



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:42 PM UTC

PDB ID : 4W1T / pdb_00004w1t
Title : Structure of the Ssl1 laccase mutant H99Y with depleted type-2 copper ion
Authors : Gunne, M.; Hoepfner, 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

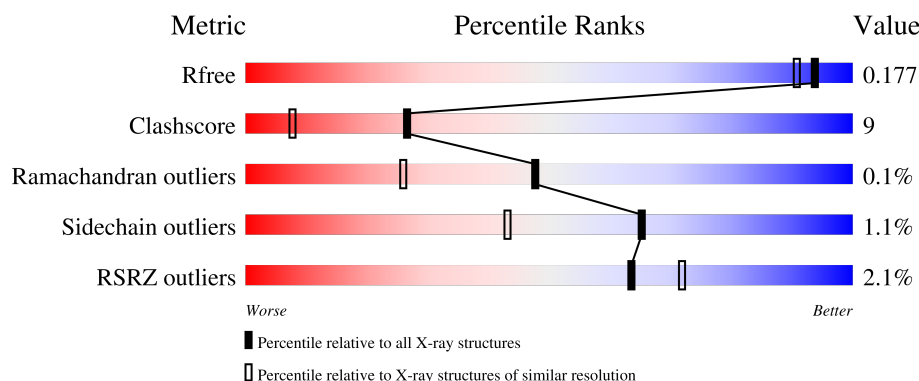
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (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 $\leq 5\%$. 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	% 75% 16% • 7%
1	B	293	3% 75% 15% • 8%
1	C	293	% 80% 14% • 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:

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:

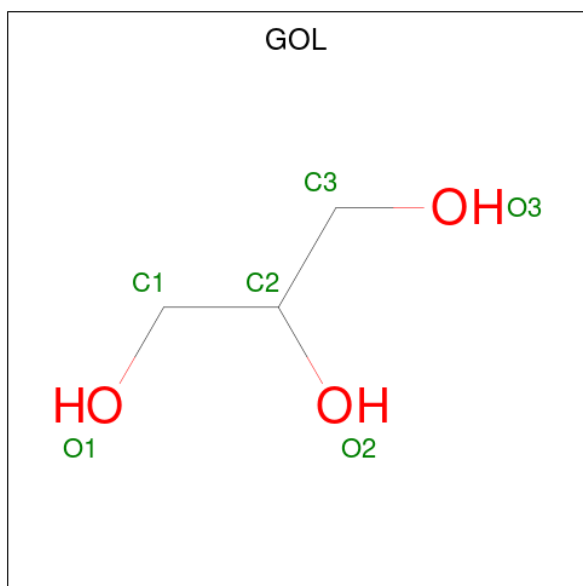
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	initiating methionine	UNP B5HSR1
A	34	HIS	-	expression tag	UNP B5HSR1
A	35	HIS	-	expression tag	UNP B5HSR1
A	36	HIS	-	expression tag	UNP B5HSR1
A	37	HIS	-	expression tag	UNP B5HSR1
A	38	HIS	-	expression tag	UNP B5HSR1
A	39	HIS	-	expression tag	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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- 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

- Molecule 1: Copper oxidase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	5.38 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.149 , 0.180 (Not available) , 0.177	Depositor DCC
R_{free} test set	6427 reflections (4.99%)	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 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

