD2	2.52	0.42
1:G:92:PHE:HD2	1:G:123:VAL:HG21	1.84	0.42
1:I:115:GLY:O	1:I:159:HIS:HB3	2.19	0.42
1:J:288:HIS:HB3	1:J:300:VAL:HG13	2.01	0.42
1:I:224:MET:HE2	1:I:234:PHE:HB2	2.02	0.42
1:J:244:ASN:HB2	1:K:255:PRO:O	2.20	0.42
1:A:62:GLY:HA3	1:H:205:PRO:HB3	2.01	0.41
1:C:69:GLU:HB2	1:C:72:LYS:HD2	2.01	0.41
1:C:94:ASN:CG	1:C:100:VAL:HG12	2.45	0.41
1:K:58:ARG:NH2	7:K:403:SO4:O4	2.37	0.41
1:G:43:ALA:HB2	1:G:187:LEU:HD21	2.02	0.41
1:A:59:LEU:HD21	1:A:73:ALA:HB3	2.01	0.41
1:F:106:GLY:HA3	1:F:154:TRP:CD2	2.55	0.41
1:K:141:ARG:NH1	1:K:145:THR:OG1	2.47	0.41
1:B:111:ILE:HG13	1:B:119:ASN:ND2	2.35	0.41
1:B:118[B]:GLN:HG3	1:B:119:ASN:N	2.33	0.41
1:G:116:THR:H	1:G:121:SER:HB3	1.86	0.41
1:J:122:HIS:HB3	1:J:160:VAL:HG21	2.02	0.41
1:B:87:THR:HG23	1:B:134:ARG:HG2	2.02	0.41
4:E:403:AZI:N3	1:F:263:ILE:HG22	2.36	0.41
1:I:195:VAL:HA	1:I:225:ILE:O	2.19	0.41
1:C:242:ALA:O	1:C:247:GLY:HA2	2.20	0.41
1:G:106:GLY:HA3	1:G:154:TRP:CD2	2.56	0.41
1:E:105:HIS:CE1	1:F:235:HIS:CE1	3.09	0.41
1:J:94:ASN:CG	1:J:100:VAL:HG12	2.46	0.41
1:B:106:GLY:HA3	1:B:154:TRP:CD2	2.56	0.41
1:C:110:GLU:HG3	1:C:134:ARG:HH21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:LEU:HD12	1:F:133:TRP:HB3	2.03	0.41
1:H:264[A]:CYS:HG	1:H:270:PHE:HE1	1.69	0.41
1:K:140:ARG:HG2	1:K:146:TRP:CZ3	2.55	0.41
1:L:289:CYS:O	1:L:295:SER:HB3	2.21	0.41
1:B:206:ALA:HB1	1:B:297:MET:O	2.21	0.41
1:B:230:TYR:HB3	4:B:403:AZI:N2	2.36	0.41
1:C:242:ALA:HB2	1:C:249[B]:LEU:HD22	2.02	0.41
1:H:207:HIS:CE1	1:H:298:GLY:HA2	2.55	0.41
1:G:92:PHE:CD2	1:G:123:VAL:HG21	2.56	0.40
1:D:58:ARG:NH1	1:D:96:LEU:HD22	2.35	0.40
1:F:52:VAL:HG12	1:F:88:LEU:HD11	2.02	0.40
1:C:249[B]:LEU:HD12	1:C:254:ASP:CG	2.47	0.40
1:I:242:ALA:O	1:I:247:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/322 (87%)	274 (98%)	7 (2%)	0	100	100
1	B	277/322 (86%)	270 (98%)	6 (2%)	1 (0%)	30	22
1	C	276/322 (86%)	270 (98%)	6 (2%)	0	100	100
1	D	276/322 (86%)	270 (98%)	6 (2%)	0	100	100
1	E	278/322 (86%)	273 (98%)	5 (2%)	0	100	100
1	F	273/322 (85%)	270 (99%)	3 (1%)	0	100	100
1	G	276/322 (86%)	266 (96%)	9 (3%)	1 (0%)	30	22
1	H	277/322 (86%)	269 (97%)	8 (3%)	0	100	100
1	I	273/322 (85%)	267 (98%)	6 (2%)	0	100	100
1	J	278/322 (86%)	271 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	277/322 (86%)	271 (98%)	6 (2%)	0	100	100
1	L	273/322 (85%)	268 (98%)	5 (2%)	0	100	100
All	All	3315/3864 (86%)	3239 (98%)	74 (2%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	LYS
1	G	160	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/249 (90%)	224 (100%)	0	100	100
1	B	220/249 (88%)	219 (100%)	1 (0%)	81	84
1	C	220/249 (88%)	217 (99%)	3 (1%)	59	59
1	D	219/249 (88%)	219 (100%)	0	100	100
1	E	221/249 (89%)	216 (98%)	5 (2%)	44	40
1	F	217/249 (87%)	216 (100%)	1 (0%)	81	84
1	G	219/249 (88%)	219 (100%)	0	100	100
1	H	220/249 (88%)	219 (100%)	1 (0%)	81	84
1	I	217/249 (87%)	217 (100%)	0	100	100
1	J	221/249 (89%)	220 (100%)	1 (0%)	81	84
1	K	220/249 (88%)	218 (99%)	2 (1%)	70	73
1	L	217/249 (87%)	216 (100%)	1 (0%)	81	84
All	All	2635/2988 (88%)	2620 (99%)	15 (1%)	81	81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	224	MET
1	C	97	ASP
1	C	128[A]	THR
1	C	128[B]	THR
1	E	120	LYS
1	E	124	GLU
1	E	224	MET
1	E	233	THR
1	E	248	MET
1	F	224	MET
1	H	224	MET
1	J	224	MET
1	K	160	VAL
1	K	224	MET
1	L	224	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	292	GLN
1	B	83	ASN
1	B	122	HIS
1	C	63	GLN
1	C	83	ASN
1	C	165	HIS
1	C	261	ASN
1	C	292	GLN
1	D	292	GLN
1	E	83	ASN
1	E	207	HIS
1	E	237	HIS
1	F	83	ASN
1	F	292	GLN
1	G	292	GLN
1	H	207	HIS
1	I	83	ASN
1	I	192	HIS
1	I	292	GLN
1	J	83	ASN
1	J	165	HIS
1	J	257	GLN
1	J	292	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	83	ASN
1	K	207	HIS
1	L	83	ASN
1	L	197	ASN
1	L	207	HIS
1	L	257	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 24 are monoatomic - leaving 9 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	AZI	H	403	-	2,2,2	2.60	2 (100%)	0,1,1	-	-
7	SO4	K	403	-	4,4,4	0.41	0	6,6,6	0.11	0
4	AZI	J	403	-	2,2,2	2.70	2 (100%)	0,1,1	-	-
6	FMT	D	403	-	2,2,2	0.67	0	1,1,1	0.50	0
5	GOL	B	404	-	5,5,5	0.20	0	5,5,5	0.21	0
3	TRS	J	404	-	7,7,7	0.36	0	9,9,9	0.88	0
4	AZI	E	403	-	2,2,2	2.52	2 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRS	A	403	-	7,7,7	0.29	0	9,9,9	0.91	0
4	AZI	B	403	-	2,2,2	2.75	2 (100%)	0,1,1	-	-

