WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 10:40 pm GMT

PDB ID	:	4W1T
Title	:	Structure of the Ssl1 laccase mutant H99Y with depleted type-2 copper ion
Authors	:	Gunne, M.; Hoeppner, A.; Jaeger, V.D.; Urlacher, V.B.
Deposited on	:	2014-08-14
Resolution	:	1.55 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

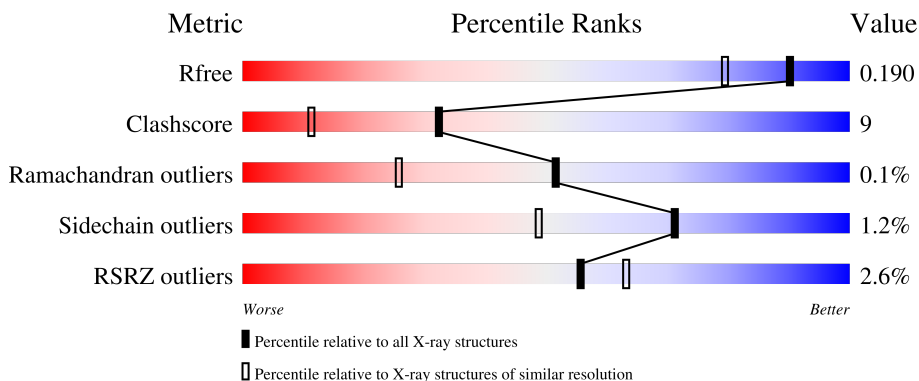|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	Percentile Ranks	Value
Rfree		0.190
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		1.2%
RSRZ outliers		2.6%

Worse — *Better*

▌ Percentile relative to all X-ray structures

⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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

Mol	Chain	Length	Quality of chain
1	A	293	% 75% 16% • 7%
1	B	293	4% 77% 13% • 8%
1	C	293	2% 80% 13% • 6%

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:

WORLDWIDE wwPDB PROTEIN DATA BANK

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	401	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7360 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	272	Total	C	N	O	S	0	2	0
			2127	1331	386	400	10			
1	B	269	Total	C	N	O	S	0	6	0
			2120	1329	381	400	10			
1	C	276	Total	C	N	O	S	0	7	0
			2178	1365	394	408	11			

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	99	TYR	HIS	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	99	TYR	HIS	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	99	TYR	HIS	engineered mutation	UNP B5HSR1

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
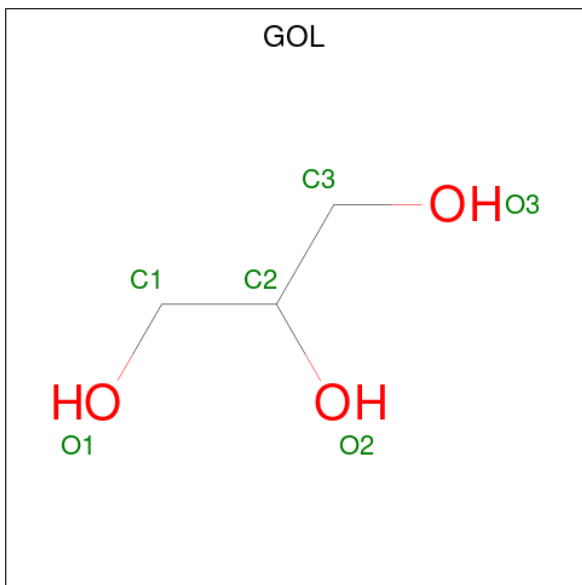
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0

• Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	Cu 5	0	0
3	B	3	Total 3	Cu 3	0	0
3	C	1	Total 1	Cu 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	305	Total 305	O 305	0	0
4	B	264	Total 264	O 264	0	0
4	C	327	Total 327	O 327	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.
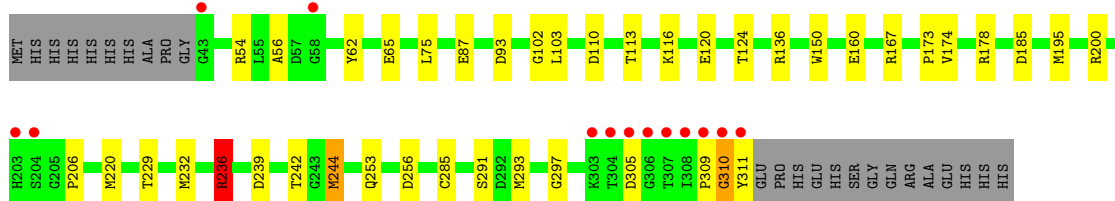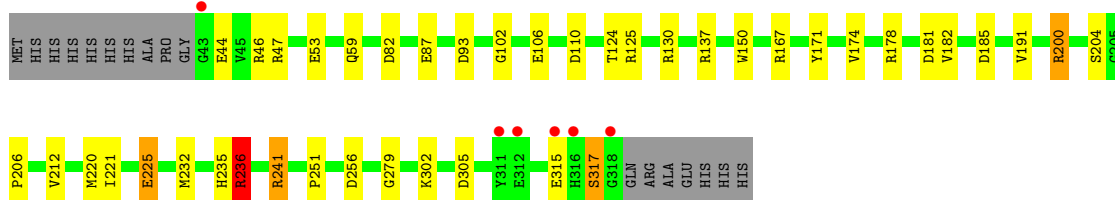
• Molecule 1: Copper oxidase
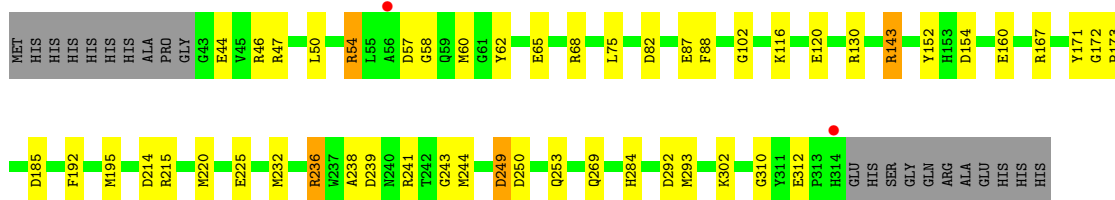
• Molecule 1: Copper oxidase