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: 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	1.64	15/2193 (0.7%)	1.43	13/2976 (0.4%)
1	B	1.58	14/2196 (0.6%)	1.36	9/2979 (0.3%)
1	C	1.52	15/2260 (0.7%)	1.30	8/3066 (0.3%)
All	All	1.58	44/6649 (0.7%)	1.37	30/9021 (0.3%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	GLY	C-O	-11.00	1.12	1.23
1	B	297	GLY	N-CA	9.45	1.54	1.45
1	C	251	PRO	N-CA	-9.44	1.38	1.47
1	A	96	ALA	N-CA	8.15	1.56	1.45
1	A	112	THR	N-CA	-7.89	1.36	1.45
1	A	173	PRO	CA-CB	-7.87	1.45	1.54
1	B	184	PRO	N-CA	-7.81	1.39	1.46
1	A	60	MET	CG-SD	-7.71	1.61	1.80
1	A	215	ARG	CA-C	-7.19	1.44	1.52
1	B	54	ARG	CZ-NH2	-6.89	1.24	1.33
1	C	279	GLY	N-CA	-6.85	1.38	1.45
1	C	250	ASP	C-N	6.62	1.38	1.33
1	B	59	GLN	N-CA	6.58	1.53	1.45
1	B	64	LEU	CA-C	6.55	1.61	1.52
1	B	75	LEU	CA-CB	-6.42	1.43	1.53
1	A	172	GLY	N-CA	-6.33	1.36	1.44
1	A	62	TYR	C-N	6.22	1.41	1.33
1	C	167	ARG	CD-NE	-6.18	1.37	1.46
1	C	309	PRO	CA-C	-6.18	1.45	1.52
1	C	305	ASP	N-CA	6.07	1.54	1.46
1	A	249	ASP	CG-OD1	6.00	1.36	1.25
1	C	184	PRO	C-O	5.79	1.30	1.23
1	C	151	HIS	CA-C	-5.63	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	ASP	N-CA	5.59	1.52	1.46
1	A	74	PRO	CA-C	5.57	1.59	1.52
1	B	118	ASP	N-CA	-5.52	1.39	1.45
1	B	197	ILE	C-O	5.49	1.30	1.24
1	A	242	THR	N-CA	-5.46	1.38	1.46
1	C	189	THR	CA-C	-5.45	1.46	1.52
1	B	90	ASN	N-CA	-5.41	1.39	1.46
1	C	156	VAL	C-O	5.35	1.30	1.24
1	C	205	GLY	N-CA	5.32	1.51	1.44
1	A	224	GLY	CA-C	-5.31	1.46	1.52
1	C	57	ASP	C-O	5.28	1.30	1.23
1	A	103	LEU	C-O	-5.25	1.16	1.23
1	A	251	PRO	CA-C	5.25	1.57	1.52
1	C	205	GLY	C-O	5.17	1.30	1.24
1	B	291	SER	N-CA	5.12	1.52	1.46
1	B	100	VAL	CA-C	5.11	1.58	1.52
1	A	264	ASP	CA-C	-5.11	1.46	1.52
1	C	75	LEU	C-O	5.09	1.29	1.24
1	B	288	GLN	N-CA	5.09	1.52	1.46
1	B	123	GLY	N-CA	-5.04	1.39	1.45
1	C	130	ARG	CZ-NH2	5.04	1.40	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	VAL	CB-CA-C	-8.49	98.95	110.42
1	A	168	LYS	N-CA-C	8.14	123.03	113.18
1	C	236	ARG	NE-CZ-NH2	-8.02	111.99	119.20
1	A	172	GLY	O-C-N	7.29	129.06	121.77
1	B	273	GLY	N-CA-C	6.08	124.06	115.30
1	B	241	ARG	N-CA-C	5.94	117.45	110.97
1	B	174	VAL	CB-CA-C	-5.93	100.91	110.28
1	B	282	MET	O-C-N	5.89	130.08	122.89
1	B	70	THR	O-C-N	5.87	130.27	123.17
1	B	236	ARG	CD-NE-CZ	5.86	132.60	124.40
1	A	170	LEU	O-C-N	5.84	130.21	122.56
1	C	250	ASP	CA-C-O	5.75	123.03	119.29
1	C	110	ASP	N-CA-C	-5.69	105.22	111.82
1	B	166	ILE	N-CA-C	5.67	115.86	110.42
1	A	174	VAL	CB-CA-C	-5.58	102.18	110.33
1	A	195	MET	CG-SD-CE	-5.58	88.63	100.90
1	A	224	GLY	N-CA-C	5.49	118.20	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ILE	CB-CA-C	5.39	114.61	109.33
1	B	244	MET	CG-SD-CE	5.37	112.72	100.90
1	A	93	ASP	N-CA-C	5.35	119.44	113.02
1	A	64	LEU	N-CA-C	-5.27	106.35	112.89
1	C	167	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	A	109	SER	CA-C-N	5.16	127.70	120.28
1	A	109	SER	C-N-CA	5.16	127.70	120.28
1	A	164	GLY	N-CA-C	5.15	119.37	112.77
1	C	236	ARG	NH1-CZ-NH2	5.10	125.94	119.30
1	B	110	ASP	O-C-N	-5.07	115.64	122.43
1	A	143	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	C	312	GLU	CA-C-N	5.00	124.66	119.56
1	C	312	GLU	C-N-CA	5.00	124.66	119.56

