Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 08:38 pm GMT

PDB ID	:	5O4Q
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:

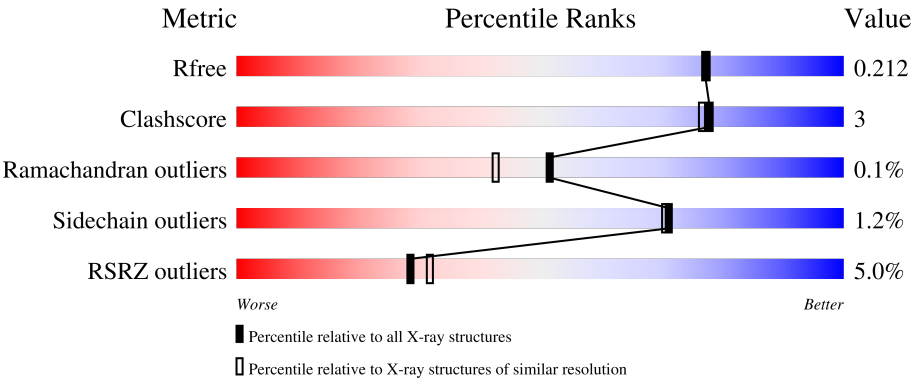
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	4% 80% 7% 13%
1	B	322	4% 77% 9% · 14%
1	C	322	4% 78% 8% 15%
1	D	322	5% 80% 6% 14%
1	E	322	3% 80% 5% · 14%

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Mol	Chain	Length	Quality of chain
1	F	322	3% 79% 7% 15%
1	G	322	6% 80% 7% 14%
1	H	322	5% 78% 8% 14%
1	I	322	5% 79% 6% 15%
1	J	322	3% 81% 6% 13%
1	K	322	4% 78% 8% 14%
1	L	322	5% 83% 15%

2 Entry composition (i)

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

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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	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

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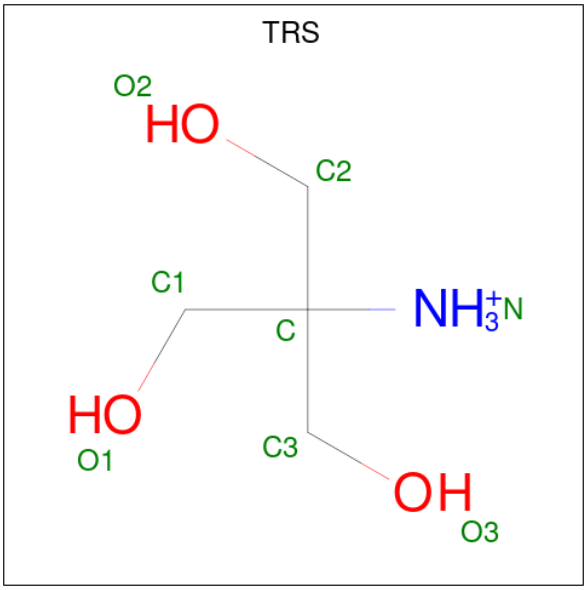
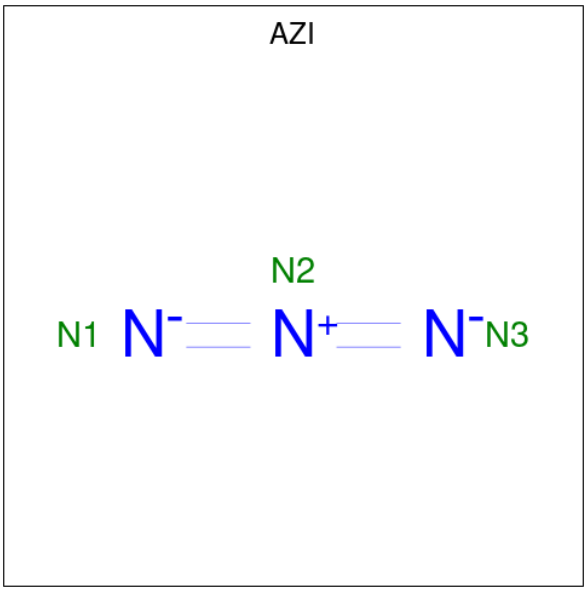
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0
2	G	2	Total Cu 2 2	0	0
2	H	2	Total Cu 2 2	0	0
2	I	2	Total Cu 2 2	0	0
2	J	2	Total Cu 2 2	0	0
2	K	2	Total Cu 2 2	0	0
2	L	2	Total Cu 2 2	0	0

