



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:40 am BST

PDB ID : 4WTQ
Title : Structure of the Ssl1 laccase mutant M295L
Authors : Gunne, M.; Hoepfner, A.; Urlacher, V.B.
Deposited on : 2014-10-30
Resolution : 1.80 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 : 2.11
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

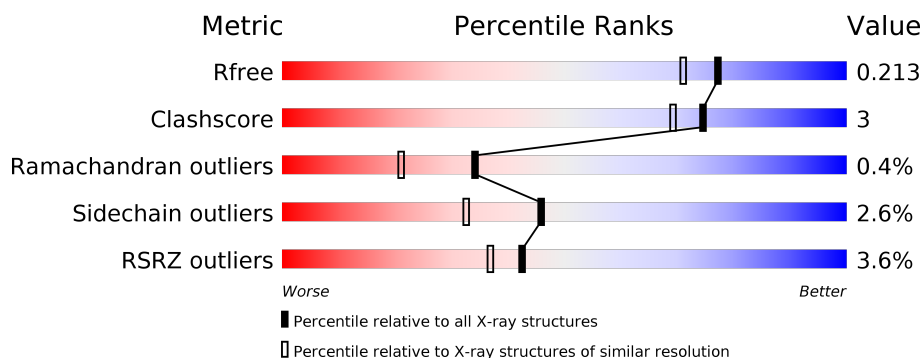
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	293	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	293	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>
1	C	293	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6718 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 Copper oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2096	1310	383	394	9			
1	B	269	Total	C	N	O	S	0	0	0
			2087	1305	382	391	9			
1	C	269	Total	C	N	O	S	0	0	0
			2087	1305	382	391	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	initiating methionine	UNP B5HSR1
A	34	HIS	-	expression tag	UNP B5HSR1
A	35	HIS	-	expression tag	UNP B5HSR1
A	36	HIS	-	expression tag	UNP B5HSR1
A	37	HIS	-	expression tag	UNP B5HSR1
A	38	HIS	-	expression tag	UNP B5HSR1
A	39	HIS	-	expression tag	UNP B5HSR1
A	295	LEU	MET	engineered mutation	UNP B5HSR1
B	33	MET	-	initiating methionine	UNP B5HSR1
B	34	HIS	-	expression tag	UNP B5HSR1
B	35	HIS	-	expression tag	UNP B5HSR1
B	36	HIS	-	expression tag	UNP B5HSR1
B	37	HIS	-	expression tag	UNP B5HSR1
B	38	HIS	-	expression tag	UNP B5HSR1
B	39	HIS	-	expression tag	UNP B5HSR1
B	295	LEU	MET	engineered mutation	UNP B5HSR1
C	33	MET	-	initiating methionine	UNP B5HSR1
C	34	HIS	-	expression tag	UNP B5HSR1
C	35	HIS	-	expression tag	UNP B5HSR1
C	36	HIS	-	expression tag	UNP B5HSR1
C	37	HIS	-	expression tag	UNP B5HSR1
C	38	HIS	-	expression tag	UNP B5HSR1
C	39	HIS	-	expression tag	UNP B5HSR1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	295	LEU	MET	engineered mutation	UNP B5HSR1

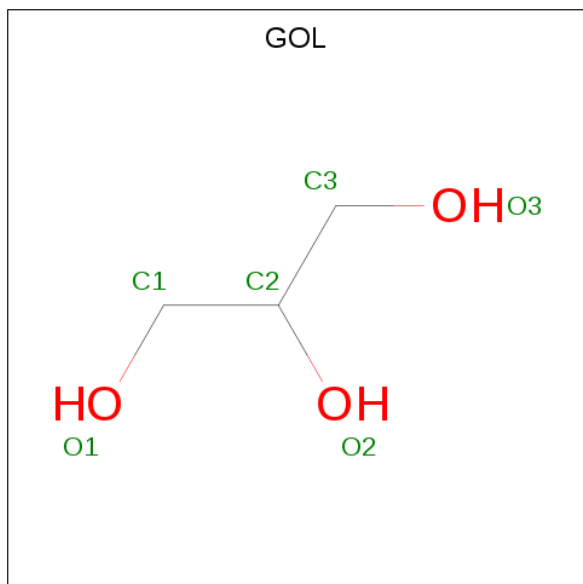
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Cu 3 3	0	0
2	A	3	Total Cu 3 3	0	0
2	C	3	Total Cu 3 3	0	0

