wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 08:22 am GMT

PDB ID	:	5O4I
Title	:	Crystal Structure of mutant M54L/M64L/M96L of Two-Domain Laccase from Streptomyces griseoflavus dialyzed against solution containing 0.25 mM copper sulfate
Authors	:	Gabdulkhakov, A.G.; Tishchenko, T.V.
Deposited on	:	2017-05-29
Resolution	:	1.80 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 (1)) were used in the production of this report:

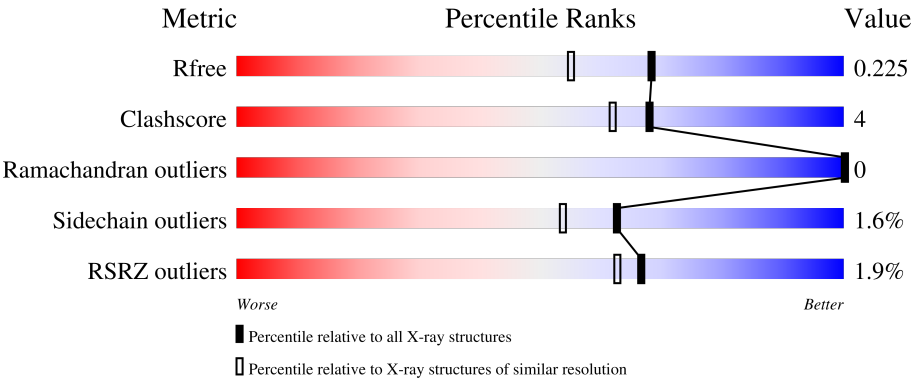
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	322	2% 75% 11% 14%
1	B	322	. 81% 6% 13%
1	C	322	2% 78% 8% 14%
1	D	322	. 77% 9% 14%
1	E	322	2% 77% 9% 14%

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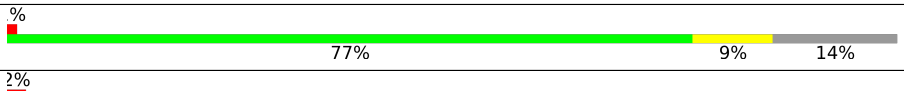
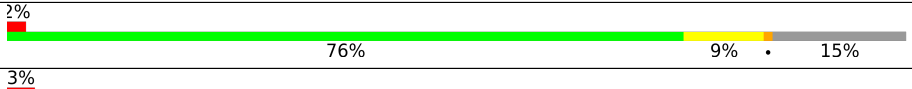
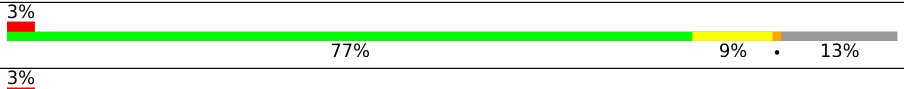
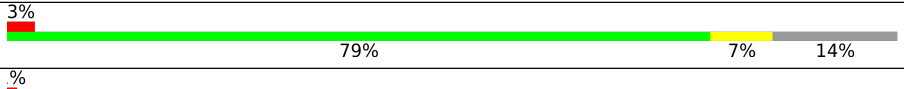
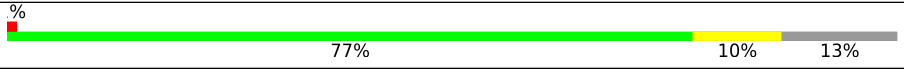
Mol	Chain	Length	Quality of chain
1	F	322	
1	G	322	
1	H	322	
1	I	322	
1	J	322	
1	K	322	
1	L	322	

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
3	GOL	G	406	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26973 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	278	Total	C	N	O	S	0	1	0
			2137	1336	390	402	9			
1	B	281	Total	C	N	O	S	0	3	0
			2181	1361	399	412	9			
1	C	277	Total	C	N	O	S	0	4	0
			2152	1347	391	404	10			
1	D	278	Total	C	N	O	S	0	2	0
			2141	1339	390	403	9			
1	E	278	Total	C	N	O	S	0	2	0
			2144	1339	391	405	9			
1	F	277	Total	C	N	O	S	0	2	0
			2140	1336	390	405	9			
1	G	278	Total	C	N	O	S	0	0	0
			2130	1331	389	401	9			
1	H	277	Total	C	N	O	S	0	0	0
			2125	1328	388	400	9			
1	I	275	Total	C	N	O	S	0	3	0
			2130	1332	388	401	9			
1	J	279	Total	C	N	O	S	0	2	0
			2155	1346	394	406	9			
1	K	278	Total	C	N	O	S	0	1	0
			2138	1335	390	404	9			
1	L	280	Total	C	N	O	S	0	0	0
			2153	1344	394	406	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 4 4	0	1
2	B	3	Total Cu 4 4	0	1
2	C	3	Total Cu 4 4	0	1
2	D	3	Total Cu 4 4	0	1

