



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 10:02 PM BST

PDB ID : 6FDJ
Title : Crystal Structure of Two-Domain Laccase mutant H165A from *Streptomyces griseoflavus* with high copper ions occupancy
Authors : Gabdulkhakov, A.G.; Tishchenko, T.V.
Deposited on : 2017-12-25
Resolution : 2.31 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

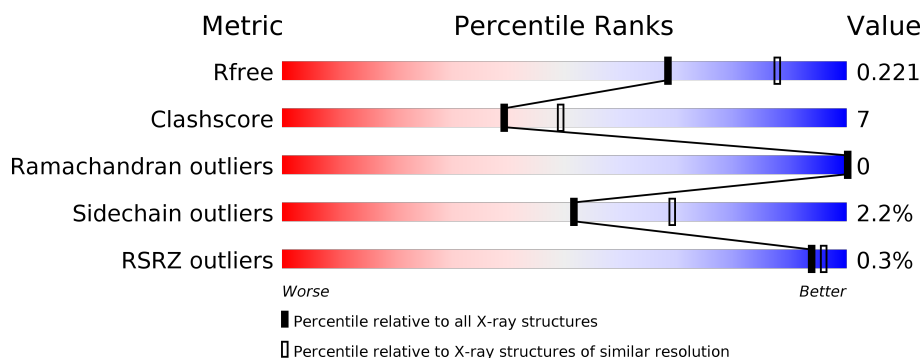
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	<div> <div></div> <div>71%15%14%</div> </div>
1	B	322	<div> <div>%</div> <div>71%15%14%</div> </div>
1	C	322	<div> <div></div> <div>71%14%15%</div> </div>
1	D	322	<div> <div></div> <div>71%15%14%</div> </div>
1	E	322	<div> <div></div> <div>70%16%14%</div> </div>
1	F	322	<div> <div></div> <div>70%15%15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	322	<div><div></div><div>74%12%14%</div></div>
1	H	322	<div><div>%</div><div></div><div>69%16%14%</div></div>
1	I	322	<div><div></div><div>67%19%14%</div></div>
1	J	322	<div><div></div><div>70%16%14%</div></div>
1	K	322	<div><div></div><div>67%18%14%</div></div>
1	L	322	<div><div></div><div>72%14%14%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25844 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	0	0
			2125	1325	387	401	12			
1	B	278	Total	C	N	O	S	0	1	0
			2132	1329	388	403	12			
1	C	275	Total	C	N	O	S	0	0	0
			2105	1313	384	396	12			
1	D	278	Total	C	N	O	S	0	0	0
			2125	1325	387	401	12			
1	E	277	Total	C	N	O	S	0	0	0
			2118	1320	386	400	12			
1	F	275	Total	C	N	O	S	0	0	0
			2105	1313	384	396	12			
1	G	278	Total	C	N	O	S	0	0	0
			2125	1325	387	401	12			
1	H	277	Total	C	N	O	S	0	0	0
			2118	1320	386	400	12			
1	I	276	Total	C	N	O	S	0	0	0
			2113	1317	385	399	12			
1	J	277	Total	C	N	O	S	0	0	0
			2120	1322	386	400	12			
1	K	276	Total	C	N	O	S	0	0	0
			2110	1316	385	397	12			
1	L	276	Total	C	N	O	S	0	0	0
			2113	1317	385	399	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
B	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
C	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
D	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
E	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81

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Chain	Residue	Modelled	Actual	Comment	Reference
F	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
G	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
H	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
I	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
J	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
K	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81
L	165	ALA	HIS	engineered mutation	UNP A0A0M4FJ81

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

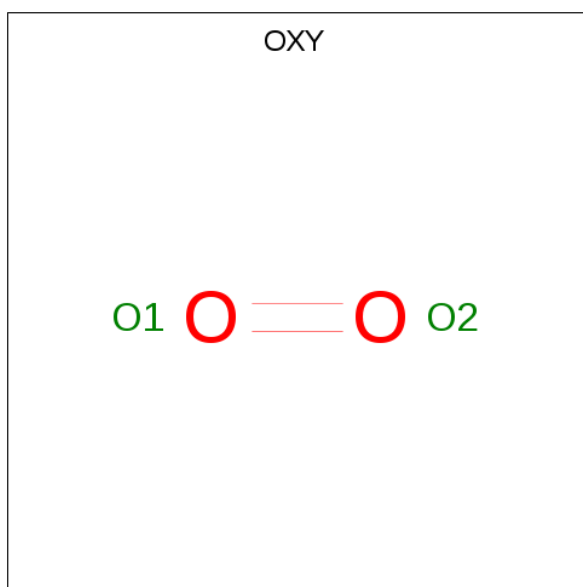
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	7	Total Cu 7 7	0	0
2	J	7	Total Cu 7 7	0	0
2	D	7	Total Cu 7 7	0	0
2	K	4	Total Cu 4 4	0	0
2	E	4	Total Cu 4 4	0	0
2	H	4	Total Cu 4 4	0	0
2	B	4	Total Cu 4 4	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	7	Total Cu 7 7	0	0
2	L	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	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	F	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	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	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			2	2		
4	G	1	Total	O	0	0
			2	2		
4	J	1	Total	O	0	0
			2	2		
4	K	1	Total	O	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	24	Total	O	0	0
			24	24		
5	C	31	Total	O	0	0
			31	31		
5	D	30	Total	O	0	0
			30	30		
5	E	32	Total	O	0	0
			32	32		
5	F	26	Total	O	0	0
			26	26		

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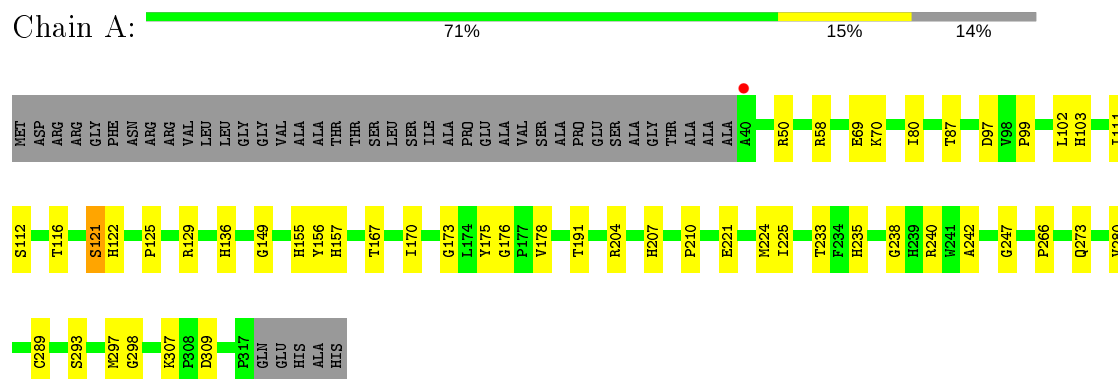
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	22	Total 22	O 22	0	0
5	H	28	Total 28	O 28	0	0
5	I	19	Total 19	O 19	0	0
5	J	26	Total 26	O 26	0	0
5	K	18	Total 18	O 18	0	0
5	L	23	Total 23	O 23	0	0

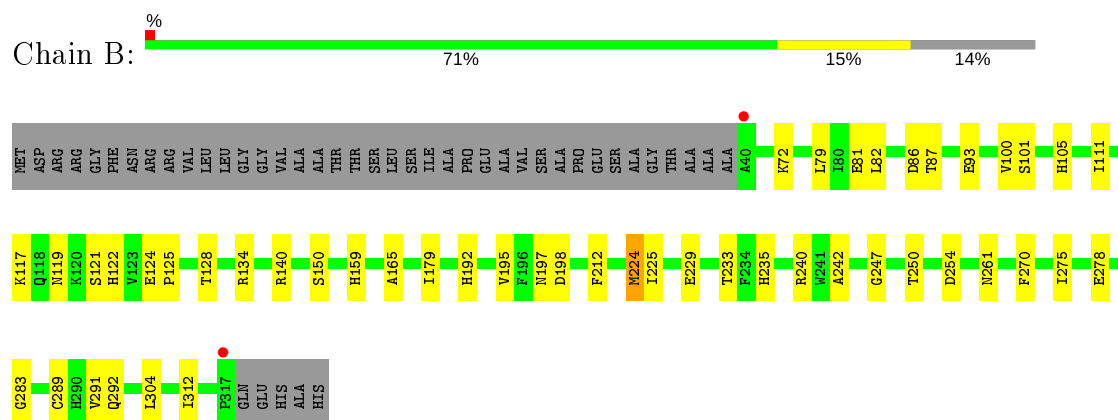
3 Residue-property plots

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.

