



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 10:14 AM JST

PDB ID : 5Z0J
Title : Crystal structure of copper-bound tyrosinase from *Streptomyces castaneoglobisporus* in complex with the caddie protein obtained by soaking in the hydroxylamine-containing solution for 2 h at 277 K
Authors : Matoba, Y.; Sugiyama, M.
Deposited on : 2017-12-19
Resolution : 1.35 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 : 4.02b-467
Mogul : 1.8.5 (274361), 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

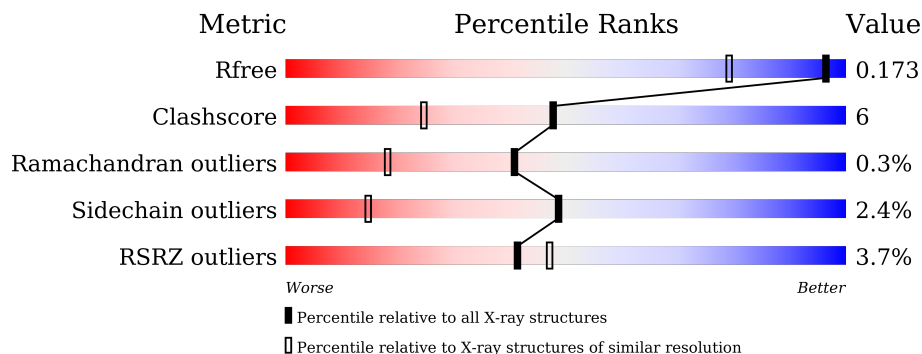
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	281	 2% 85% 11%
2	B	134	 5% 44% 10% 43%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3344 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2303	1448	427	423	5	0	16	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	SER	PHE	conflict	UNP Q83WS2
A	274	LEU	-	expression tag	UNP Q83WS2
A	275	GLU	-	expression tag	UNP Q83WS2
A	276	HIS	-	expression tag	UNP Q83WS2
A	277	HIS	-	expression tag	UNP Q83WS2
A	278	HIS	-	expression tag	UNP Q83WS2
A	279	HIS	-	expression tag	UNP Q83WS2
A	280	HIS	-	expression tag	UNP Q83WS2
A	281	HIS	-	expression tag	UNP Q83WS2

- Molecule 2 is a protein called MelC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	77	610	385	111	112	2	0	6	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	DAH	TYR	see sequence details	UNP Q83WS1
B	127	LEU	-	expression tag	UNP Q83WS1
B	128	GLU	-	expression tag	UNP Q83WS1
B	129	HIS	-	expression tag	UNP Q83WS1
B	130	HIS	-	expression tag	UNP Q83WS1
B	131	HIS	-	expression tag	UNP Q83WS1
B	132	HIS	-	expression tag	UNP Q83WS1

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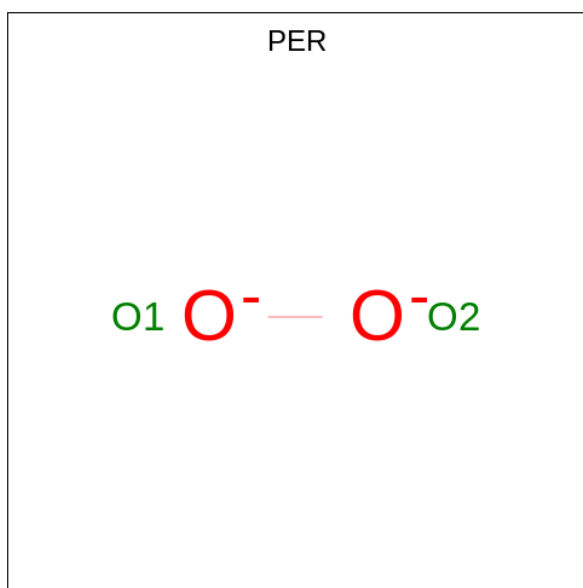
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Chain	Residue	Modelled	Actual	Comment	Reference
B	133	HIS	-	expression tag	UNP Q83WS1
B	134	HIS	-	expression tag	UNP Q83WS1

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

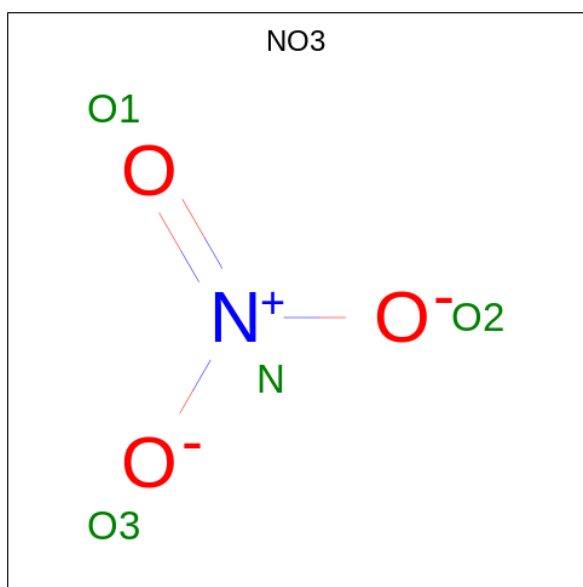
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cu 6 6	0	2
3	B	1	Total Cu 2 2	0	1

