



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:37 am BST

PDB ID : 6RH9  
Title : Crystal Structure of Two-Domain Laccase mutant I170F from *Streptomyces griseoflavus*  
Authors : Gabdulkhakov, A.G.; Tishchenko, T.V.; Kolyadenko, I.A.  
Deposited on : 2019-04-19  
Resolution : 1.85 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](mailto: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.

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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 : 2.11  
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) : 2.11

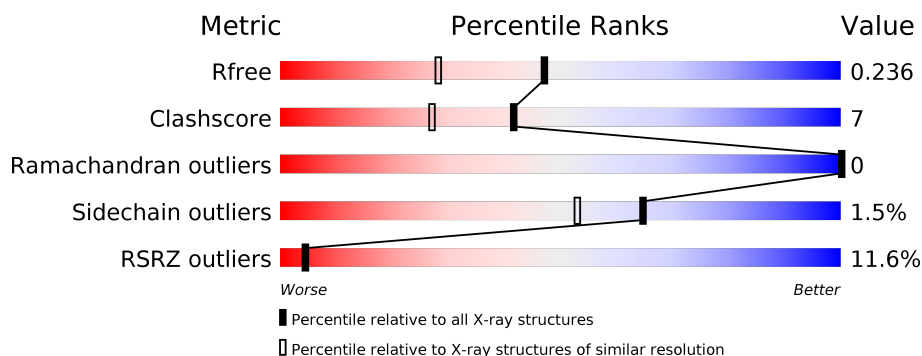
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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>6%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>14%</div> </div> </div>
1	B	322	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>14%</div> </div> </div>
1	C	322	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>14%</div> </div> </div>
1	D	322	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>14%</div> </div> </div>
1	E	322	<div> <div>9%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>14%</div> </div> </div>
1	F	322	<div> <div>17%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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
2	CU	G	403	-	-	-	X
3	EDO	D	405	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26209 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	5	0
			2171	1353	396	409	13			
1	B	278	Total	C	N	O	S	0	0	0
			2133	1331	389	401	12			
1	C	277	Total	C	N	O	S	0	0	0
			2128	1328	388	400	12			
1	D	278	Total	C	N	O	S	0	0	0
			2133	1331	389	401	12			
1	E	277	Total	C	N	O	S	0	1	0
			2136	1333	389	401	13			
1	F	276	Total	C	N	O	S	0	2	0
			2132	1331	388	400	13			
1	G	279	Total	C	N	O	S	0	1	0
			2151	1341	392	406	12			
1	H	278	Total	C	N	O	S	0	1	0
			2141	1336	390	402	13			
1	I	275	Total	C	N	O	S	0	2	0
			2123	1326	387	397	13			
1	J	278	Total	C	N	O	S	0	0	0
			2133	1331	389	401	12			
1	K	278	Total	C	N	O	S	0	3	0
			2155	1344	394	404	13			
1	L	275	Total	C	N	O	S	0	0	0
			2113	1319	386	396	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	LEU	conflict	UNP A0A0M4FJ81
A	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
B	21	PHE	LEU	conflict	UNP A0A0M4FJ81
B	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
C	21	PHE	LEU	conflict	UNP A0A0M4FJ81

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Chain	Residue	Modelled	Actual	Comment	Reference
C	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
D	21	PHE	LEU	conflict	UNP A0A0M4FJ81
D	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
E	21	PHE	LEU	conflict	UNP A0A0M4FJ81
E	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
F	21	PHE	LEU	conflict	UNP A0A0M4FJ81
F	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
G	21	PHE	LEU	conflict	UNP A0A0M4FJ81
G	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
H	21	PHE	LEU	conflict	UNP A0A0M4FJ81
H	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
I	21	PHE	LEU	conflict	UNP A0A0M4FJ81
I	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
J	21	PHE	LEU	conflict	UNP A0A0M4FJ81
J	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
K	21	PHE	LEU	conflict	UNP A0A0M4FJ81
K	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81
L	21	PHE	LEU	conflict	UNP A0A0M4FJ81
L	170	PHE	ILE	engineered mutation	UNP A0A0M4FJ81

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	5	Total Cu 5 5	0	0
2	J	4	Total Cu 4 4	0	0
2	D	4	Total Cu 4 4	0	0
2	K	4	Total Cu 4 4	0	0
2	E	4	Total Cu 4 4	0	0
2	H	3	Total Cu 3 3	0	0
2	B	4	Total Cu 4 4	0	0
2	I	4	Total Cu 4 4	0	0
2	C	4	Total Cu 4 4	0	0
2	A	4	Total Cu 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	4	Total	Cu	0	0
			4	4		
2	F	4	Total	Cu	0	0
			4	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



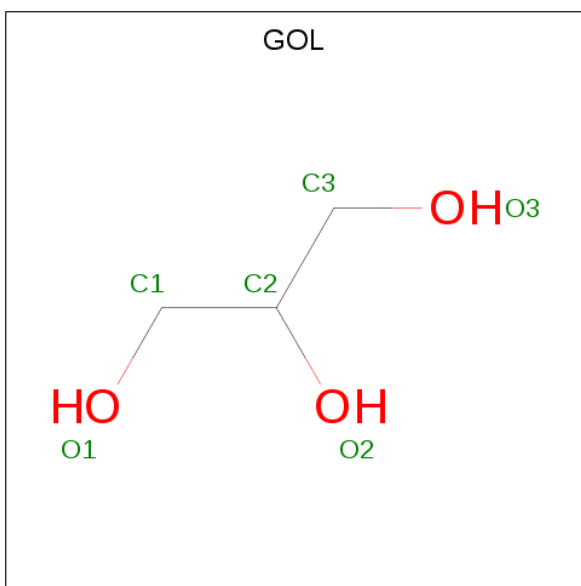
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



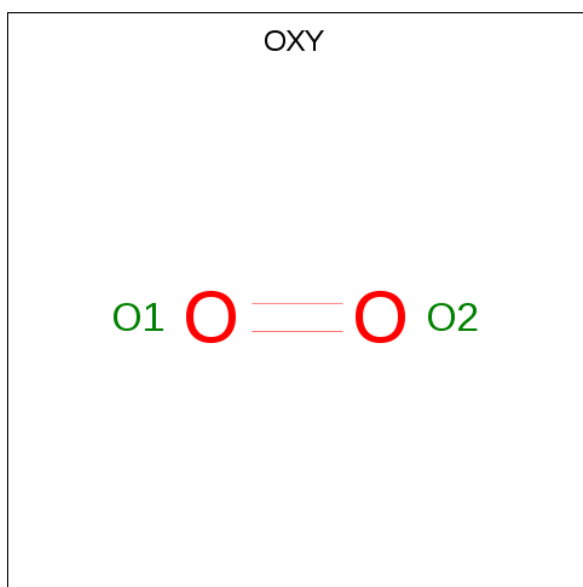
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total O 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	40	Total O 40 40	0	0
7	B	43	Total O 43 43	0	0
7	C	43	Total O 43 43	0	0
7	D	45	Total O 45 45	0	0
7	E	41	Total O 41 41	0	0
7	F	23	Total O 23 23	0	0
7	G	51	Total O 51 51	0	0
7	H	51	Total O 51 51	0	0
7	I	34	Total O 34 34	0	0
7	J	38	Total O 38 38	0	0
7	K	32	Total O 32 32	0	0

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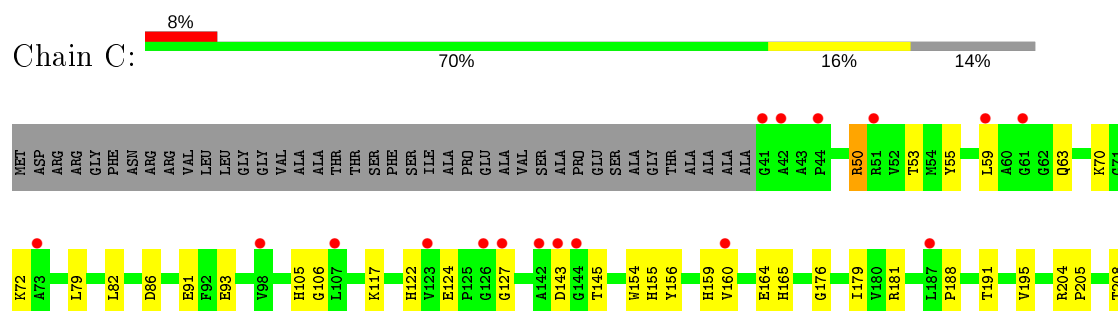


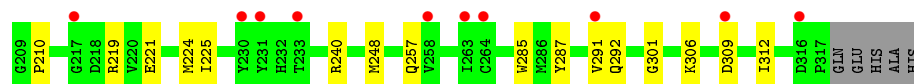
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	30	Total	O	0	0
			30	30		