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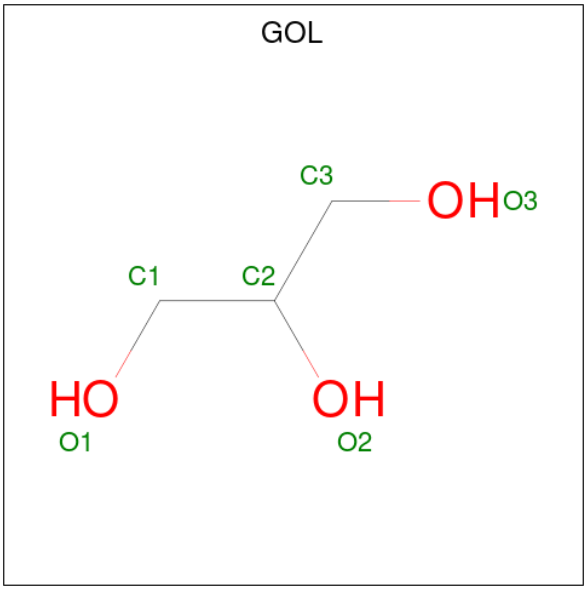
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	3	Total Cu 4 4	0	1
2	F	3	Total Cu 4 4	0	1
2	G	3	Total Cu 4 4	0	1
2	H	3	Total Cu 3 3	0	0
2	I	3	Total Cu 3 3	0	0
2	J	3	Total Cu 4 4	0	1
2	K	3	Total Cu 3 3	0	0
2	L	3	Total Cu 4 4	0	1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

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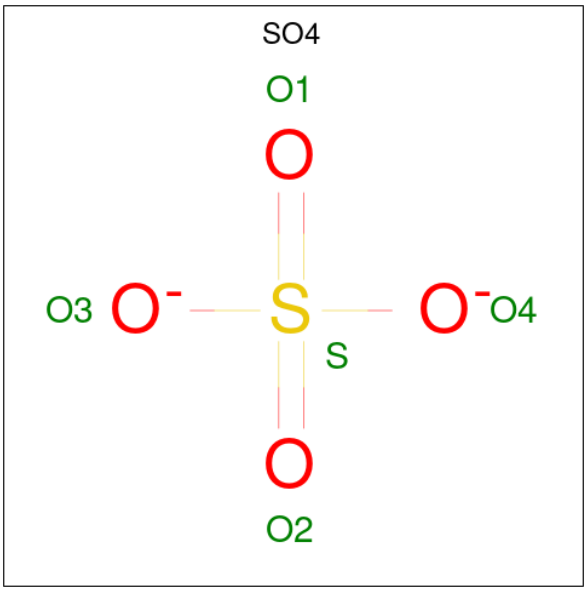
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	85	Total O 85 85	0	0
5	B	94	Total O 94 94	0	0
5	C	86	Total O 86 86	0	0
5	D	90	Total O 90 90	0	0
5	E	82	Total O 82 82	0	0
5	F	78	Total O 78 78	0	0
5	G	79	Total O 79 79	0	0
5	H	65	Total O 65 65	0	0

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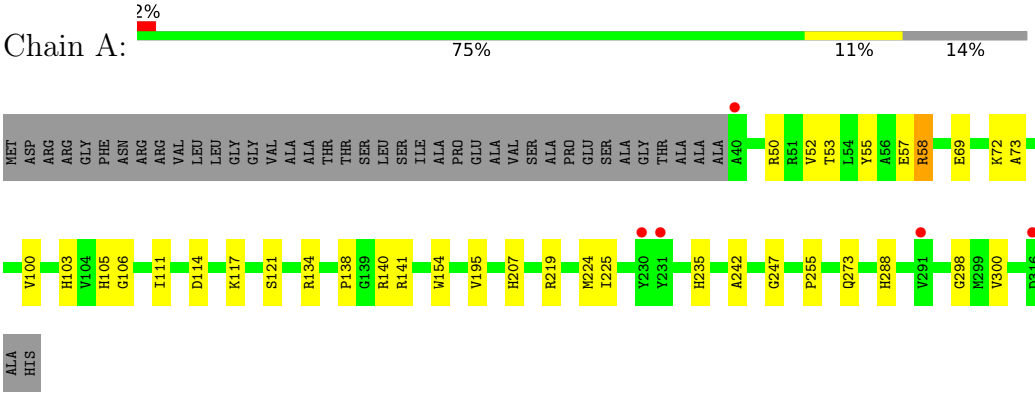
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	65	Total O 65 65	0	0
5	J	72	Total O 72 72	0	0
5	K	58	Total O 58 58	0	0
5	L	70	Total O 70 70	0	0

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.

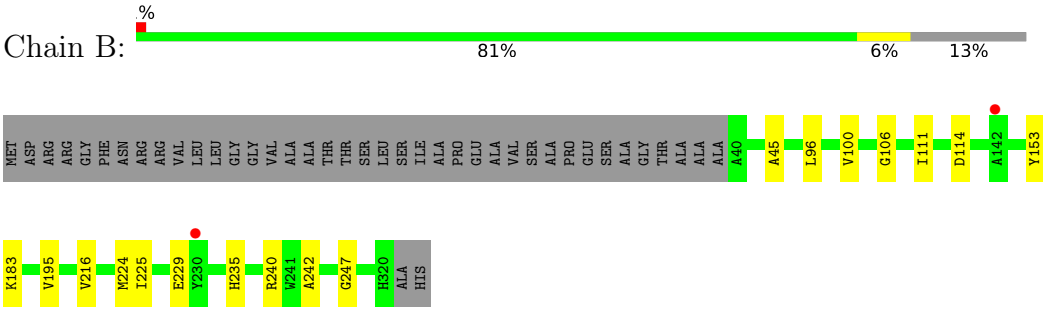
• Molecule 1: Two-domain laccase

Chain A:



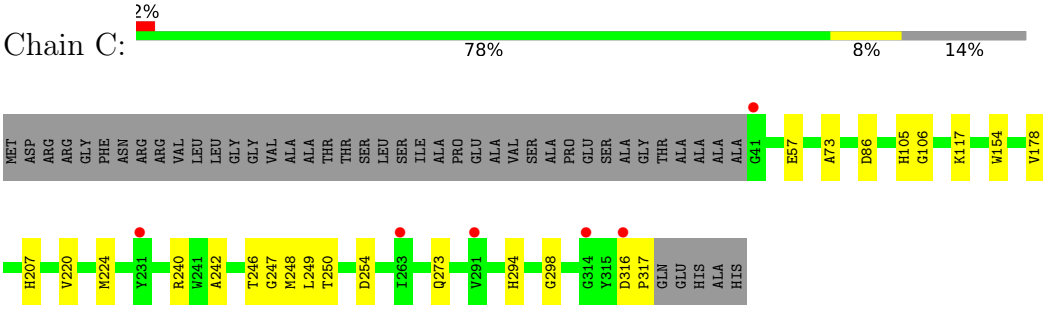
• Molecule 1: Two-domain laccase

Chain B:



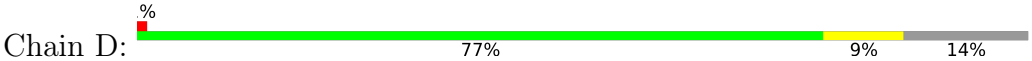
• Molecule 1: Two-domain laccase

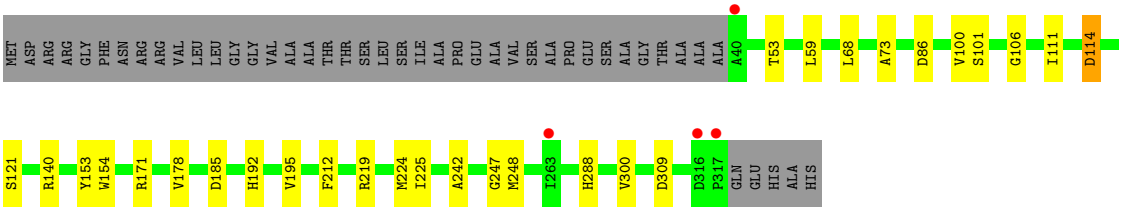
Chain C:



• Molecule 1: Two-domain laccase

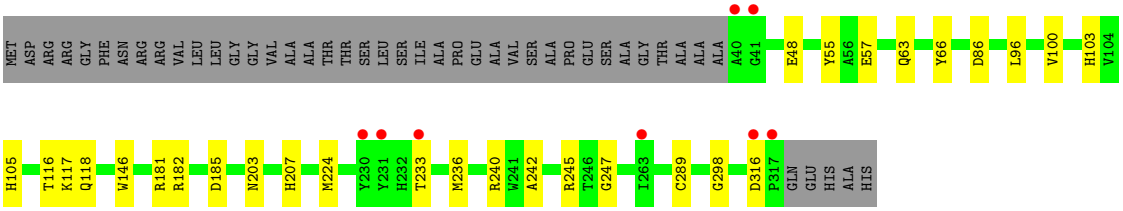
Chain D:





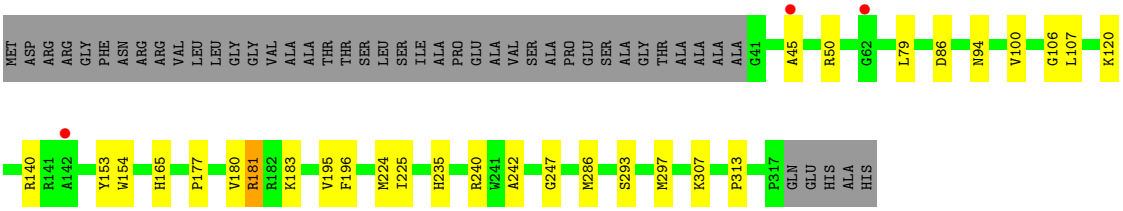
• Molecule 1: Two-domain laccase

Chain E:



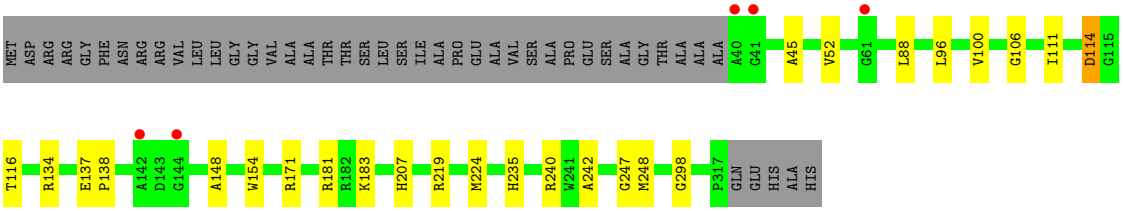
• Molecule 1: Two-domain laccase

Chain F:



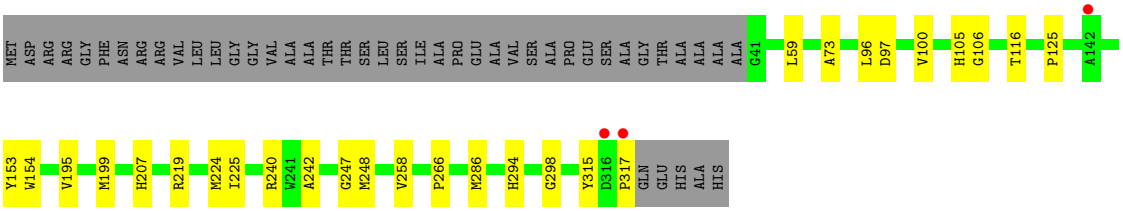
• Molecule 1: Two-domain laccase

Chain G:



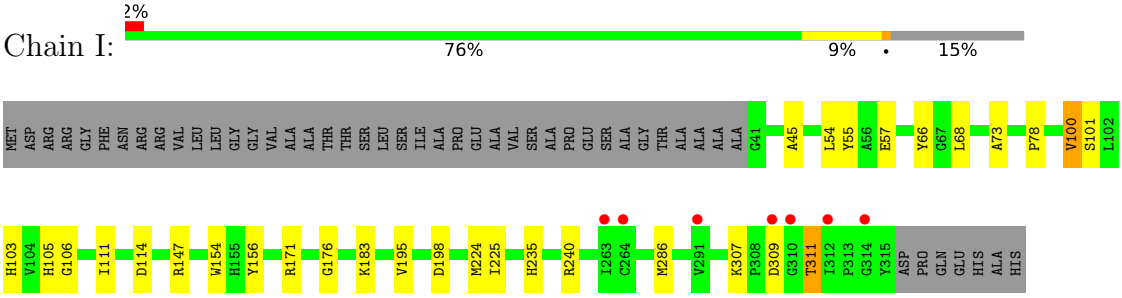
• Molecule 1: Two-domain laccase

Chain H:



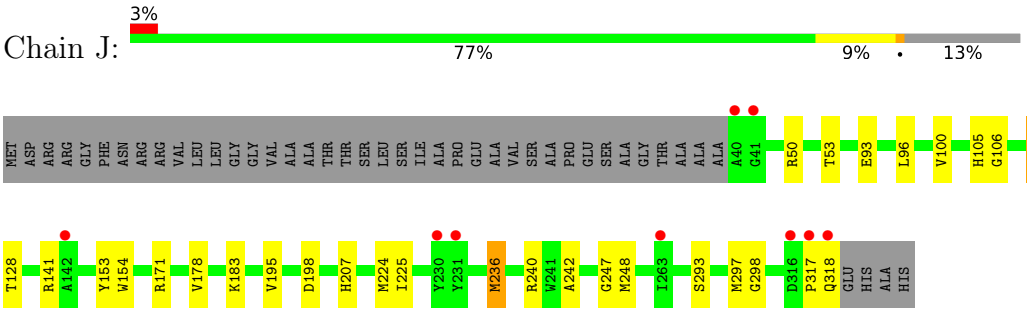
• Molecule 1: Two-domain laccase

Chain I:



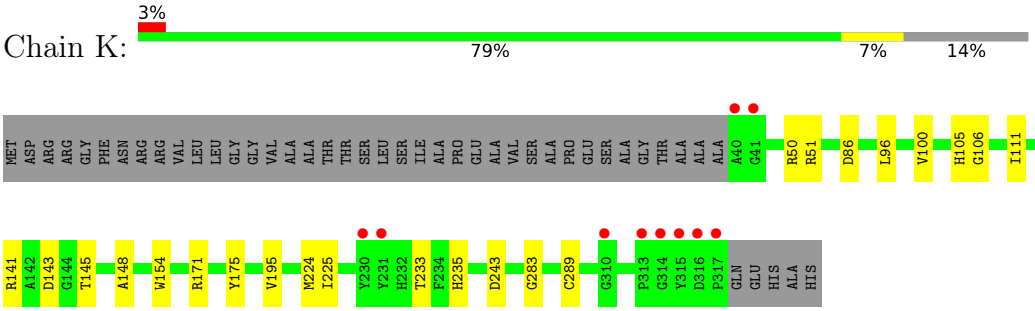
• Molecule 1: Two-domain laccase

Chain J:



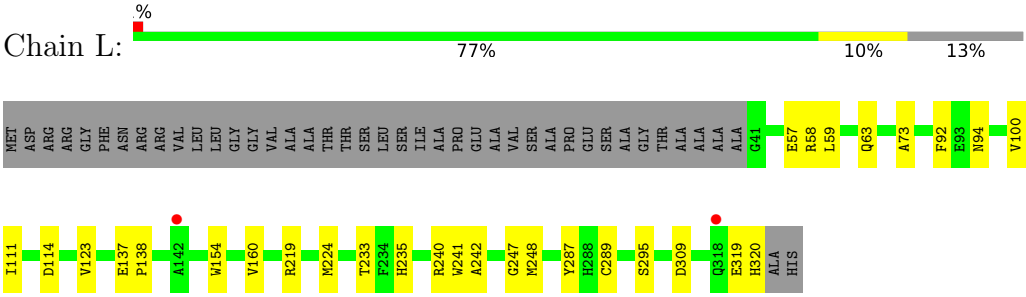
• Molecule 1: Two-domain laccase

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	76.93Å 94.93Å 116.59Å 90.08° 90.20° 91.65°	Depositor
Resolution (Å)	50.00 – 1.80 47.45 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.6 (50.00-1.80) 92.6 (47.45-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.177 , 0.222 0.186 , 0.225	Depositor DCC
R_{free} test set	13997 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l 0.118 for -h,k,-l 0.096 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26973	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: GOL, CU, SO4

