



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:29 PM UTC

PDB ID : 5F7B / pdb_00005f7b
Title : Resting state structure of CuNiR form *Alcaligenes faecalis* determined at 293 K
Authors : Fukuda, Y.; Tse, K.M.; Nakane, T.; Nakatsu, T.; Suzuki, M.; Sugahara, M.; Inoue, S.; Masuda, T.; Yumoto, F.; Matsugaki, N.; Nango, E.; Tono, K.; Joti, Y.; Kameshima, T.; Song, C.; Hatsui, T.; Yabashi, M.; Nureki, O.; Murphy, M.E.P.; Inoue, T.; Iwata, S.; Mizohata, E.
Deposited on : 2015-12-07
Resolution : 1.56 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
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)	:	Engl & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

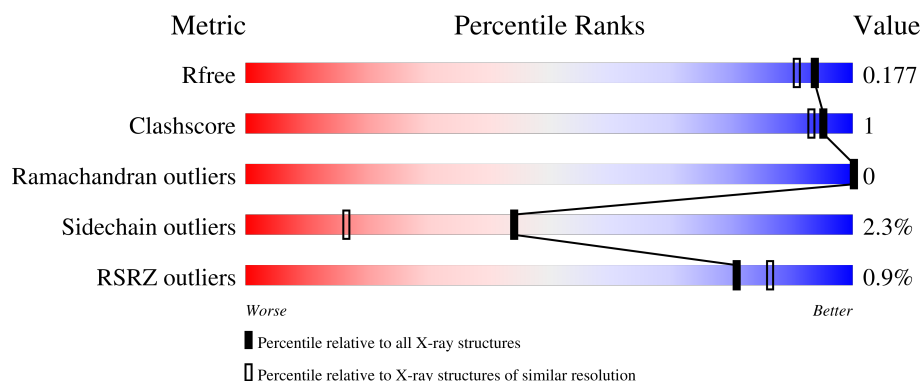
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	342	% 88% 10% ..
1	B	342	% 89% 8% ..
1	C	342	% 90% 7% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8248 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-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	3	0
			2587	1655	436	483	13			
1	B	337	Total	C	N	O	S	0	6	0
			2624	1675	444	493	12			
1	C	336	Total	C	N	O	S	0	2	0
			2578	1650	435	482	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	expression tag	UNP P38501
A	341	LEU	-	expression tag	UNP P38501
A	342	VAL	-	expression tag	UNP P38501
A	343	PRO	-	expression tag	UNP P38501
A	344	ARG	-	expression tag	UNP P38501
B	3	MET	-	expression tag	UNP P38501
B	341	LEU	-	expression tag	UNP P38501
B	342	VAL	-	expression tag	UNP P38501
B	343	PRO	-	expression tag	UNP P38501
B	344	ARG	-	expression tag	UNP P38501
C	3	MET	-	expression tag	UNP P38501
C	341	LEU	-	expression tag	UNP P38501
C	342	VAL	-	expression tag	UNP P38501
C	343	PRO	-	expression tag	UNP P38501
C	344	ARG	-	expression tag	UNP P38501

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

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

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

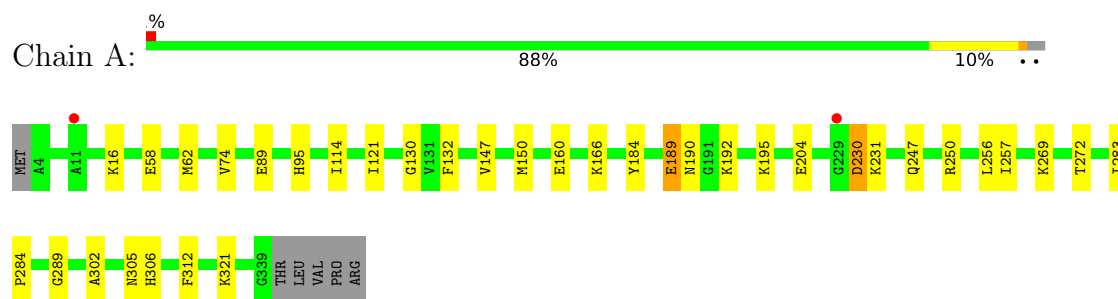
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	3
			125	125		
3	B	151	Total	O	0	4
			155	155		
3	C	168	Total	O	0	5
			173	173		