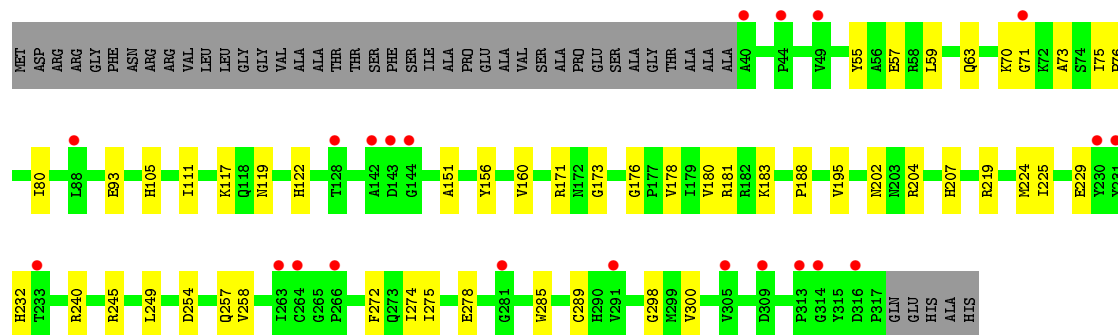


- Molecule 1: Two-domain laccase

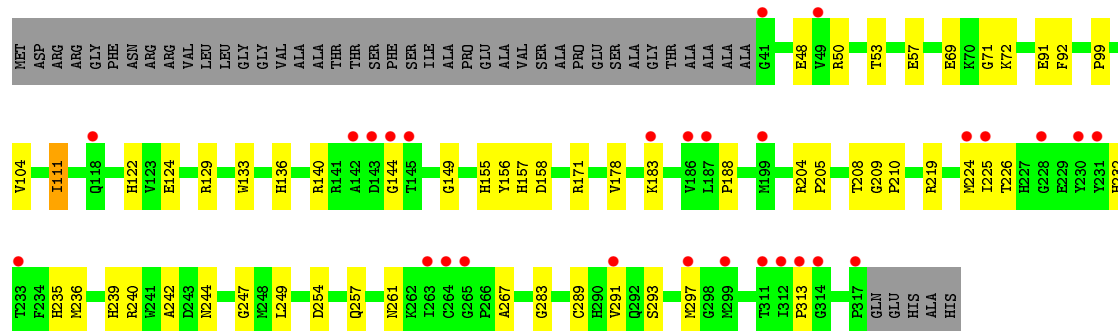




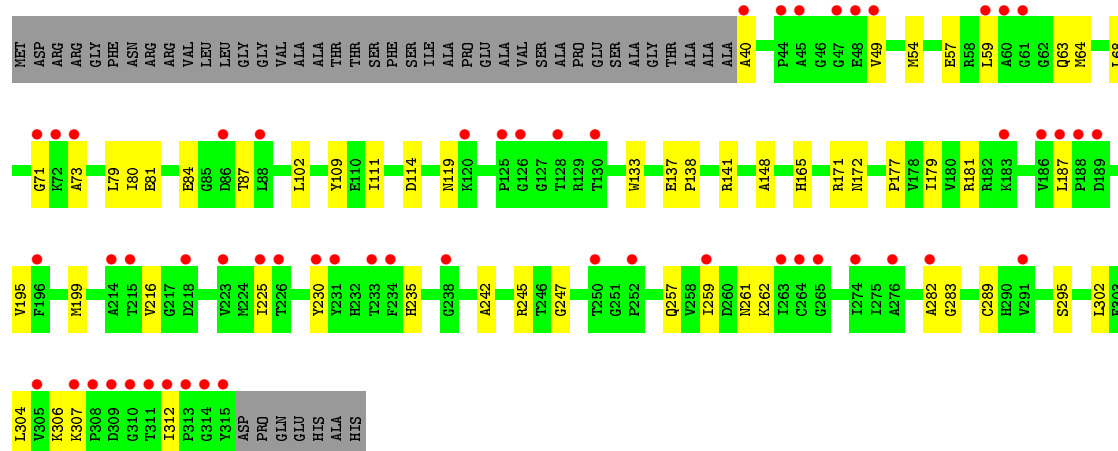
• Molecule 1: Two-domain laccase



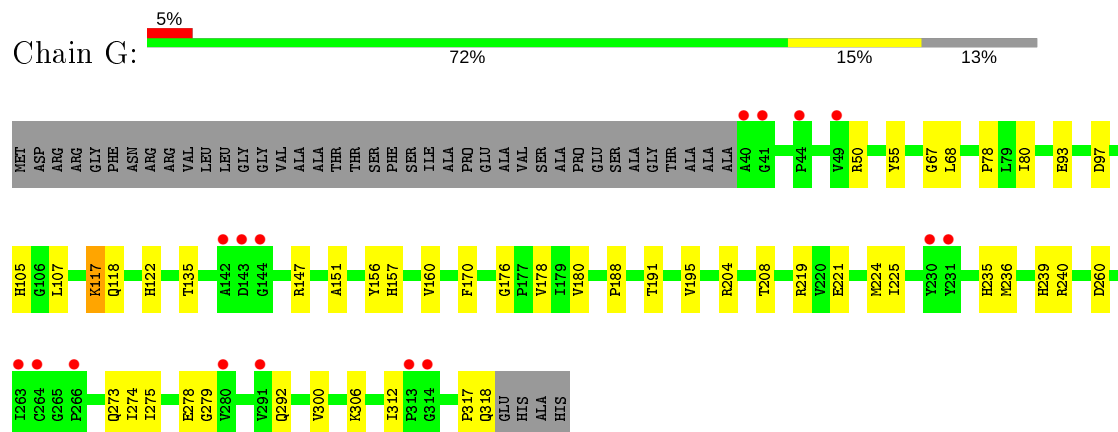
• Molecule 1: Two-domain laccase



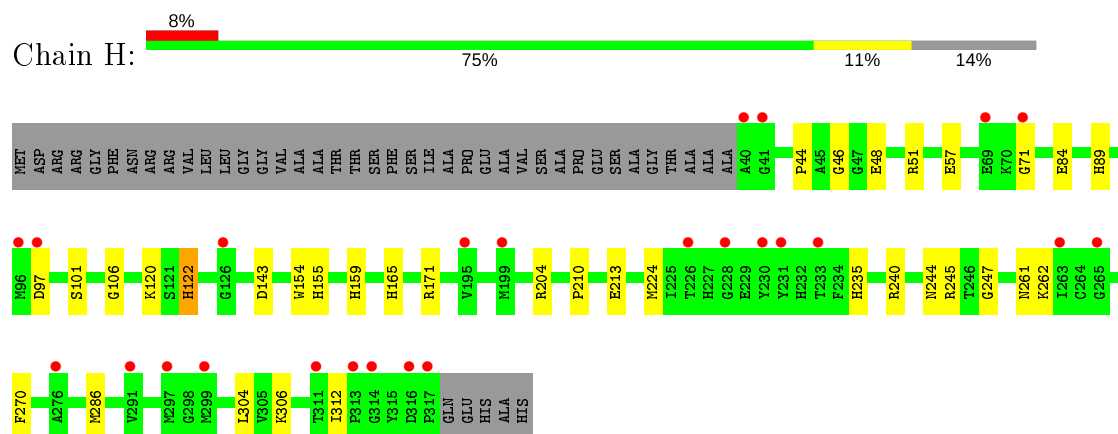
• Molecule 1: Two-domain laccase



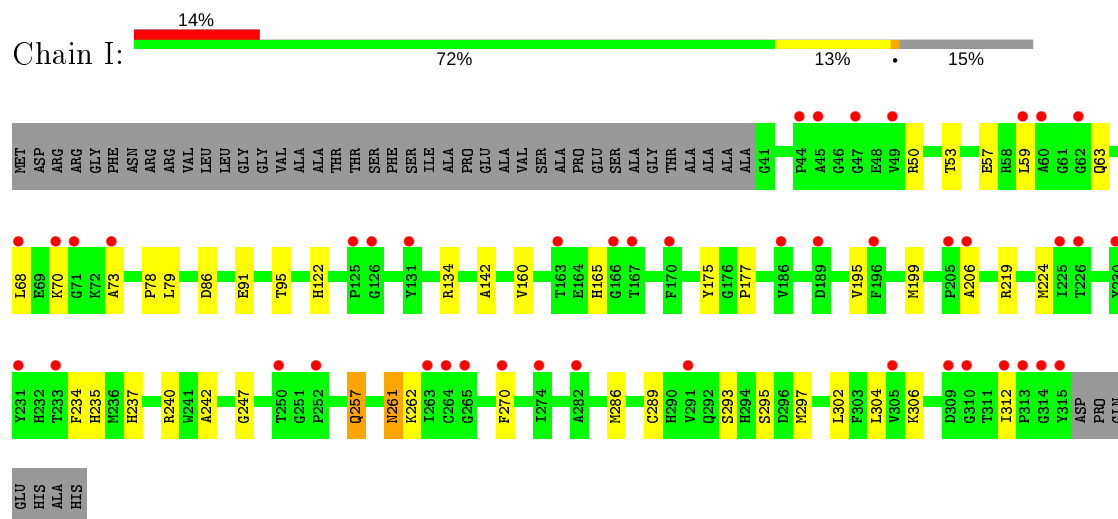
- Molecule 1: Two-domain laccase



- Molecule 1: Two-domain laccase

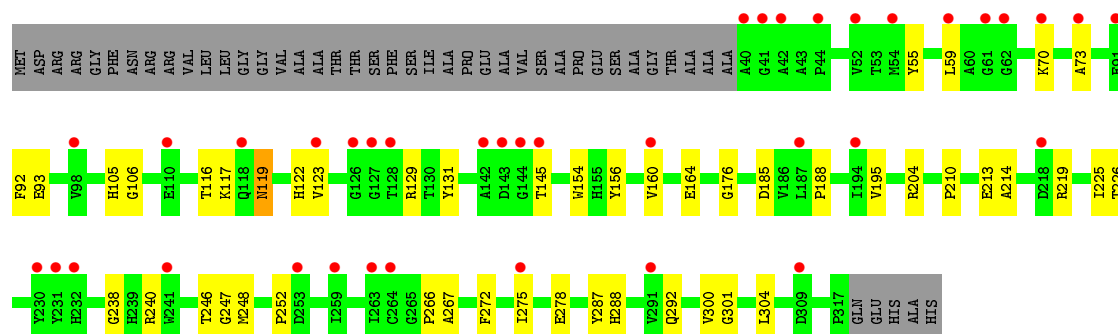


- Molecule 1: Two-domain laccase

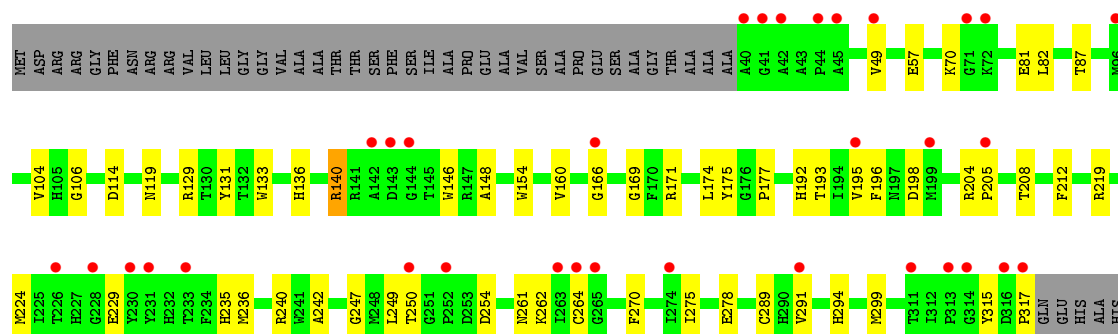


- Molecule 1: Two-domain laccase

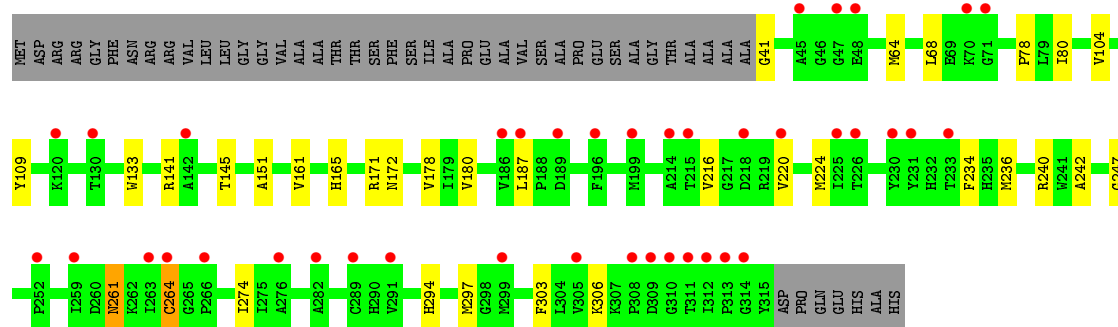




• Molecule 1: Two-domain laccase



• Molecule 1: Two-domain laccase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.25Å 94.77Å 116.18Å 90.13° 89.95° 92.56°	Depositor
Resolution (Å)	47.34 – 1.85 47.34 – 1.85	Depositor EDS
% Data completeness (in resolution range)	91.3 (47.34-1.85) 91.4 (47.34-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.178 , 0.237 0.179 , 0.236	Depositor DCC
$R_{free}$ test set	12841 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l 0.097 for -h,k,-l 0.065 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	26209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, OXY, CU, EDO

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	0/2235	0.57	0/3036
1	B	0.45	0/2196	0.58	0/2983
1	C	0.39	0/2191	0.57	0/2976
1	D	0.42	0/2196	0.56	0/2983
1	E	0.47	0/2199	0.59	0/2986
1	F	0.41	0/2197	0.58	0/2983
1	G	0.46	0/2214	0.59	0/3008
1	H	0.43	0/2204	0.57	0/2993
1	I	0.40	0/2188	0.57	0/2971
1	J	0.40	0/2196	0.54	0/2983
1	K	0.40	0/2219	0.58	0/3013
1	L	0.43	0/2175	0.59	0/2953
All	All	0.42	0/26410	0.57	0/35868