• Molecule 1: Copper oxidase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.49Å 104.56Å 163.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.28 – 1.55 52.28 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.28-1.55) 100.0 (52.28-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.38 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.149 , 0.180 0.163 , 0.190	Depositor DCC
R_{free} test set	6427 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	11.9	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.4	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7360	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	1.29	6/2193 (0.3%)	1.39	21/2976 (0.7%)
1	B	1.25	5/2196 (0.2%)	1.32	16/2979 (0.5%)
1	C	1.23	8/2260 (0.4%)	1.32	23/3066 (0.8%)
All	All	1.26	19/6649 (0.3%)	1.34	60/9021 (0.7%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	MET	CG-SD	-7.57	1.61	1.81
1	A	310	GLY	C-O	-6.94	1.12	1.23
1	A	172	GLY	N-CA	-6.67	1.36	1.46
1	B	54	ARG	CZ-NH2	-6.58	1.24	1.33
1	C	317	SER	CB-OG	-6.41	1.33	1.42
1	C	225	GLU	CD-OE2	-6.40	1.18	1.25
1	B	291	SER	CB-OG	-6.33	1.34	1.42
1	C	171	TYR	CE1-CZ	-5.86	1.30	1.38
1	B	297	GLY	N-CA	5.74	1.54	1.46
1	A	171	TYR	CG-CD2	5.67	1.46	1.39
1	A	62	TYR	CE1-CZ	5.60	1.45	1.38
1	C	251	PRO	N-CA	-5.48	1.38	1.47
1	C	130	ARG	CZ-NH2	5.35	1.40	1.33
1	B	62	TYR	CG-CD1	-5.33	1.32	1.39
1	C	279	GLY	N-CA	-5.23	1.38	1.46
1	C	167	ARG	CD-NE	-5.21	1.37	1.46
1	A	62	TYR	CZ-OH	-5.09	1.29	1.37
1	C	106	GLU	CD-OE1	-5.06	1.20	1.25
1	B	65	GLU	CG-CD	5.00	1.59	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	236	ARG	NE-CZ-NH2	-16.63	111.99	120.30
1	A	249	ASP	CB-CG-OD2	-12.01	107.49	118.30
1	C	167	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	A	249	ASP	CB-CG-OD1	11.07	128.26	118.30
1	C	167	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	B	236	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	C	178	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	B	236	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	B	54	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	A	154	ASP	CB-CG-OD2	9.59	126.93	118.30
1	A	185	ASP	CB-CG-OD2	9.26	126.63	118.30
1	B	54	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	C	256	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	A	152	TYR	CB-CG-CD2	8.92	126.35	121.00
1	B	178	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	C	125	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	244	MET	CG-SD-CE	7.82	112.72	100.20
1	A	167	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	136	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	195	MET	CG-SD-CE	-7.23	88.63	100.20
1	C	256	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	143	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	B	103	LEU	CB-CG-CD1	6.80	122.55	111.00
1	A	82	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	130	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	C	241	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	305	ASP	CB-CG-OD1	6.65	124.29	118.30
1	C	174	VAL	CB-CA-C	-6.55	98.95	111.40
1	A	292	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	236	ARG	CD-NE-CZ	6.43	132.60	123.60
1	B	256	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	239	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	250	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	152	TYR	CD1-CE1-CZ	6.05	125.25	119.80
1	B	167	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	236	ARG	NH1-CZ-NH2	5.94	125.94	119.40
1	A	241	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	192	PHE	CB-CG-CD1	5.89	124.92	120.80
1	A	62	TYR	CZ-CE2-CD2	5.86	125.07	119.80
1	C	178	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	214	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	93	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	185	ASP	CB-CG-OD2	5.74	123.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	200	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	302	LYS	CD-CE-NZ	5.68	124.75	111.70
1	C	125	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	174	VAL	CB-CA-C	-5.52	100.91	111.40
1	A	82	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	C	137	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	130	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	C	130	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	C	185	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	181	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	54	ARG	CG-CD-NE	5.23	122.78	111.80
1	B	195	MET	CG-SD-CE	-5.20	91.88	100.20
1	C	82	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	C	93	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	A	239	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	200	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	241	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	2127	0	2008	34	0
1	B	2120	0	2014	38	0
1	C	2178	0	2073	35	0
2	A	6	0	8	1	0
2	B	18	0	24	1	0
2	C	6	0	8	5	0
3	A	5	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
4	A	305	0	0	23	6
4	B	264	0	0	23	0
4	C	327	0	0	35	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7360	0	6135	111	6

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 9.