- Molecule 4 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	1

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N O 4 1 3	0	0
5	A	1	Total N O 4 1 3	0	0
5	A	1	Total N O 4 1 3	0	0
5	A	1	Total N O 4 1 3	0	0
5	B	1	Total N O 4 1 3	0	1
5	B	1	Total N O 4 1 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	292	Total O 292 292	0	1
6	B	105	Total O 105 105	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.77Å 96.97Å 54.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.35 38.81 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-1.35) 98.6 (38.81-1.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.35Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.134 , 0.178 0.131 , 0.173	Depositor DCC
R_{free} test set	3779 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3344	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NO3, DAH, CU, PER

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	0.62	0/2434	1.32	24/3318 (0.7%)
2	B	0.63	0/632	1.56	9/855 (1.1%)
All	All	0.62	0/3066	1.37	33/4173 (0.8%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	ARG	NE-CZ-NH1	-13.29	113.65	120.30
2	B	70	GLY	C-N-CA	13.22	150.06	122.30
2	B	53	ARG	NE-CZ-NH1	-11.60	114.50	120.30
2	B	105	ARG	NE-CZ-NH2	11.20	125.90	120.30
1	A	178	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	17[A]	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	17[B]	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	136[A]	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	136[B]	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	17[A]	ARG	CD-NE-CZ	9.18	136.46	123.60
1	A	17[B]	ARG	CD-NE-CZ	9.18	136.46	123.60
1	A	140	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	A	229	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	92	ARG	NE-CZ-NH2	-7.59	116.50	120.30
2	B	52	ARG	NE-CZ-NH1	-7.09	116.76	120.30
2	B	105	ARG	CD-NE-CZ	7.08	133.51	123.60
1	A	91	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	132	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	136[A]	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	136[B]	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	B	88	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	235	TYR	CB-CG-CD2	6.54	124.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	CD-NE-CZ	6.15	132.22	123.60
1	A	229	ARG	NH1-CZ-NH2	6.09	126.10	119.40
1	A	16	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	B	57	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	114	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	229	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	140	ARG	NH1-CZ-NH2	5.39	125.33	119.40
1	A	229	ARG	CD-NE-CZ	-5.39	116.05	123.60
1	A	109	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	53	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	269	TYR	CB-CG-CD2	-5.05	117.97	121.00

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	2303	0	2178	27	0
2	B	610	0	563	15	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
4	A	2	0	0	1	0
5	A	16	0	0	0	0
5	B	8	0	0	1	0
6	A	292	0	0	1	0
6	B	105	0	0	1	0
All	All	3344	0	2741	35	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 6.

All (35) 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:157:GLU:OE1	1:A:229:ARG:NH2	1.68	1.24
4:A:304[A]:PER:O1	2:B:98[A]:DAH:OE2	2.06	0.74
2:B:68:HIS:NE2	2:B:70:GLY:HA3	2.03	0.73
1:A:95:ARG:HB2	1:A:95:ARG:HH11	1.54	0.71
1:A:136[A]:ARG:HD2	1:A:138:TYR:OH	1.95	0.67
1:A:275:GLU:HG3	1:A:276:HIS:O	2.04	0.57
1:A:42[B]:ILE:HG12	1:A:54[B]:HIS:CE1	2.41	0.55
2:B:68:HIS:CE1	2:B:70:GLY:HA3	2.42	0.55
1:A:157:GLU:CD	1:A:229:ARG:HH22	2.09	0.53
1:A:185[A]:ARG:NH2	2:B:88:ASP:HB3	2.27	0.50
1:A:38[B]:HIS:CE1	1:A:42[B]:ILE:HG13	2.47	0.50
1:A:42[A]:ILE:HG12	2:B:97[A]:HIS:NE2	2.28	0.49
2:B:67:GLU:N	6:B:306:HOH:O	2.47	0.48
1:A:39:ASN:HA	1:A:42[A]:ILE:HG22	1.96	0.48
1:A:83[B]:LEU:HD11	1:A:213:TRP:HB3	1.96	0.47
2:B:92:ILE:HG13	5:B:202[A]:NO3:O2	2.15	0.47
1:A:134[B]:ASP:HB2	2:B:119:PRO:O	2.15	0.46
1:A:17[B]:ARG:NH1	6:A:412:HOH:O	2.49	0.46
1:A:93:THR:OG1	1:A:95:ARG:NH1	2.49	0.46
1:A:42[A]:ILE:HG12	2:B:97[A]:HIS:CD2	2.51	0.46
1:A:134[B]:ASP:CA	2:B:121:LEU:HG	2.47	0.45
2:B:45:PHE:CE2	2:B:56:GLY:HA3	2.52	0.44
1:A:42[A]:ILE:HD12	1:A:54[A]:HIS:NE2	2.33	0.43
1:A:201[A]:MET:HG2	1:A:209:ASP:HB3	2.00	0.43
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.84	0.42
1:A:242:PRO:O	1:A:243:ASP:HB2	2.19	0.42
2:B:67:GLU:HB2	2:B:82[A]:HIS:NE2	2.34	0.42
1:A:134[B]:ASP:C	2:B:121:LEU:HG	2.40	0.42
1:A:192:ARG:HH11	1:A:192:ARG:HD2	1.74	0.42
2:B:68:HIS:CD2	2:B:70:GLY:HA3	2.54	0.42
1:A:113:GLY:O	1:A:140:ARG:HA	2.21	0.41
1:A:16:ARG:HG2	1:A:16:ARG:NH1	2.35	0.41
1:A:56:SER:O	1:A:178:ARG:HD3	2.21	0.41
1:A:42[B]:ILE:HG21	1:A:42[B]:ILE:HD12	1.89	0.40
1:A:136[B]:ARG:NH2	2:B:114:GLU:OE1	2.52	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	290/281 (103%)	279 (96%)	11 (4%)	0	100	100
2	B	77/134 (58%)	72 (94%)	4 (5%)	1 (1%)	12	1
All	All	367/415 (88%)	351 (96%)	15 (4%)	1 (0%)	41	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	71	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	251/240 (105%)	246 (98%)	5 (2%)	55	21
2	B	63/93 (68%)	61 (97%)	2 (3%)	39	8
All	All	314/333 (94%)	307 (98%)	7 (2%)	49	18

