



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 10:05 pm BST

PDB ID : 6G5M  
Title : The structure of thiocyanate dehydrogenase from Thioalkalivibrio paradoxus complex with CU(I) ions.  
Authors : Polyakov, K.M.; Tsallagov, S.I.; Tikhkonova, T.V.; Popov, V.O.  
Deposited on : 2018-03-29  
Resolution : 2.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	2.11
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)	:	2.11

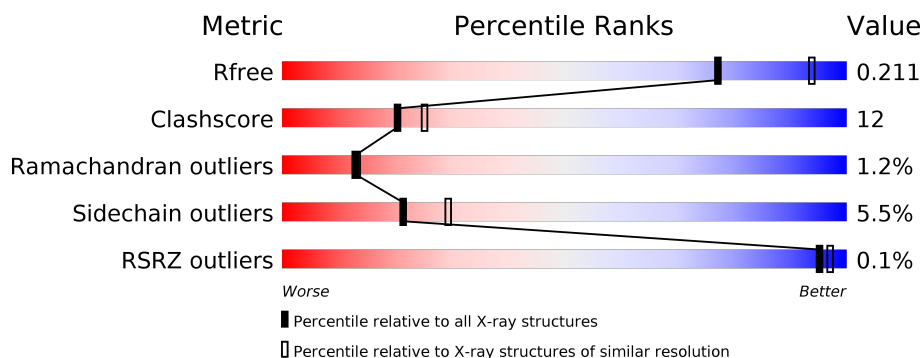
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	467	<div> <div>70%</div> <div>25%</div> <div>••</div> </div>
1	B	467	<div> <div>70%</div> <div>27%</div> <div>•</div> </div>
1	C	467	<div> <div>73%</div> <div>24%</div> <div>•</div> </div>
1	D	467	<div> <div>72%</div> <div>26%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSD	B	131[B]	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15507 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 thiocyanate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	5	0
			3626	2316	602	689	19			
1	B	466	Total	C	N	O	S	0	7	0
			3639	2321	606	690	22			
1	C	467	Total	C	N	O	S	0	6	0
			3653	2331	608	692	22			
1	D	466	Total	C	N	O	S	0	8	0
			3648	2326	606	696	20			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Cu	0	0
			6	6		
2	A	7	Total	Cu	0	0
			7	7		
2	D	8	Total	Cu	0	0
			8	8		
2	C	8	Total	Cu	0	0
			8	8		

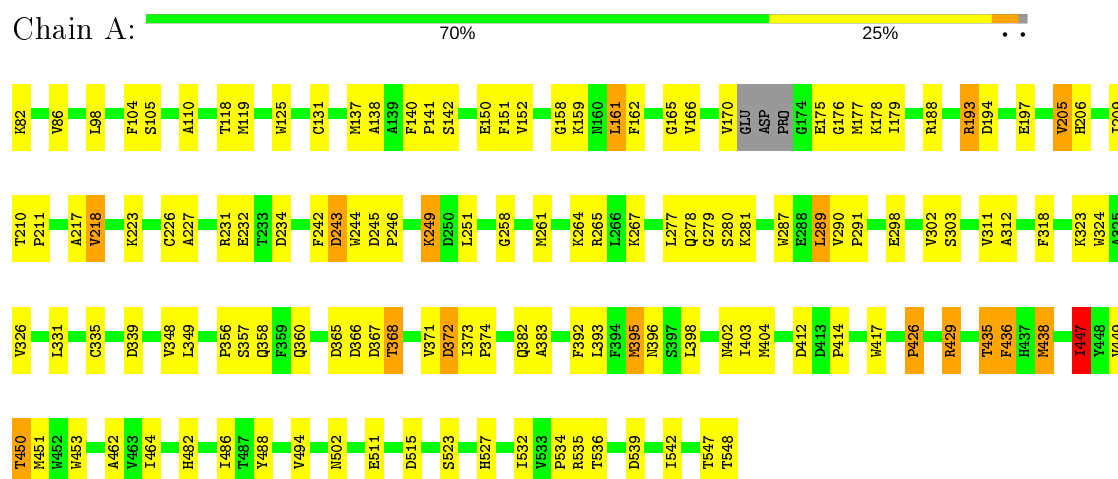
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total	O	0	0
			234	234		
3	B	217	Total	O	0	0
			217	217		
3	C	222	Total	O	0	0
			222	222		
3	D	239	Total	O	0	0
			239	239		

