



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:30 PM UTC

PDB ID : 9LZ7 / pdb_00009lz7
Title : Reductive-half reaction intermediate of copper amine oxidase from *Arthrobacter globiformis* captured with short-a-axis diffraction data by mix-and-inject serial crystallography at 22-ms time delay
Authors : Murakawa, T.; Okajima, T.
Deposited on : 2025-02-21
Resolution : 2.22 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

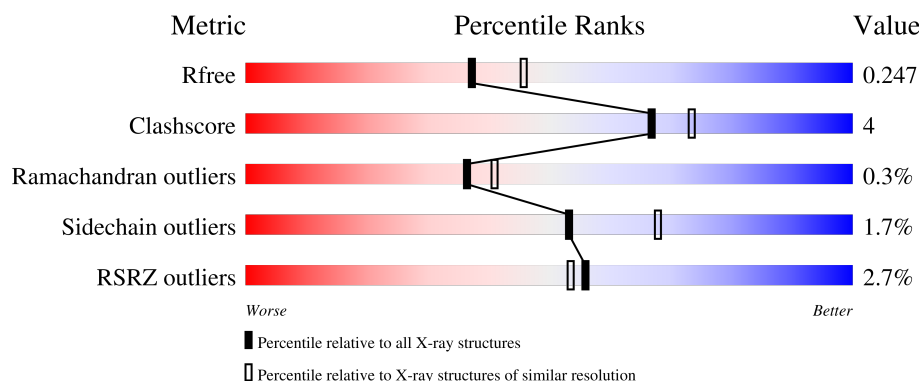
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

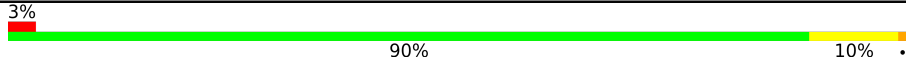
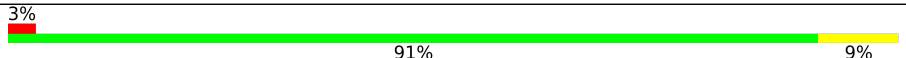
The reported resolution of this entry is 2.22 Å.

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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	620	
1	B	620	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10600 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	6	0
			4909	3107	862	931	9			
1	B	620	Total	C	N	O	S	0	2	0
			4888	3090	859	930	9			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

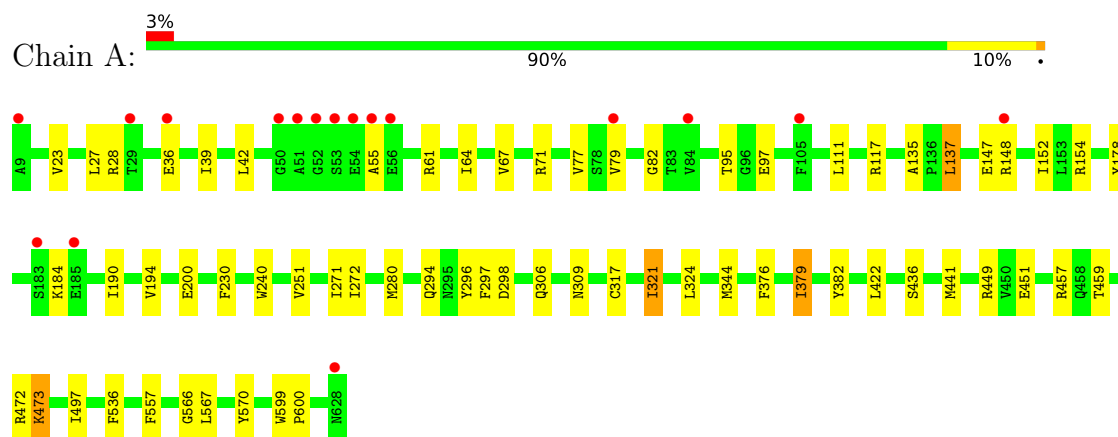
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	404	Total	O	0	0
			404	404		
4	B	395	Total	O	0	0
			395	395		

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: Phenylethylamine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.05Å 64.89Å 158.72Å 90.00° 116.83° 90.00°	Depositor
Resolution (Å)	29.84 – 2.22 29.84 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.84-2.22) 88.4 (29.84-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.28 (at 1.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.211 , 0.248 0.211 , 0.247	Depositor DCC
R_{free} test set	16780 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	5.1	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	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	0.94	EDS
Total number of atoms	10600	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2081e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 2TY, CU, NA

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	0.31	0/5026	0.52	0/6842
1	B	0.32	0/4993	0.52	0/6798
All	All	0.32	0/10019	0.52	0/13640

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4909	0	4755	39	0
1	B	4888	0	4715	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	404	0	0	15	0
4	B	395	0	0	6	0
All	All	10600	0	9470	72	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 4.