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	0.86	1/2199 (0.0%)	0.94	5/2991 (0.2%)
1	B	0.91	1/2244 (0.0%)	0.92	1/3052 (0.0%)
1	C	0.88	0/2217	0.90	3/3015 (0.1%)
1	D	0.90	1/2206 (0.0%)	0.99	9/3001 (0.3%)
1	E	0.89	1/2209 (0.0%)	0.92	4/3004 (0.1%)
1	F	0.87	0/2202	0.92	3/2995 (0.1%)
1	G	0.84	0/2192	0.92	5/2981 (0.2%)
1	H	0.82	0/2187	0.89	0/2974
1	I	0.81	0/2194	0.87	0/2983
1	J	0.83	0/2217	0.86	3/3015 (0.1%)
1	K	0.80	0/2200	0.89	3/2992 (0.1%)
1	L	0.85	2/2216 (0.1%)	0.91	2/3013 (0.1%)
All	All	0.86	6/26483 (0.0%)	0.91	38/36016 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	ASP	CB-CG	-6.15	1.38	1.51
1	E	146	TRP	CB-CG	-5.66	1.40	1.50
1	L	241	TRP	CB-CG	5.57	1.60	1.50
1	L	287	TYR	CG-CD2	5.11	1.45	1.39
1	A	121	SER	CB-OG	-5.07	1.35	1.42

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	309	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	134	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	D	309	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	140	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	E	245	ARG	NE-CZ-NH1	6.57	123.58	120.30

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	2137	0	2015	24	0
1	B	2181	0	2049	9	0
1	C	2152	0	2036	15	0
1	D	2141	0	2022	16	0
1	E	2144	0	2018	18	0
1	F	2140	0	2011	16	0
1	G	2130	0	2007	13	0
1	H	2125	0	2002	20	0
1	I	2130	0	2011	21	0
1	J	2155	0	2030	18	0
1	K	2138	0	2010	17	0
1	L	2153	0	2023	17	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	4	0	0	0	0
2	K	3	0	0	0	0
2	L	4	0	0	0	0
3	A	12	0	16	2	0
3	B	24	0	32	2	0
3	C	24	0	32	2	0
3	D	30	0	40	1	0
3	E	36	0	48	3	0
3	F	18	0	24	2	0
3	G	30	0	40	2	0
3	H	12	0	16	3	0
3	I	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	24	0	32	2	0
3	K	24	0	32	1	0
3	L	6	0	8	0	0
4	B	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	J	5	0	0	0	0
5	A	85	0	0	2	0
5	B	94	0	0	0	0
5	C	86	0	0	1	0
5	D	90	0	0	3	0
5	E	82	0	0	6	0
5	F	78	0	0	0	0
5	G	79	0	0	1	0
5	H	65	0	0	0	0
5	I	65	0	0	1	0
5	J	72	0	0	3	0
5	K	58	0	0	3	0
5	L	70	0	0	4	0
All	All	26973	0	24578	192	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 4.

The worst 5 of 192 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:I:103:HIS:ND1	5:I:501:HOH:O	1.97	0.95
3:B:406:GOL:O2	3:C:407:GOL:H12	1.69	0.93
1:L:103:HIS:HD2	5:L:505:HOH:O	1.52	0.91
1:K:143:ASP:OD1	1:K:145:THR:HG22	1.77	0.84
1:K:141:ARG:HH11	1:K:145:THR:HG23	1.42	0.83

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	277/322 (86%)	269 (97%)	8 (3%)	0	100	100
1	B	282/322 (88%)	276 (98%)	6 (2%)	0	100	100
1	C	279/322 (87%)	274 (98%)	5 (2%)	0	100	100
1	D	278/322 (86%)	270 (97%)	8 (3%)	0	100	100
1	E	278/322 (86%)	272 (98%)	6 (2%)	0	100	100
1	F	277/322 (86%)	272 (98%)	5 (2%)	0	100	100
1	G	276/322 (86%)	270 (98%)	6 (2%)	0	100	100
1	H	275/322 (85%)	267 (97%)	8 (3%)	0	100	100
1	I	276/322 (86%)	272 (99%)	4 (1%)	0	100	100
1	J	279/322 (87%)	270 (97%)	9 (3%)	0	100	100
1	K	277/322 (86%)	270 (98%)	7 (2%)	0	100	100
1	L	278/322 (86%)	270 (97%)	8 (3%)	0	100	100
All	All	3332/3864 (86%)	3252 (98%)	80 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	220/249 (88%)	217 (99%)	3 (1%)	67	59
1	B	225/249 (90%)	223 (99%)	2 (1%)	78	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	223/249 (90%)	220 (99%)	3 (1%)	69	62
1	D	221/249 (89%)	220 (100%)	1 (0%)	88	87
1	E	221/249 (89%)	216 (98%)	5 (2%)	50	37
1	F	221/249 (89%)	217 (98%)	4 (2%)	59	48
1	G	219/249 (88%)	217 (99%)	2 (1%)	78	75
1	H	219/249 (88%)	216 (99%)	3 (1%)	67	59
1	I	220/249 (88%)	214 (97%)	6 (3%)	44	31
1	J	222/249 (89%)	216 (97%)	6 (3%)	44	31
1	K	220/249 (88%)	218 (99%)	2 (1%)	78	75
1	L	222/249 (89%)	217 (98%)	5 (2%)	50	37
All	All	2653/2988 (89%)	2611 (98%)	42 (2%)	62	54