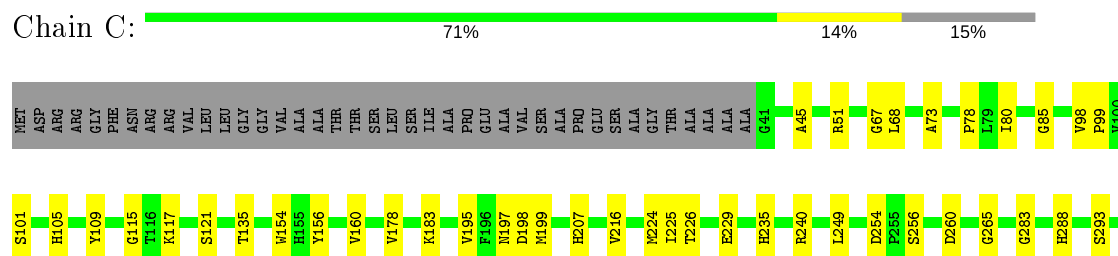
• Molecule 1: Two-domain laccase

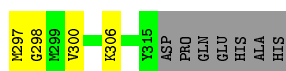


• Molecule 1: Two-domain laccase



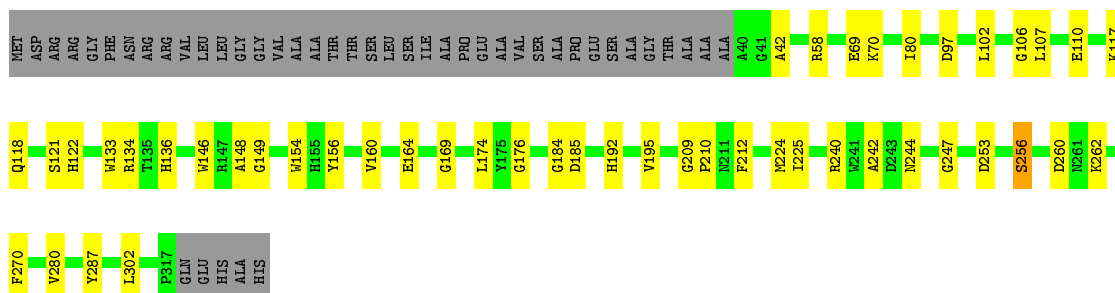
• Molecule 1: Two-domain laccase





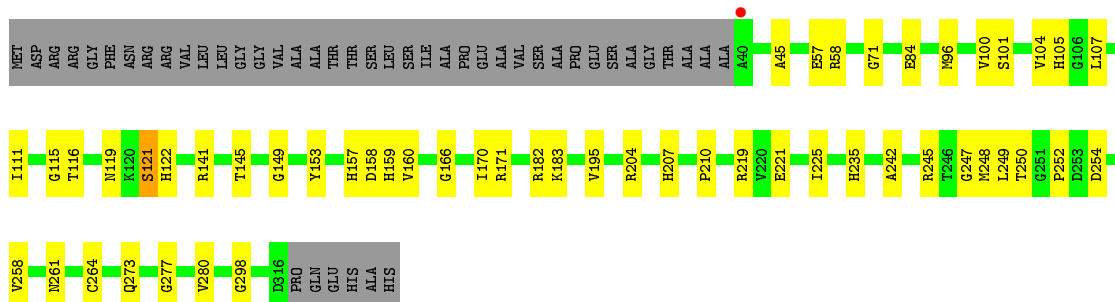
- Molecule 1: Two-domain laccase

Chain D:



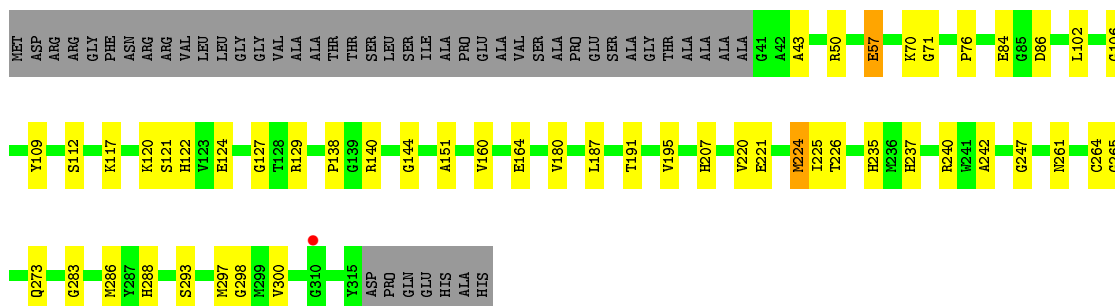
- Molecule 1: Two-domain laccase

Chain E:



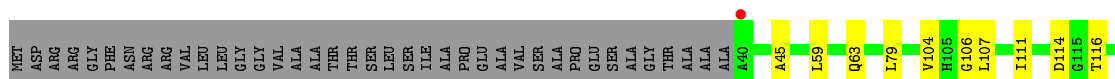
- Molecule 1: Two-domain laccase

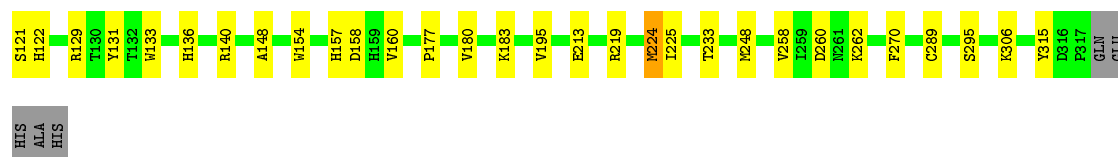
Chain F:



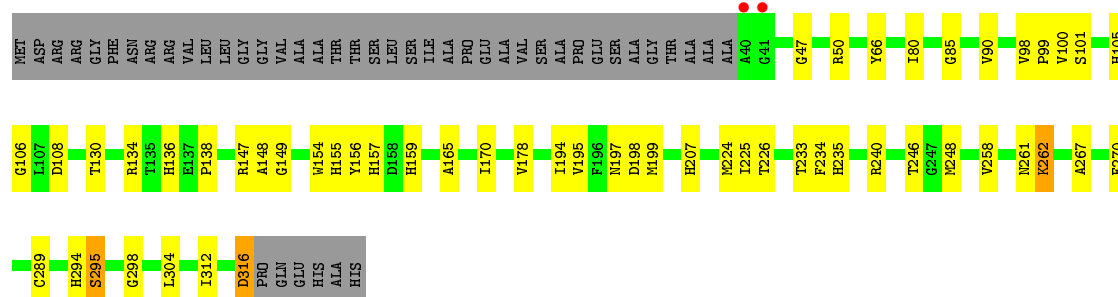
- Molecule 1: Two-domain laccase

Chain G:

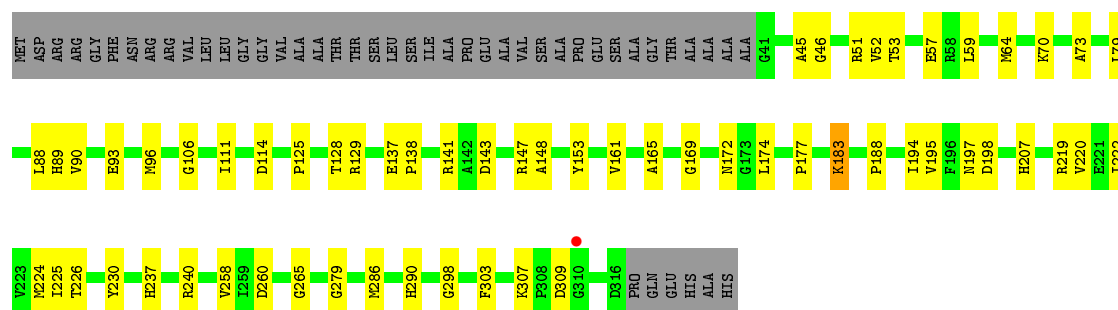




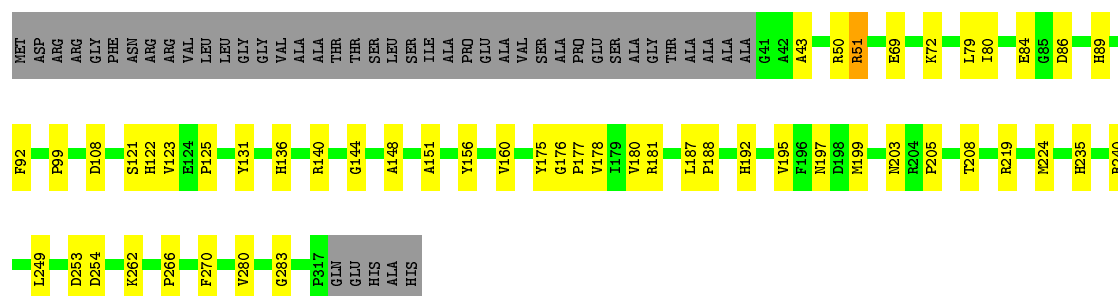
- Molecule 1: Two-domain laccase



- Molecule 1: Two-domain laccase

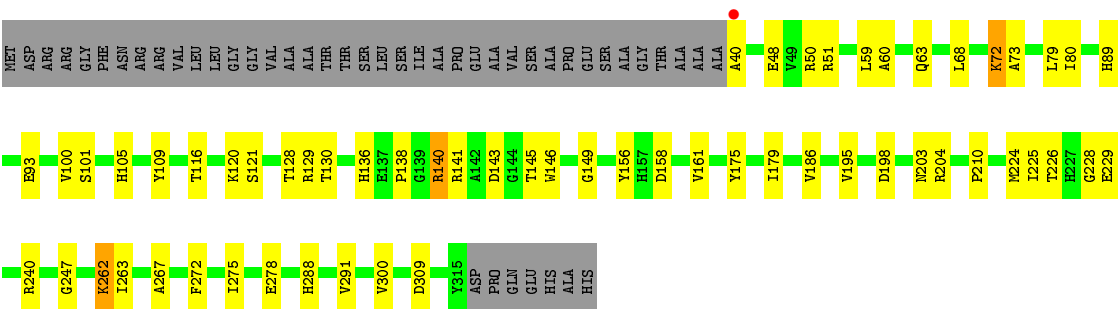


- Molecule 1: Two-domain laccase

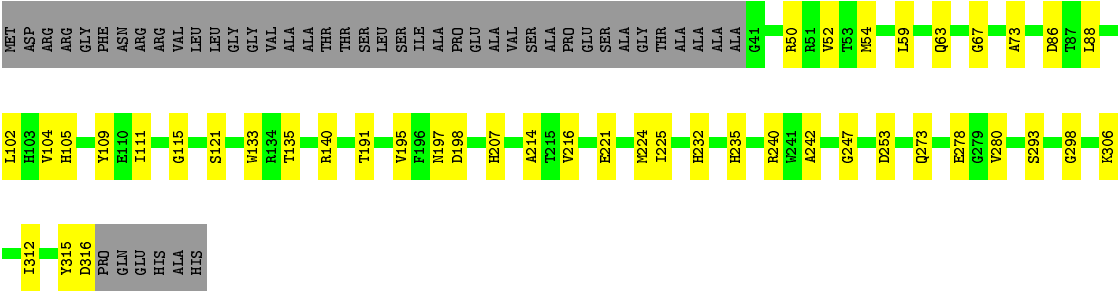


- Molecule 1: Two-domain laccase





● 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	77.37Å 95.12Å 116.47Å 90.13° 90.11° 91.85°	Depositor
Resolution (Å)	49.71 – 2.31 49.71 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.71-2.31) 97.5 (49.71-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.171 , 0.222 0.171 , 0.221	Depositor DCC
R_{free} test set	7160 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l 0.158 for -h,k,-l 0.205 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25844	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

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

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	0.41	0/2186	0.61	0/2970
1	B	0.45	0/2193	0.64	0/2980
1	C	0.42	0/2165	0.62	0/2940
1	D	0.44	0/2186	0.62	0/2970
1	E	0.45	0/2178	0.62	0/2958
1	F	0.42	0/2165	0.63	0/2940
1	G	0.42	0/2186	0.62	0/2970
1	H	0.42	0/2178	0.61	0/2958
1	I	0.38	0/2173	0.59	0/2951
1	J	0.44	0/2181	0.61	0/2963
1	K	0.44	0/2170	0.64	0/2947
1	L	0.44	0/2173	0.61	0/2951
All	All	0.43	0/26134	0.62	0/35498

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	2125	0	1999	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2132	0	2006	34	0
1	C	2105	0	1983	29	0
1	D	2125	0	1999	29	0
1	E	2118	0	1993	37	0
1	F	2105	0	1983	32	0
1	G	2125	0	1999	32	0
1	H	2118	0	1992	37	0
1	I	2113	0	1987	40	0
1	J	2120	0	1994	31	0
1	K	2110	0	1988	40	0
1	L	2113	0	1987	29	0
2	A	7	0	0	0	0
2	B	4	0	0	1	0
2	C	1	0	0	0	0
2	D	7	0	0	0	0
2	E	4	0	0	0	0
2	F	1	0	0	0	0
2	G	7	0	0	0	0
2	H	4	0	0	0	0
2	I	1	0	0	0	0
2	J	7	0	0	0	0
2	K	4	0	0	0	0
2	L	1	0	0	0	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
3	E	12	0	16	2	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
3	I	6	0	8	1	0
3	J	12	0	16	0	0
3	K	6	0	8	0	0
3	L	6	0	8	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
5	A	24	0	0	0	0
5	B	24	0	0	0	0
5	C	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	30	0	0	1	0
5	E	32	0	0	1	0
5	F	26	0	0	1	0
5	G	22	0	0	1	0
5	H	28	0	0	1	0
5	I	19	0	0	2	0
5	J	26	0	0	3	0
5	K	18	0	0	0	0
5	L	23	0	0	0	0
All	All	25844	0	24006	365	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 7.