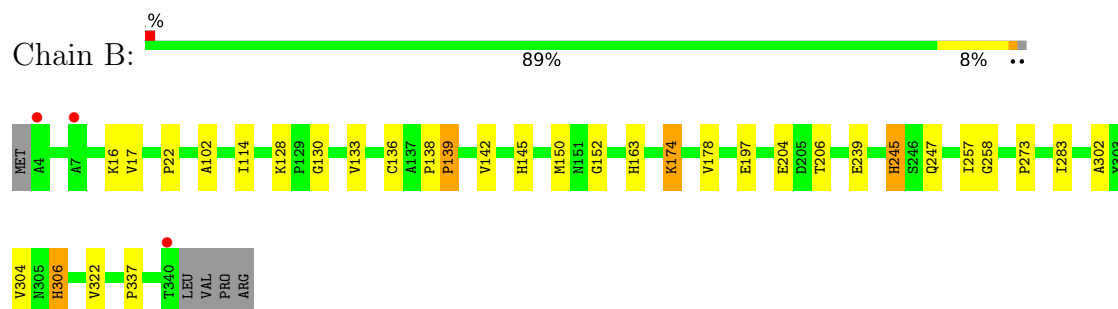
3 Residue-property plots [i](#)

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.

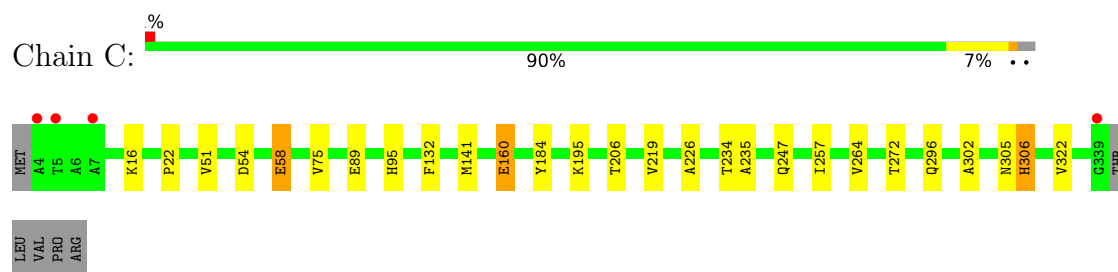
- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.84Å 103.51Å 147.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 1.56 48.83 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.83-1.56) 99.3 (48.83-1.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.149 , 0.177 0.150 , 0.177	Depositor DCC
R_{free} test set	6714 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8248	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: 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	1.46	14/2658 (0.5%)	1.33	5/3622 (0.1%)
1	B	1.47	17/2695 (0.6%)	1.33	7/3672 (0.2%)
1	C	1.48	13/2649 (0.5%)	1.32	6/3612 (0.2%)
All	All	1.47	44/8002 (0.5%)	1.33	18/10906 (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
1	B	0	1
1	C	0	3
All	All	0	5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	305	ASN	C-O	-6.97	1.15	1.24
1	A	74	VAL	C-O	6.45	1.31	1.24
1	B	114	ILE	C-O	6.45	1.30	1.24
1	A	289	GLY	N-CA	6.35	1.51	1.44
1	B	22	PRO	CA-C	6.26	1.55	1.51
1	A	62	MET	C-O	-6.23	1.16	1.24
1	B	283	ILE	N-CA	6.16	1.51	1.46
1	B	322	VAL	N-CA	6.11	1.53	1.46
1	C	22	PRO	C-O	6.04	1.29	1.24
1	B	273	PRO	CA-C	5.99	1.55	1.51
1	B	17	VAL	C-O	-5.96	1.17	1.24
1	B	130	GLY	N-CA	5.96	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	ASN	C-O	-5.82	1.17	1.24
1	B	304	VAL	C-O	-5.81	1.17	1.23
1	B	152	GLY	N-CA	5.80	1.50	1.45
1	C	206	THR	N-CA	5.77	1.53	1.46
1	A	250	ARG	C-O	-5.72	1.16	1.23
1	B	174	LYS	C-O	-5.71	1.17	1.23
1	C	219	VAL	CA-C	-5.66	1.46	1.52
1	A	130	GLY	N-CA	5.62	1.50	1.45
1	C	95	HIS	C-O	-5.58	1.16	1.23
1	C	51	VAL	C-O	-5.51	1.17	1.24
1	A	256	LEU	N-CA	5.50	1.53	1.46
1	A	121	ILE	N-CA	-5.47	1.39	1.46
1	C	132	PHE	C-O	-5.41	1.17	1.23