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	311	THR
1	K	51	ARG
1	J	50	ARG
1	J	224	MET
1	L	58	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	103	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 92 ligands modelled in this entry, 45 are monoatomic - leaving 47 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	K	405	-	5,5,5	0.37	0	5,5,5	0.53	0
3	GOL	B	405	-	5,5,5	0.69	0	5,5,5	0.71	0
3	GOL	G	407	-	5,5,5	1.18	1 (20%)	5,5,5	1.33	0
3	GOL	L	404	-	5,5,5	0.85	0	5,5,5	0.83	0
3	GOL	H	404	-	5,5,5	0.63	0	5,5,5	0.36	0
3	GOL	H	405	-	5,5,5	0.88	0	5,5,5	1.30	0
3	GOL	C	406	-	5,5,5	0.47	0	5,5,5	0.76	0
4	SO4	J	408	-	4,4,4	0.42	0	6,6,6	0.39	0
3	GOL	C	404	-	5,5,5	0.30	0	5,5,5	0.83	0
3	GOL	G	405	-	5,5,5	0.56	0	5,5,5	0.65	0
3	GOL	A	404	-	5,5,5	0.24	0	5,5,5	0.62	0
4	SO4	G	409	-	4,4,4	0.50	0	6,6,6	0.26	0
3	GOL	E	404	-	5,5,5	0.65	0	5,5,5	0.93	0
3	GOL	K	404	-	5,5,5	0.68	0	5,5,5	0.57	0
3	GOL	B	404	-	5,5,5	0.59	0	5,5,5	0.96	0
3	GOL	B	407	-	5,5,5	0.29	0	5,5,5	0.46	0
3	GOL	D	407	-	5,5,5	0.33	0	5,5,5	1.66	1 (20%)
3	GOL	B	406	-	5,5,5	0.48	0	5,5,5	1.07	0
3	GOL	E	408	-	5,5,5	0.47	0	5,5,5	1.53	1 (20%)
3	GOL	D	406	-	5,5,5	0.36	0	5,5,5	0.99	0
3	GOL	D	404	-	5,5,5	0.59	0	5,5,5	1.03	0
3	GOL	E	406	-	5,5,5	0.33	0	5,5,5	0.97	0
3	GOL	C	407	-	5,5,5	0.55	0	5,5,5	1.02	0
3	GOL	G	404	-	5,5,5	0.59	0	5,5,5	0.72	0
3	GOL	J	407	-	5,5,5	0.71	0	5,5,5	0.71	0
3	GOL	E	405	-	5,5,5	0.97	0	5,5,5	0.95	0
3	GOL	J	404	-	5,5,5	0.34	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	J	406	-	5,5,5	1.07	0	5,5,5	0.98	0
3	GOL	E	409	-	5,5,5	0.79	0	5,5,5	1.27	0
3	GOL	G	406	-	5,5,5	0.74	0	5,5,5	1.76	2 (40%)
3	GOL	F	405	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	I	405	-	5,5,5	0.51	0	5,5,5	1.23	0
3	GOL	I	404	-	5,5,5	0.52	0	5,5,5	0.28	0
3	GOL	G	408	-	5,5,5	0.72	0	5,5,5	0.96	0
3	GOL	I	406	-	5,5,5	0.65	0	5,5,5	0.77	0
3	GOL	E	407	-	5,5,5	0.57	0	5,5,5	0.87	0
3	GOL	F	406	-	5,5,5	0.36	0	5,5,5	0.73	0
3	GOL	A	405	-	5,5,5	0.54	0	5,5,5	0.62	0
3	GOL	J	405	-	5,5,5	0.64	0	5,5,5	1.27	0
4	SO4	F	407	-	4,4,4	0.44	0	6,6,6	0.38	0
3	GOL	K	407	-	5,5,5	0.87	0	5,5,5	0.81	0
4	SO4	B	408	-	4,4,4	0.44	0	6,6,6	0.52	0
3	GOL	K	406	-	5,5,5	0.62	0	5,5,5	0.46	0
3	GOL	C	405	-	5,5,5	1.35	0	5,5,5	0.96	0
3	GOL	D	408	-	5,5,5	0.61	0	5,5,5	1.24	0
3	GOL	D	405	-	5,5,5	0.84	0	5,5,5	1.36	2 (40%)
3	GOL	F	404	-	5,5,5	0.55	0	5,5,5	1.06	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
3	GOL	K	405	-	-	0/4/4/4	-
3	GOL	B	405	-	-	2/4/4/4	-
3	GOL	G	407	-	-	2/4/4/4	-
3	GOL	L	404	-	-	0/4/4/4	-
3	GOL	H	404	-	-	0/4/4/4	-
3	GOL	H	405	-	-	3/4/4/4	-
3	GOL	C	406	-	-	0/4/4/4	-
3	GOL	C	404	-	-	2/4/4/4	-
3	GOL	G	405	-	-	0/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	E	404	-	-	0/4/4/4	-
3	GOL	K	404	-	-	0/4/4/4	-
3	GOL	B	404	-	-	3/4/4/4	-
3	GOL	B	407	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	407	-	-	4/4/4/4	-
3	GOL	B	406	-	-	3/4/4/4	-
3	GOL	E	408	-	-	4/4/4/4	-
3	GOL	D	406	-	-	2/4/4/4	-
3	GOL	D	404	-	-	2/4/4/4	-
3	GOL	E	406	-	-	2/4/4/4	-
3	GOL	C	407	-	-	2/4/4/4	-
3	GOL	G	404	-	-	0/4/4/4	-
3	GOL	J	407	-	-	2/4/4/4	-
3	GOL	E	405	-	-	0/4/4/4	-
3	GOL	J	404	-	-	0/4/4/4	-
3	GOL	J	406	-	-	4/4/4/4	-
3	GOL	E	409	-	-	2/4/4/4	-
3	GOL	G	406	-	-	4/4/4/4	-
3	GOL	F	405	-	-	0/4/4/4	-
3	GOL	I	405	-	-	2/4/4/4	-
3	GOL	I	404	-	-	0/4/4/4	-
3	GOL	G	408	-	-	0/4/4/4	-
3	GOL	I	406	-	-	2/4/4/4	-
3	GOL	E	407	-	-	2/4/4/4	-
3	GOL	F	406	-	-	2/4/4/4	-
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	J	405	-	-	4/4/4/4	-
3	GOL	K	407	-	-	1/4/4/4	-
3	GOL	K	406	-	-	0/4/4/4	-
3	GOL	C	405	-	-	0/4/4/4	-
3	GOL	D	408	-	-	3/4/4/4	-
3	GOL	D	405	-	-	0/4/4/4	-
3	GOL	F	404	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	407	GOL	O2-C2	2.07	1.49	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	406	GOL	O3-C3-C2	2.91	124.16	110.20
3	D	407	GOL	C3-C2-C1	-2.65	101.39	111.70
3	E	408	GOL	O2-C2-C3	2.28	119.18	109.12
3	D	405	GOL	C3-C2-C1	-2.11	103.49	111.70
3	D	405	GOL	O2-C2-C1	2.08	118.26	109.12