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



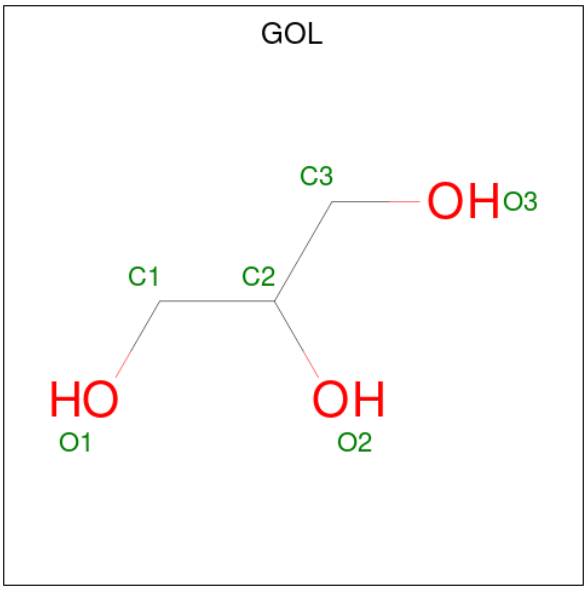
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 4 1 3	0	0
3	J	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N_3).



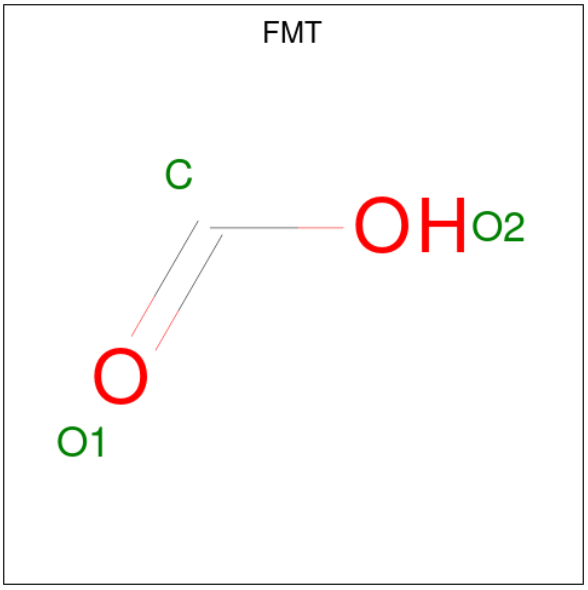
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total N 3 3	0	0
4	E	1	Total N 3 3	0	0
4	H	1	Total N 3 3	0	0
4	J	1	Total N 3 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



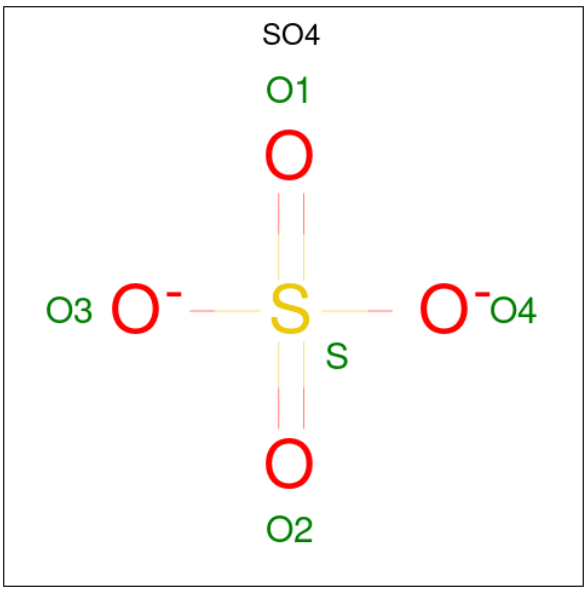
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is water.

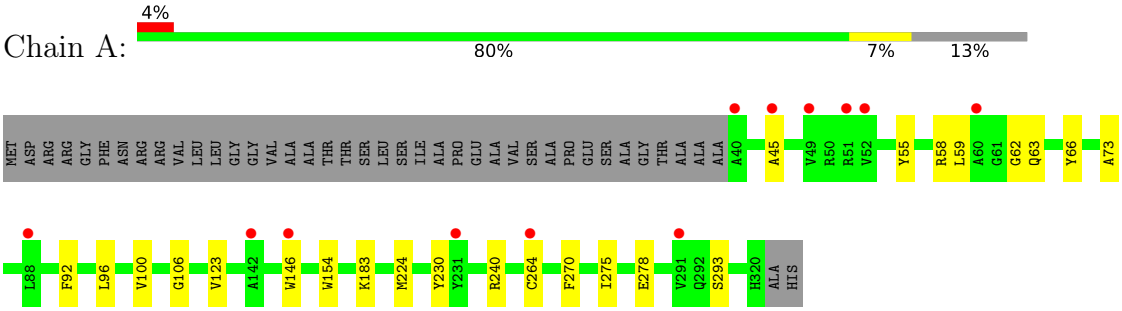
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	74	Total O 74 74	0	0
8	B	68	Total O 68 68	0	0
8	C	59	Total O 59 59	0	0
8	D	56	Total O 56 56	0	0
8	E	76	Total O 76 76	0	0
8	F	73	Total O 73 73	0	0
8	G	61	Total O 61 61	0	0
8	H	55	Total O 55 55	0	0
8	I	46	Total O 46 46	0	0
8	J	66	Total O 66 66	0	0
8	K	71	Total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