All (365) 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:K:158:ASP:OD2	1:K:161:VAL:HG12	1.66	0.96
1:B:289:CYS:HG	2:B:401:CU:CU	0.68	0.94
1:C:80:ILE:HB	1:C:178:VAL:HG12	1.51	0.93
1:J:151:ALA:HA	1:J:180:VAL:HG23	1.56	0.86
1:B:124:GLU:HG3	1:B:125:PRO:HD2	1.58	0.84
1:J:199:MET:HB2	5:J:510:HOH:O	1.78	0.82
1:A:80:ILE:HD12	1:A:156:TYR:CE1	2.20	0.77
1:C:199:MET:HB2	5:C:519:HOH:O	1.84	0.76
1:A:80:ILE:CD1	1:A:156:TYR:CE1	2.69	0.75
1:F:57:GLU:OE2	1:F:70:LYS:HD2	1.88	0.74
1:F:288:HIS:HB3	1:F:300:VAL:HG12	1.72	0.71
1:H:262:LYS:HD2	1:H:270:PHE:CE2	2.26	0.71
1:G:136:HIS:NE2	1:G:148:ALA:O	2.22	0.69
1:K:93:GLU:HB2	1:K:128:THR:HG22	1.74	0.69
1:I:46:GLY:H	1:I:183:LYS:NZ	1.93	0.67
1:J:192:HIS:NE2	5:J:502:HOH:O	2.28	0.67
1:L:191:THR:HG23	1:L:221:GLU:HG2	1.75	0.67
1:E:84:GLU:OE2	1:E:182:ARG:NH2	2.25	0.66
1:I:59:LEU:HD21	1:I:73:ALA:HB3	1.78	0.66
1:A:80:ILE:HD12	1:A:156:TYR:HE1	1.57	0.66
1:I:64:MET:HG3	1:I:172:ASN:HB3	1.77	0.66
1:K:59:LEU:HD21	1:K:73:ALA:HB3	1.78	0.66
1:H:224:MET:HG2	1:H:270:PHE:CZ	2.30	0.66
1:E:57:GLU:OE2	1:E:71:GLY:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:LYS:HD3	1:G:270:PHE:CE1	2.32	0.65
1:J:197:ASN:ND2	1:J:203:ASN:OD1	2.27	0.65
1:J:188:PRO:HA	1:J:219:ARG:HG2	1.79	0.64
1:E:245:ARG:NH1	3:E:404:GOL:O3	2.31	0.64
1:A:280:VAL:HG12	1:C:109:TYR:H	1.63	0.64
1:C:99:PRO:HD2	1:H:98:VAL:HG12	1.78	0.64
1:C:288:HIS:HB3	1:C:300:VAL:HG12	1.80	0.63
1:B:195:VAL:HG22	1:B:225:ILE:HB	1.81	0.62
1:K:60:ALA:O	1:K:63:GLN:HG3	2.00	0.62
1:E:219:ARG:HH12	1:E:248:MET:CE	2.13	0.61
1:L:52:VAL:HG22	1:L:88:LEU:HD11	1.81	0.61
1:A:156:TYR:CZ	1:A:176:GLY:HA3	2.36	0.61
1:K:143:ASP:OD1	1:K:145:THR:HG22	2.01	0.60
1:D:122:HIS:HB3	1:D:160:VAL:HG21	1.84	0.60
1:H:304:LEU:HB3	1:H:312:ILE:HD13	1.84	0.60
1:L:221:GLU:HB2	1:L:273:GLN:HG2	1.83	0.60
1:F:117:LYS:HD3	1:F:164:GLU:HG2	1.84	0.60
1:F:57:GLU:OE2	1:F:70:LYS:HA	2.02	0.59
1:F:50:ARG:NH1	1:F:86:ASP:OD2	2.35	0.59
1:C:297:MET:HG2	1:I:230:TYR:OH	2.02	0.59
1:K:79:LEU:HD11	1:K:179:ILE:HG13	1.84	0.59
1:E:115:GLY:H	1:E:121:SER:HB3	1.68	0.58
1:D:136:HIS:NE2	1:D:148:ALA:O	2.23	0.58
1:H:154:TRP:HB2	1:H:178:VAL:HG23	1.84	0.58
1:D:156:TYR:CZ	1:D:176:GLY:HA3	2.39	0.58
1:J:140:ARG:NH1	1:J:144:GLY:O	2.33	0.58
1:E:219:ARG:HH12	1:E:248:MET:HE3	1.69	0.57
1:K:141:ARG:HH11	1:K:145:THR:CG2	2.17	0.57
1:A:307:LYS:HB2	1:A:309:ASP:OD1	2.04	0.57
1:B:233:THR:OG1	1:B:261:ASN:OD1	2.21	0.57
1:K:51:ARG:HG2	1:K:89:HIS:HB2	1.86	0.57
1:A:103:HIS:NE2	4:A:407:OXY:O2	2.37	0.57
1:K:68:LEU:H	1:K:72:LYS:HE2	1.69	0.57
1:E:104:VAL:HG21	1:E:107:LEU:HD22	1.87	0.57
1:G:262:LYS:CD	1:G:270:PHE:CZ	2.87	0.57
1:H:207:HIS:CE1	1:H:298:GLY:HA2	2.39	0.57
1:J:280:VAL:HG12	1:L:109:TYR:H	1.69	0.57
1:B:229:GLU:OE2	1:C:293:SER:OG	2.23	0.56
1:E:45:ALA:HB2	1:E:183:LYS:HE2	1.86	0.56
1:B:111:ILE:HG13	1:B:119:ASN:ND2	2.20	0.56
1:I:197:ASN:O	1:I:198:ASP:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:ALA:HA	1:F:180:VAL:HB	1.87	0.56
1:E:122:HIS:HB3	1:E:160:VAL:HG21	1.88	0.56
1:K:141:ARG:NH2	1:L:278:GLU:OE1	2.34	0.56
1:B:242:ALA:O	1:B:247:GLY:HA2	2.05	0.56
1:H:289:CYS:O	1:H:295:SER:HB3	2.06	0.56
1:A:207:HIS:CD2	1:A:298:GLY:HA2	2.41	0.56
1:J:156:TYR:HD1	1:J:178:VAL:HG23	1.70	0.56
1:K:141:ARG:HH21	1:L:278:GLU:CD	2.08	0.56
1:D:58:ARG:NH2	1:D:97:ASP:OD1	2.39	0.56
1:I:45:ALA:HA	1:I:183:LYS:HG3	1.89	0.55
1:E:242:ALA:O	1:E:247:GLY:HA2	2.05	0.55
1:G:122:HIS:HB3	1:G:160:VAL:HG21	1.88	0.55
1:G:258:VAL:HG21	1:I:148:ALA:HB1	1.88	0.55
1:L:54:MET:HE2	1:L:102:LEU:HD22	1.88	0.55
1:A:111:ILE:HG21	1:B:283:GLY:HA3	1.89	0.55
1:D:42:ALA:HA	1:D:185:ASP:O	2.06	0.55
1:F:207:HIS:CE1	1:F:298:GLY:HA2	2.41	0.55
1:I:52:VAL:HG12	1:I:88:LEU:HD21	1.89	0.55
1:L:86:ASP:O	1:L:135:THR:OG1	2.25	0.55
1:E:207:HIS:CE1	1:E:298:GLY:HA2	2.43	0.54
1:A:157:HIS:ND1	1:A:170:ILE:HD11	2.23	0.54
1:B:124:GLU:CG	1:B:125:PRO:HD2	2.35	0.54
1:J:136:HIS:NE2	1:J:148:ALA:O	2.30	0.54
1:L:216:VAL:HG23	1:L:306:LYS:O	2.08	0.54
1:B:197:ASN:O	1:B:198:ASP:HB2	2.08	0.54
1:E:250:THR:HG22	1:E:254:ASP:HB2	1.89	0.54
1:G:116:THR:H	1:G:121:SER:HB3	1.71	0.54
1:A:99:PRO:HG3	1:A:125:PRO:HD3	1.90	0.53
1:G:224:MET:SD	1:G:224:MET:C	2.86	0.53
1:L:312:ILE:HB	1:L:315:TYR:HB3	1.91	0.53
1:E:111:ILE:HG21	1:F:283:GLY:HA3	1.91	0.53
1:B:93:GLU:HB2	1:B:128[A]:THR:HG22	1.90	0.53
1:G:106:GLY:HA3	1:G:154:TRP:CD2	2.44	0.53
1:G:262:LYS:CD	1:G:270:PHE:CE1	2.91	0.53
1:G:262:LYS:HD2	1:G:270:PHE:CZ	2.43	0.53
1:L:207:HIS:CE1	1:L:298:GLY:HA2	2.44	0.53
1:D:148:ALA:HB1	1:E:258:VAL:HG21	1.90	0.53
1:E:195:VAL:HA	1:E:225:ILE:O	2.09	0.53
1:F:84:GLU:OE1	1:F:138:PRO:HD3	2.08	0.53
1:D:80:ILE:HD12	1:D:156:TYR:CE1	2.44	0.52
1:G:79:LEU:HA	1:G:177:PRO:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:ASN:O	1:H:198:ASP:HB2	2.09	0.52
1:I:79:LEU:HA	1:I:177:PRO:HG2	1.90	0.52
1:D:117:LYS:HD2	1:D:164:GLU:OE2	2.10	0.52
1:D:244:ASN:HB3	1:D:256:SER:OG	2.09	0.52
1:G:195:VAL:HA	1:G:225:ILE:O	2.09	0.52
1:G:260:ASP:OD2	1:I:106:GLY:N	2.42	0.52
1:B:117:LYS:HD3	1:B:122:HIS:CD2	2.45	0.52
1:E:221:GLU:HB2	1:E:273:GLN:HG2	1.92	0.52
1:B:111:ILE:HD12	1:C:283:GLY:HA3	1.90	0.52
1:D:262:LYS:HD3	1:D:270:PHE:CE1	2.45	0.52
1:K:158:ASP:OD2	1:K:161:VAL:CG1	2.51	0.52
1:G:262:LYS:HD3	1:G:270:PHE:CZ	2.45	0.51
1:G:262:LYS:HE2	1:G:270:PHE:CG	2.44	0.51
1:J:205:PRO:HG2	1:J:208:THR:HG21	1.91	0.51
1:J:266:PRO:HG2	1:K:291:VAL:HG22	1.91	0.51
1:I:88:LEU:HD23	1:I:89:HIS:N	2.24	0.51
1:B:79:LEU:HD11	1:B:179:ILE:HG13	1.93	0.51
1:E:157:HIS:ND1	1:E:158:ASP:O	2.42	0.51
1:K:138:PRO:HB2	1:K:146:TRP:CZ2	2.46	0.51
1:D:110:GLU:HG3	1:D:134:ARG:HH21	1.76	0.51
1:F:124:GLU:OE1	1:F:127:GLY:HA3	2.10	0.51
1:L:214:ALA:O	1:L:306:LYS:N	2.37	0.51
1:B:235:HIS:HB2	1:B:261:ASN:ND2	2.26	0.50
1:B:275:ILE:HB	1:B:278:GLU:HB2	1.94	0.50