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 [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	2171	0	2029	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2133	0	1999	21	0
1	C	2128	0	1994	37	0
1	D	2133	0	1999	36	0
1	E	2136	0	2002	33	0
1	F	2132	0	2002	44	0
1	G	2151	0	2013	27	0
1	H	2141	0	2007	25	0
1	I	2123	0	1996	30	0
1	J	2133	0	1999	32	0
1	K	2155	0	2016	40	0
1	L	2113	0	1983	30	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	5	0	0	0	0
2	H	3	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	C	4	0	6	1	0
3	D	4	0	6	6	0
3	G	8	0	12	0	0
3	J	4	0	6	1	0
3	L	8	0	12	1	0
4	D	5	0	0	0	0
5	G	6	0	8	1	0
6	I	2	0	0	0	0
7	A	40	0	0	0	0
7	B	43	0	0	0	0
7	C	43	0	0	7	0
7	D	45	0	0	1	0
7	E	41	0	0	1	0
7	F	23	0	0	4	0
7	G	51	0	0	4	0
7	H	51	0	0	1	0
7	I	34	0	0	1	0
7	J	38	0	0	4	0
7	K	32	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	30	0	0	1	0
All	All	26209	0	24089	349	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 (349) 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:F:282:ALA:HB2	1:F:307:LYS:HE3	1.40	1.02
1:F:282:ALA:CB	1:F:307:LYS:HE3	1.92	0.98
1:L:220:VAL:HG21	1:L:303:PHE:HZ	1.45	0.80
1:K:250:THR:HG22	1:K:254:ASP:HB2	1.64	0.79
1:F:216:VAL:HG21	1:F:307:LYS:NZ	1.99	0.77
1:I:59:LEU:HD21	1:I:73:ALA:HB3	1.68	0.76
1:L:64:MET:HG3	1:L:172:ASN:HB3	1.68	0.76
1:J:246:THR:HG23	1:J:248:MET:H	1.52	0.74
1:F:59:LEU:HD21	1:F:73:ALA:HB3	1.70	0.74
1:F:84:GLU:HB2	7:F:518:HOH:O	1.88	0.73
1:B:98:VAL:HG12	1:E:99:PRO:HD2	1.69	0.73
1:F:111:ILE:O	1:F:119:ASN:ND2	2.21	0.73
1:F:307:LYS:HE2	1:F:307:LYS:HA	1.70	0.73
1:J:122:HIS:HB3	1:J:160:VAL:HG21	1.70	0.72
1:F:102:LEU:HD11	1:F:133:TRP:HZ2	1.55	0.71
1:E:111:ILE:HD13	1:F:283:GLY:HA3	1.72	0.71
1:F:282:ALA:HB2	1:F:307:LYS:CE	2.19	0.70
1:B:216:VAL:HG21	1:B:307:LYS:HE2	1.72	0.70
1:F:257:GLN:HG2	1:F:259:ILE:HG23	1.74	0.70
1:F:49:VAL:HG22	1:F:87:THR:HB	1.75	0.69
7:J:502:HOH:O	1:L:165:HIS:HB3	1.92	0.68
1:K:205:PRO:O	1:K:208:THR:HG22	1.93	0.68
1:D:245:ARG:NH1	3:D:405:EDO:H22	2.09	0.67
1:E:57:GLU:OE2	1:E:71:GLY:N	2.20	0.67
1:B:307:LYS:HD3	1:B:308:PRO:HD2	1.75	0.67
1:F:282:ALA:HB3	1:F:307:LYS:HE3	1.76	0.67
1:C:257:GLN:HB3	7:C:542:HOH:O	1.94	0.67
1:G:317:PRO:O	1:G:318:GLN:HB3	1.94	0.66
1:K:205:PRO:HD2	1:K:208:THR:HG21	1.78	0.66
1:C:117:LYS:HD3	1:C:164:GLU:HG2	1.79	0.64
1:K:140:ARG:HG2	1:K:146:TRP:CE3	2.32	0.64
1:E:236:MET:HE2	1:E:239:HIS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:NH1	1:C:248:MET:SD	2.66	0.63
1:C:292:GLN:NE2	7:C:502:HOH:O	2.31	0.62
1:L:220:VAL:HG21	1:L:303:PHE:CZ	2.33	0.62
1:L:220:VAL:HG23	1:L:274:ILE:HG13	1.82	0.62
1:G:80:ILE:HB	1:G:178:VAL:HG22	1.82	0.61
1:D:257:GLN:HG3	1:F:245:ARG:HA	1.83	0.61
1:C:124:GLU:HG2	1:C:127:GLY:HA3	1.81	0.61
1:C:181:ARG:HA	3:C:405:EDO:H11	1.83	0.61
1:I:59:LEU:N	1:I:63:GLN:O	2.34	0.61
1:F:102:LEU:HD11	1:F:133:TRP:CZ2	2.36	0.60
1:E:249:LEU:HD22	1:E:254:ASP:HB3	1.84	0.59
1:G:156:TYR:CZ	1:G:176:GLY:HA3	2.38	0.59
1:A:42:ALA:HB1	1:A:184:GLY:HA2	1.84	0.58
1:H:51:ARG:HG2	1:H:89:HIS:HB2	1.85	0.58
1:J:226:THR:O	1:J:267:ALA:N	2.34	0.58
1:D:245:ARG:HH12	3:D:405:EDO:H22	1.68	0.58
1:D:181:ARG:HH11	3:D:405:EDO:H11	1.68	0.57
1:K:315:TYR:O	1:K:317:PRO:HD3	2.05	0.57
1:L:68:LEU:HD21	1:L:78:PRO:CB	2.35	0.57
1:D:275:ILE:HB	1:D:278:GLU:HB2	1.87	0.57
1:H:244:ASN:OD1	1:H:247:GLY:N	2.35	0.57
1:K:171:ARG:CD	1:K:198:ASP:OD2	2.53	0.56
1:B:51:ARG:HH11	1:B:51:ARG:HB3	1.71	0.56
1:H:57:GLU:OE2	1:H:71:GLY:N	2.29	0.56
1:L:64:MET:CE	1:L:161:VAL:HG11	2.35	0.56
1:G:195:VAL:HA	1:G:225:ILE:O	2.06	0.56
1:E:122:HIS:NE2	1:E:124:GLU:OE2	2.39	0.56
1:J:292:GLN:NE2	7:J:502:HOH:O	2.39	0.56
1:D:156:TYR:CZ	1:D:176:GLY:HA3	2.41	0.55
1:F:40:ALA:N	1:F:187:LEU:HB2	2.21	0.55
1:K:171:ARG:HH12	1:K:229:GLU:HG2	1.71	0.55
1:A:106:GLY:HA3	1:A:154:TRP:CD2	2.41	0.55
1:B:165:HIS:HB3	7:C:502:HOH:O	2.07	0.55
1:E:293:SER:O	1:E:297:MET:HG2	2.07	0.55
1:A:124[A]:GLU:OE1	1:A:124[A]:GLU:N	2.37	0.54
1:I:293:SER:O	1:I:297:MET:HG3	2.07	0.54
1:C:50:ARG:NH2	1:C:86:ASP:OD2	2.40	0.54
1:E:283:GLY:HA2	1:E:313:PRO:HD2	1.89	0.54
1:C:204:ARG:HD3	1:C:210:PRO:HD3	1.88	0.54
1:J:117:LYS:HG3	1:J:160:VAL:HG22	1.89	0.54
1:K:171:ARG:HD3	7:K:504:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:GLU:OE1	1:E:50:ARG:NH1	2.41	0.53
1:H:106:GLY:HA3	1:H:154:TRP:CD2	2.43	0.53
1:F:79:LEU:HA	1:F:177:PRO:HG2	1.89	0.53
1:F:59:LEU:N	1:F:63:GLN:O	2.39	0.53
1:K:204:ARG:HB3	1:K:208:THR:CG2	2.38	0.53
1:L:64:MET:HE2	1:L:161:VAL:HG11	1.90	0.53
1:D:181:ARG:NH1	3:D:405:EDO:H11	2.24	0.53
1:D:122:HIS:HB3	1:D:160:VAL:HG21	1.90	0.53
1:B:45:ALA:HB2	1:B:183:LYS:HD3	1.89	0.53
1:A:235:HIS:HB2	1:A:261:ASN:OD1	2.09	0.53
1:B:165:HIS:CB	7:C:502:HOH:O	2.57	0.52
1:J:117:LYS:HD3	1:J:164:GLU:HG2	1.90	0.52
1:F:216:VAL:HG21	1:F:307:LYS:HZ1	1.72	0.52
1:I:289:CYS:O	1:I:295:SER:HB3	2.10	0.52
1:L:80:ILE:HB	1:L:178:VAL:HG22	1.91	0.52
1:A:183:LYS:HD2	1:A:183:LYS:O	2.09	0.52
1:J:300:VAL:HG21	1:L:165:HIS:CE1	2.44	0.52
1:A:249:LEU:HD22	1:A:254:ASP:HB3	1.92	0.52
1:K:140:ARG:HG2	1:K:146:TRP:HE3	1.75	0.52
1:D:249:LEU:HD22	1:D:254:ASP:HB3	1.91	0.51
1:L:294:HIS:NE2	3:L:405:EDO:O2	2.39	0.51
1:J:116:THR:HG23	1:J:119:ASN:H	1.75	0.51
1:E:235:HIS:HB2	1:E:261:ASN:OD1	2.10	0.51
1:H:262:LYS:HD3	1:H:270:PHE:CE1	2.45	0.51
1:B:289:CYS:O	1:B:295:SER:HB3	2.09	0.51
1:K:129:ARG:HD3	1:K:131:TYR:CZ	2.45	0.51
1:D:55:TYR:HA	1:D:93:GLU:O	2.11	0.51
1:F:81:GLU:OE2	1:F:181:ARG:NH2	2.39	0.50
1:G:292:GLN:NE2	7:G:507:HOH:O	2.41	0.50
1:L:64:MET:HE1	1:L:161:VAL:HG21	1.93	0.50
1:K:204:ARG:HE	1:K:208:THR:HG23	1.76	0.50
1:C:309:ASP:N	7:C:504:HOH:O	2.35	0.50
1:E:242:ALA:O	1:E:247:GLY:HA2	2.11	0.50
1:H:48:GLU:OE1	1:H:48:GLU:N	2.44	0.50
1:K:166[B]:GLY:O	1:K:169:GLY:N	2.45	0.50
1:D:180:VAL:O	3:D:405:EDO:H21	2.12	0.50
1:H:159:HIS:CE1	1:H:165:HIS:HA	2.47	0.50
1:I:70:LYS:HE2	1:I:95:THR:HG21	1.94	0.50