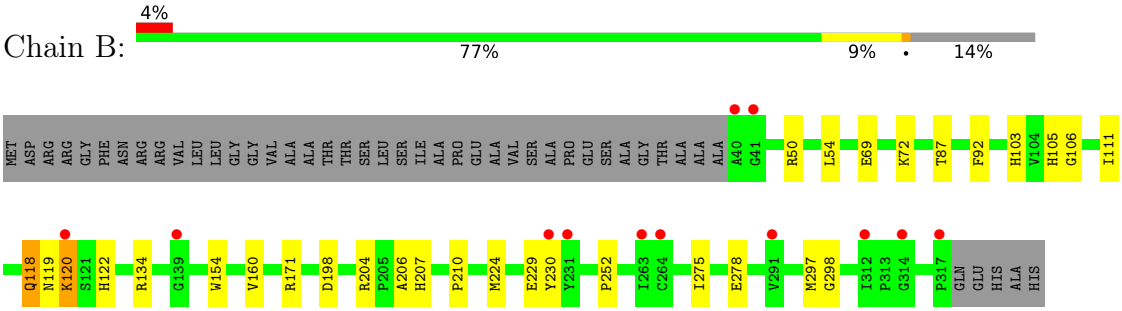
• Molecule 1: Two-domain laccase

Chain A:



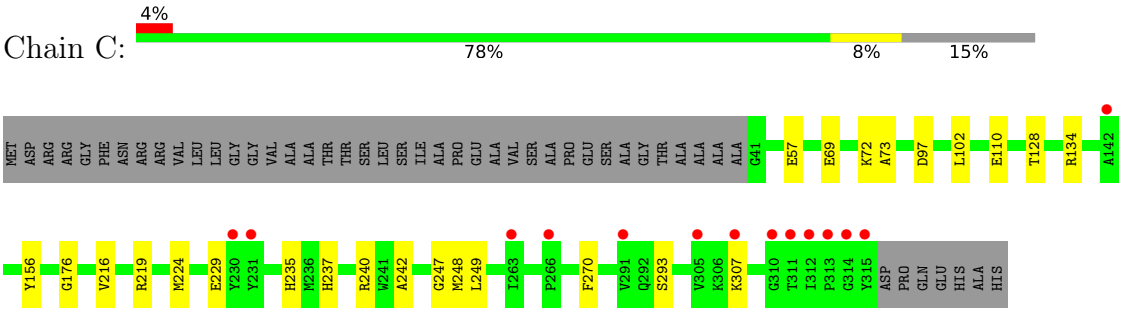
• Molecule 1: Two-domain laccase

Chain B:



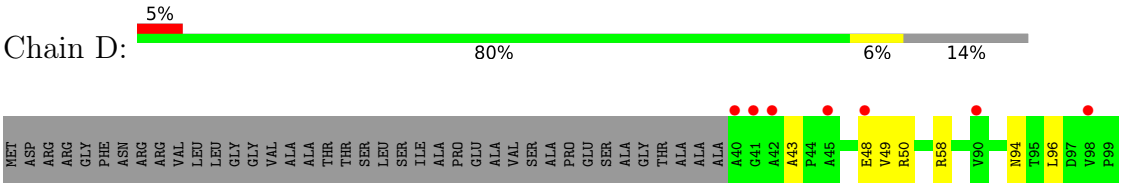
• Molecule 1: Two-domain laccase

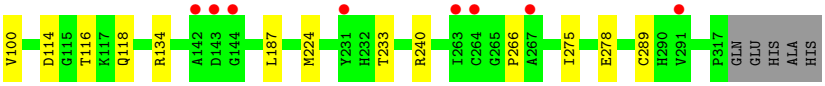
Chain C:



• Molecule 1: Two-domain laccase

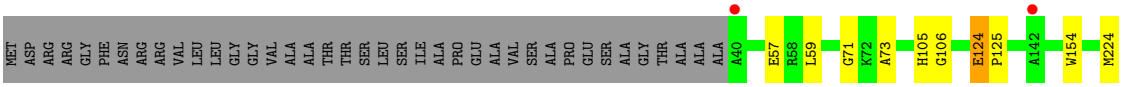
Chain D:

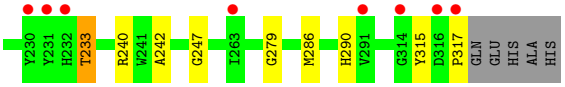




• Molecule 1: Two-domain laccase

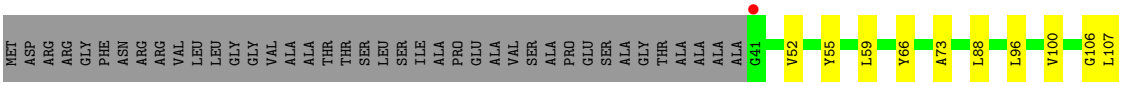
Chain E:

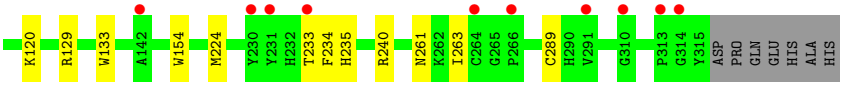




• Molecule 1: Two-domain laccase

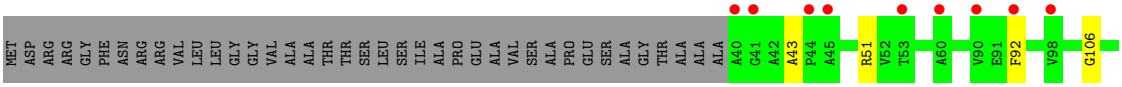
Chain F:

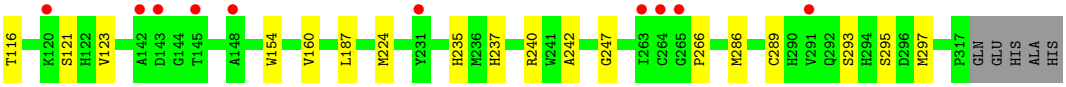




• Molecule 1: Two-domain laccase

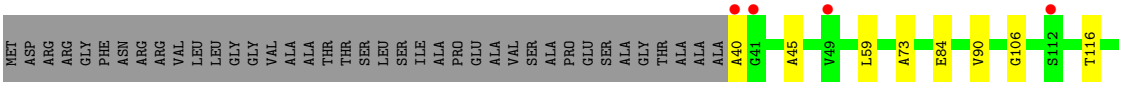
Chain G:





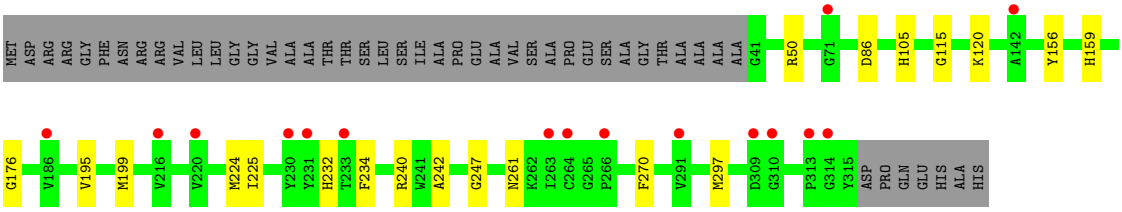
• Molecule 1: Two-domain laccase

Chain H:

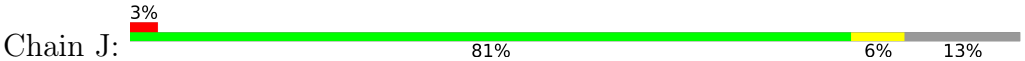


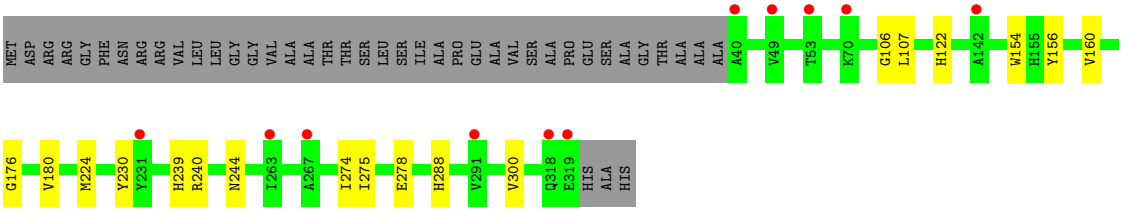
• Molecule 1: Two-domain laccase

Chain I:

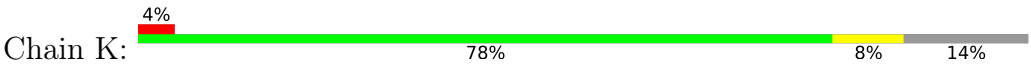


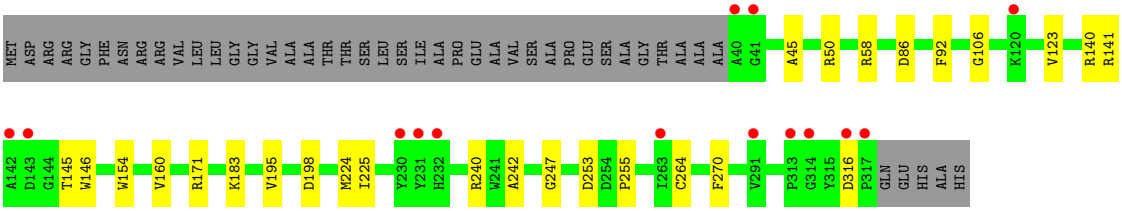
• Molecule 1: Two-domain laccase



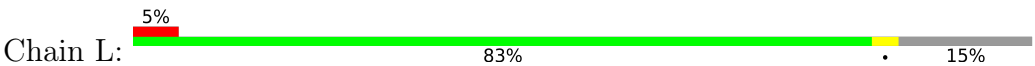


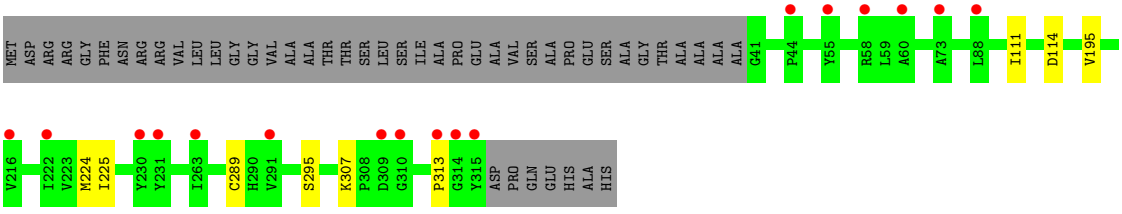
• Molecule 1: Two-domain laccase





• Molecule 1: Two-domain laccase





4 Data and refinement statistics (i)

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 49.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-1.90) 95.7 (49.69-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.03%)	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 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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.*

[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, FMT, SO4, AZI, TRS, GOL

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	0.35	0/2234	0.58	0/3038
1	B	0.34	0/2201	0.54	0/2993
1	C	0.33	0/2194	0.56	0/2983
1	D	0.34	0/2192	0.57	0/2981
1	E	0.38	0/2206	0.58	0/3001
1	F	0.36	0/2171	0.59	0/2951
1	G	0.32	0/2192	0.54	0/2981
1	H	0.34	0/2198	0.55	0/2989
1	I	0.32	0/2171	0.54	0/2951
1	J	0.36	0/2210	0.57	0/3005
1	K	0.33	0/2198	0.55	0/2989
1	L	0.32	0/2171	0.55	0/2951
All	All	0.34	0/26338	0.56	0/35813

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2139	0	2014	19	0
1	C	2133	0	2010	17	0
1	D	2130	0	2007	12	0
1	E	2144	0	2023	11	0
1	F	2110	0	1991	11	0
1	G	2130	0	2007	12	0
1	H	2133	0	2012	21	0
1	I	2110	0	1991	13	0
1	J	2148	0	2021	11	0
1	K	2133	0	2012	13	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	1	0
8	D	56	0	0	0	0
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	1	0
8	J	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	K	71	0	0	0	0
8	L	46	0	0	0	0
All	All	26408	0	24152	146	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 (146) 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
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:D:116:THR:HG21	1:E:286:MET:HE3	1.73	0.70
1:C:224:MET:HE2	1:C:270:PHE:CE1	2.30	0.67
3:A:403:TRS:H32	1:H:230:TYR:OH	1.96	0.65
1:K:264[A]:CYS:HG	1:K:270:PHE:HE1	1.42	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:E:59:LEU:HD21	1:E:73:ALA:HB3	1.83	0.61
1:B:160:VAL:O	5:B:404:GOL:O3	2.15	0.61
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:C:219:ARG:HH22	1:C:248:MET:HE1	1.71	0.56
1:E:315:TYR:O	1:E:317:PRO:HD3	2.06	0.55
1:H:90:VAL:HG13	1:H:131:TYR:HB2	1.88	0.54
1:I:224:MET:HE2	1:I:270:PHE:CE1	2.43	0.54
1:K:316:ASP:OD1	1:K:316:ASP:N	2.39	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:J:107:LEU:CD2	1:J:180:VAL:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ARG:HD3	1:B:198:ASP:OD2	2.11	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:I:224:MET:HE2	1:I:270:PHE:CZ	2.46	0.49
1:I:224:MET:HE3	8:I:526:HOH:O	2.11	0.49
1:H:137:GLU:HG2	1:H:183:LYS:HZ2	1.78	0.49
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: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:D:94:ASN:CG	1:D:100:VAL:HG12	2.34	0.47
1:F:55:TYR:O	1:F:66:TYR:HA	2.15	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:H:195:VAL:HA	1:H:225:ILE:O	2.16	0.45
1:C:224:MET:HE3	8:C:542:HOH: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:57:GLU:CD	1:E:71:GLY:H	2.21	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: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: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:B:118[B]:GLN:HG3	1:B:119:ASN:N	2.33	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:G:286:MET:HB3	1:G:286:MET:HE2	1.81	0.43
1:D:43:ALA:HB2	1:D:187:LEU:HD21	2.00	0.43
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:C:229:GLU:HG2	1:I:297:MET:HE1	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:HIS:HB3	1:J:300:VAL:HG13	2.01	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: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: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:I:199:MET:HE1	1:I:232:HIS:HE1	1.85	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
1:F:107:LEU:HD12	1:F:133:TRP:HB3	2.03	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:B:229:GLU:OE2	1:C:293:SER:OG	2.36	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%)	34	24
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%)	34	24
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
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%)	51	42