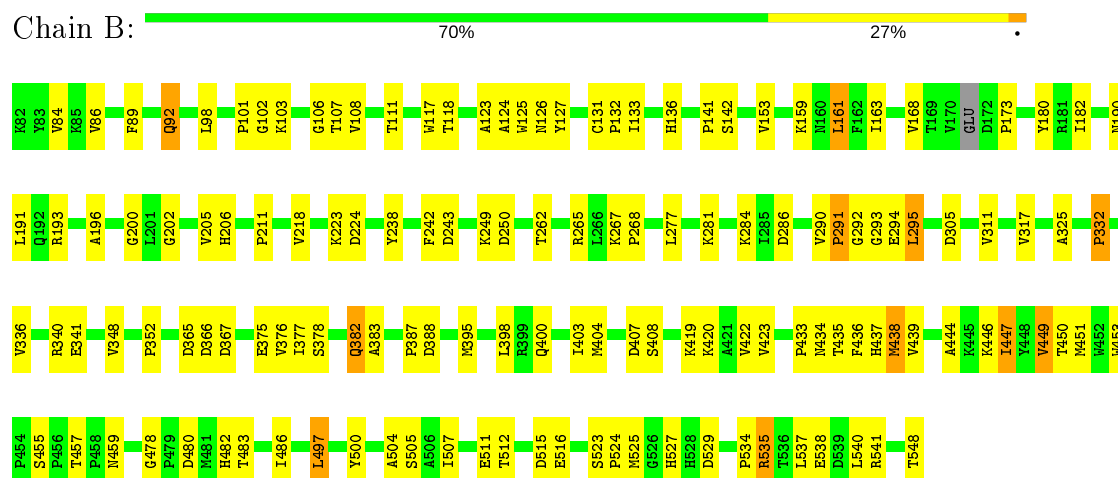
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: thiocyanate dehydrogenase