1:E:115:GLY:H	1:E:121:SER:CB	2.24	0.50
1:H:226:THR:O	1:H:267:ALA:N	2.38	0.50
1:I:237:HIS:CE1	1:I:286:MET:HE2	2.47	0.50
1:K:105:HIS:CE1	1:L:235:HIS:CE1	2.99	0.50
1:A:116:THR:H	1:A:121:SER:HB3	1.76	0.50
1:A:242:ALA:O	1:A:247:GLY:HA2	2.12	0.50
1:G:111:ILE:O	1:G:114:ASP:HB2	2.11	0.50
1:K:275:ILE:HB	1:K:278:GLU:HB2	1.93	0.50
1:B:82:LEU:HB3	1:B:86:ASP:HB2	1.92	0.50
1:K:229:GLU:OE2	1:L:293:SER:OG	2.29	0.50
1:I:64:MET:HE2	1:I:161:VAL:HG11	1.94	0.50
1:L:140:ARG:HG3	1:L:140:ARG:HH11	1.75	0.50
1:C:80:ILE:HD12	1:C:156:TYR:CE1	2.47	0.50
1:I:57:GLU:HG2	1:I:70:LYS:HE3	1.94	0.50
1:J:79:LEU:HA	1:J:177:PRO:HG2	1.93	0.50
1:C:115:GLY:H	1:C:121:SER:HB2	1.77	0.50
1:L:59:LEU:N	1:L:63:GLN:O	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ILE:HB	1:E:119:ASN:ND2	2.26	0.50
1:G:224:MET:SD	5:G:517:HOH:O	2.60	0.50
1:I:153:TYR:O	3:I:402:GOL:H12	2.11	0.50
1:G:157:HIS:ND1	1:G:158:ASP:O	2.37	0.49
1:D:195:VAL:HA	1:D:225:ILE:O	2.12	0.49
1:B:233:THR:HG22	1:B:291:VAL:HG23	1.94	0.49
1:G:262:LYS:HE2	1:G:270:PHE:CD1	2.47	0.49
1:H:199:MET:HE1	1:H:294:HIS:HA	1.95	0.49
1:E:166:GLY:O	1:E:170:ILE:HG13	2.12	0.49
1:D:242:ALA:O	1:D:247:GLY:HA2	2.11	0.49
1:J:50:ARG:NH1	1:J:86:ASP:OD2	2.44	0.49
1:A:293:SER:HB3	1:C:229:GLU:OE2	2.13	0.49
1:K:140:ARG:CD	1:K:146:TRP:HE3	2.26	0.49
1:D:280:VAL:HG12	1:F:109:TYR:H	1.78	0.48
1:F:288:HIS:CB	1:F:300:VAL:HG12	2.40	0.48
1:A:221:GLU:HB2	1:A:273:GLN:HG2	1.94	0.48
1:E:235:HIS:HB2	1:E:261:ASN:OD1	2.12	0.48
1:I:111:ILE:O	1:I:114:ASP:HB2	2.14	0.48
1:E:149:GLY:HA3	1:E:182:ARG:HH21	1.78	0.48
1:A:293:SER:O	1:A:297:MET:HG3	2.14	0.48
1:E:58:ARG:HG3	1:E:96:MET:HG2	1.96	0.48
1:D:192:HIS:HB3	1:D:212:PHE:CE1	2.49	0.48
1:F:57:GLU:OE2	1:F:71:GLY:N	2.43	0.48
1:F:226:THR:HB	1:F:265:GLY:O	2.13	0.48
1:H:233:THR:O	1:H:289:CYS:HA	2.14	0.48
1:D:210:PRO:HD2	1:D:287:TYR:OH	2.13	0.48
1:H:235:HIS:HB2	1:H:261:ASN:OD1	2.14	0.48
1:H:195:VAL:HA	1:H:225:ILE:O	2.14	0.47
1:H:194:ILE:O	1:H:224:MET:HA	2.14	0.47
1:G:262:LYS:HD2	1:G:270:PHE:CE2	2.48	0.47
1:J:51:ARG:HA	1:J:89:HIS:O	2.14	0.47
1:G:116:THR:N	1:G:121:SER:HB3	2.29	0.47
1:H:157:HIS:ND1	1:H:170:ILE:HD11	2.30	0.47
1:B:198:ASP:OD1	1:B:229:GLU:N	2.44	0.47
1:E:277:GLY:HA2	1:E:280:VAL:HG23	1.96	0.47
1:I:64:MET:HE1	1:I:161:VAL:HG21	1.96	0.47
1:K:141:ARG:HH11	1:K:145:THR:HG23	1.78	0.47
1:D:106:GLY:HA3	1:D:154:TRP:CD2	2.49	0.47
1:D:260:ASP:OD2	1:F:106:GLY:N	2.47	0.47
1:G:233:THR:O	1:G:289:CYS:HA	2.15	0.47
1:J:80:ILE:HB	1:J:178:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:120:LYS:HA	1:K:120:LYS:HD2	1.73	0.47
1:G:315:TYR:O	1:K:309:ASP:HB3	2.14	0.47
1:C:85:GLY:N	1:C:135:THR:OG1	2.47	0.46
1:E:116:THR:H	1:E:121:SER:HB3	1.80	0.46
1:I:194:ILE:HD12	1:I:222:ILE:HG23	1.97	0.46
1:J:69:GLU:HB2	1:J:72:LYS:HD3	1.97	0.46
1:L:104:VAL:HB	1:L:133:TRP:CZ2	2.51	0.46
1:H:148:ALA:HB1	1:I:258:VAL:HG21	1.98	0.46
1:L:115:GLY:N	1:L:121:SER:OG	2.48	0.46
1:B:100:VAL:HG22	1:B:101:SER:H	1.79	0.46
1:A:266:PRO:O	1:B:233:THR:HG21	2.15	0.46
1:C:207:HIS:CE1	1:C:298:GLY:HA2	2.51	0.46
1:B:195:VAL:HA	1:B:225:ILE:O	2.16	0.46
1:H:156:TYR:HD2	1:H:178:VAL:HG13	1.80	0.46
1:L:195:VAL:HA	1:L:225:ILE:O	2.16	0.46
1:C:67:GLY:HA3	1:C:73:ALA:HA	1.97	0.46
1:H:134:ARG:NH1	1:I:279:GLY:O	2.29	0.46
1:C:235:HIS:HE1	1:C:260:ASP:OD2	1.98	0.46
1:E:249:LEU:HD22	1:E:254:ASP:HB3	1.98	0.46
1:H:105:HIS:CD2	1:H:155:HIS:CE1	3.04	0.46
1:J:92:PHE:CD1	1:J:123:VAL:HG21	2.51	0.46
1:B:192:HIS:HB3	1:B:212:PHE:CE1	2.51	0.45
1:E:105:HIS:CE1	1:F:235:HIS:CE1	3.04	0.45
1:E:141:ARG:HB2	1:E:145:THR:O	2.15	0.45
1:E:149:GLY:HA3	1:E:182:ARG:NH2	2.31	0.45
1:L:306:LYS:HG2	1:L:312:ILE:HD11	1.97	0.45
1:K:116:THR:H	1:K:121:SER:HB3	1.81	0.45
1:K:141:ARG:HH11	1:K:145:THR:HG21	1.81	0.45
1:K:175:TYR:OH	1:K:203:ASN:OD1	2.22	0.45
1:L:67:GLY:HA3	1:L:73:ALA:HA	1.99	0.45
1:B:159:HIS:CE1	1:B:165:ALA:HA	2.51	0.45
1:C:154:TRP:HB2	1:C:178:VAL:HG23	1.98	0.45
1:D:136:HIS:CD2	1:D:149:GLY:HA2	2.51	0.45
1:K:100:VAL:HG22	1:K:101:SER:H	1.80	0.45
1:I:165:ALA:HB1	5:I:511:HOH:O	2.17	0.45
1:K:40:ALA:HB3	1:K:186:VAL:HG13	1.99	0.45
1:E:84:GLU:OE2	1:E:149:GLY:HA3	2.16	0.45
1:F:293:SER:O	1:F:297:MET:HG2	2.17	0.45
1:I:96:MET:O	1:I:125:PRO:HB3	2.17	0.45
1:D:195:VAL:HG22	1:D:225:ILE:HB	1.99	0.44
1:F:112:SER:O	1:F:129:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:VAL:HG23	1:H:178:VAL:O	2.17	0.44
1:I:46:GLY:H	1:I:183:LYS:HZ2	1.62	0.44
1:K:141:ARG:HB2	1:K:145:THR:HG22	1.98	0.44
1:A:235:HIS:CE1	1:C:105:HIS:CE1	3.06	0.44
1:E:104:VAL:HG12	5:E:522:HOH:O	2.16	0.44
1:F:242:ALA:O	1:F:247:GLY:HA2	2.18	0.44
1:B:121:SER:O	1:B:121:SER:OG	2.34	0.44
1:B:304:LEU:HB3	1:B:312:ILE:HD13	2.00	0.44
1:B:87:THR:HG23	1:B:134:ARG:HG2	1.98	0.44
1:I:183:LYS:CD	1:I:183:LYS:H	2.30	0.44
1:K:48:GLU:HG2	1:K:50:ARG:HG3	1.99	0.44
1:B:229:GLU:OE1	1:C:293:SER:N	2.42	0.44
1:B:105:HIS:CE1	1:C:235:HIS:CE1	3.06	0.44
1:F:195:VAL:HA	1:F:225:ILE:O	2.17	0.44
1:F:237:HIS:CE1	1:F:286:MET:HE2	2.52	0.44
1:H:80:ILE:HB	1:H:178:VAL:HG12	2.00	0.44
1:K:195:VAL:HA	1:K:225:ILE:O	2.18	0.44
1:D:253:ASP:HB2	5:D:521:HOH:O	2.17	0.44
1:E:115:GLY:N	1:E:121:SER:HB3	2.33	0.44
1:I:188:PRO:HA	1:I:219:ARG:HG2	1.99	0.44
1:J:108:ASP:OD2	1:J:136:HIS:ND1	2.50	0.44
1:H:316:ASP:OD1	1:H:316:ASP:N	2.46	0.44
1:I:207:HIS:CE1	1:I:298:GLY:HA2	2.53	0.44
1:J:235:HIS:CE1	1:L:105:HIS:CE1	3.05	0.44
1:H:246:THR:HG23	1:H:248:MET:H	1.82	0.44
1:I:138:PRO:HA	1:I:147:ARG:O	2.18	0.44
1:J:249:LEU:HD22	1:J:254:ASP:HB3	2.00	0.44
1:A:116:THR:N	1:A:121:SER:HB3	2.33	0.43
1:F:191:THR:OG1	1:F:221:GLU:OE1	2.31	0.43
1:L:253:ASP:OD1	1:L:253:ASP:N	2.30	0.43
1:C:197:ASN:O	1:C:198:ASP:HB2	2.18	0.43
1:C:216:VAL:HG23	1:C:306:LYS:O	2.19	0.43
1:I:141:ARG:HB2	1:I:143:ASP:OD1	2.16	0.43
1:A:156:TYR:HD1	1:A:178:VAL:CG2	2.31	0.43