All (2) Ramachandran outliers are listed below:

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

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	224/249 (90%)	222 (99%)	2 (1%)	78	79
1	B	220/249 (88%)	216 (98%)	4 (2%)	59	55
1	C	220/249 (88%)	216 (98%)	4 (2%)	59	55
1	D	219/249 (88%)	216 (99%)	3 (1%)	67	65
1	E	221/249 (89%)	217 (98%)	4 (2%)	59	55
1	F	217/249 (87%)	215 (99%)	2 (1%)	78	79
1	G	219/249 (88%)	215 (98%)	4 (2%)	59	55
1	H	220/249 (88%)	218 (99%)	2 (1%)	78	79
1	I	217/249 (87%)	215 (99%)	2 (1%)	78	79
1	J	221/249 (89%)	219 (99%)	2 (1%)	78	79
1	K	220/249 (88%)	216 (98%)	4 (2%)	59	55
1	L	217/249 (87%)	216 (100%)	1 (0%)	88	89
All	All	2635/2988 (88%)	2601 (99%)	34 (1%)	71	68

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	MET
1	A	240	ARG
1	B	50	ARG
1	B	118[A]	GLN
1	B	118[B]	GLN
1	B	224	MET
1	C	97	ASP
1	C	128[A]	THR
1	C	128[B]	THR
1	C	240	ARG
1	D	114	ASP
1	D	224	MET
1	D	240	ARG
1	E	124	GLU
1	E	224	MET
1	E	233	THR
1	E	240	ARG
1	F	224	MET
1	F	240	ARG
1	G	51	ARG
1	G	224	MET
1	G	237	HIS

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Mol	Chain	Res	Type
1	G	240	ARG
1	H	224	MET
1	H	240	ARG
1	I	120	LYS
1	I	240	ARG
1	J	224	MET
1	J	240	ARG
1	K	160	VAL
1	K	224	MET
1	K	240	ARG
1	K	253	ASP
1	L	224	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	122	HIS
1	E	237	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	-	0,2,2	-	-	0,1,1	-	-
6	FMT	D	403	-	2,2,2	0.70	0	1,1,1	0.50	0
4	AZI	J	403	-	0,2,2	-	-	0,1,1	-	-
4	AZI	E	403	-	0,2,2	-	-	0,1,1	-	-
3	TRS	A	403	-	7,7,7	0.28	0	9,9,9	0.77	0
7	SO4	K	403	-	4,4,4	0.30	0	6,6,6	0.08	0
4	AZI	B	403	-	0,2,2	-	-	0,1,1	-	-
5	GOL	B	404	-	5,5,5	0.20	0	5,5,5	0.20	0
3	TRS	J	404	-	7,7,7	0.35	0	9,9,9	0.76	0

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	-

There are no bond length outliers.