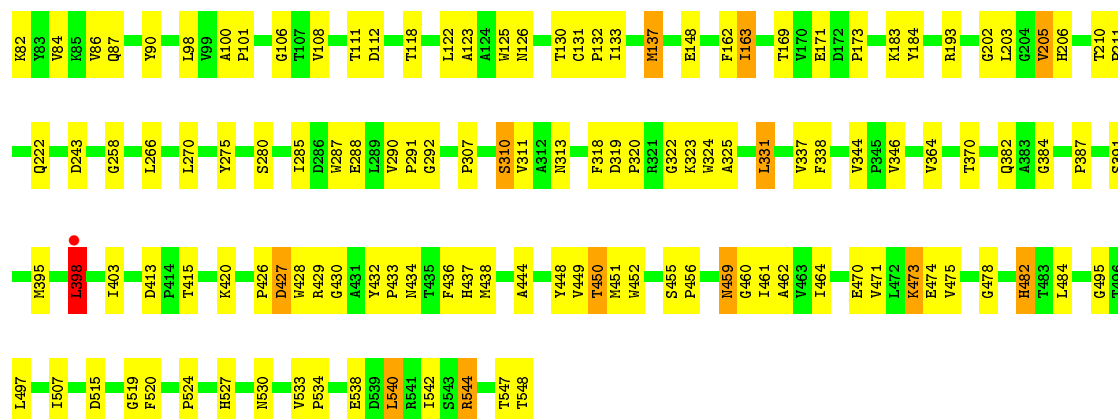


- Molecule 1: thiocyanate dehydrogenase



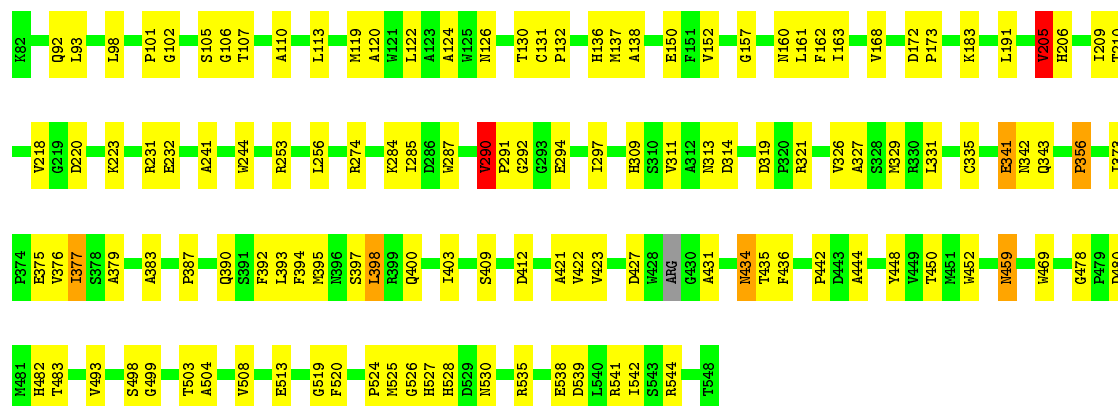
- Molecule 1: thiocyanate dehydrogenase





• Molecule 1: thiocyanate dehydrogenase

Chain D:  72% 26%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.64Å 162.37Å 90.71Å 90.00° 119.64° 90.00°	Depositor
Resolution (Å)	45.58 – 2.31 45.58 – 2.31	Depositor EDS
% Data completeness (in resolution range)	95.8 (45.58-2.31) 95.9 (45.58-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.132 , 0.206 0.138 , 0.211	Depositor DCC
$R_{free}$ test set	4591 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 22.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.059 for -h-l,k,h 0.059 for l,k,-h-l 0.069 for h,-k,-h-l 0.054 for -h-l,-k,l 0.459 for l,-k,h	Xtriage
Reported twinning fraction	0.474 for H, K, L 0.526 for L, -K, H	Depositor
Outliers	0 of 95620 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CSD, 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	0.92	0/3746	1.06	9/5108 (0.2%)
1	B	0.90	0/3767	1.01	5/5140 (0.1%)
1	C	0.90	0/3778	1.04	5/5154 (0.1%)
1	D	0.89	0/3786	1.04	8/5164 (0.2%)
All	All	0.90	0/15077	1.04	27/20566 (0.1%)

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	161	LEU	CB-CG-CD2	-7.28	98.62	111.00
1	D	480	ASP	CB-CG-OD1	7.15	124.74	118.30
1	C	430	GLY	N-CA-C	-7.10	95.34	113.10
1	D	231	ARG	NE-CZ-NH1	7.05	123.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	497	LEU	Peptide
1	C	427	ASP	Peptide

## 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	3626	0	3506	86	0
1	B	3639	0	3502	107	0
1	C	3653	0	3528	89	0
1	D	3648	0	3500	91	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
2	C	8	0	0	1	0
2	D	8	0	0	0	0
3	A	234	0	0	12	0
3	B	217	0	0	6	0
3	C	222	0	0	6	0
3	D	239	0	0	10	0
All	All	15507	0	14036	357	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 12.

The worst 5 of 357 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:D:398:LEU:HB3	3:D:823:HOH:O	1.45	1.15
1:B:131[A]:CSD:SG	1:B:161:LEU:HD22	2.02	1.00
1:B:131[A]:CSD:SG	1:B:161:LEU:CD2	2.54	0.96
1:B:131[B]:CSD:SG	1:B:161:LEU:HD23	2.08	0.93
1:C:451[B]:MET:HE3	1:C:462:ALA:HB2	1.55	0.87

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	464/467 (99%)	416 (90%)	43 (9%)	5 (1%)	14	15
1	B	467/467 (100%)	427 (91%)	36 (8%)	4 (1%)	17	19
1	C	469/467 (100%)	419 (89%)	41 (9%)	9 (2%)	8	6
1	D	469/467 (100%)	434 (92%)	31 (7%)	4 (1%)	17	19
All	All	1869/1868 (100%)	1696 (91%)	151 (8%)	22 (1%)	13	13

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	398	LEU
1	A	312	ALA
1	A	398	LEU
1	B	366	ASP
1	C	429	ARG

### 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	392/391 (100%)	369 (94%)	23 (6%)	19	26
1	B	393/391 (100%)	370 (94%)	23 (6%)	19	26
1	C	396/391 (101%)	373 (94%)	23 (6%)	20	27
1	D	396/391 (101%)	377 (95%)	19 (5%)	25	35
All	All	1577/1564 (101%)	1489 (94%)	88 (6%)	21	29

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	449	VAL
1	C	163	ILE
1	D	427	ASP
1	B	455[A]	SER
1	B	505[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	390	GLN
1	C	401	ASN
1	D	342	ASN
1	C	278	GLN
1	D	192	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	CSD	B	131[B]	-	4,5,8	1.02	0	1,5,10	1.26	0
1	CSD	D	131	1	3,6,8	1.18	0	0,6,10	0.00	-
1	CSD	C	131[A]	-	4,5,8	1.54	1 (25%)	1,5,10	1.51	0
1	CSD	C	131[B]	-	4,5,8	1.49	1 (25%)	1,5,10	2.06	1 (100%)
1	CSD	A	131	1	3,7,8	1.07	0	1,8,10	2.01	1 (100%)
1	CSD	B	131[A]	-	4,5,8	0.69	0	1,5,10	0.32	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
1	CSD	B	131[B]	-	-	1/1/4/8	-
1	CSD	D	131	1	-	1/1/5/8	-
1	CSD	C	131[A]	-	-	1/1/4/8	-
1	CSD	C	131[B]	-	-	1/1/4/8	-
1	CSD	A	131	1	-	2/2/6/8	-
1	CSD	B	131[A]	-	-	1/1/4/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131[A]	CSD	CB-CA	2.44	1.55	1.53
1	C	131[B]	CSD	CB-CA	2.44	1.55	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131[B]	CSD	CA-CB-SG	-2.06	110.00	114.44
1	A	131	CSD	OD1-SG-CB	-2.01	101.70	105.54