1:A:58:ARG:NH1	1:A:97:ASP:OD1	2.51	0.43
1:B:224:MET:HB3	1:B:270:PHE:CE1	2.54	0.43
1:H:138:PRO:HD3	1:H:149:GLY:HA3	2.00	0.43
1:I:195:VAL:HA	1:I:225:ILE:O	2.18	0.43
1:J:84:GLU:HG3	1:J:181:ARG:O	2.19	0.43
1:A:112:SER:O	1:A:129:ARG:NH2	2.52	0.43
1:J:122:HIS:HB3	1:J:160:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:VAL:HG22	1:G:225:ILE:HB	2.00	0.43
1:J:43:ALA:HB2	1:J:187:LEU:HD21	2.00	0.43
1:K:129:ARG:HG2	1:K:130:THR:N	2.33	0.43
1:K:80:ILE:HD12	1:K:156:TYR:CE2	2.54	0.43
1:C:195:VAL:HA	1:C:225:ILE:O	2.19	0.43
1:G:129:ARG:HD3	1:G:131:TYR:CZ	2.54	0.42
1:B:250:THR:HB	1:B:254:ASP:HB2	2.00	0.42
1:C:226:THR:HB	1:C:265:GLY:O	2.19	0.42
1:F:43:ALA:HB2	1:F:187:LEU:HD21	2.00	0.42
1:H:246:THR:HG22	5:H:528:HOH:O	2.19	0.42
1:J:121:SER:O	1:J:131:TYR:OH	2.23	0.42
1:L:198:ASP:O	1:L:232:HIS:CE1	2.72	0.42
1:A:155:HIS:HB3	1:A:225:ILE:HD13	2.02	0.42
1:B:81:GLU:HA	1:B:179:ILE:O	2.19	0.42
1:A:167:THR:OG1	1:B:292:GLN:HB3	2.19	0.42
1:D:209:GLY:HA3	1:D:210:PRO:HA	1.84	0.42
1:J:175:TYR:CE1	1:J:195:VAL:HG11	2.54	0.42
1:A:173:GLY:HA2	1:A:175:TYR:CE2	2.54	0.42
1:A:191:THR:HA	1:A:221:GLU:O	2.20	0.42
1:D:107:LEU:HD12	1:D:133:TRP:HB3	2.02	0.42
1:A:136:HIS:CD2	1:A:149:GLY:HA2	2.54	0.42
1:F:235:HIS:HB2	1:F:261:ASN:OD1	2.20	0.42
1:J:262:LYS:HD3	1:J:270:PHE:CE2	2.54	0.42
1:F:120:LYS:HA	1:F:120:LYS:HD3	1.75	0.42
1:F:140:ARG:NH2	1:F:144:GLY:O	2.51	0.42
1:G:107:LEU:HD21	1:G:180:VAL:HG21	2.00	0.42
1:K:262:LYS:HD3	1:K:263:ILE:O	2.20	0.42
1:B:72:LYS:HB3	1:B:72:LYS:HE3	1.88	0.42
1:D:302:LEU:HD23	1:D:302:LEU:HA	1.88	0.42
1:E:153:TYR:CZ	3:E:404:GOL:H2	2.54	0.42
1:D:146:TRP:CH2	1:E:252:PRO:HG3	2.55	0.42
1:H:234:PHE:O	1:H:261:ASN:HA	2.19	0.42
1:I:88:LEU:HD22	1:I:90:VAL:HG23	2.02	0.42
1:A:50:ARG:HG2	1:A:87:THR:O	2.20	0.42
1:D:106:GLY:HA3	1:D:154:TRP:CE3	2.55	0.42
1:H:267:ALA:HB2	1:I:290:HIS:CE1	2.55	0.42
1:C:45:ALA:HB2	1:C:183:LYS:HD2	2.01	0.41
1:C:68:LEU:HG	1:C:78:PRO:HG3	2.02	0.41
1:H:90:VAL:O	1:H:130:THR:HA	2.19	0.41
1:I:93:GLU:HB2	1:I:128:THR:HG22	2.01	0.41
1:I:52:VAL:HG22	1:I:53:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:TYR:H	1:L:280:VAL:HG12	1.85	0.41
1:D:169:GLY:O	1:D:174:LEU:HB2	2.20	0.41
1:G:45:ALA:HA	1:G:183:LYS:HB2	2.02	0.41
1:H:100:VAL:HG22	1:H:101:SER:H	1.85	0.41
1:K:204:ARG:HD3	1:K:210:PRO:HD3	2.01	0.41
1:I:226:THR:HB	1:I:265:GLY:O	2.20	0.41
1:L:197:ASN:O	1:L:198:ASP:HB2	2.20	0.41
1:D:69:GLU:HG2	1:D:70:LYS:N	2.35	0.41
1:F:224:MET:SD	5:F:516:HOH:O	2.62	0.41
1:I:96:MET:HB3	1:I:96:MET:HE3	1.73	0.41
1:E:204:ARG:HD3	1:E:210:PRO:HD3	2.02	0.41
1:F:140:ARG:HH21	1:F:140:ARG:HG3	1.86	0.41
1:F:220:VAL:O	1:F:273:GLN:HA	2.20	0.41
1:I:169:GLY:O	1:I:174:LEU:HB2	2.21	0.41
1:J:253:ASP:N	1:J:253:ASP:OD1	2.52	0.41
1:K:136:HIS:CD2	1:K:149:GLY:HA2	2.56	0.41
1:H:108:ASP:OD2	1:H:136:HIS:ND1	2.47	0.41
1:I:137:GLU:HG2	1:I:183:LYS:HE2	2.01	0.41
1:L:306:LYS:HG2	1:L:312:ILE:CD1	2.50	0.41
1:C:249:LEU:HD22	1:C:254:ASP:HB3	2.03	0.41
1:F:224:MET:C	1:F:224:MET:SD	2.99	0.41
1:G:219:ARG:HH12	1:G:248:MET:HE3	1.86	0.41
1:I:260:ASP:OD2	5:I:501:HOH:O	2.22	0.41
1:K:226:THR:O	1:K:267:ALA:N	2.41	0.41
1:G:104:VAL:HB	1:G:133:TRP:CZ2	2.56	0.41
1:G:213:GLU:HB3	1:G:306:LYS:HE2	2.02	0.41
1:J:99:PRO:HG3	1:J:125:PRO:HD3	2.03	0.41
1:J:283:GLY:HA3	1:L:111:ILE:HD13	2.01	0.41
1:G:148:ALA:HB1	1:H:258:VAL:HG21	2.02	0.41
1:K:198:ASP:OD1	1:K:228:GLY:HA3	2.21	0.41
1:A:204:ARG:HD3	1:A:210:PRO:HD3	2.03	0.40
1:H:106:GLY:HA3	1:H:154:TRP:CD2	2.57	0.40
1:H:66:TYR:CD2	1:H:156:TYR:HE1	2.39	0.40
1:J:262:LYS:HD2	5:J:508:HOH:O	2.20	0.40
1:D:42:ALA:HB1	1:D:184:GLY:HA2	2.02	0.40
1:E:159:HIS:CE1	1:F:286:MET:HE1	2.56	0.40
1:G:59:LEU:HB2	1:G:63:GLN:HB2	2.03	0.40
1:I:220:VAL:HG21	1:I:303:PHE:HZ	1.86	0.40
1:L:242:ALA:O	1:L:247:GLY:HA2	2.21	0.40
1:C:156:TYR:HD1	1:C:178:VAL:HG13	1.87	0.40
1:C:249:LEU:HD23	1:C:256:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:HIS:HB3	1:F:160:VAL:HG11	2.03	0.40
1:H:138:PRO:HA	1:H:147:ARG:O	2.20	0.40
1:H:159:HIS:CE1	1:H:165:ALA:HA	2.56	0.40
1:C:98:VAL:HG12	1:H:99:PRO:HD2	2.03	0.40
1:J:156:TYR:CZ	1:J:176:GLY:HA3	2.56	0.40
1:A:233:THR:O	1:A:289:CYS:HA	2.20	0.40
1:E:100:VAL:HG22	1:E:101:SER:H	1.86	0.40
1:K:140:ARG:HD2	1:K:146:TRP:HE3	1.86	0.40
1:A:238:GLY:O	1:A:280:VAL:HG21	2.22	0.40
1:H:47:GLY:HA2	1:H:85:GLY:O	2.21	0.40
1:I:307:LYS:O	1:I:309:ASP:N	2.54	0.40
1:K:247:GLY:HA3	1:K:272:PHE:CB	2.52	0.40
1:K:288:HIS:HB3	1:K:300:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	276/322 (86%)	269 (98%)	7 (2%)	0	100	100
1	B	277/322 (86%)	261 (94%)	16 (6%)	0	100	100
1	C	273/322 (85%)	255 (93%)	18 (7%)	0	100	100
1	D	276/322 (86%)	261 (95%)	15 (5%)	0	100	100
1	E	275/322 (85%)	257 (94%)	18 (6%)	0	100	100
1	F	273/322 (85%)	256 (94%)	17 (6%)	0	100	100
1	G	276/322 (86%)	259 (94%)	17 (6%)	0	100	100
1	H	275/322 (85%)	264 (96%)	11 (4%)	0	100	100
1	I	274/322 (85%)	255 (93%)	19 (7%)	0	100	100
1	J	275/322 (85%)	266 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	274/322 (85%)	258 (94%)	16 (6%)	0	100	100
1	L	274/322 (85%)	262 (96%)	12 (4%)	0	100	100
All	All	3298/3864 (85%)	3123 (95%)	175 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	218/248 (88%)	211 (97%)	7 (3%)	39	54
1	B	219/248 (88%)	215 (98%)	4 (2%)	59	75
1	C	216/248 (87%)	210 (97%)	6 (3%)	43	60
1	D	218/248 (88%)	212 (97%)	6 (3%)	43	60
1	E	217/248 (88%)	214 (99%)	3 (1%)	67	81
1	F	216/248 (87%)	209 (97%)	7 (3%)	39	54
1	G	218/248 (88%)	215 (99%)	3 (1%)	67	81
1	H	217/248 (88%)	212 (98%)	5 (2%)	50	67
1	I	217/248 (88%)	212 (98%)	5 (2%)	50	67
1	J	218/248 (88%)	215 (99%)	3 (1%)	67	81
1	K	216/248 (87%)	211 (98%)	5 (2%)	50	67
1	L	217/248 (88%)	213 (98%)	4 (2%)	59	75
All	All	2607/2976 (88%)	2549 (98%)	58 (2%)	52	69