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	133	Total 133	O 133	0	0
5	B	134	Total 134	O 134	0	0
5	C	164	Total 164	O 164	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.53Å 104.80Å 164.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.58 – 1.80 24.58 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (24.58-1.80) 98.2 (24.58-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.171 , 0.208 0.180 , 0.213	Depositor DCC
R_{free} test set	4083 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6718	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, O, 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	1.06	3/2154 (0.1%)	1.04	8/2923 (0.3%)
1	B	0.98	1/2145 (0.0%)	0.97	2/2911 (0.1%)
1	C	0.99	0/2145	1.01	6/2911 (0.2%)
All	All	1.01	4/6444 (0.1%)	1.01	16/8745 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	PRO	C-N	-14.40	1.00	1.34
1	A	249	ASP	C-N	-10.53	1.09	1.34
1	B	76	ILE	C-N	-7.43	1.17	1.34
1	A	206	PRO	N-CD	5.34	1.55	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASP	O-C-N	-7.70	110.38	122.70
1	C	137	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	248	PRO	C-N-CA	6.58	138.14	121.70
1	C	110	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	250	ASP	CB-CG-OD1	6.11	123.79	118.30
1	A	177	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ASP	CB-CG-OD2	5.87	123.59	118.30
1	B	178	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	250	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	93	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	241	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	249	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	177	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	244	MET	CG-SD-CE	5.17	108.48	100.20
1	B	264	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	174	VAL	CB-CA-C	-5.06	101.79	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	HIS	Peptide

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	2096	0	1978	14	0
1	B	2087	0	1973	12	0
1	C	2087	0	1974	15	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	C	6	0	8	1	0
5	A	133	0	0	0	0
5	B	134	0	0	0	0
5	C	164	0	0	4	0
All	All	6718	0	5933	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (39) 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:C:311:TYR:OH	5:C:501:HOH:O	2.00	0.78
1:A:202:ALA:HA	1:A:203:HIS:C	2.08	0.74
1:C:310:GLY:O	1:C:311:TYR:HB2	1.86	0.72
1:B:290:HIS:HB3	1:B:295:LEU:HD12	1.72	0.70
1:A:201:PRO:O	1:A:202:ALA:HB3	1.95	0.66
1:A:200:ARG:HB3	1:A:201:PRO:HD2	1.77	0.65
1:A:201:PRO:O	1:A:202:ALA:CB	2.49	0.61
1:A:289:SER:OG	1:C:225:GLU:OE2	2.19	0.61
1:B:57:ASP:N	1:B:57:ASP:OD1	2.33	0.60
1:C:47:ARG:NE	5:C:626:HOH:O	2.25	0.57
1:C:310:GLY:O	1:C:311:TYR:CB	2.53	0.57
1:C:195:MET:HE2	1:C:293:MET:SD	2.45	0.56
1:B:225:GLU:OE2	1:C:289:SER:OG	2.24	0.55
1:B:56:ALA:C	1:B:57:ASP:OD1	2.45	0.55
1:A:202:ALA:HA	1:A:204:SER:N	2.25	0.51
1:C:180:GLY:H	4:C:404:GOL:H32	1.76	0.50
1:C:290:HIS:HB3	1:C:295:LEU:HD12	1.93	0.49
1:A:200:ARG:CB	1:A:201:PRO:HD2	2.41	0.48
1:B:75:LEU:HA	1:B:173:PRO:HG2	1.96	0.47
1:A:155:HIS:O	1:A:160:GLU:O	2.32	0.47
1:C:229:THR:O	1:C:285:CYS:HA	2.16	0.46
1:B:88:PHE:HD2	1:B:119:VAL:HG21	1.82	0.45
1:B:230:PHE:O	1:B:257:ASN:HA	2.18	0.44
1:A:47:ARG:NE	1:A:87:GLU:OE1	2.49	0.43
1:B:195:MET:O	1:B:295:LEU:HD21	2.18	0.43
1:B:202:ALA:O	1:B:204:SER:N	2.52	0.43
1:B:179:LYS:HD2	1:B:180:GLY:N	2.33	0.43
1:C:87:GLU:HG2	5:C:659:HOH:O	2.18	0.42
1:A:154:ASP:OD2	1:A:157:VAL:HB	2.19	0.42
1:B:88:PHE:CD2	1:B:119:VAL:HG21	2.55	0.42
1:C:160:GLU:HG3	5:C:607:HOH:O	2.20	0.42
1:A:195:MET:HE2	1:A:293:MET:SD	2.61	0.41
1:C:201:PRO:O	1:C:203:HIS:N	2.53	0.41
1:B:229:THR:O	1:B:285:CYS:HA	2.20	0.41
1:C:195:MET:CE	1:C:293:MET:SD	3.09	0.41
1:A:229:THR:O	1:A:285:CYS:HA	2.20	0.41
1:A:65:GLU:HB2	1:A:68:ARG:HG3	2.03	0.41
1:A:48:ILE:O	1:A:48:ILE:HG13	2.20	0.40
1:C:230:PHE:O	1:C:257:ASN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/293 (92%)	258 (96%)	9 (3%)	1 (0%)	34	21
1	B	267/293 (91%)	255 (96%)	10 (4%)	2 (1%)	22	10
1	C	267/293 (91%)	257 (96%)	10 (4%)	0	100	100
All	All	802/879 (91%)	770 (96%)	29 (4%)	3 (0%)	34	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	57	ASP
1	B	203	HIS
1	A	202	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/236 (92%)	210 (97%)	7 (3%)	39	25
1	B	216/236 (92%)	213 (99%)	3 (1%)	67	59
1	C	216/236 (92%)	209 (97%)	7 (3%)	39	25
All	All	649/708 (92%)	632 (97%)	17 (3%)	46	32