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

Mol	Chain	Res	Type
1	A	88	TRP
1	A	95	ARG
1	A	103	PHE
1	A	190	HIS
1	A	233	SER

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Mol	Chain	Res	Type
2	B	67	GLU
2	B	68	HIS

Sometimes 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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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
5	NO3	A	308	-	1,3,3	0.39	0	0,3,3	-	-
4	PER	A	304[A]	3	0,1,1	-	-	-	-	-
5	NO3	B	203	-	1,3,3	0.67	0	0,3,3	-	-
5	NO3	A	306	-	1,3,3	0.35	0	0,3,3	-	-
5	NO3	B	202[A]	-	1,3,3	0.57	0	0,3,3	-	-
5	NO3	A	307	-	1,3,3	0.30	0	0,3,3	-	-
5	NO3	A	305	-	1,3,3	0.16	0	0,3,3	-	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304[A]	PER	1	0
5	B	202[A]	NO3	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 [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	276/281 (98%)	-0.35	6 (2%) 62 68	9, 14, 28, 58	0
2	B	76/134 (56%)	0.31	7 (9%) 9 10	9, 15, 51, 59	0
All	All	352/415 (84%)	-0.21	13 (3%) 41 47	9, 14, 29, 59	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	69	GLY	14.1
2	B	123	PHE	10.7
1	A	276	HIS	9.5
2	B	70	GLY	9.3
2	B	68	HIS	8.7
2	B	67	GLU	5.7
2	B	40	ALA	4.5
1	A	277	HIS	4.0
1	A	275	GLU	3.4
1	A	148	ALA	3.2
2	B	59	ALA	2.7
1	A	95	ARG	2.6
1	A	48	SER	2.2

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(Å ²)	Q<0.9
2	DAH	B	98[A]	13/14	0.97	0.06	12,15,15,15	1

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
5	NO3	B	202[A]	4/4	0.83	0.24	19,22,23,26	4
5	NO3	A	307	4/4	0.90	0.13	26,32,33,36	0
5	NO3	A	305	4/4	0.94	0.14	18,20,22,25	0
5	NO3	A	308	4/4	0.95	0.16	28,29,30,35	0
5	NO3	A	306	4/4	0.97	0.05	20,22,23,32	0
4	PER	A	304[A]	2/2	0.97	0.18	14,14,14,15	2
5	NO3	B	203	4/4	0.98	0.08	22,24,29,29	0
3	CU	A	303	1/1	0.99	0.14	44,44,44,44	1
3	CU	A	301[A]	1/1	0.99	0.11	13,13,13,13	1
3	CU	A	301[B]	1/1	0.99	0.11	13,13,13,13	1
3	CU	A	301[C]	1/1	0.99	0.11	14,14,14,14	1
3	CU	B	201[B]	1/1	1.00	0.05	17,17,17,17	1
3	CU	A	302[B]	1/1	1.00	0.08	11,11,11,11	1
3	CU	A	302[A]	1/1	1.00	0.08	11,11,11,11	1
3	CU	B	201[A]	1/1	1.00	0.05	22,22,22,22	1

6.5 Other polymers [i](#)

There are no such residues in this entry.