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	2127	0	2008	36	0
1	B	2120	0	2014	39	0
1	C	2178	0	2073	37	0
2	A	6	0	8	1	0
2	B	18	0	24	2	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	25	6
4	B	264	0	0	24	0
4	C	327	0	0	36	3
All	All	7360	0	6135	117	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 (117) 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
1:A:225[B]:GLU:CD	4:A:708:HOH:O	2.27	0.71
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:B:242:THR:HB	1:B:244:MET:HE3	1.74	0.68
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
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:A:293:MET:HE3	4:A:544:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:235:HIS:C	1:C:236:ARG:HD3	2.25	0.62
1:A:244:MET:HE2	4:A:761:HOH:O	2.01	0.61
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:C:59:GLN:CD	4:C:792:HOH:O	2.32	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
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: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: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:B:305:ASP:C	1:B:305:ASP:OD1	2.56	0.48
1:C:59:GLN:OE1	4:C:792:HOH:O	2.19	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:GOL:O3	4:B:699:HOH:O	1.98	0.46
1:A:225[B]:GLU:CG	4:A:708:HOH:O	2.59	0.46
1:B:229:THR:O	1:B:285:CYS:HA	2.15	0.46
1:A:57:ASP:C	1:A:57:ASP:OD1	2.58	0.46
1:C:236:ARG:NE	4:C:689:HOH:O	2.49	0.46
1:B:309:PRO:O	1:B:310:GLY:C	2.59	0.45
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: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:C:195:MET:HE3	1:C:195:MET:HB3	1.92	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:195:MET:HE1	1:B:290:HIS:CD2	2.56	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:C:47[B]:ARG:HB3	1:C:47[B]:ARG:HH11	1.86	0.40
1:A:195:MET:HE3	4:A:692:HOH:O	2.21	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 [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	272/293 (93%)	268 (98%)	4 (2%)	0	100	100
1	B	273/293 (93%)	264 (97%)	8 (3%)	1 (0%)	30	13
1	C	281/293 (96%)	277 (99%)	4 (1%)	0	100	100
All	All	826/879 (94%)	809 (98%)	16 (2%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	GLY

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	221/236 (94%)	219 (99%)	2 (1%)	70	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	222/236 (94%)	219 (99%)	3 (1%)	59	33
1	C	229/236 (97%)	227 (99%)	2 (1%)	70	51
All	All	672/708 (95%)	665 (99%)	7 (1%)	65	47

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	220	MET
1	B	66	LYS
1	B	220	MET
1	B	236	ARG
1	C	220	MET
1	C	315	GLU

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

Mol	Chain	Res	Type
1	C	288	GLN

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 oligosaccharides 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	B	402	-	5,5,5	1.41	1 (20%)	5,5,5	0.60	0
2	GOL	B	403	-	5,5,5	1.25	1 (20%)	5,5,5	2.17	2 (40%)
2	GOL	A	401	-	5,5,5	0.48	0	5,5,5	0.92	0
2	GOL	C	401	-	5,5,5	0.91	0	5,5,5	1.46	1 (20%)
2	GOL	B	401	-	5,5,5	0.92	0	5,5,5	1.15	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	B	402	-	-	1/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	C	401	-	-	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	2.75	1.54	1.42
2	B	403	GOL	O2-C2	2.26	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	GOL	O2-C2-C1	3.79	124.88	109.18
2	C	401	GOL	O2-C2-C1	2.77	120.63	109.18
2	B	403	GOL	C3-C2-C1	-2.22	103.67	111.80

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
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 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	GOL	2	0
2	A	401	GOL	1	0
2	C	401	GOL	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.02	4 (1%)	72 79	6, 13, 28, 50	2 (0%)
1	B	269/293 (91%)	0.13	9 (3%)	49 57	6, 15, 33, 46	6 (2%)
1	C	276/293 (94%)	-0.36	4 (1%)	73 80	5, 10, 24, 43	7 (2%)
All	All	817/879 (92%)	-0.07	17 (2%)	63 72	5, 13, 30, 50	15 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ALA	4.2
1	B	311	TYR	3.9
1	A	45	VAL	3.2
1	A	314	HIS	3.1
1	B	56	ALA	3.1
1	A	43	GLY	3.1
1	B	308	ILE	2.9
1	C	318	GLY	2.7
1	B	309	PRO	2.5
1	C	43	GLY	2.5
1	B	293	MET	2.5
1	B	310	GLY	2.4
1	B	43	GLY	2.4
1	C	312	GLU	2.4
1	C	314	HIS	2.2
1	B	67	GLY	2.1
1	B	58	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	GOL	B	401	6/6	0.85	0.13	24,37,38,40	0
2	GOL	A	401	6/6	0.87	0.14	25,39,40,45	0
2	GOL	B	403	6/6	0.94	0.10	18,24,25,33	0
2	GOL	B	402	6/6	0.95	0.07	12,13,15,16	0
2	GOL	C	401	6/6	0.96	0.07	16,20,22,30	0
3	CU	A	405	1/1	0.97	0.04	15,15,15,15	1
3	CU	A	404	1/1	0.98	0.03	10,10,10,10	1
3	CU	B	405	1/1	0.98	0.03	6,6,6,6	1
3	CU	B	406	1/1	0.98	0.03	11,11,11,11	1
3	CU	B	404	1/1	0.99	0.02	10,10,10,10	0
3	CU	A	402	1/1	1.00	0.01	6,6,6,6	0
3	CU	A	403	1/1	1.00	0.01	9,9,9,9	0
3	CU	A	406	1/1	1.00	0.01	3,3,3,3	1
3	CU	C	402	1/1	1.00	0.01	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.