1:H:143:ASP:OD2	1:I:219:ARG:NH2	2.41	0.49
1:L:224:MET:HE1	1:L:264:CYS:SG	2.52	0.49
1:D:258:VAL:HG21	1:F:148:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:VAL:HG21	1:I:165:HIS:CE1	2.47	0.49
1:I:50:ARG:NH1	1:I:86:ASP:OD2	2.45	0.49
1:K:196:PHE:CE2	1:K:289:CYS:HB2	2.47	0.49
1:C:105:HIS:HA	7:C:508:HOH:O	2.12	0.49
1:E:188:PRO:HA	1:E:219:ARG:HG2	1.94	0.49
1:J:105:HIS:CE1	1:K:235:HIS:CE1	3.00	0.49
1:A:199[B]:MET:SD	1:D:171:ARG:NH2	2.86	0.49
1:L:68:LEU:H	1:L:68:LEU:HD22	1.78	0.49
1:F:216:VAL:HG21	1:F:307:LYS:CE	2.43	0.49
1:E:111:ILE:O	1:E:111:ILE:HG13	2.12	0.49
1:A:199[B]:MET:SD	1:D:171:ARG:NH1	2.86	0.48
1:L:41:GLY:C	1:L:187:LEU:HD23	2.33	0.48
1:L:297:MET:SD	7:L:520:HOH:O	2.60	0.48
1:D:76:PRO:HD3	1:D:202:ASN:HB3	1.96	0.48
1:E:236:MET:HE3	7:E:523:HOH:O	2.12	0.48
1:F:54:MET:HE1	1:F:80:ILE:HD11	1.96	0.48
1:J:156:TYR:CZ	1:J:176:GLY:HA3	2.48	0.48
1:F:306:LYS:HG2	1:F:312:ILE:HG12	1.95	0.48
1:G:157:HIS:CG	1:G:170:PHE:CZ	3.02	0.48
1:K:235:HIS:HB2	1:K:261:ASN:OD1	2.12	0.48
1:K:249:LEU:HD22	1:K:254:ASP:HB3	1.95	0.48
1:K:49:VAL:HG13	1:K:87:THR:HG23	1.95	0.48
1:F:242:ALA:O	1:F:247:GLY:HA2	2.14	0.48
1:I:79:LEU:HA	1:I:177:PRO:HG2	1.94	0.48
1:A:51:ARG:HG2	1:A:89:HIS:HB2	1.96	0.48
1:C:122:HIS:HB3	1:C:160:VAL:HG11	1.96	0.48
7:G:510:HOH:O	1:I:165:HIS:HB3	2.14	0.48
1:G:279:GLY:O	1:I:134:ARG:NH2	2.45	0.47
1:F:289:CYS:O	1:F:295:SER:HB3	2.14	0.47
1:H:101:SER:OG	1:H:159:HIS:N	2.36	0.47
1:J:188:PRO:HA	1:J:219:ARG:HG2	1.96	0.47
1:J:275:ILE:HB	1:J:278:GLU:HB2	1.96	0.47
1:K:81:GLU:O	1:K:82:LEU:HD23	2.14	0.47
1:D:80:ILE:HB	1:D:178:VAL:HG22	1.95	0.47
1:H:120:LYS:HD2	1:H:122:HIS:CE1	2.50	0.47
1:J:185:ASP:OD2	3:J:405:EDO:H11	2.14	0.47
1:J:214:ALA:HB2	7:J:526:HOH:O	2.14	0.47
1:C:50:ARG:NH2	1:C:82:LEU:HD23	2.30	0.47
1:H:97:ASP:N	1:H:97:ASP:OD1	2.47	0.47
1:E:205:PRO:HD2	1:E:208:THR:OG1	2.15	0.47
1:F:79:LEU:HD11	1:F:179:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ARG:HH12	5:G:408:GOL:H31	1.79	0.47
1:I:306:LYS:HG2	1:I:312:ILE:HG12	1.96	0.47
1:I:53:THR:HG22	1:I:91:GLU:HB2	1.97	0.47
1:K:171:ARG:HH12	1:K:229:GLU:CG	2.27	0.47
1:C:287:TYR:CE2	1:C:301:GLY:HA3	2.50	0.46
1:F:141:ARG:NH2	7:F:501:HOH:O	2.24	0.46
1:D:117:LYS:HG3	1:D:122:HIS:CE1	2.51	0.46
1:G:188:PRO:HA	1:G:219:ARG:HG2	1.97	0.46
1:A:242:ALA:O	1:A:247:GLY:HA2	2.15	0.46
1:H:120:LYS:HD2	1:H:122:HIS:HE1	1.78	0.46
1:H:245:ARG:HA	1:I:257:GLN:HG2	1.97	0.46
1:C:106:GLY:HA3	1:C:154:TRP:CD2	2.50	0.46
1:D:300:VAL:HG21	1:F:165:HIS:CE1	2.50	0.46
1:E:156:TYR:HD2	1:E:178:VAL:HG22	1.80	0.46
1:I:199:MET:HE1	7:I:517:HOH:O	2.16	0.46
1:I:304:LEU:HB3	1:I:312:ILE:HD13	1.97	0.46
1:C:72:LYS:HD3	1:H:44:PRO:HG3	1.97	0.46
1:G:105:HIS:CE1	1:H:235:HIS:CE1	3.03	0.46
1:J:213:GLU:HA	1:J:304:LEU:O	2.15	0.46
1:D:75:ILE:HD13	1:D:173:GLY:HA3	1.96	0.46
1:F:302:LEU:HD13	1:F:304:LEU:HD21	1.97	0.46
1:K:136:HIS:NE2	1:K:148:ALA:O	2.40	0.46
1:A:111:ILE:O	1:A:114:ASP:HB2	2.16	0.46
1:D:59:LEU:HD21	1:D:73:ALA:HB3	1.97	0.46
1:J:106:GLY:HA3	1:J:154:TRP:CD2	2.51	0.46
1:K:236:MET:HE3	7:K:529:HOH:O	2.16	0.46
1:A:111:ILE:HG13	1:B:283:GLY:HA3	1.98	0.46
1:F:235:HIS:HB2	1:F:261:ASN:OD1	2.17	0.45
1:J:287:TYR:CE2	1:J:301:GLY:HA3	2.51	0.45
1:K:171:ARG:HD3	1:K:198:ASP:OD2	2.15	0.45
1:D:151:ALA:HA	1:D:180:VAL:HB	1.97	0.45
1:D:207:HIS:CD2	1:D:298:GLY:HA2	2.50	0.45
1:K:114:ASP:OD2	1:K:119:ASN:ND2	2.43	0.45
1:L:64:MET:HG3	1:L:172:ASN:CB	2.43	0.45
1:A:121:SER:HA	1:A:129:ARG:CZ	2.47	0.45
1:C:205:PRO:O	1:C:208:THR:OG1	2.20	0.45
1:C:55:TYR:HA	1:C:93:GLU:O	2.16	0.45
1:F:230:TYR:HB3	7:F:506:HOH:O	2.16	0.45
1:G:55:TYR:HA	1:G:93:GLU:O	2.17	0.45
1:L:242:ALA:O	1:L:247:GLY:HA2	2.17	0.45
1:C:117:LYS:HE2	1:C:117:LYS:HB3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:O	1:B:247:GLY:HA2	2.16	0.45
1:J:219:ARG:NH1	1:J:248:MET:SD	2.85	0.45
1:D:111:ILE:HD11	1:D:119:ASN:ND2	2.31	0.45
1:H:120:LYS:NZ	1:H:122:HIS:CE1	2.85	0.45
1:F:195:VAL:HA	1:F:225:ILE:O	2.17	0.45
7:G:514:HOH:O	1:H:286:MET:HG3	2.17	0.45
1:K:106:GLY:HA3	1:K:154:TRP:CD2	2.51	0.45
1:I:68:LEU:HD21	1:I:78:PRO:CB	2.48	0.44
1:J:105:HIS:HA	7:J:504:HOH:O	2.16	0.44
1:K:160:VAL:HG12	7:K:501:HOH:O	2.17	0.44
1:B:102:LEU:HB3	1:B:131:TYR:CE2	2.52	0.44
1:J:204:ARG:HD3	1:J:210:PRO:HD3	1.98	0.44
1:L:68:LEU:N	1:L:68:LEU:HD22	2.32	0.44
1:H:46:GLY:HA3	1:H:84:GLU:O	2.17	0.44
1:I:302:LEU:HD23	1:I:302:LEU:HA	1.76	0.44
1:B:266:PRO:HG2	1:C:291:VAL:HG22	1.99	0.44
1:G:191:THR:HA	1:G:221:GLU:O	2.17	0.44
1:D:195:VAL:HA	1:D:225:ILE:O	2.18	0.44
1:G:275:ILE:HB	1:G:278:GLU:HB2	2.00	0.44
1:F:307:LYS:CE	1:F:307:LYS:HA	2.43	0.44
1:A:136:HIS:CD2	1:A:149:GLY:HA2	2.53	0.44
1:E:157:HIS:ND1	1:E:158:ASP:O	2.39	0.44
1:E:226:THR:O	1:E:267:ALA:N	2.47	0.44
1:G:117:LYS:HG3	1:G:118:GLN:OE1	2.17	0.44
1:L:68:LEU:HD21	1:L:78:PRO:HB3	2.00	0.44
1:C:53:THR:HG22	1:C:91:GLU:HG3	1.99	0.44
1:E:244:ASN:OD1	1:E:247:GLY:N	2.50	0.44
1:F:199:MET:HE1	7:F:513:HOH:O	2.18	0.44
1:I:142:ALA:O	1:J:252:PRO:HB3	2.18	0.44
1:F:64:MET:H	1:F:172:ASN:HB3	1.82	0.43
1:G:204:ARG:NH2	1:G:208:THR:O	2.51	0.43
1:G:97:ASP:N	1:G:97:ASP:OD1	2.40	0.43
1:I:235:HIS:HB2	1:I:261:ASN:OD1	2.18	0.43
1:B:216:VAL:HG23	1:B:306:LYS:O	2.18	0.43
1:C:59:LEU:HB2	1:C:63:GLN:HB2	1.99	0.43
1:F:216:VAL:HG21	1:F:307:LYS:HZ3	1.82	0.43
1:J:129:ARG:HD3	1:J:131:TYR:CZ	2.53	0.43
1:J:59:LEU:HD21	1:J:73:ALA:HB3	2.00	0.43
1:C:195:VAL:HA	1:C:225:ILE:O	2.18	0.43
1:C:204:ARG:NH2	1:C:208:THR:O	2.51	0.43
1:J:55:TYR:HA	1:J:93:GLU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ASP:OD1	1:C:145:THR:OG1	2.31	0.43
1:E:69:GLU:HB2	1:E:72:LYS:HD2	2.01	0.43
1:A:122:HIS:HB3	1:A:160:VAL:HG21	1.99	0.43
1:A:108:ASP:OD2	1:A:136:HIS:ND1	2.51	0.43
1:E:155:HIS:HB3	1:E:225:ILE:HD13	2.00	0.43
1:K:192:HIS:HB3	1:K:212:PHE:CE1	2.54	0.43
1:C:188:PRO:HA	1:C:219:ARG:HG2	2.01	0.43
1:D:181:ARG:HA	3:D:405:EDO:H21	2.00	0.43