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	131[B]	CSD	N-CA-CB-SG
1	D	131	CSD	N-CA-CB-SG
1	C	131[A]	CSD	N-CA-CB-SG
1	C	131[B]	CSD	N-CA-CB-SG
1	A	131	CSD	N-CA-CB-SG

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	131[B]	CSD	5	0
1	D	131	CSD	1	0
1	C	131[B]	CSD	1	0
1	A	131	CSD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	131[A]	CSD	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 29 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	463/467 (99%)	-0.73	0 100 100	23, 36, 55, 88	0
1	B	465/467 (99%)	-0.73	0 100 100	21, 36, 58, 83	0
1	C	466/467 (99%)	-0.76	1 (0%) 95 97	23, 36, 51, 81	0
1	D	465/467 (99%)	-0.79	0 100 100	24, 36, 50, 82	0
All	All	1859/1868 (99%)	-0.75	1 (0%) 95 97	21, 36, 53, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	398	LEU	2.5

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSD	B	131[B]	6/9	0.94	0.12	27,34,39,50	2
1	CSD	B	131[A]	6/9	0.94	0.12	27,31,34,37	2
1	CSD	C	131[B]	6/9	0.95	0.09	38,40,43,44	1
1	CSD	C	131[A]	6/9	0.95	0.09	38,40,43,44	1
1	CSD	A	131	8/9	0.96	0.11	25,35,39,44	0
1	CSD	D	131	7/9	0.96	0.08	36,41,46,55	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CU	A	606	1/1	0.91	0.13	60,60,60,60	1
2	CU	D	606	1/1	0.94	0.13	31,31,31,31	1
2	CU	C	608	1/1	0.97	0.12	36,36,36,36	1
2	CU	D	607	1/1	0.98	0.17	43,43,43,43	1
2	CU	A	607	1/1	0.98	0.12	41,41,41,41	1
2	CU	A	603	1/1	0.98	0.10	29,29,29,29	1
2	CU	D	603	1/1	0.98	0.12	23,23,23,23	1
2	CU	C	603	1/1	0.99	0.08	30,30,30,30	1
2	CU	B	603	1/1	0.99	0.11	26,26,26,26	1
2	CU	B	606	1/1	0.99	0.14	32,32,32,32	1
2	CU	C	606	1/1	0.99	0.09	25,25,25,25	1
2	CU	A	605	1/1	0.99	0.17	19,19,19,19	1
2	CU	C	607	1/1	0.99	0.17	35,35,35,35	1
2	CU	B	605	1/1	0.99	0.15	16,16,16,16	1
2	CU	D	608	1/1	0.99	0.12	26,26,26,26	1
2	CU	D	604	1/1	1.00	0.11	39,39,39,39	1
2	CU	B	601	1/1	1.00	0.10	36,36,36,36	0
2	CU	D	601	1/1	1.00	0.07	41,41,41,41	0
2	CU	C	601	1/1	1.00	0.08	36,36,36,36	0
2	CU	D	602	1/1	1.00	0.15	35,35,35,35	1
2	CU	A	601	1/1	1.00	0.10	41,41,41,41	0
2	CU	A	602	1/1	1.00	0.15	26,26,26,26	1
2	CU	B	602	1/1	1.00	0.17	22,22,22,22	1
2	CU	C	602	1/1	1.00	0.15	35,35,35,35	1
2	CU	C	605	1/1	1.00	0.21	18,18,18,18	1
2	CU	B	604	1/1	1.00	0.15	35,35,35,35	1
2	CU	A	604	1/1	1.00	0.14	40,40,40,40	1
2	CU	C	604	1/1	1.00	0.13	29,29,29,29	1
2	CU	D	605	1/1	1.00	0.13	31,31,31,31	1

## 6.5 Other polymers

There are no such residues in this entry.