1	B	206	THR	N-CA	5.39	1.53	1.46
1	B	245	HIS	N-CA	5.37	1.52	1.46
1	C	234	THR	N-CA	5.35	1.52	1.45
1	A	283	ILE	N-CA	5.25	1.50	1.46
1	C	272	THR	C-O	-5.23	1.17	1.24
1	C	141	MET	C-O	-5.23	1.17	1.24
1	C	296	GLN	N-CA	5.22	1.52	1.45
1	A	284	PRO	C-O	5.21	1.29	1.23
1	C	75	VAL	CA-C	-5.20	1.48	1.52
1	B	22	PRO	CA-CB	5.15	1.58	1.53
1	A	147	VAL	C-O	-5.12	1.18	1.24
1	B	128	LYS	CA-C	5.10	1.56	1.52
1	B	133	VAL	CA-CB	5.09	1.61	1.54
1	A	312	PHE	CA-C	-5.09	1.45	1.52
1	B	145	HIS	CA-C	5.09	1.59	1.52
1	B	102	ALA	N-CA	5.07	1.51	1.45
1	C	264	VAL	N-CA	5.07	1.52	1.46
1	A	114	ILE	N-CA	5.06	1.52	1.46
1	A	231	LYS	CA-C	5.00	1.60	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	TYR	CA-C-N	-8.06	115.62	123.04
1	C	184	TYR	C-N-CA	-8.06	115.62	123.04
1	C	226	ALA	N-CA-C	5.92	118.52	111.71
1	A	272	THR	CA-C-N	-5.65	115.59	119.66
1	A	272	THR	C-N-CA	-5.65	115.59	119.66
1	B	306	HIS	CA-C-N	-5.65	114.91	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	HIS	C-N-CA	-5.65	114.91	122.42
1	A	184	TYR	CA-C-N	-5.52	117.96	123.04
1	A	184	TYR	C-N-CA	-5.52	117.96	123.04
1	C	141	MET	CG-SD-CE	-5.35	89.14	100.90
1	B	197	GLU	N-CA-C	5.25	116.81	111.14
1	C	306	HIS	CA-C-N	-5.25	115.44	122.42
1	C	306	HIS	C-N-CA	-5.25	115.44	122.42
1	B	142	VAL	CA-C-N	-5.24	113.64	119.19
1	B	142	VAL	C-N-CA	-5.24	113.64	119.19
1	B	22	PRO	N-CA-CB	-5.13	100.32	103.19
1	A	204	GLU	N-CA-C	5.07	116.50	111.07
1	B	258	GLY	N-CA-C	-5.07	108.33	114.92

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	HIS	Peptide
1	B	306	HIS	Peptide
1	C	306	HIS	Peptide
1	C	58	GLU	Mainchain

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	2587	0	2513	6	1
1	B	2624	0	2541	7	0
1	C	2578	0	2505	5	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	125	0	0	0	0
3	B	155	0	0	2	0
3	C	173	0	0	1	0
All	All	8248	0	7559	18	1

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 1.