1:J:247:GLY:HA3	1:J:272:PHE:HA	2.01	0.43
1:J:145:THR:HG21	1:K:219:ARG:NH2	2.34	0.43
1:D:55:TYR:CZ	1:D:70:LYS:HG2	2.52	0.43
1:G:235:HIS:HA	1:G:260:ASP:O	2.19	0.43
1:B:259:ILE:HD12	1:B:262:LYS:HB2	2.01	0.43
1:F:57:GLU:CD	1:F:71:GLY:H	2.22	0.43
1:K:104:VAL:HB	1:K:133:TRP:CZ2	2.53	0.43
1:E:140:ARG:NH1	1:E:144:GLY:O	2.48	0.43
1:E:204:ARG:HD3	1:E:210:PRO:HD3	2.00	0.43
1:F:114:ASP:HB3	1:F:119:ASN:HD22	1.82	0.43
1:I:237:HIS:CE1	1:I:286:MET:HE3	2.54	0.43
1:K:275:ILE:HB	1:K:278:GLU:HB2	2.01	0.43
1:L:234:PHE:CZ	1:L:236:MET:HG3	2.54	0.43
1:B:109:TYR:CE2	1:C:285:TRP:HZ3	2.36	0.43
1:H:120:LYS:CD	1:H:122:HIS:HE1	2.32	0.43
1:L:216:VAL:HG23	1:L:306:LYS:O	2.19	0.43
1:C:287:TYR:CZ	1:C:301:GLY:HA3	2.54	0.42
1:C:72:LYS:HD2	1:C:72:LYS:HA	1.88	0.42
1:I:175:TYR:CE1	1:I:195:VAL:HG21	2.54	0.42
1:K:175:TYR:CE1	1:K:195:VAL:HG11	2.53	0.42
1:C:155:HIS:HB3	1:C:225:ILE:HD13	2.02	0.42
1:I:68:LEU:H	1:I:68:LEU:HD22	1.84	0.42
1:K:140:ARG:HG2	1:K:146:TRP:CZ3	2.53	0.42
1:L:68:LEU:HD22	1:L:78:PRO:HG3	2.01	0.42
1:A:275:ILE:HB	1:A:278:GLU:HB2	2.02	0.42
1:B:237:HIS:CE1	1:B:286:MET:HE3	2.54	0.42
1:C:70:LYS:HB2	1:C:70:LYS:HE3	1.95	0.42
1:H:171:ARG:HD2	1:H:171:ARG:HA	1.82	0.42
1:H:204:ARG:HD3	1:H:210:PRO:HD3	2.01	0.42
1:H:235:HIS:HB2	1:H:261:ASN:OD1	2.19	0.42
1:C:79:LEU:HD11	1:C:179:ILE:HG13	2.01	0.42
1:D:232:HIS:HB3	1:D:289:CYS:SG	2.60	0.42
1:E:92:PHE:HB3	1:E:129:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:LEU:HD23	1:E:249:LEU:HA	1.83	0.42
1:D:188:PRO:HA	1:D:219:ARG:HG2	2.02	0.42
1:F:40:ALA:N	1:F:187:LEU:CB	2.82	0.42
1:K:242:ALA:O	1:K:247:GLY:HA2	2.18	0.42
1:D:229:GLU:OE1	1:E:291:VAL:HG12	2.19	0.42
1:K:174:LEU:HA	1:K:174:LEU:HD23	1.93	0.42
1:C:159:HIS:CE1	1:C:165:HIS:HA	2.55	0.42
1:G:239:HIS:CD2	1:G:274:ILE:HD12	2.55	0.42
1:L:151:ALA:HA	1:L:180:VAL:HB	2.00	0.42
1:G:122:HIS:HB3	1:G:160:VAL:HG11	2.01	0.42
1:B:307:LYS:HD3	1:B:308:PRO:CD	2.46	0.42
1:C:191:THR:HA	1:C:221:GLU:O	2.20	0.42
1:I:206:ALA:HB1	1:I:297:MET:O	2.20	0.42
1:J:195:VAL:HA	1:J:225:ILE:O	2.20	0.42
1:A:106:GLY:HA3	1:A:154:TRP:CE3	2.55	0.41
1:L:141:ARG:HD2	1:L:145:THR:OG1	2.19	0.41
1:B:51:ARG:NH1	1:B:51:ARG:HB3	2.34	0.41
1:D:285:TRP:HZ3	1:F:109:TYR:CE2	2.37	0.41
1:J:238:GLY:N	1:L:109:TYR:OH	2.47	0.41
1:A:229:GLU:OE2	1:B:293:SER:OG	2.38	0.41
1:A:232:HIS:HB3	1:A:289:CYS:SG	2.61	0.41
1:I:57:GLU:OE1	1:I:70:LYS:HA	2.20	0.41
1:J:266:PRO:HG2	1:K:291:VAL:HG22	2.02	0.41
1:K:224:MET:HE1	1:K:264:CYS:SG	2.60	0.41
1:I:234:PHE:O	1:I:261:ASN:HA	2.20	0.41
1:K:57:GLU:OE1	1:K:70:LYS:HA	2.20	0.41
1:A:110:GLU:HG3	1:A:134:ARG:HH21	1.86	0.41
1:D:272:PHE:HD1	1:D:274:ILE:HG23	1.84	0.41
1:D:59:LEU:HB2	1:D:63:GLN:HB2	2.02	0.41
1:G:107:LEU:HG	1:G:135:THR:HG22	2.03	0.41
1:D:105:HIS:CE1	1:E:235:HIS:CE1	3.09	0.41
1:F:257:GLN:HG2	1:F:259:ILE:CG2	2.45	0.41
1:J:92:PHE:CD2	1:J:123:VAL:HG21	2.56	0.41
1:I:262:LYS:HD3	1:I:270:PHE:CE1	2.55	0.41
1:K:294:HIS:HB3	1:K:299:MET:HE2	2.03	0.41
1:E:209:GLY:HA3	1:E:210:PRO:HA	1.95	0.41
1:E:232:HIS:HB3	1:E:289:CYS:SG	2.61	0.41
1:G:67:GLY:HA3	7:G:521:HOH:O	2.21	0.41
1:I:306:LYS:HG2	1:I:312:ILE:CG1	2.50	0.41
1:C:106:GLY:HA3	1:C:154:TRP:CE3	2.56	0.41
1:D:245:ARG:HA	1:E:257:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:GLU:OE2	1:D:71:GLY:N	2.48	0.41
1:F:137:GLU:HG3	1:F:138:PRO:HD2	2.02	0.41
1:H:155:HIS:HB2	7:H:519:HOH:O	2.21	0.41
1:I:122:HIS:HB3	1:I:160:VAL:HG11	2.02	0.41
1:I:242:ALA:O	1:I:247:GLY:HA2	2.19	0.41
1:K:262:LYS:HD3	1:K:270:PHE:CZ	2.55	0.41
1:G:236:MET:HB3	1:G:236:MET:HE2	1.75	0.41
1:C:156:TYR:CZ	1:C:176:GLY:HA3	2.57	0.41
1:C:306:LYS:HG2	1:C:312:ILE:HD11	2.02	0.41
1:F:68:LEU:HD23	1:F:68:LEU:HA	1.82	0.41
1:H:306:LYS:HG2	1:H:312:ILE:HG13	2.03	0.41
1:L:224:MET:CE	1:L:264:CYS:SG	3.09	0.41
1:G:306:LYS:HG2	1:G:312:ILE:CG1	2.50	0.40
1:B:165:HIS:HB2	7:C:502:HOH:O	2.21	0.40
1:G:151:ALA:HA	1:G:180:VAL:HB	2.03	0.40
1:G:68:LEU:HG	1:G:78:PRO:HG3	2.03	0.40
1:H:213:GLU:HA	1:H:304:LEU:O	2.21	0.40
1:L:64:MET:HE1	1:L:161:VAL:HG11	2.02	0.40
1:A:299:MET:HB3	1:A:299:MET:HE2	1.97	0.40
1:E:53:THR:HG22	1:E:91:GLU:HG2	2.03	0.40
1:G:219:ARG:HD3	1:G:273:GLN:OE1	2.22	0.40
1:J:288:HIS:CB	1:J:300:VAL:HG22	2.51	0.40
1:L:234:PHE:O	1:L:261:ASN:HA	2.22	0.40
1:D:105:HIS:HA	7:D:502:HOH:O	2.20	0.40
1:E:104:VAL:HB	1:E:133:TRP:CZ2	2.56	0.40
1:J:288:HIS:HB3	1:J:300:VAL:HG13	2.03	0.40
1:K:177:PRO:HG3	1:K:193:THR:OG1	2.22	0.40
1:B:228:GLY:O	1:C:292:GLN:HG2	2.21	0.40
1:E:136:HIS:CD2	1:E:149:GLY:HA2	2.56	0.40
1:L:104:VAL:HB	1:L:133:TRP:CZ2	2.56	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	281/322 (87%)	270 (96%)	11 (4%)	0	100	100
1	B	276/322 (86%)	266 (96%)	10 (4%)	0	100	100
1	C	275/322 (85%)	265 (96%)	10 (4%)	0	100	100
1	D	276/322 (86%)	269 (98%)	7 (2%)	0	100	100
1	E	276/322 (86%)	266 (96%)	10 (4%)	0	100	100
1	F	276/322 (86%)	264 (96%)	12 (4%)	0	100	100
1	G	278/322 (86%)	272 (98%)	6 (2%)	0	100	100
1	H	277/322 (86%)	267 (96%)	10 (4%)	0	100	100
1	I	275/322 (85%)	263 (96%)	12 (4%)	0	100	100
1	J	276/322 (86%)	265 (96%)	11 (4%)	0	100	100
1	K	279/322 (87%)	271 (97%)	8 (3%)	0	100	100
1	L	273/322 (85%)	259 (95%)	14 (5%)	0	100	100
All	All	3318/3864 (86%)	3197 (96%)	121 (4%)	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	223/249 (90%)	220 (99%)	3 (1%)	69	58
1	B	219/249 (88%)	217 (99%)	2 (1%)	78	72
1	C	219/249 (88%)	216 (99%)	3 (1%)	67	55
1	D	219/249 (88%)	215 (98%)	4 (2%)	59	45
1	E	220/249 (88%)	214 (97%)	6 (3%)	44	29
1	F	219/249 (88%)	217 (99%)	2 (1%)	78	72
1	G	221/249 (89%)	217 (98%)	4 (2%)	59	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	220/249 (88%)	217 (99%)	3 (1%)	67	55
1	I	219/249 (88%)	215 (98%)	4 (2%)	59	45
1	J	219/249 (88%)	216 (99%)	3 (1%)	67	55
1	K	221/249 (89%)	219 (99%)	2 (1%)	78	72
1	L	217/249 (87%)	213 (98%)	4 (2%)	59	45
All	All	2636/2988 (88%)	2596 (98%)	40 (2%)	65	53