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	GOL	B	404	-	-	4/4/4/4	-
3	TRS	A	403	-	-	6/9/9/9	-
3	TRS	J	404	-	-	9/9/9/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	403	AZI	N1-N2	2.97	1.29	1.23
4	B	403	AZI	N3-N2	2.84	1.28	1.23
4	E	403	AZI	N1-N2	2.77	1.28	1.23
4	B	403	AZI	N1-N2	2.66	1.28	1.23
4	H	403	AZI	N3-N2	2.63	1.28	1.23
4	H	403	AZI	N1-N2	2.57	1.28	1.23
4	J	403	AZI	N3-N2	2.39	1.28	1.23
4	E	403	AZI	N3-N2	2.23	1.27	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	TRS	C2-C-C1-O1
3	A	403	TRS	C3-C-C1-O1
3	A	403	TRS	N-C-C1-O1
3	A	403	TRS	C1-C-C2-O2
3	A	403	TRS	N-C-C2-O2
3	J	404	TRS	C2-C-C1-O1
3	J	404	TRS	C3-C-C1-O1
3	J	404	TRS	N-C-C3-O3
5	B	404	GOL	O1-C1-C2-C3
5	B	404	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	404	GOL	C1-C2-C3-O3
3	J	404	TRS	C3-C-C2-O2
3	J	404	TRS	C2-C-C3-O3
3	A	403	TRS	C3-C-C2-O2
3	J	404	TRS	N-C-C2-O2
5	B	404	GOL	O2-C2-C3-O3
3	J	404	TRS	C1-C-C3-O3
3	J	404	TRS	N-C-C1-O1
3	J	404	TRS	C1-C-C2-O2