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

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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
4	E	403	AZI	1	0
3	A	403	TRS	4	0
7	K	403	SO4	1	0
4	B	403	AZI	1	0
5	B	404	GOL	1	0
3	J	404	TRS	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.39	12 (4%)	35	38	15, 27, 40, 57	2 (0%)
1	B	278/322 (86%)	0.52	12 (4%)	35	38	16, 30, 48, 74	2 (0%)
1	C	275/322 (85%)	0.51	14 (5%)	28	31	16, 31, 47, 58	3 (1%)
1	D	278/322 (86%)	0.46	15 (5%)	25	29	15, 29, 46, 65	5 (1%)
1	E	278/322 (86%)	0.38	10 (3%)	42	45	16, 26, 40, 70	3 (1%)
1	F	275/322 (85%)	0.39	11 (4%)	38	41	15, 27, 41, 66	4 (1%)
1	G	278/322 (86%)	0.53	19 (6%)	17	19	17, 32, 49, 62	4 (1%)
1	H	278/322 (86%)	0.52	15 (5%)	25	29	17, 32, 49, 73	3 (1%)
1	I	275/322 (85%)	0.57	16 (5%)	23	25	17, 35, 49, 61	2 (0%)
1	J	280/322 (86%)	0.42	11 (3%)	39	42	15, 28, 41, 65	3 (1%)
1	K	278/322 (86%)	0.45	14 (5%)	28	32	14, 28, 47, 76	2 (0%)
1	L	275/322 (85%)	0.52	17 (6%)	20	23	18, 34, 50, 58	4 (1%)
All	All	3329/3864 (86%)	0.47	166 (4%)	28	32	14, 30, 47, 76	37 (1%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	40	ALA	8.8
1	E	40	ALA	8.0
1	D	40	ALA	7.1
1	E	317	PRO	7.1
1	B	317	PRO	7.0
1	G	40	ALA	5.8
1	K	40	ALA	5.4
1	B	314	GLY	5.3
1	J	142	ALA	5.3
1	J	40	ALA	5.1
1	F	314	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	H	317	PRO	4.7
1	G	142	ALA	4.6
1	K	317	PRO	4.6
1	D	142	ALA	4.6
1	B	40	ALA	4.4
1	F	142	ALA	4.4
1	C	314	GLY	4.4
1	I	313	PRO	4.1
1	H	314	GLY	4.1
1	C	313	PRO	4.1
1	A	142	ALA	4.1
1	I	314	GLY	4.1
1	H	41	GLY	4.0
1	J	319	GLU	3.9
1	L	216	VAL	3.8
1	F	291	VAL	3.6
1	J	318	GLN	3.6
1	I	142	ALA	3.5
1	I	291	VAL	3.5
1	A	264[A]	CYS	3.5
1	C	310	GLY	3.4
1	L	313	PRO	3.4
1	I	310	GLY	3.3
1	L	291	VAL	3.2
1	L	315	TYR	3.1
1	L	231	TYR	3.1
1	K	313	PRO	3.1
1	G	143	ASP	3.0
1	D	291	VAL	3.0
1	L	88	LEU	3.0
1	G	60	ALA	3.0
1	B	230	TYR	3.0
1	E	230	TYR	3.0
1	A	291	VAL	3.0
1	G	90	VAL	3.0
1	D	45	ALA	3.0
1	G	44	PRO	3.0
1	K	314	GLY	3.0
1	D	98	VAL	3.0
1	D	90	VAL	2.9
1	C	315	TYR	2.8
1	D	41	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	263	ILE	2.8
1	F	310	GLY	2.8
1	C	291	VAL	2.8
1	B	231	TYR	2.8
1	I	231	TYR	2.8
1	F	264	CYS	2.7
1	J	231	TYR	2.7
1	C	231	TYR	2.7
1	E	316	ASP	2.7
1	D	231	TYR	2.7
1	K	230	TYR	2.7
1	K	231	TYR	2.7
1	B	291	VAL	2.7
1	D	264	CYS	2.7
1	I	264	CYS	2.7
1	I	266	PRO	2.7
1	F	41	GLY	2.7
1	G	41	GLY	2.7
1	E	263	ILE	2.6
1	K	263	ILE	2.6
1	H	230	TYR	2.6
1	A	146	TRP	2.6
1	A	88	LEU	2.6
1	D	263	ILE	2.6
1	G	98	VAL	2.6
1	H	313	PRO	2.5
1	K	143	ASP	2.5
1	A	40	ALA	2.5
1	G	53	THR	2.5
1	A	49	VAL	2.5
1	G	231	TYR	2.5
1	L	314	GLY	2.5
1	C	307	LYS	2.5
1	J	49	VAL	2.5
1	A	231	TYR	2.5
1	J	263	ILE	2.4
1	H	49	VAL	2.4
1	K	291	VAL	2.4
1	F	233	THR	2.4