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	A	70	LYS
1	A	102	LEU
1	A	121	SER

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Mol	Chain	Res	Type
1	A	122	HIS
1	A	224	MET
1	A	240	ARG
1	B	140	ARG
1	B	150	SER
1	B	224	MET
1	B	240	ARG
1	C	51	ARG
1	C	101	SER
1	C	117	LYS
1	C	160	VAL
1	C	224	MET
1	C	240	ARG
1	D	102	LEU
1	D	118	GLN
1	D	121	SER
1	D	224	MET
1	D	240	ARG
1	D	256	SER
1	E	121	SER
1	E	171	ARG
1	E	264	CYS
1	F	57	GLU
1	F	76	PRO
1	F	102	LEU
1	F	121	SER
1	F	224	MET
1	F	240	ARG
1	F	264	CYS
1	G	140	ARG
1	G	224	MET
1	G	295	SER
1	H	50	ARG
1	H	240	ARG
1	H	262	LYS
1	H	295	SER
1	H	316	ASP
1	I	51	ARG
1	I	129	ARG
1	I	183	LYS
1	I	224	MET
1	I	240	ARG

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Mol	Chain	Res	Type
1	J	51	ARG
1	J	224	MET
1	J	240	ARG
1	K	72	LYS
1	K	140	ARG
1	K	224	MET
1	K	240	ARG
1	K	262	LYS
1	L	50	ARG
1	L	224	MET
1	L	240	ARG
1	L	316	ASP

