



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2017 – 01:28 PM EST

PDB ID : 5HZT  
Title : Crystal structure of Dronpa-Cu<sup>2+</sup>  
Authors : Hwang, K.Y.; Nam, K.H.  
Deposited on : 2016-02-03  
Resolution : 2.84 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

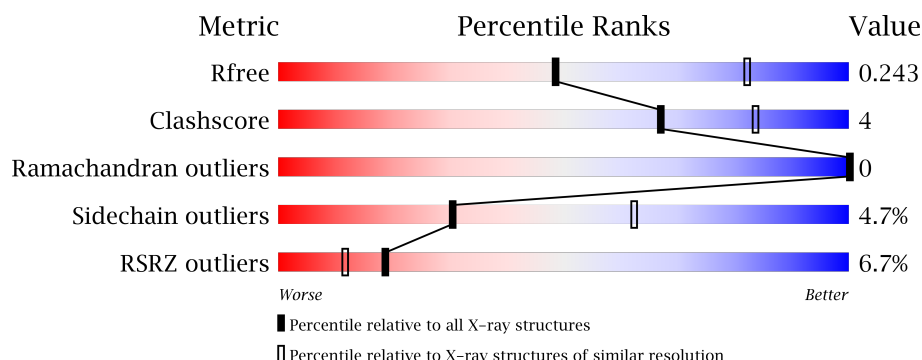
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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))
$R_{free}$	100719	3466 (2.88-2.80)
Clashscore	112137	3975 (2.88-2.80)
Ramachandran outliers	110173	3902 (2.88-2.80)
Sidechain outliers	110143	3905 (2.88-2.80)
RSRZ outliers	101464	3501 (2.88-2.80)

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. 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	215	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	215	<div> <div>16%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>••</div> </div> </div>
1	C	215	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>
1	D	215	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
1	E	215	<div> <div></div> <div> <div></div> <div>87%</div> <div>12%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	215	<div> <div>8%</div> <div>85%</div> <div>14%</div> </div>
1	G	215	<div> <div>10%</div> <div>87%</div> <div>13%</div> </div>
1	H	215	<div> <div>%</div> <div>87%</div> <div>13%</div> </div>
1	I	215	<div> <div>5%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	J	215	<div> <div>10%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	K	215	<div> <div>6%</div> <div>77%</div> <div>10%</div> <div>•</div> <div>12%</div> </div>
1	L	215	<div> <div>3%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20400 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 Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1551	985	265	292	9			
1	B	210	Total	C	N	O	S	0	0	0
			1698	1084	286	319	9			
1	C	214	Total	C	N	O	S	0	0	0
			1727	1103	291	324	9			
1	D	215	Total	C	N	O	S	0	0	0
			1736	1108	292	327	9			
1	E	215	Total	C	N	O	S	0	0	0
			1736	1108	292	327	9			
1	F	214	Total	C	N	O	S	0	0	0
			1730	1105	291	325	9			
1	G	214	Total	C	N	O	S	0	0	0
			1727	1103	291	324	9			
1	H	215	Total	C	N	O	S	0	0	0
			1736	1108	292	327	9			
1	I	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	J	211	Total	C	N	O	S	0	0	0
			1704	1087	287	321	9			
1	K	189	Total	C	N	O	S	0	0	0
			1519	967	258	285	9			
1	L	214	Total	C	N	O	S	0	0	0
			1730	1105	291	325	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	chromophore	UNP Q5TLG6
A	?	-	TYR	chromophore	UNP Q5TLG6
A	62	GYS	GLY	chromophore	UNP Q5TLG6
B	?	-	CYS	chromophore	UNP Q5TLG6
B	?	-	TYR	chromophore	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	62	GYS	GLY	chromophore	UNP Q5TLG6
C	?	-	CYS	chromophore	UNP Q5TLG6
C	?	-	TYR	chromophore	UNP Q5TLG6
C	62	GYS	GLY	chromophore	UNP Q5TLG6
D	?	-	CYS	chromophore	UNP Q5TLG6
D	?	-	TYR	chromophore	UNP Q5TLG6
D	62	GYS	GLY	chromophore	UNP Q5TLG6
E	?	-	CYS	chromophore	UNP Q5TLG6
E	?	-	TYR	chromophore	UNP Q5TLG6
E	62	GYS	GLY	chromophore	UNP Q5TLG6
F	?	-	CYS	chromophore	UNP Q5TLG6
F	?	-	TYR	chromophore	UNP Q5TLG6
F	62	GYS	GLY	chromophore	UNP Q5TLG6
G	?	-	CYS	chromophore	UNP Q5TLG6
G	?	-	TYR	chromophore	UNP Q5TLG6
G	62	GYS	GLY	chromophore	UNP Q5TLG6
H	?	-	CYS	chromophore	UNP Q5TLG6
H	?	-	TYR	chromophore	UNP Q5TLG6
H	62	GYS	GLY	chromophore	UNP Q5TLG6
I	?	-	CYS	chromophore	UNP Q5TLG6
I	?	-	TYR	chromophore	UNP Q5TLG6
I	62	GYS	GLY	chromophore	UNP Q5TLG6
J	?	-	CYS	chromophore	UNP Q5TLG6
J	?	-	TYR	chromophore	UNP Q5TLG6
J	62	GYS	GLY	chromophore	UNP Q5TLG6
K	?	-	CYS	chromophore	UNP Q5TLG6
K	?	-	TYR	chromophore	UNP Q5TLG6
K	62	GYS	GLY	chromophore	UNP Q5TLG6
L	?	-	CYS	chromophore	UNP Q5TLG6
L	?	-	TYR	chromophore	UNP Q5TLG6
L	62	GYS	GLY	chromophore	UNP Q5TLG6