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	124	THR
1	A	206	PRO
1	A	220	MET
1	A	236	ARG
1	A	295	LEU
1	A	312	GLU
1	B	57	ASP
1	B	220	MET
1	B	282	MET
1	C	98	LEU
1	C	204	SER
1	C	220	MET
1	C	282	MET
1	C	293	MET
1	C	309	PRO
1	C	311	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	C	404	-	5,5,5	1.42	1 (20%)	5,5,5	1.20	1 (20%)

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
4	GOL	C	404	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	404	GOL	O2-C2	2.15	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	404	GOL	C3-C2-C1	-2.07	103.66	111.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	76:ILE	C	77:GLU	N	1.17
1	A	249:ASP	C	250:ASP	N	1.09
1	A	248:PRO	C	249:ASP	N	1.00

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	270/293 (92%)	-0.06	12 (4%) 34 28	16, 26, 50, 97	0
1	B	269/293 (91%)	-0.09	11 (4%) 37 31	17, 27, 53, 92	0
1	C	269/293 (91%)	-0.28	6 (2%) 62 57	14, 22, 41, 65	0
All	All	808/879 (91%)	-0.15	29 (3%) 42 37	14, 25, 50, 97	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	HIS	7.0
1	A	56	ALA	5.7
1	B	203	HIS	4.4
1	A	202	ALA	4.4
1	B	202	ALA	4.1
1	C	43	GLY	4.0
1	A	204	SER	3.6
1	A	201	PRO	3.6
1	C	311	TYR	3.4
1	B	56	ALA	3.2
1	A	43	GLY	3.0
1	A	45	VAL	2.9
1	B	45	VAL	2.9
1	B	311	TYR	2.8
1	B	44	GLU	2.8
1	C	100	VAL	2.7
1	C	202	ALA	2.7
1	C	68	ARG	2.6
1	B	204	SER	2.5
1	A	44	GLU	2.4
1	B	310	GLY	2.4
1	C	203	HIS	2.3
1	A	68	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	304	THR	2.2
1	A	100	VAL	2.2
1	B	43	GLY	2.1
1	A	138	SER	2.1
1	A	160	GLU	2.1
1	B	309	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	404	6/6	0.63	0.20	35,43,45,45	0
3	O	A	404	1/1	0.98	0.12	32,32,32,32	0
2	CU	C	402	1/1	0.99	0.04	21,21,21,21	0
2	CU	C	401	1/1	0.99	0.06	21,21,21,21	0
2	CU	B	403	1/1	0.99	0.05	29,29,29,29	1
2	CU	B	401	1/1	0.99	0.07	25,25,25,25	0
2	CU	A	402	1/1	0.99	0.06	23,23,23,23	0
2	CU	B	402	1/1	0.99	0.07	22,22,22,22	0
3	O	B	404	1/1	0.99	0.14	31,31,31,31	0
2	CU	A	403	1/1	0.99	0.05	26,26,26,26	1
2	CU	C	403	1/1	0.99	0.07	22,22,22,22	1
2	CU	A	401	1/1	1.00	0.04	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.