All (72) 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:A:271:ILE:HG22	1:A:272:ILE:HG13	1.67	0.77
1:B:56:GLU:HG3	1:B:58:ARG:HG2	1.68	0.74
1:B:294:GLN:NE2	1:B:296:TYR:OH	2.21	0.73
1:A:294:GLN:NE2	1:A:296:TYR:OH	2.15	0.68
1:A:317:CYS:HB3	1:A:321[A]:ILE:HG12	1.77	0.66
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.31	0.66
1:A:117:ARG:NH1	4:A:1111:HOH:O	2.29	0.65
1:B:271:ILE:HG22	1:B:272:ILE:HG13	1.79	0.65
1:B:22:GLU:OE1	4:B:1101:HOH:O	2.14	0.64
1:A:324:LEU:HG	1:A:344:MET:HE2	1.80	0.64
1:B:20:ILE:HD12	1:B:327:VAL:HG12	1.82	0.60
1:A:111:LEU:HD21	1:A:184:LYS:HB3	1.84	0.59
1:B:453:GLU:OE2	1:B:513:LYS:NZ	2.34	0.59
1:B:153:LEU:HD12	1:B:181:VAL:HG11	1.85	0.56
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.41	0.55
1:A:309:ASN:ND2	4:A:1126:HOH:O	2.40	0.54
1:A:298:ASP:OD1	4:A:1103:HOH:O	2.19	0.53
1:A:135:ALA:O	1:A:137:LEU:HD22	2.09	0.53
1:B:242:LYS:NZ	4:B:1105:HOH:O	2.27	0.51
1:B:148:ARG:NH2	4:B:1122:HOH:O	2.43	0.51
1:A:200:GLU:OE1	4:A:1102:HOH:O	2.18	0.51
1:A:111:LEU:HD11	1:A:184:LYS:HA	1.93	0.50
1:A:280:MET:O	1:A:297:PHE:HA	2.11	0.50
1:A:147:GLU:HG2	1:A:152:ILE:HG13	1.95	0.49
1:B:230:PHE:HB3	1:B:240:TRP:HB2	1.93	0.49
1:A:230:PHE:HB3	1:A:240:TRP:CD1	2.48	0.49
1:A:251:VAL:CG2	1:A:306:GLN:HB3	2.43	0.48
1:A:566:GLY:HA2	1:A:570:TYR:CZ	2.49	0.48
1:A:117:ARG:NE	4:A:1114:HOH:O	2.34	0.48
1:A:23:VAL:HG11	1:A:42:LEU:HD11	1.95	0.48
1:A:451:GLU:OE1	4:A:1101:HOH:O	2.19	0.48
1:A:473:LYS:HG3	4:A:1191:HOH:O	2.13	0.48
1:A:61:ARG:NH1	4:A:1107:HOH:O	2.26	0.47
1:B:71:ARG:HG2	1:B:90:LEU:O	2.14	0.47
1:B:148:ARG:HA	1:B:148:ARG:CZ	2.45	0.47
1:A:97:GLU:OE2	4:A:1104:HOH:O	2.21	0.47
1:A:449:ARG:NH1	4:A:1143:HOH:O	2.48	0.47
1:B:457:ARG:HE	1:B:457:ARG:HB3	1.50	0.47
1:B:144:TYR:HB2	1:B:147:GLU:HG3	1.96	0.46
1:A:567:LEU:HD23	1:A:567:LEU:HA	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:HG22	1:B:306:GLN:HB3	1.98	0.46
1:A:599:TRP:CE3	1:A:600:PRO:HA	2.51	0.45
1:B:154:ARG:HD2	1:B:293:TRP:CE3	2.51	0.45
1:A:28[B]:ARG:NH1	4:A:1122:HOH:O	2.45	0.45
1:B:26:ILE:HD11	1:B:82:GLY:HA2	1.99	0.44
1:B:266:ASP:OD1	1:B:266:ASP:N	2.44	0.44
1:A:441:MET:HG3	1:A:497:ILE:HG21	2.00	0.43
1:B:401:LYS:HG2	1:B:606:THR:HG22	2.01	0.43
1:B:479:ARG:O	1:B:482:GLU:HG2	2.19	0.43
1:A:36:GLU:O	1:A:67:VAL:HG12	2.18	0.43
1:B:9:ALA:N	4:B:1143:HOH:O	2.51	0.43
1:A:27:LEU:HD13	1:A:64:ILE:HD11	2.01	0.43
1:B:185:GLU:OE1	1:B:185:GLU:HA	2.18	0.42
1:A:148:ARG:NH1	4:A:1133:HOH:O	2.45	0.42
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.90	0.42
1:A:457:ARG:NH1	4:A:1106:HOH:O	2.25	0.42
1:B:282:VAL:HG21	4:B:1106:HOH:O	2.20	0.42
1:A:379:ILE:O	1:A:382:2TY:HD2	2.20	0.42
1:A:154:ARG:HD3	1:A:178:TYR:CE1	2.55	0.42
1:A:422:LEU:HD13	1:A:599:TRP:HB2	2.01	0.41
1:A:71:ARG:NH1	4:A:1109:HOH:O	2.52	0.41
1:B:9:ALA:N	4:B:1150:HOH:O	2.53	0.41
1:B:19:GLU:O	1:B:23:VAL:HG23	2.21	0.41
1:B:160:GLN:HG2	1:B:162:PHE:O	2.21	0.41
1:A:436:SER:HB2	1:A:536:PHE:CE2	2.56	0.40
1:A:95:THR:O	1:A:557:PHE:HB2	2.21	0.40
1:B:453:GLU:HA	1:B:473:LYS:O	2.21	0.40
1:B:41:TYR:HB3	1:B:63:PHE:CD2	2.57	0.40
1:B:280:MET:HE3	1:B:435:PHE:CE2	2.56	0.40
1:B:280:MET:O	1:B:297:PHE:HA	2.20	0.40
1:A:117:ARG:NH2	4:A:1114:HOH:O	2.51	0.40
1:B:268:LEU:HD12	1:B:268:LEU:HA	1.88	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	623/620 (100%)	600 (96%)	21 (3%)	2 (0%)	36	41
1	B	619/620 (100%)	596 (96%)	21 (3%)	2 (0%)	36	41
All	All	1242/1240 (100%)	1196 (96%)	42 (3%)	4 (0%)	36	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	B	55	ALA
1	A	82	GLY
1	B	303	LEU