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	B	405	GOL	C1-C2-C3-O3
3	B	406	GOL	O1-C1-C2-C3
3	C	404	GOL	O1-C1-C2-C3

There are no ring outliers.

16 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	404	GOL	2	0
3	H	405	GOL	1	0
3	C	406	GOL	1	0
3	B	404	GOL	1	0
3	B	406	GOL	1	0
3	E	408	GOL	3	0
3	D	406	GOL	1	0
3	C	407	GOL	1	0
3	J	406	GOL	1	0
3	G	408	GOL	2	0
3	I	406	GOL	2	0
3	F	406	GOL	1	0
3	A	405	GOL	2	0
3	J	405	GOL	1	0
3	K	407	GOL	1	0
3	F	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	278/322 (86%)	-0.18	6 (2%)	62	57	14, 25, 41, 79	2 (0%)
1	B	281/322 (87%)	-0.21	2 (0%)	87	86	14, 23, 37, 57	2 (0%)
1	C	277/322 (86%)	-0.19	6 (2%)	62	57	14, 24, 41, 63	3 (1%)
1	D	278/322 (86%)	-0.21	4 (1%)	75	72	15, 24, 39, 73	3 (1%)
1	E	278/322 (86%)	-0.14	8 (2%)	51	46	16, 24, 40, 85	1 (0%)
1	F	277/322 (86%)	-0.21	3 (1%)	80	78	14, 25, 42, 55	3 (1%)
1	G	278/322 (86%)	-0.13	5 (1%)	68	64	16, 26, 44, 66	3 (1%)
1	H	277/322 (86%)	-0.10	3 (1%)	80	78	15, 28, 44, 77	2 (0%)
1	I	275/322 (85%)	-0.07	7 (2%)	57	52	16, 28, 44, 56	2 (0%)
1	J	279/322 (86%)	-0.06	9 (3%)	47	41	16, 26, 43, 83	2 (0%)
1	K	278/322 (86%)	0.04	10 (3%)	42	37	18, 30, 46, 82	3 (1%)
1	L	280/322 (86%)	-0.18	2 (0%)	87	86	16, 25, 42, 70	3 (1%)
All	All	3336/3864 (86%)	-0.14	65 (1%)	66	63	14, 25, 43, 85	29 (0%)

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	ALA	8.5
1	K	317	PRO	6.8
1	E	317	PRO	6.2
1	K	40	ALA	6.1
1	J	40	ALA	5.8