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Cu 2 2	0	0
2	J	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	K	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Cu 2	0	0
2	H	2	Total 2	Cu 2	0	0
2	B	2	Total 2	Cu 2	0	0
2	I	2	Total 2	Cu 2	0	0
2	C	2	Total 2	Cu 2	0	0
2	A	2	Total 2	Cu 2	0	0
2	L	2	Total 2	Cu 2	0	0
2	F	2	Total 2	Cu 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	3	Total 3	O 3	0	0
3	C	3	Total 3	O 3	0	0
3	D	3	Total 3	O 3	0	0
3	E	6	Total 6	O 6	0	0
3	F	2	Total 2	O 2	0	0
3	G	3	Total 3	O 3	0	0
3	H	7	Total 7	O 7	0	0
3	I	5	Total 5	O 5	0	0
3	J	3	Total 3	O 3	0	0
3	K	10	Total 10	O 10	0	0

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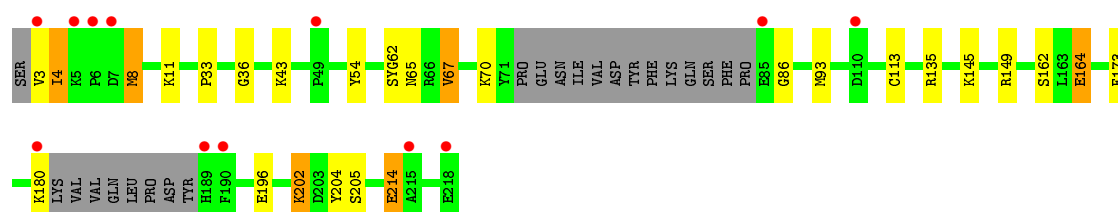
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	4	Total	O	0	0
			4	4		

### 3 Residue-property plots [i](#)


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.

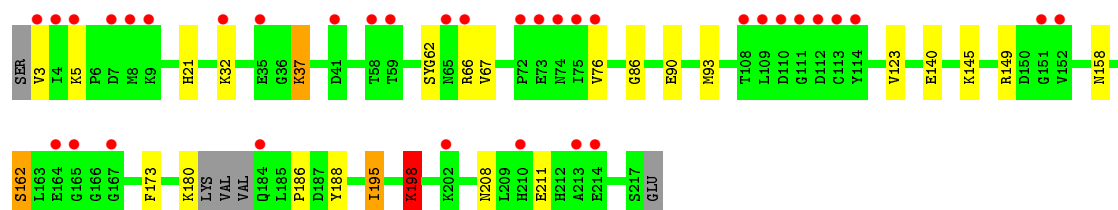
#### • Molecule 1: Fluorescent protein Dronpa

Chain A: 




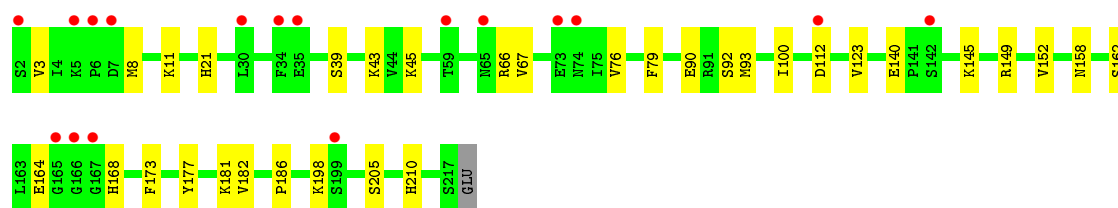
#### • Molecule 1: Fluorescent protein Dronpa