All (111) 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:B:293:MET:HG2	4:B:714:HOH:O	1.29	1.31
1:C:59:GLN:HG2	4:C:792:HOH:O	1.04	1.21
1:B:110:ASP:HB3	4:B:663:HOH:O	1.03	1.18
1:C:110:ASP:HB3	4:C:759:HOH:O	0.99	1.17
1:A:236:ARG:HD2	4:C:757:HOH:O	1.43	1.14
1:C:124[B]:THR:CG2	4:C:718:HOH:O	1.94	1.13
1:A:225[B]:GLU:OE2	4:A:708:HOH:O	1.73	1.04
1:B:120:GLU:OE1	4:B:754:HOH:O	1.74	1.03
1:A:293:MET:HG3	4:A:741:HOH:O	1.63	0.98
1:C:225:GLU:OE2	4:C:823:HOH:O	1.81	0.96
1:A:54:ARG:HG3	4:A:504:HOH:O	1.63	0.96
1:A:236:ARG:HD3	4:C:756:HOH:O	1.63	0.96
1:A:58:GLY:O	4:A:712:HOH:O	1.86	0.93
1:B:160:GLU:HG3	4:B:701:HOH:O	1.69	0.92
1:A:232:MET:HG3	4:A:760:HOH:O	1.72	0.88
1:A:120:GLU:HG3	4:A:520:HOH:O	1.72	0.88
1:C:124[B]:THR:HG23	4:C:718:HOH:O	1.67	0.87
4:A:657:HOH:O	1:B:244:MET:HG2	1.76	0.86
1:A:54:ARG:CG	4:A:504:HOH:O	2.24	0.82
1:B:311:TYR:HD1	4:B:627:HOH:O	1.62	0.82
1:A:312:GLU:OE1	4:A:501:HOH:O	1.97	0.81
1:B:56:ALA:O	4:B:683:HOH:O	2.01	0.79
1:A:160:GLU:HG2	4:A:775:HOH:O	1.81	0.79
1:B:116:LYS:CE	4:B:753:HOH:O	2.34	0.75
1:A:232:MET:CG	4:A:760:HOH:O	2.30	0.73
1:B:160:GLU:OE1	4:B:661:HOH:O	2.06	0.73
1:C:47[B]:ARG:NH1	4:C:721:HOH:O	1.82	0.72
2:C:401:GOL:C1	4:C:700:HOH:O	2.38	0.70
1:A:249:ASP:OD1	4:A:502:HOH:O	2.09	0.70
4:A:657:HOH:O	1:B:244:MET:CG	2.36	0.69
1:C:47[A]:ARG:NH2	4:C:801:HOH:O	2.25	0.69
1:C:236:ARG:HG2	4:C:689:HOH:O	1.92	0.68
1:B:232:MET:HG3	4:B:720:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253[A]:GLN:HG3	4:A:740:HOH:O	1.94	0.67
1:C:59:GLN:CG	4:C:792:HOH:O	1.87	0.67
1:C:44:GLU:OE1	1:C:46:ARG:NH2	2.27	0.67
1:C:53:GLU:OE1	4:C:709:HOH:O	2.13	0.67
1:C:232[A]:MET:CG	4:C:735:HOH:O	2.44	0.65
1:C:235:HIS:O	1:C:236:ARG:HD3	1.97	0.65
1:B:160:GLU:CG	4:B:701:HOH:O	2.34	0.65
2:C:401:GOL:H12	4:C:700:HOH:O	1.96	0.65
1:B:116:LYS:HE2	4:B:753:HOH:O	1.97	0.63
1:B:242:THR:HB	1:B:244:MET:HE3	1.79	0.63
1:B:116:LYS:HE3	4:B:753:HOH:O	2.00	0.60
1:A:120:GLU:CG	4:A:520:HOH:O	2.40	0.60
1:A:244:MET:CE	4:A:761:HOH:O	2.48	0.60
1:A:236:ARG:CD	4:C:757:HOH:O	2.22	0.60
1:C:317:SER:HB2	4:C:504:HOH:O	2.03	0.59
1:A:244:MET:HE2	4:A:761:HOH:O	2.01	0.59
1:B:236:ARG:NE	4:B:721:HOH:O	2.34	0.59
1:B:232:MET:CG	4:B:720:HOH:O	2.50	0.58
1:C:87:GLU:HG2	4:C:718:HOH:O	2.03	0.58
1:C:235:HIS:C	1:C:236:ARG:HD3	2.25	0.57
4:A:746:HOH:O	1:B:236:ARG:HD3	2.03	0.57
1:A:44:GLU:OE1	1:A:46:ARG:NH2	2.38	0.57
1:B:113:THR:OG1	1:B:160:GLU:OE2	2.18	0.57
1:B:113:THR:CB	1:B:160:GLU:OE2	2.53	0.56
1:B:124:THR:HB	4:B:751:HOH:O	2.04	0.56
1:C:232[A]:MET:HG3	4:C:735:HOH:O	2.05	0.56