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	A	224	MET
1	A	240	ARG
1	B	224	MET
1	B	240	ARG
1	C	50	ARG
1	C	224	MET
1	C	240	ARG
1	D	183	LYS
1	D	204	ARG
1	D	224	MET
1	D	240	ARG
1	E	111	ILE
1	E	171	ARG
1	E	183	LYS
1	E	224[A]	MET
1	E	224[B]	MET
1	E	240	ARG
1	F	171	ARG
1	F	262	LYS
1	G	50	ARG
1	G	117	LYS
1	G	224	MET
1	G	240	ARG
1	H	122	HIS
1	H	224	MET
1	H	240	ARG
1	I	224	MET
1	I	240	ARG
1	I	257	GLN

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Mol	Chain	Res	Type
1	I	261	ASN
1	J	70	LYS
1	J	119	ASN
1	J	240	ARG
1	K	140	ARG
1	K	240	ARG
1	L	171	ARG
1	L	240	ARG
1	L	261	ASN
1	L	264	CYS

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

Mol	Chain	Res	Type
1	E	119	ASN
1	F	119	ASN
1	F	165	HIS
1	H	122	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 48 are monoatomic - leaving 10 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	EDO	G	407	-	3,3,3	0.44	0	2,2,2	0.48	0
3	EDO	G	406	-	3,3,3	0.46	0	2,2,2	0.34	0
4	SO4	D	406	-	4,4,4	0.17	0	6,6,6	0.13	0
3	EDO	C	405	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	L	405	-	3,3,3	0.44	0	2,2,2	0.37	0
6	OXY	I	402	2	1,1,1	0.14	0	-		
5	GOL	G	408	-	5,5,5	0.34	0	5,5,5	0.40	0
3	EDO	D	405	-	3,3,3	0.43	0	2,2,2	0.20	0
3	EDO	J	405	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	L	406	-	3,3,3	0.36	0	2,2,2	0.89	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	EDO	G	407	-	-	0/1/1/1	-
3	EDO	G	406	-	-	0/1/1/1	-
3	EDO	C	405	-	-	0/1/1/1	-
3	EDO	L	405	-	-	0/1/1/1	-
5	GOL	G	408	-	-	2/4/4/4	-
3	EDO	D	405	-	-	0/1/1/1	-
3	EDO	J	405	-	-	1/1/1/1	-
3	EDO	L	406	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	408	GOL	O1-C1-C2-O2
5	G	408	GOL	O1-C1-C2-C3
3	J	405	EDO	O1-C1-C2-O2
3	L	406	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	405	EDO	1	0
3	L	405	EDO	1	0
5	G	408	GOL	1	0
3	D	405	EDO	6	0
3	J	405	EDO	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	278/322 (86%)	0.74	19 (6%)	17 16	24, 37, 53, 82	2 (0%)
1	B	278/322 (86%)	0.93	37 (13%)	3 3	24, 38, 60, 104	2 (0%)
1	C	277/322 (86%)	0.81	27 (9%)	7 7	24, 39, 56, 70	2 (0%)
1	D	278/322 (86%)	0.71	22 (7%)	12 12	24, 38, 53, 66	3 (1%)
1	E	277/322 (86%)	0.87	28 (10%)	7 6	25, 38, 55, 80	4 (1%)
1	F	276/322 (85%)	1.22	56 (20%)	1 1	28, 46, 64, 76	6 (2%)
1	G	279/322 (86%)	0.72	16 (5%)	23 23	23, 36, 53, 72	3 (1%)
1	H	278/322 (86%)	0.84	25 (8%)	9 9	23, 36, 51, 86	3 (1%)
1	I	275/322 (85%)	1.00	44 (16%)	1 2	26, 41, 60, 69	4 (1%)
1	J	278/322 (86%)	0.94	38 (13%)	3 3	25, 42, 60, 77	3 (1%)
1	K	278/322 (86%)	0.96	33 (11%)	4 4	25, 41, 59, 86	3 (1%)
1	L	275/322 (85%)	1.08	40 (14%)	2 2	26, 42, 59, 82	1 (0%)
All	All	3327/3864 (86%)	0.90	385 (11%)	4 4	23, 39, 58, 104	36 (1%)

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	PRO	9.6
1	B	40	ALA	8.7
1	A	316	ASP	8.1
1	K	314	GLY	8.0
1	B	314	GLY	7.6
1	K	40	ALA	7.5
1	A	40	ALA	7.1
1	J	40	ALA	6.6
1	E	317	PRO	6.2
1	F	40	ALA	6.1
1	L	130	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	252	PRO	5.6
1	L	314	GLY	5.4
1	F	314	GLY	5.2
1	H	317	PRO	5.1
1	K	143	ASP	5.1
1	B	316	ASP	5.1
1	K	317	PRO	5.0
1	I	59	LEU	4.9
1	H	40	ALA	4.9
1	I	264[A]	CYS	4.8
1	K	316	ASP	4.8
1	F	186	VAL	4.8
1	L	47	GLY	4.7
1	J	42	ALA	4.7
1	C	142	ALA	4.5
1	J	142	ALA	4.5
1	C	98	VAL	4.4
1	B	309	ASP	4.4
1	F	313	PRO	4.4
1	F	310	GLY	4.3
1	L	309	ASP	4.2
1	I	167	THR	4.2
1	L	310	GLY	4.2
1	I	315	TYR	4.2
1	F	250	THR	4.2
1	L	313	PRO	4.1
1	I	313	PRO	4.1
1	L	230	TYR	4.1
1	E	142	ALA	4.1
1	L	45	ALA	4.1
1	L	291	VAL	4.0
1	L	308	PRO	4.0
1	E	314	GLY	4.0
1	B	142	ALA	4.0
1	G	314	GLY	4.0
1	F	215	THR	3.9
1	K	41	GLY	3.9
1	A	317	PRO	3.9
1	F	264	CYS	3.9
1	J	41	GLY	3.9
1	H	199[A]	MET	3.9
1	H	313	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	K	313	PRO	3.9
1	A	143	ASP	3.8
1	J	143	ASP	3.8
1	L	311	THR	3.8
1	C	291	VAL	3.8
1	F	71	GLY	3.8
1	H	316	ASP	3.8
1	E	313	PRO	3.8
1	I	291	VAL	3.8
1	F	214	ALA	3.7
1	H	263	ILE	3.7
1	F	312	ILE	3.7
1	D	49	VAL	3.7
1	G	313	PRO	3.6
1	B	310	GLY	3.6
1	L	142	ALA	3.6
1	F	291	VAL	3.6
1	L	252	PRO	3.6
1	A	314	GLY	3.6
1	D	40	ALA	3.6
1	K	72	LYS	3.6
1	L	312	ILE	3.5
1	H	291	VAL	3.5
1	B	263	ILE	3.5
1	D	314	GLY	3.5
1	A	199[A]	MET	3.5
1	C	143	ASP	3.4
1	E	230	TYR	3.4
1	G	142	ALA	3.4
1	K	230	TYR	3.4
1	B	291	VAL	3.4
1	D	291	VAL	3.4
1	B	199	MET	3.4
1	K	263	ILE	3.4
1	I	71	GLY	3.4
1	K	142	ALA	3.4
1	I	312	ILE	3.4
1	J	264	CYS	3.4
1	K	199[A]	MET	3.4
1	H	230	TYR	3.3
1	C	42	ALA	3.3
1	F	45	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	143	ASP	3.3
1	I	309	ASP	3.3
1	G	49	VAL	3.3
1	F	263	ILE	3.3
1	B	205	PRO	3.3
1	L	196	PHE	3.3
1	F	309	ASP	3.3
1	F	47	GLY	3.2
1	L	264	CYS	3.2
1	F	44	PRO	3.2
1	B	313	PRO	3.2
1	D	44	PRO	3.2
1	E	291	VAL	3.2
1	C	231	TYR	3.2
1	L	231	TYR	3.2
1	L	215	THR	3.1
1	A	263	ILE	3.1