Chain B: 




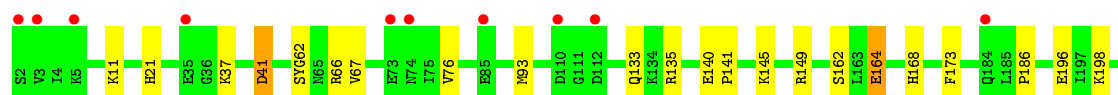
#### • Molecule 1: Fluorescent protein Dronpa

Chain C: 



#### • Molecule 1: Fluorescent protein Dronpa

Chain D: 







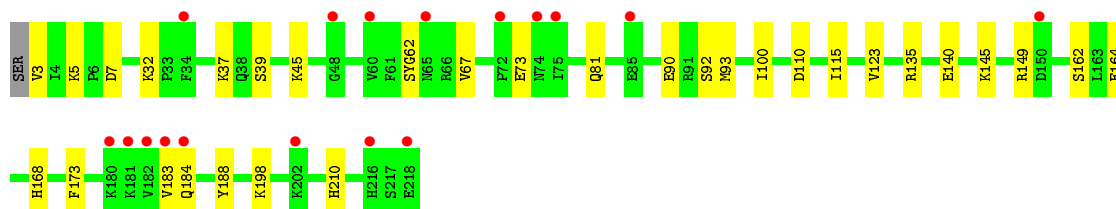
- Molecule 1: Fluorescent protein Dronpa

Chain E: 87% 12%



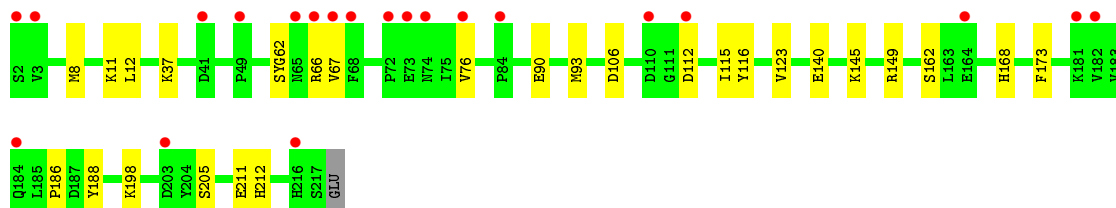
- Molecule 1: Fluorescent protein Dronpa

Chain F: 8% 85% 14%



- Molecule 1: Fluorescent protein Dronpa

Chain G: 10% 87% 13%



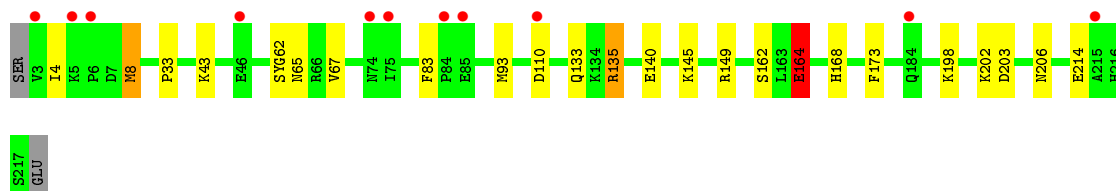
- Molecule 1: Fluorescent protein Dronpa