All (18) 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:257:ILE:HD12	1:C:302:ALA:HB3	1.75	0.67
1:A:189:GLU:CD	1:A:189:GLU:H	2.03	0.66
1:A:257:ILE:HD12	1:A:302:ALA:HB3	1.84	0.60
1:B:174:LYS:HD2	1:B:239:GLU:OE2	2.07	0.55
1:A:189:GLU:CD	1:A:189:GLU:N	2.64	0.55
1:B:257:ILE:HD12	1:B:302:ALA:HB3	1.92	0.51
1:C:89:GLU:HG2	3:C:604:HOH:O	2.10	0.51
1:B:178:VAL:O	1:B:245:HIS:HA	2.16	0.46
1:B:163:HIS:HD2	3:B:687[A]:HOH:O	1.98	0.45
1:A:58:GLU:CD	1:A:195:LYS:HE3	2.42	0.45
1:C:235:ALA:O	1:C:322:VAL:HA	2.16	0.45
1:B:136:CYS:HB2	1:B:150:MET:HG2	1.98	0.44
1:C:58:GLU:CD	1:C:195:LYS:HE3	2.43	0.43
1:C:160:GLU:H	1:C:160:GLU:CD	2.27	0.43
1:B:163:HIS:CD2	3:B:687[A]:HOH:O	2.73	0.41
1:B:138:PRO:HA	1:B:139:PRO:HD3	1.97	0.41
1:A:132:PHE:CE2	1:A:269:LYS:HE3	2.56	0.41
1:A:95:HIS:HB3	1:A:150:MET:HE1	2.03	0.40

All (1) 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)
1:A:230:ASP:OD2	1:C:54:ASP:OD1[3_444]	2.02	0.18

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	337/342 (98%)	334 (99%)	3 (1%)	0	100	100
1	B	341/342 (100%)	338 (99%)	3 (1%)	0	100	100
1	C	336/342 (98%)	334 (99%)	2 (1%)	0	100	100
All	All	1014/1026 (99%)	1006 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	267/270 (99%)	257 (96%)	10 (4%)	30	6
1	B	271/270 (100%)	266 (98%)	5 (2%)	51	24
1	C	266/270 (98%)	263 (99%)	3 (1%)	65	43
All	All	804/810 (99%)	786 (98%)	18 (2%)	44	18

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	89	GLU
1	A	160	GLU
1	A	166	LYS
1	A	189	GLU
1	A	190	ASN
1	A	192	LYS
1	A	230	ASP
1	A	247	GLN
1	A	321	LYS
1	B	16	LYS
1	B	139	PRO
1	B	204	GLU
1	B	247	GLN
1	B	337	PRO

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Mol	Chain	Res	Type
1	C	16	LYS
1	C	160	GLU
1	C	247	GLN

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

Mol	Chain	Res	Type
1	B	115	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 ⓘ

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	336/342 (98%)	-0.10	2 (0%) 85 89	13, 25, 49, 83	3 (0%)
1	B	337/342 (98%)	-0.20	3 (0%) 81 86	8, 22, 51, 78	6 (1%)
1	C	336/342 (98%)	-0.35	4 (1%) 76 83	12, 20, 42, 70	2 (0%)
All	All	1009/1026 (98%)	-0.22	9 (0%) 81 86	8, 22, 49, 83	11 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ALA	4.2
1	C	4	ALA	4.0
1	A	229	GLY	3.4
1	C	7	ALA	2.7
1	B	340	THR	2.4
1	C	339	GLY	2.4
1	C	5	THR	2.4
1	A	11	ALA	2.2
1	B	7	ALA	2.2

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(Å ²)	Q<0.9
2	CU	A	501	1/1	1.00	0.01	21,21,21,21	0
2	CU	A	502	1/1	1.00	0.01	18,18,18,18	0
2	CU	B	501	1/1	1.00	0.01	22,22,22,22	0
2	CU	B	502	1/1	1.00	0.02	19,19,19,19	0
2	CU	C	501	1/1	1.00	0.01	16,16,16,16	0
2	CU	C	502	1/1	1.00	0.01	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.