1:B:200:ARG:HD3	1:B:206:PRO:HD3	1.88	0.55
1:A:225[B]:GLU:CD	4:A:708:HOH:O	2.27	0.55
1:B:253[A]:GLN:HG3	4:B:738:HOH:O	2.05	0.55
1:B:253[B]:GLN:HG3	4:B:723:HOH:O	2.06	0.55
1:C:236:ARG:CG	4:C:689:HOH:O	2.53	0.54
1:A:253[B]:GLN:HG3	4:A:682:HOH:O	2.08	0.54
1:B:75:LEU:HA	1:B:173:PRO:HG2	1.90	0.53
2:C:401:GOL:H31	4:C:700:HOH:O	2.08	0.53
1:C:87:GLU:CG	4:C:718:HOH:O	2.56	0.53
1:B:242:THR:HG22	2:B:403:GOL:H32	1.92	0.51
1:A:225[B]:GLU:CG	4:A:708:HOH:O	2.59	0.51
1:C:47[B]:ARG:CZ	4:C:721:HOH:O	2.44	0.51
1:C:232[A]:MET:HG2	4:C:735:HOH:O	2.10	0.50
1:C:47[B]:ARG:NH2	4:C:721:HOH:O	2.45	0.49
1:C:59:GLN:OE1	4:C:792:HOH:O	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:HG2	4:C:700:HOH:O	2.12	0.48
1:C:182[A]:VAL:CG2	4:C:556:HOH:O	2.62	0.48
1:B:113:THR:HB	1:B:160:GLU:OE2	2.14	0.48
1:A:238:ALA:O	1:A:243:GLY:HA2	2.14	0.47
1:B:253[A]:GLN:CG	4:B:738:HOH:O	2.62	0.47
1:B:229:THR:O	1:B:285:CYS:HA	2.15	0.46
1:C:236:ARG:NE	4:C:689:HOH:O	2.49	0.46
2:C:401:GOL:O1	4:C:700:HOH:O	2.20	0.45
1:B:311:TYR:CD1	4:B:627:HOH:O	2.48	0.45
1:C:102:GLY:HA3	1:C:150:TRP:CD2	2.51	0.45
1:C:124[B]:THR:HG22	4:C:718:HOH:O	1.87	0.45
1:C:236:ARG:HB2	4:C:689:HOH:O	2.16	0.45
2:C:401:GOL:C3	4:C:700:HOH:O	2.66	0.44
1:B:87[B]:GLU:CG	4:B:751:HOH:O	2.66	0.44
1:B:305:ASP:C	1:B:305:ASP:OD1	2.56	0.44
1:A:50:LEU:O	1:A:88:PHE:HA	2.18	0.43
1:A:253[B]:GLN:HA	4:A:682:HOH:O	2.18	0.43
1:C:212[A]:VAL:HG23	1:C:302:LYS:O	2.19	0.43
1:A:215:ARG:HD3	1:A:269:GLN:OE1	2.19	0.42
1:C:191:VAL:HA	1:C:221:ILE:O	2.20	0.42
1:B:253[B]:GLN:HA	4:B:738:HOH:O	2.19	0.42
1:A:65:GLU:HB2	1:A:68:ARG:HG3	2.00	0.42
1:A:75:LEU:HA	1:A:173:PRO:HG2	2.01	0.42
1:C:200:ARG:HD3	1:C:206:PRO:HD3	2.01	0.42
1:A:284:HIS:CE1	4:C:772:HOH:O	2.72	0.42
1:A:57:ASP:C	1:A:57:ASP:OD1	2.58	0.41
1:C:124[A]:THR:HG23	4:C:765:HOH:O	2.20	0.41
1:A:102:GLY:O	1:B:236:ARG:HD2	2.19	0.41
1:B:236:ARG:HD3	4:B:721:HOH:O	2.21	0.41
1:A:253[A]:GLN:HA	4:A:682:HOH:O	2.21	0.41
1:B:102:GLY:HA3	1:B:150:TRP:CD2	2.55	0.41
1:B:253[A]:GLN:HA	4:B:738:HOH:O	2.20	0.41
1:A:143:ARG:HH12	2:A:401:GOL:H12	1.86	0.41
1:A:47:ARG:NH1	1:A:87:GLU:OE1	2.47	0.40
1:B:309:PRO:O	1:B:310:GLY:C	2.59	0.40
1:C:47[B]:ARG:HB3	1:C:47[B]:ARG:HH11	1.86	0.40
1:C:200:ARG:HB3	1:C:204[B]:SER:OG	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:530:HOH:O	4:A:555:HOH:O[1_455]	1.83	0.37
4:A:553:HOH:O	4:A:560:HOH:O[4_547]	1.93	0.27
4:A:517:HOH:O	4:C:510:HOH:O[1_455]	1.99	0.21
4:A:555:HOH:O	4:A:557:HOH:O[1_655]	2.10	0.10
4:A:539:HOH:O	4:C:533:HOH:O[4_447]	2.11	0.09
4:A:505:HOH:O	4:C:532:HOH:O[1_455]	2.17	0.03