1	F	130	THR	3.1
1	I	230	TYR	3.1
1	H	97	ASP	3.1
1	B	264	CYS	3.1
1	D	264	CYS	3.1
1	J	291	VAL	3.1
1	B	144	GLY	3.1
1	E	263	ILE	3.1
1	D	231	TYR	3.1
1	B	230	TYR	3.0
1	I	186	VAL	3.0
1	K	49	VAL	3.0
1	F	59	LEU	3.0
1	B	45	ALA	3.0
1	I	196	PHE	3.0
1	J	73	ALA	3.0
1	K	264	CYS	3.0
1	K	144	GLY	3.0
1	D	142	ALA	3.0
1	A	264	CYS	3.0
1	B	228	GLY	3.0
1	J	62	GLY	3.0
1	E	297	MET	3.0
1	I	45	ALA	3.0
1	I	263	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	145	THR	3.0
1	F	311	THR	3.0
1	J	231	TYR	3.0
1	D	309	ASP	3.0
1	J	309	ASP	3.0
1	L	282	ALA	2.9
1	I	62	GLY	2.9
1	B	233	THR	2.9
1	G	231	TYR	2.9
1	B	47	GLY	2.9
1	E	144	GLY	2.9
1	F	120	LYS	2.9
1	F	308	PRO	2.9
1	E	231	TYR	2.9
1	H	314	GLY	2.9
1	E	143	ASP	2.9
1	G	291	VAL	2.9
1	L	299	MET	2.9
1	F	265	GLY	2.9
1	K	228	GLY	2.9
1	H	231	TYR	2.8
1	F	88	LEU	2.8
1	I	250	THR	2.8
1	K	226	THR	2.8
1	A	142	ALA	2.8
1	J	253	ASP	2.8
1	D	313	PRO	2.8
1	H	126	GLY	2.8
1	D	230	TYR	2.8
1	F	72	LYS	2.8
1	C	41	GLY	2.8
1	H	265	GLY	2.8
1	J	98	VAL	2.8
1	L	266	PRO	2.8
1	C	123	VAL	2.8
1	F	48	GLU	2.8
1	F	233	THR	2.7
1	C	264	CYS	2.7
1	F	231	TYR	2.7
1	H	233	THR	2.7
1	I	47	GLY	2.7
1	C	144	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	205	PRO	2.7
1	L	189	ASP	2.7
1	B	196	PHE	2.7
1	F	60	ALA	2.7
1	J	230	TYR	2.7
1	L	305	VAL	2.7
1	D	144	GLY	2.7
1	G	40	ALA	2.7
1	I	49	VAL	2.7
1	L	187	LEU	2.7
1	F	86	ASP	2.6
1	K	42	ALA	2.6
1	E	265	GLY	2.6
1	F	259	ILE	2.6
1	I	166	GLY	2.6
1	J	126	GLY	2.6
1	B	231	TYR	2.6
1	C	230	TYR	2.6
1	K	44	PRO	2.6
1	F	187	LEU	2.6
1	I	70	LYS	2.6
1	F	225	ILE	2.6
1	L	225	ILE	2.6
1	I	189	ASP	2.6
1	H	297	MET	2.6
1	I	270	PHE	2.6
1	F	128	THR	2.6
1	F	282	ALA	2.6
1	H	228	GLY	2.6
1	K	45	ALA	2.6
1	E	199	MET	2.6
1	L	289	CYS	2.6
1	F	276	ALA	2.6
1	B	72	LYS	2.6
1	I	205	PRO	2.6
1	A	274	ILE	2.6
1	J	123	VAL	2.6
1	B	234	PHE	2.5
1	A	71	GLY	2.5
1	G	264	CYS	2.5
1	A	231	TYR	2.5
1	B	315	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	206	ALA	2.5
1	G	44	PRO	2.5
1	H	96	MET	2.5
1	I	233	THR	2.5
1	B	225	ILE	2.5
1	L	259	ILE	2.5
1	G	230	TYR	2.5
1	E	187	LEU	2.5
1	L	263	ILE	2.5
1	E	49	VAL	2.5
1	G	266	PRO	2.5
1	L	276	ALA	2.5
1	B	289	CYS	2.5
1	J	61	GLY	2.5
1	D	128	THR	2.5
1	I	44	PRO	2.5
1	J	259	ILE	2.5
1	F	315	TYR	2.5
1	I	231	TYR	2.5
1	L	226	THR	2.5
1	B	308	PRO	2.4
1	F	307	LYS	2.4
1	E	186	VAL	2.4
1	K	233	THR	2.4
1	F	226	THR	2.4
1	J	145	THR	2.4
1	I	68	LEU	2.4
1	K	265	GLY	2.4
1	A	226	THR	2.4
1	K	291	VAL	2.4
1	D	316	ASP	2.4
1	I	170	PHE	2.4
1	B	299	MET	2.4
1	E	264	CYS	2.4
1	H	311	THR	2.4
1	G	144	GLY	2.4
1	I	126	GLY	2.4
1	L	186	VAL	2.4
1	J	70	LYS	2.4
1	E	118	GLN	2.4
1	C	187	LEU	2.4
1	A	230	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	230	TYR	2.4
1	C	309	ASP	2.4
1	L	214	ALA	2.4
1	E	311	THR	2.4
1	J	91	GLU	2.4
1	D	263	ILE	2.4
1	H	195	VAL	2.4
1	C	126	GLY	2.3
1	F	238	GLY	2.3
1	G	41	GLY	2.3
1	A	195	VAL	2.3
1	C	233	THR	2.3
1	I	131	TYR	2.3
1	K	71	GLY	2.3
1	F	125	PRO	2.3
1	L	218	ASP	2.3
1	C	217	GLY	2.3
1	J	127	GLY	2.3
1	I	226	THR	2.3
1	F	183	LYS	2.3
1	L	70	LYS	2.3
1	A	126	GLY	2.3
1	B	162	GLY	2.3
1	J	263	ILE	2.3
1	K	96	MET	2.3
1	C	73	ALA	2.3
1	I	60	ALA	2.3
1	H	71	GLY	2.3
1	B	297	MET	2.3
1	F	49	VAL	2.3
1	K	195	VAL	2.3
1	B	266	PRO	2.3
1	J	44	PRO	2.3
1	A	120	LYS	2.3
1	D	88	LEU	2.3
1	D	143	ASP	2.3
1	F	61	GLY	2.2
1	H	41	GLY	2.2
1	K	311	THR	2.2
1	L	233	THR	2.2
1	K	274	ILE	2.2
1	I	310	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	144	GLY	2.2
1	J	118	GLN	2.2
1	F	234	PHE	2.2
1	I	252	PRO	2.2
1	L	199	MET	2.2
1	B	226	THR	2.2
1	F	218	ASP	2.2
1	J	52	VAL	2.2
1	G	263	ILE	2.2
1	I	225	ILE	2.2
1	D	71	GLY	2.2
1	E	228	GLY	2.2
1	C	107	LEU	2.2
1	B	311	THR	2.2
1	F	189	ASP	2.2
1	C	160	VAL	2.2
1	F	223	VAL	2.2
1	K	166[A]	GLY	2.2
1	J	59	LEU	2.2
1	K	252	PRO	2.2
1	E	299	MET	2.2
1	J	128	THR	2.2
1	F	73	ALA	2.2
1	I	73	ALA	2.2
1	G	280	VAL	2.2
1	J	160	VAL	2.2
1	E	225	ILE	2.2
1	E	183	LYS	2.2
1	C	127	GLY	2.2
1	I	265	GLY	2.2
1	I	282	ALA	2.2
1	F	196	PHE	2.2
1	A	266	PRO	2.1
1	B	295	SER	2.1
1	J	54	MET	2.1
1	J	187	LEU	2.1
1	I	314	GLY	2.1
1	L	71	GLY	2.1
1	D	305	VAL	2.1
1	A	119	ASN	2.1
1	C	316	ASP	2.1
1	D	233	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	250	THR	2.1
1	J	241	TRP	2.1
1	F	305	VAL	2.1
1	L	220	VAL	2.1
1	F	126	GLY	2.1
1	H	299	MET	2.1
1	L	120	LYS	2.1
1	I	125	PRO	2.1
1	D	281	GLY	2.1
1	L	48	GLU	2.1
1	E	233	THR	2.1
1	H	226	THR	2.1
1	C	263	ILE	2.1
1	E	312	ILE	2.1
1	I	274	ILE	2.1
1	J	194	ILE	2.1
1	B	189	ASP	2.1
1	B	265	GLY	2.1
1	E	41	GLY	2.1
1	K	231	TYR	2.1
1	C	258	VAL	2.1
1	I	305	VAL	2.1
1	C	44	PRO	2.1
1	D	266	PRO	2.1
1	F	274	ILE	2.1
1	J	275	ILE	2.1
1	C	61	GLY	2.1
1	E	224[A]	MET	2.0
1	J	110	GLU	2.0
1	J	218	ASP	2.0
1	H	276	ALA	2.0
1	C	59	LEU	2.0
1	H	69	GLU	2.0
1	I	163	THR	2.0
1	J	232	HIS	2.0
1	F	188	PRO	2.0
1	B	312	ILE	2.0
1	C	51	ARG	2.0