1	E	142	ALA	2.4
1	B	263	ILE	2.4
1	J	291	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	70	LYS	2.4
1	F	231	TYR	2.4
1	I	309	ASP	2.4
1	A	60	ALA	2.4
1	K	316	ASP	2.4
1	I	186	VAL	2.4
1	K	120	LYS	2.4
1	L	60	ALA	2.4
1	B	41	GLY	2.4
1	B	120	LYS	2.3
1	G	265	GLY	2.3
1	F	313	PRO	2.3
1	I	220	VAL	2.3
1	D	42	ALA	2.3
1	C	230	TYR	2.3
1	C	263	ILE	2.3
1	I	216	VAL	2.3
1	C	142	ALA	2.3
1	H	233	THR	2.3
1	G	120	LYS	2.3
1	H	266	PRO	2.3
1	H	316	ASP	2.3
1	E	231	TYR	2.3
1	E	291	VAL	2.3
1	L	263	ILE	2.3
1	L	309	ASP	2.3
1	I	233	THR	2.2
1	H	142	ALA	2.2
1	D	48	GLU	2.2
1	K	41	GLY	2.2
1	L	44	PRO	2.2
1	G	145	THR	2.2
1	G	45	ALA	2.2
1	B	139	GLY	2.2
1	L	222	ILE	2.2
1	H	231	TYR	2.2
1	D	267	ALA	2.2
1	D	144	GLY	2.2
1	J	267	ALA	2.2
1	L	310	GLY	2.2
1	G	291	VAL	2.2
1	G	263	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	53	THR	2.1
1	G	148	ALA	2.1
1	F	266	PRO	2.1
1	A	45	ALA	2.1
1	C	266	PRO	2.1
1	C	305	VAL	2.1
1	C	312	ILE	2.1
1	A	51	ARG	2.1
1	L	58	ARG	2.1
1	G	92	PHE	2.1
1	A	52	VAL	2.1
1	B	264	CYS	2.1
1	G	264	CYS	2.1
1	I	263	ILE	2.1
1	I	71	GLY	2.1
1	I	230	TYR	2.1
1	C	311	THR	2.1
1	L	230	TYR	2.0
1	K	232	HIS	2.0
1	L	73	ALA	2.0
1	B	312	ILE	2.0
1	D	143	ASP	2.0
1	H	112	SER	2.0
1	F	230	TYR	2.0
1	L	55	TYR	2.0
1	E	314	GLY	2.0
1	K	142	ALA	2.0
1	H	143	ASP	2.0
1	E	232	HIS	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
3	TRS	J	404	8/8	0.84	0.33	33,35,39,41	0
3	TRS	A	403	8/8	0.88	0.32	32,35,40,44	0
4	AZI	J	403	3/3	0.90	0.26	22,22,23,30	0
4	AZI	E	403	3/3	0.91	0.22	28,28,30,31	0
5	GOL	B	404	6/6	0.91	0.15	35,38,42,43	0
6	FMT	D	403	3/3	0.92	0.13	34,34,40,40	0
4	AZI	H	403	3/3	0.94	0.27	19,19,22,25	0
4	AZI	B	403	3/3	0.95	0.25	19,19,25,27	0
7	SO4	K	403	5/5	0.97	0.29	66,66,69,70	0
2	CU	I	401	1/1	0.99	0.09	32,32,32,32	1
2	CU	J	402	1/1	0.99	0.10	39,39,39,39	0
2	CU	L	401	1/1	0.99	0.10	33,33,33,33	1
2	CU	D	402	1/1	0.99	0.10	32,32,32,32	0
2	CU	G	402	1/1	1.00	0.10	32,32,32,32	0
2	CU	H	401	1/1	1.00	0.11	20,20,20,20	0
2	CU	H	402	1/1	1.00	0.11	33,33,33,33	1
2	CU	A	402	1/1	1.00	0.11	29,29,29,29	1
2	CU	I	402	1/1	1.00	0.13	22,22,22,22	0
2	CU	J	401	1/1	1.00	0.12	21,21,21,21	0
2	CU	B	401	1/1	1.00	0.14	23,23,23,23	0
2	CU	K	401	1/1	1.00	0.13	21,21,21,21	0
2	CU	K	402	1/1	1.00	0.10	30,30,30,30	1
2	CU	B	402	1/1	1.00	0.10	34,34,34,34	1
2	CU	L	402	1/1	1.00	0.12	25,25,25,25	0
2	CU	C	401	1/1	1.00	0.09	29,29,29,29	1
2	CU	C	402	1/1	1.00	0.13	22,22,22,22	0
2	CU	D	401	1/1	1.00	0.13	22,22,22,22	0
2	CU	A	401	1/1	1.00	0.14	18,18,18,18	0
2	CU	E	401	1/1	1.00	0.11	20,20,20,20	0
2	CU	E	402	1/1	1.00	0.13	24,24,24,24	1
2	CU	F	401	1/1	1.00	0.10	28,28,28,28	1
2	CU	F	402	1/1	1.00	0.12	21,21,21,21	0
2	CU	G	401	1/1	1.00	0.12	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.