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
3	GOL	K	407	6/6	0.84	0.16	31,42,51,55	0
3	GOL	E	409	6/6	0.85	0.17	34,41,44,48	0
3	GOL	I	406	6/6	0.88	0.11	37,40,45,46	0
3	GOL	C	407	6/6	0.89	0.20	34,36,40,40	0
3	GOL	G	408	6/6	0.89	0.17	33,34,35,38	0
3	GOL	J	407	6/6	0.90	0.18	36,44,46,47	0
3	GOL	A	405	6/6	0.91	0.14	39,45,49,52	0
3	GOL	J	406	6/6	0.92	0.11	29,33,37,42	0
3	GOL	D	407	6/6	0.92	0.20	36,40,42,43	0
3	GOL	C	404	6/6	0.92	0.16	23,25,28,29	0
4	SO4	G	409	5/5	0.92	0.16	66,70,74,81	0
3	GOL	E	408	6/6	0.93	0.14	27,36,39,45	0
4	SO4	F	407	5/5	0.93	0.23	60,62,64,69	0
3	GOL	D	408	6/6	0.93	0.15	32,37,43,50	0
3	GOL	G	407	6/6	0.94	0.12	29,30,34,34	0
3	GOL	C	405	6/6	0.94	0.12	21,25,25,27	0
4	SO4	B	408	5/5	0.94	0.30	59,61,68,75	0
3	GOL	E	405	6/6	0.94	0.10	21,22,24,25	0
3	GOL	F	406	6/6	0.94	0.13	34,36,36,37	0
4	SO4	J	408	5/5	0.94	0.27	66,68,72,72	0
3	GOL	E	406	6/6	0.95	0.10	25,31,32,34	0
3	GOL	H	405	6/6	0.95	0.13	24,24,26,27	0
3	GOL	I	405	6/6	0.95	0.08	30,31,32,32	0
3	GOL	E	407	6/6	0.95	0.12	26,32,36,37	0
3	GOL	J	405	6/6	0.95	0.12	21,25,28,28	0
3	GOL	B	406	6/6	0.95	0.12	23,28,30,30	0
3	GOL	G	406	6/6	0.96	0.13	20,24,25,25	0
3	GOL	D	404	6/6	0.96	0.14	23,26,27,28	0
3	GOL	D	406	6/6	0.96	0.09	27,31,34,37	0
3	GOL	B	407	6/6	0.96	0.16	32,36,38,52	0
3	GOL	I	404	6/6	0.96	0.11	22,23,24,28	0
3	GOL	C	406	6/6	0.96	0.09	31,35,39,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	404	6/6	0.96	0.12	21,23,25,27	0
3	GOL	J	404	6/6	0.96	0.12	21,25,27,30	0
3	GOL	H	404	6/6	0.97	0.15	23,23,26,26	0
3	GOL	F	405	6/6	0.97	0.10	23,24,27,27	0
3	GOL	K	404	6/6	0.97	0.13	21,23,27,28	0
3	GOL	K	406	6/6	0.97	0.14	24,29,31,31	0
3	GOL	A	404	6/6	0.97	0.10	19,21,21,22	0
3	GOL	L	404	6/6	0.97	0.08	23,23,24,25	0
3	GOL	G	404	6/6	0.97	0.12	22,25,25,28	0
3	GOL	D	405	6/6	0.97	0.10	17,18,19,21	0
3	GOL	E	404	6/6	0.97	0.14	21,22,24,24	0
3	GOL	B	405	6/6	0.97	0.12	21,23,25,29	0
3	GOL	G	405	6/6	0.98	0.08	22,24,25,26	0
2	CU	K	403	1/1	0.98	0.09	28,28,28,28	0
3	GOL	K	405	6/6	0.98	0.13	23,23,24,29	0
2	CU	G	402	1/1	0.98	0.06	26,26,26,26	1
3	GOL	F	404	6/6	0.98	0.12	20,21,23,24	0
2	CU	L	403	1/1	0.99	0.06	30,30,30,30	1
2	CU	A	403[B]	1/1	0.99	0.11	22,22,22,22	1
2	CU	B	402	1/1	0.99	0.07	28,28,28,28	1
2	CU	C	403	1/1	0.99	0.04	27,27,27,27	1
2	CU	D	402	1/1	0.99	0.04	27,27,27,27	1
2	CU	E	402	1/1	0.99	0.05	25,25,25,25	1
2	CU	F	403	1/1	0.99	0.04	29,29,29,29	1
2	CU	A	402	1/1	0.99	0.07	27,27,27,27	1
2	CU	G	403[A]	1/1	0.99	0.10	23,23,23,23	1
2	CU	G	403[B]	1/1	0.99	0.10	22,22,22,22	1
2	CU	H	402	1/1	0.99	0.04	27,27,27,27	1
2	CU	H	403	1/1	0.99	0.07	28,28,28,28	0
2	CU	I	401	1/1	0.99	0.08	28,28,28,28	0
2	CU	I	403	1/1	0.99	0.06	29,29,29,29	1
2	CU	K	402	1/1	0.99	0.08	31,31,31,31	1
2	CU	A	403[A]	1/1	0.99	0.11	22,22,22,22	1
2	CU	K	401	1/1	1.00	0.10	21,21,21,21	0
2	CU	D	403[B]	1/1	1.00	0.11	21,21,21,21	1
2	CU	E	401	1/1	1.00	0.10	18,18,18,18	0
2	CU	L	401[A]	1/1	1.00	0.10	23,23,23,23	1
2	CU	L	401[B]	1/1	1.00	0.10	21,21,21,21	1
2	CU	L	402	1/1	1.00	0.10	16,16,16,16	0
2	CU	B	403[A]	1/1	1.00	0.12	23,23,23,23	1
2	CU	E	403[A]	1/1	1.00	0.11	23,23,23,23	1
2	CU	E	403[B]	1/1	1.00	0.11	24,24,24,24	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	F	401[A]	1/1	1.00	0.10	20,20,20,20	1
2	CU	F	401[B]	1/1	1.00	0.10	19,19,19,19	1
2	CU	F	402	1/1	1.00	0.11	18,18,18,18	0
2	CU	B	403[B]	1/1	1.00	0.12	21,21,21,21	1
2	CU	G	401	1/1	1.00	0.10	17,17,17,17	0
2	CU	C	401[A]	1/1	1.00	0.09	24,24,24,24	1
2	CU	C	401[B]	1/1	1.00	0.09	22,22,22,22	1
2	CU	C	402	1/1	1.00	0.12	17,17,17,17	0
2	CU	H	401	1/1	1.00	0.11	17,17,17,17	0
2	CU	B	401	1/1	1.00	0.11	15,15,15,15	0
2	CU	D	401	1/1	1.00	0.10	17,17,17,17	0
2	CU	A	401	1/1	1.00	0.11	18,18,18,18	0
2	CU	I	402	1/1	1.00	0.12	20,20,20,20	0
2	CU	D	403[A]	1/1	1.00	0.11	24,24,24,24	1
2	CU	J	401	1/1	1.00	0.10	18,18,18,18	0
2	CU	J	402	1/1	1.00	0.06	26,26,26,26	1
2	CU	J	403[A]	1/1	1.00	0.10	27,27,27,27	1
2	CU	J	403[B]	1/1	1.00	0.10	25,25,25,25	1

6.5 Other polymers (i)

There are no such residues in this entry.