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	519/513 (101%)	505 (97%)	14 (3%)	39	52
1	B	515/513 (100%)	509 (99%)	6 (1%)	63	76
All	All	1034/1026 (101%)	1014 (98%)	20 (2%)	53	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	77	VAL
1	A	79	VAL
1	A	137	LEU
1	A	190	ILE
1	A	194	VAL
1	A	321[A]	ILE
1	A	321[B]	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	376	PHE
1	A	379	ILE
1	A	459	THR
1	A	472[A]	ARG
1	A	472[B]	ARG
1	A	473	LYS
1	B	56	GLU
1	B	138	SER
1	B	376	PHE
1	B	379	ILE
1	B	472[A]	ARG
1	B	472[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	345	HIS
1	A	418	ASN
1	A	458	GLN
1	A	573	GLN
1	B	81	ASN
1	B	294	GLN
1	B	306	GLN
1	B	363	ASN
1	B	418	ASN
1	B	458	GLN
1	B	518	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	2TY	A	382	1	21,23,24	1.04	0	23,30,32	1.02	0
1	2TY	B	382	1	21,23,24	1.20	2 (9%)	23,30,32	1.17	2 (8%)

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
1	2TY	A	382	1	-	1/11/12/14	0/2/2/2
1	2TY	B	382	1	-	1/11/12/14	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	2TY	CB-CG	-2.43	1.47	1.51
1	B	382	2TY	CZ-CE2	2.15	1.43	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	2TY	OH-CZ-CE2	2.63	126.77	120.44
1	B	382	2TY	OH-CZ-CE1	-2.60	112.45	119.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	382	2TY	N-CA-CB-CG
1	A	382	2TY	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382	2TY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	619/620 (99%)	0.30	17 (2%) 56 53	13, 28, 48, 129	6 (0%)
1	B	619/620 (99%)	0.19	17 (2%) 56 53	14, 27, 45, 116	2 (0%)
All	All	1238/1240 (99%)	0.25	34 (2%) 56 53	13, 28, 47, 129	8 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	SER	5.3
1	A	55	ALA	5.2
1	A	51	ALA	5.1
1	B	55	ALA	5.0
1	B	52	GLY	4.7
1	A	53	SER	4.7
1	B	51	ALA	4.4
1	A	54	GLU	4.4
1	A	52	GLY	4.1
1	B	54	GLU	4.1
1	B	628	ASN	4.0
1	B	50	GLY	3.1
1	B	148	ARG	3.0
1	A	50	GLY	3.0
1	B	9	ALA	3.0
1	B	56	GLU	3.0
1	A	56	GLU	2.9
1	A	29	THR	2.8
1	A	9	ALA	2.6
1	B	150	ARG	2.5
1	A	628	ASN	2.5
1	B	105	PHE	2.4
1	B	562	SER	2.4
1	A	148	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	36	GLU	2.3
1	A	84	VAL	2.3
1	B	266	ASP	2.2
1	A	183	SER	2.2
1	A	105	PHE	2.1
1	B	627	ALA	2.1
1	B	208	GLU	2.1
1	A	79	VAL	2.1
1	B	358	LEU	2.0
1	A	185	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	2TY	A	382	22/23	0.91	0.12	21,26,36,43	0
1	2TY	B	382	22/23	0.91	0.11	20,27,35,40	0

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	CU	A	1001	1/1	0.96	0.04	18,18,18,18	0
3	NA	A	1002	1/1	0.97	0.12	16,16,16,16	0
3	NA	B	1002	1/1	0.97	0.06	14,14,14,14	0
2	CU	B	1001	1/1	0.99	0.03	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.