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	403	SO4	1	0
5	B	404	GOL	1	0
3	J	404	TRS	1	0
4	E	403	AZI	1	0
3	A	403	TRS	4	0
4	B	403	AZI	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	281/322 (87%)	-0.23	2 (0%) 84 86	8, 27, 40, 57	4 (1%)
1	B	278/322 (86%)	-0.05	3 (1%) 78 80	16, 29, 48, 74	2 (0%)
1	C	275/322 (85%)	-0.01	2 (0%) 84 86	13, 30, 47, 58	5 (1%)
1	D	278/322 (86%)	-0.11	2 (0%) 84 86	15, 29, 46, 65	5 (1%)
1	E	278/322 (86%)	-0.23	3 (1%) 78 80	12, 26, 40, 70	3 (1%)
1	F	275/322 (85%)	-0.16	1 (0%) 88 90	15, 27, 41, 66	3 (1%)
1	G	278/322 (86%)	-0.02	2 (0%) 84 86	17, 32, 48, 62	4 (1%)
1	H	278/322 (86%)	0.03	4 (1%) 73 76	16, 32, 49, 73	2 (0%)
1	I	275/322 (85%)	0.08	2 (0%) 84 86	17, 35, 49, 61	2 (0%)
1	J	280/322 (86%)	-0.14	3 (1%) 78 80	15, 27, 41, 65	3 (1%)
1	K	278/322 (86%)	-0.11	3 (1%) 78 80	14, 28, 46, 76	3 (1%)
1	L	275/322 (85%)	0.09	2 (0%) 84 86	18, 34, 50, 58	3 (1%)
All	All	3329/3864 (86%)	-0.07	29 (0%) 81 83	8, 29, 47, 76	39 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	40	ALA	5.2
1	K	317	PRO	4.4
1	B	317	PRO	4.1
1	H	317	PRO	4.1
1	F	142	ALA	4.0
1	J	319	GLU	3.9
1	D	142	ALA	3.6
1	K	40	ALA	3.6
1	J	318	GLN	3.5
1	H	40	ALA	3.4
1	E	40	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	40	ALA	3.3
1	D	40	ALA	3.2
1	E	317	PRO	3.1
1	H	45	ALA	2.9
1	B	40	ALA	2.8
1	C	142	ALA	2.7
1	B	142	ALA	2.6
1	G	142	ALA	2.6
1	A	142	ALA	2.5
1	C	315	TYR	2.4
1	H	41	GLY	2.4
1	L	297	MET	2.4
1	I	310	GLY	2.3
1	K	41	GLY	2.3
1	I	47	GLY	2.1
1	A	40	ALA	2.1
1	E	60	ALA	2.1
1	L	41	GLY	2.1

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
6	FMT	D	403	3/3	0.90	0.12	34,34,40,40	0
7	SO4	K	403	5/5	0.90	0.07	66,66,69,70	0
3	TRS	A	403	8/8	0.91	0.10	32,35,40,44	0
5	GOL	B	404	6/6	0.92	0.09	35,38,42,43	0
3	TRS	J	404	8/8	0.93	0.09	33,35,39,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AZI	J	403	3/3	0.94	0.10	22,22,23,30	0
4	AZI	E	403	3/3	0.95	0.07	28,28,30,31	0
4	AZI	B	403	3/3	0.96	0.07	19,19,25,27	0
4	AZI	H	403	3/3	0.97	0.07	19,19,22,25	0
2	CU	J	402	1/1	0.99	0.03	39,39,39,39	0
2	CU	F	401	1/1	1.00	0.02	28,28,28,28	1
2	CU	F	402	1/1	1.00	0.01	21,21,21,21	0
2	CU	G	401	1/1	1.00	0.01	22,22,22,22	0
2	CU	G	402	1/1	1.00	0.01	32,32,32,32	0
2	CU	H	401	1/1	1.00	0.02	20,20,20,20	0
2	CU	H	402	1/1	1.00	0.01	33,33,33,33	1
2	CU	I	401	1/1	1.00	0.02	32,32,32,32	1
2	CU	I	402	1/1	1.00	0.02	22,22,22,22	0
2	CU	J	401	1/1	1.00	0.02	21,21,21,21	0
2	CU	A	401	1/1	1.00	0.01	18,18,18,18	0
2	CU	K	401	1/1	1.00	0.01	21,21,21,21	0
2	CU	K	402	1/1	1.00	0.01	30,30,30,30	1
2	CU	L	401	1/1	1.00	0.01	33,33,33,33	1
2	CU	L	402	1/1	1.00	0.02	25,25,25,25	0
2	CU	A	402	1/1	1.00	0.01	29,29,29,29	1
2	CU	B	401	1/1	1.00	0.01	23,23,23,23	0
2	CU	B	402	1/1	1.00	0.02	34,34,34,34	1
2	CU	C	401	1/1	1.00	0.01	29,29,29,29	1
2	CU	C	402	1/1	1.00	0.01	22,22,22,22	0
2	CU	D	401	1/1	1.00	0.01	22,22,22,22	0
2	CU	D	402	1/1	1.00	0.02	32,32,32,32	0
2	CU	E	401	1/1	1.00	0.02	20,20,20,20	0
2	CU	E	402	1/1	1.00	0.01	24,24,24,24	1

6.5 Other polymers ⓘ

There are no such residues in this entry.