## 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CU	B	403	1/1	0.48	0.17	99,99,99,99	1
2	CU	F	404	1/1	0.61	0.18	97,97,97,97	1
2	CU	L	404	1/1	0.75	0.18	116,116,116,116	1
2	CU	G	403	1/1	0.79	0.50	219,219,219,219	1
5	GOL	G	408	6/6	0.83	0.22	51,52,54,57	0
2	CU	G	405	1/1	0.84	0.12	71,71,71,71	1
2	CU	D	403	1/1	0.87	0.99	207,207,207,207	1
4	SO4	D	406	5/5	0.88	0.27	77,78,82,84	0
3	EDO	L	405	4/4	0.89	0.57	52,56,56,56	0
2	CU	C	404	1/1	0.89	0.19	38,38,38,38	1
2	CU	K	403	1/1	0.89	0.17	59,59,59,59	1
3	EDO	C	405	4/4	0.90	0.20	53,54,55,55	0
3	EDO	G	406	4/4	0.91	0.52	38,40,41,44	0
2	CU	I	405	1/1	0.92	0.22	58,58,58,58	1
2	CU	J	403	1/1	0.92	0.18	65,65,65,65	1
3	EDO	L	406	4/4	0.94	0.10	38,40,43,45	0
3	EDO	J	405	4/4	0.94	0.16	32,33,39,45	0
3	EDO	G	407	4/4	0.95	0.18	38,40,42,43	0
3	EDO	D	405	4/4	0.95	0.19	47,48,49,51	0
2	CU	E	403	1/1	0.96	0.12	82,82,82,82	1
2	CU	A	403	1/1	0.96	0.26	100,100,100,100	1
6	OXY	I	402	2/2	0.97	0.52	57,57,57,59	0
2	CU	F	402	1/1	0.99	0.16	38,38,38,38	0
2	CU	L	402	1/1	0.99	0.14	34,34,34,34	0
2	CU	G	404	1/1	0.99	0.11	29,29,29,29	0
2	CU	J	404	1/1	0.99	0.11	37,37,37,37	0
2	CU	F	401	1/1	0.99	0.10	39,39,39,39	0
2	CU	J	401	1/1	0.99	0.12	31,31,31,31	0
2	CU	G	402	1/1	0.99	0.08	37,37,37,37	1
2	CU	E	404	1/1	0.99	0.13	37,37,37,37	0
2	CU	E	402	1/1	0.99	0.13	39,39,39,39	0
2	CU	J	402	1/1	0.99	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	C	403	1/1	1.00	0.12	38,38,38,38	0
2	CU	F	403	1/1	1.00	0.12	38,38,38,38	0
2	CU	K	404	1/1	1.00	0.13	33,33,33,33	0
2	CU	I	404	1/1	1.00	0.11	42,42,42,42	0
2	CU	H	401	1/1	1.00	0.13	31,31,31,31	0
2	CU	K	401	1/1	1.00	0.12	30,30,30,30	0
2	CU	A	401	1/1	1.00	0.11	30,30,30,30	0
2	CU	A	404	1/1	1.00	0.13	30,30,30,30	0
2	CU	C	402	1/1	1.00	0.13	29,29,29,29	0
2	CU	B	401	1/1	1.00	0.13	31,31,31,31	0
2	CU	G	401	1/1	1.00	0.13	31,31,31,31	0
2	CU	D	401	1/1	1.00	0.13	30,30,30,30	0
2	CU	C	401	1/1	1.00	0.12	39,39,39,39	0
2	CU	A	402	1/1	1.00	0.11	36,36,36,36	0
2	CU	D	404	1/1	1.00	0.10	29,29,29,29	0
2	CU	I	401	1/1	1.00	0.10	35,35,35,35	0
2	CU	I	403	1/1	1.00	0.15	31,31,31,31	0
2	CU	H	402	1/1	1.00	0.11	43,43,43,43	0
2	CU	L	403	1/1	1.00	0.11	40,40,40,40	0
2	CU	B	402	1/1	1.00	0.12	40,40,40,40	0
2	CU	L	401	1/1	1.00	0.12	33,33,33,33	0
2	CU	E	401	1/1	1.00	0.15	32,32,32,32	0
2	CU	K	402	1/1	1.00	0.10	37,37,37,37	0
2	CU	D	402	1/1	1.00	0.07	36,36,36,36	1
2	CU	B	404	1/1	1.00	0.12	36,36,36,36	0
2	CU	H	403	1/1	1.00	0.12	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.