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

Mol	Chain	Res	Type
1	A	172	ASN
1	I	172	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 48 are monoatomic - leaving 18 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	H	403	-	5,5,5	0.44	0	5,5,5	0.61	0
3	GOL	K	403	-	5,5,5	0.31	0	5,5,5	0.52	0
3	GOL	J	407	-	5,5,5	0.50	0	5,5,5	0.30	0
3	GOL	D	406	-	5,5,5	0.51	0	5,5,5	0.17	0
3	GOL	F	402	-	5,5,5	0.44	0	5,5,5	0.41	0
4	OXY	K	404	2	1,1,1	0.10	0	-		
4	OXY	J	409	2	1,1,1	0.07	0	-		
3	GOL	G	405	-	5,5,5	0.46	0	5,5,5	0.38	0
3	GOL	J	406	-	5,5,5	0.42	0	5,5,5	0.29	0
3	GOL	L	402	-	5,5,5	0.58	0	5,5,5	0.56	0
4	OXY	G	406	2	1,1,1	0.11	0	-		
4	OXY	A	407	2	1,1,1	0.09	0	-		
3	GOL	A	406	-	5,5,5	0.48	0	5,5,5	0.46	0
3	GOL	I	402	-	5,5,5	0.48	0	5,5,5	0.33	0
4	OXY	B	403	2	1,1,1	0.18	0	-		
4	OXY	D	407	2	1,1,1	0.05	0	-		
3	GOL	E	404	-	5,5,5	0.26	0	5,5,5	0.28	0
3	GOL	E	403	-	5,5,5	0.27	0	5,5,5	0.51	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	H	403	-	-	2/4/4/4	-
3	GOL	K	403	-	-	0/4/4/4	-
3	GOL	J	407	-	-	2/4/4/4	-
3	GOL	D	406	-	-	2/4/4/4	-
3	GOL	F	402	-	-	2/4/4/4	-
3	GOL	G	405	-	-	0/4/4/4	-
3	GOL	J	406	-	-	0/4/4/4	-
3	GOL	L	402	-	-	3/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-
3	GOL	I	402	-	-	0/4/4/4	-
3	GOL	E	404	-	-	2/4/4/4	-
3	GOL	E	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	403	GOL	O1-C1-C2-C3
3	A	406	GOL	O1-C1-C2-O2
3	H	403	GOL	O1-C1-C2-C3
3	F	402	GOL	O1-C1-C2-C3
3	L	402	GOL	O1-C1-C2-C3
3	H	403	GOL	O1-C1-C2-O2
3	J	407	GOL	C1-C2-C3-O3
3	A	406	GOL	O1-C1-C2-C3
3	E	404	GOL	O1-C1-C2-C3
3	L	402	GOL	C1-C2-C3-O3
3	E	404	GOL	O1-C1-C2-O2
3	F	402	GOL	O1-C1-C2-O2
3	E	403	GOL	O1-C1-C2-O2
3	L	402	GOL	O1-C1-C2-O2
3	J	407	GOL	O2-C2-C3-O3
3	D	406	GOL	O2-C2-C3-O3
3	D	406	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407	OXY	1	0
3	I	402	GOL	1	0
3	E	404	GOL	2	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	278/322 (86%)	-0.40	1 (0%) 92 95	17, 33, 48, 69	3 (1%)
1	B	278/322 (86%)	-0.41	2 (0%) 87 91	19, 31, 47, 89	3 (1%)
1	C	275/322 (85%)	-0.38	0 100 100	21, 33, 52, 65	3 (1%)
1	D	278/322 (86%)	-0.41	0 100 100	18, 30, 45, 61	1 (0%)
1	E	277/322 (86%)	-0.45	1 (0%) 92 95	19, 30, 48, 79	2 (0%)
1	F	275/322 (85%)	-0.34	1 (0%) 92 95	21, 34, 49, 54	2 (0%)
1	G	278/322 (86%)	-0.40	1 (0%) 92 95	21, 33, 47, 78	0
1	H	277/322 (86%)	-0.36	2 (0%) 87 91	21, 34, 52, 70	2 (0%)
1	I	276/322 (85%)	-0.15	1 (0%) 92 95	27, 42, 57, 76	2 (0%)
1	J	277/322 (86%)	-0.41	0 100 100	20, 33, 50, 62	0
1	K	276/322 (85%)	-0.34	1 (0%) 92 95	21, 35, 52, 69	3 (1%)
1	L	276/322 (85%)	-0.29	0 100 100	23, 37, 54, 62	2 (0%)
All	All	3321/3864 (85%)	-0.36	10 (0%) 94 96	17, 34, 51, 89	23 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	40	ALA	4.9
1	E	40	ALA	4.5
1	B	40	ALA	3.7
1	A	40	ALA	3.4
1	K	40	ALA	2.8
1	I	310	GLY	2.8
1	F	310	GLY	2.7
1	H	41	GLY	2.5
1	B	317	PRO	2.4
1	H	40	ALA	2.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	CU	B	405	1/1	0.88	0.23	34,34,34,34	1
3	GOL	K	403	6/6	0.90	0.13	30,31,34,41	0
3	GOL	E	404	6/6	0.92	0.23	34,37,46,52	0
2	CU	D	405	1/1	0.93	0.10	39,39,39,39	1
3	GOL	J	406	6/6	0.94	0.10	34,38,41,45	0
3	GOL	E	403	6/6	0.95	0.11	23,28,28,30	0
4	OXY	G	406	2/2	0.95	0.16	28,28,28,31	2
3	GOL	D	406	6/6	0.96	0.11	21,24,27,27	0
2	CU	D	403	1/1	0.96	0.06	37,37,37,37	1
2	CU	G	402	1/1	0.96	0.09	45,45,45,45	0
3	GOL	H	403	6/6	0.96	0.11	31,32,35,36	0
2	CU	J	408	1/1	0.96	0.09	39,39,39,39	0
3	GOL	L	402	6/6	0.96	0.12	24,29,35,39	0
3	GOL	J	407	6/6	0.96	0.09	26,28,29,34	0
2	CU	G	409	1/1	0.97	0.09	47,47,47,47	1
3	GOL	F	402	6/6	0.97	0.10	26,30,32,33	0
4	OXY	K	404	2/2	0.97	0.09	34,34,34,39	0
2	CU	E	406	1/1	0.97	0.13	36,36,36,36	1
3	GOL	I	402	6/6	0.97	0.10	27,33,34,34	0
3	GOL	G	405	6/6	0.97	0.10	28,30,32,32	0
2	CU	J	403	1/1	0.97	0.05	42,42,42,42	1
2	CU	B	404	1/1	0.97	0.10	44,44,44,44	1
2	CU	A	405	1/1	0.98	0.07	42,42,42,42	1
2	CU	H	405	1/1	0.98	0.06	42,42,42,42	1
2	CU	K	405	1/1	0.98	0.10	43,43,43,43	1
2	CU	G	408	1/1	0.98	0.10	39,39,39,39	0
3	GOL	A	406	6/6	0.98	0.12	24,29,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OXY	B	403	2/2	0.98	0.07	22,22,22,28	0
2	CU	K	406	1/1	0.98	0.14	56,56,56,56	1
4	OXY	D	407	2/2	0.98	0.14	23,23,23,29	2
2	CU	D	409	1/1	0.98	0.14	37,37,37,37	0
2	CU	H	401	1/1	0.99	0.12	27,27,27,27	0
2	CU	F	401	1/1	0.99	0.12	31,31,31,31	0
2	CU	B	402	1/1	0.99	0.07	34,34,34,34	0
2	CU	B	401	1/1	0.99	0.12	27,27,27,27	0
2	CU	A	404	1/1	0.99	0.14	32,32,32,32	0
2	CU	G	404	1/1	0.99	0.05	36,36,36,36	1
2	CU	A	403	1/1	0.99	0.04	41,41,41,41	1
2	CU	J	404	1/1	0.99	0.10	30,30,30,30	0
2	CU	J	410	1/1	0.99	0.12	39,39,39,39	0
2	CU	J	405	1/1	0.99	0.07	37,37,37,37	1
2	CU	G	403	1/1	0.99	0.11	29,29,29,29	0
2	CU	A	409	1/1	0.99	0.15	37,37,37,37	0
2	CU	J	401	1/1	0.99	0.09	26,26,26,26	0
2	CU	J	402	1/1	0.99	0.15	41,41,41,41	0
2	CU	E	405	1/1	0.99	0.12	42,42,42,42	0
2	CU	L	401	1/1	0.99	0.14	36,36,36,36	0
4	OXY	J	409	2/2	0.99	0.09	27,27,27,28	0
2	CU	D	404	1/1	0.99	0.14	32,32,32,32	0
2	CU	H	404	1/1	0.99	0.11	47,47,47,47	0
2	CU	A	402	1/1	0.99	0.14	37,37,37,37	0
4	OXY	A	407	2/2	0.99	0.11	24,24,24,26	2
2	CU	H	402	1/1	0.99	0.11	40,40,40,40	0
2	CU	E	402	1/1	1.00	0.10	32,32,32,32	0
2	CU	G	401	1/1	1.00	0.11	26,26,26,26	0
2	CU	E	401	1/1	1.00	0.08	22,22,22,22	0
2	CU	I	401	1/1	1.00	0.11	35,35,35,35	0
2	CU	D	401	1/1	1.00	0.12	28,28,28,28	0
2	CU	K	401	1/1	1.00	0.10	25,25,25,25	0
2	CU	D	408	1/1	1.00	0.09	40,40,40,40	0
2	CU	G	407	1/1	1.00	0.09	37,37,37,37	0
2	CU	A	408	1/1	1.00	0.10	35,35,35,35	0
2	CU	K	402	1/1	1.00	0.09	40,40,40,40	0
2	CU	A	401	1/1	1.00	0.11	26,26,26,26	0
2	CU	C	401	1/1	1.00	0.13	34,34,34,34	0
2	CU	D	402	1/1	1.00	0.15	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.