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	272/293 (93%)	268 (98%)	4 (2%)	0	100	100
1	B	273/293 (93%)	264 (97%)	8 (3%)	1 (0%)	34	14
1	C	281/293 (96%)	277 (99%)	4 (1%)	0	100	100
All	All	826/879 (94%)	809 (98%)	16 (2%)	1 (0%)	51	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	GLY

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	221/236 (94%)	218 (99%)	3 (1%)	67	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	222/236 (94%)	220 (99%)	2 (1%)	78	61
1	C	229/236 (97%)	226 (99%)	3 (1%)	69	44
All	All	672/708 (95%)	664 (99%)	8 (1%)	71	49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	220	MET
1	A	236	ARG
1	B	220	MET
1	B	236	ARG
1	C	220	MET
1	C	236	ARG
1	C	315	GLU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	#$|Z| > 2$
2	GOL	A	401	-	5,5,5	0.46	0	5,5,5	0.88	0
2	GOL	B	402	-	5,5,5	1.41	1 (20%)	5,5,5	0.57	0
2	GOL	C	401	-	5,5,5	0.89	0	5,5,5	1.37	1 (20%)
2	GOL	B	403	-	5,5,5	1.20	1 (20%)	5,5,5	2.05	2 (40%)
2	GOL	B	401	-	5,5,5	0.88	0	5,5,5	1.10	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
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	B	402	-	-	1/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	GOL	O3-C3	2.74	1.54	1.42
2	B	403	GOL	O2-C2	2.19	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	403	GOL	O2-C2-C1	3.58	124.88	109.12
2	C	401	GOL	O2-C2-C1	2.61	120.63	109.12
2	B	403	GOL	C3-C2-C1	-2.07	103.67	111.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	O1-C1-C2-O2
2	B	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	B	402	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
2	C	401	GOL	5	0
2	B	403	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	272/293 (92%)	-0.16	2 (0%)	87	90	6, 13, 28, 50	0
1	B	269/293 (91%)	-0.04	13 (4%)	30	35	6, 15, 33, 46	0
1	C	276/293 (94%)	-0.27	6 (2%)	62	67	5, 11, 24, 43	0
All	All	817/879 (92%)	-0.16	21 (2%)	56	63	5, 13, 30, 50	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ALA	4.7
1	C	43	GLY	3.9
1	B	204	SER	3.8
1	B	310	GLY	3.6
1	B	311	TYR	3.4
1	C	315	GLU	3.1
1	C	318	GLY	3.1
1	B	309	PRO	3.0
1	B	308	ILE	2.8
1	B	305	ASP	2.8
1	B	58	GLY	2.8
1	B	203	HIS	2.7
1	B	307	THR	2.6
1	B	304	THR	2.6
1	C	312	GLU	2.5
1	B	43	GLY	2.4
1	A	314	HIS	2.3
1	C	316	HIS	2.1
1	B	303	LYS	2.1
1	B	306	GLY	2.0
1	C	311	TYR	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 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	GOL	B	401	6/6	0.88	0.17	24,37,38,40	0
2	GOL	A	401	6/6	0.92	0.11	25,39,40,45	0
2	GOL	B	403	6/6	0.93	0.12	18,24,25,33	0
2	GOL	B	402	6/6	0.95	0.08	12,13,15,16	0
2	GOL	C	401	6/6	0.96	0.12	16,20,22,30	0
3	CU	A	404	1/1	0.98	0.05	10,10,10,10	1
3	CU	A	405	1/1	0.98	0.06	15,15,15,15	1
3	CU	B	405	1/1	0.98	0.09	6,6,6,6	1
3	CU	B	404	1/1	0.99	0.06	10,10,10,10	0
3	CU	A	403	1/1	0.99	0.06	9,9,9,9	0
3	CU	B	406	1/1	0.99	0.07	11,11,11,11	1
3	CU	A	406	1/1	1.00	0.08	3,3,3,3	1
3	CU	A	402	1/1	1.00	0.07	6,6,6,6	0
3	CU	C	402	1/1	1.00	0.07	6,6,6,6	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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