Chain H: 0% 87% 13%

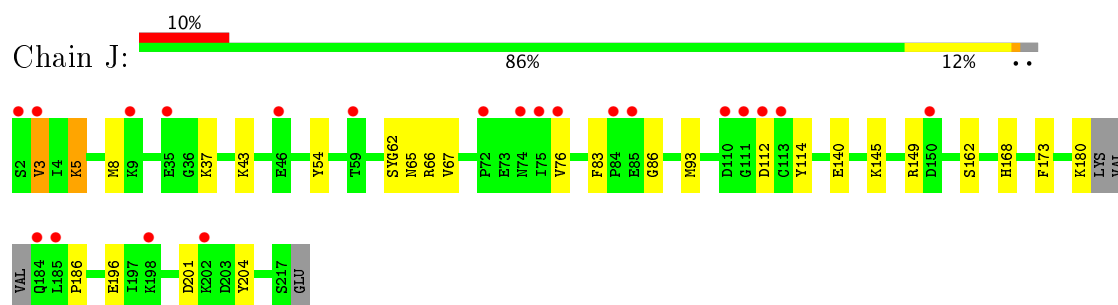


- Molecule 1: Fluorescent protein Dronpa

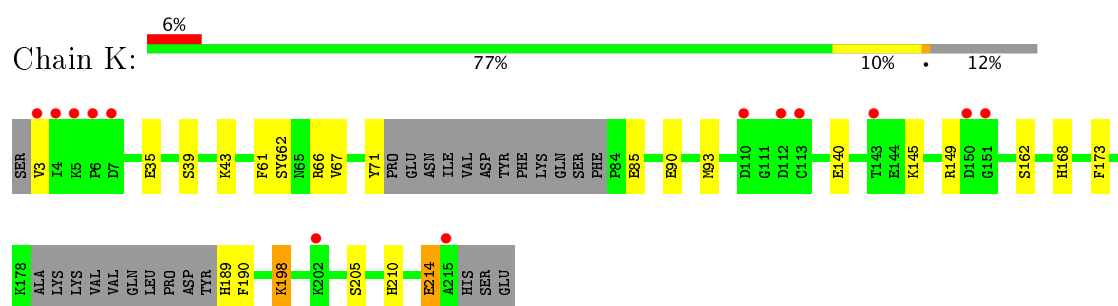
Chain I: 5% 88% 10%



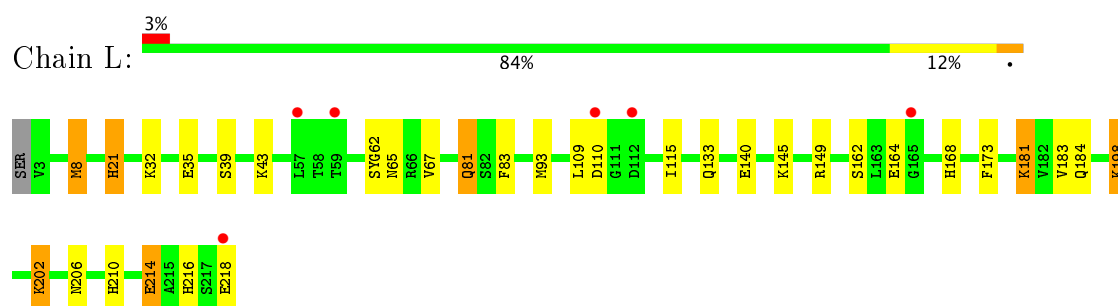
- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.27Å 105.96Å 108.03Å 115.89° 107.68° 94.12°	Depositor
Resolution (Å)	29.94 – 2.84 29.92 – 2.84	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.94-2.84) 77.9 (29.92-2.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.214 , 0.245 0.216 , 0.243	Depositor DCC
$R_{free}$ test set	2936 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	20400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GYS, 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	0.64	1/1566 (0.1%)	0.79	3/2106 (0.1%)
1	B	0.54	1/1721 (0.1%)	0.76	2/2321 (0.1%)
1	C	0.51	0/1751	0.74	2/2363 (0.1%)
1	D	0.62	1/1760 (0.1%)	0.79	6/2375 (0.3%)
1	E	0.59	0/1760	0.73	1/2375 (0.0%)
1	F	0.59	0/1754	0.78	4/2367 (0.2%)
1	G	0.54	0/1751	0.75	3/2363 (0.1%)
1	H	0.59	0/1760	0.74	1/2375 (0.0%)
1	I	0.58	1/1745 (0.1%)	0.80	6/2355 (0.3%)
1	J	0.53	0/1727	0.79	4/2329 (0.2%)
1	K	0.67	0/1534	0.82	2/2064 (0.1%)
1	L	0.66	1/1754 (0.1%)	0.84	8/2367 (0.3%)
All	All	0.59	5/20583 (0.0%)	0.78	42/27760 (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	G	0	1
1	K	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	41	ASP	CB-CG	9.06	1.70	1.51
1	B	162	SER	CB-OG	-5.90	1.34	1.42
1	L	214	GLU	CG-CD	5.34	1.59	1.51
1	A	214	GLU	CG-CD	5.17	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	214	GLU	CD-OE2	-5.06	1.20	1.25

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	198	LYS	CD-CE-NZ	9.22	132.90	111.70
1	C	198	LYS	CD-CE-NZ	9.18	132.81	111.70
1	I	198	LYS	CD-CE-NZ	9.17	132.78	111.70
1	E	198	LYS	CD-CE-NZ	9.15	132.76	111.70
1	F	198	LYS	CD-CE-NZ	9.15	132.74	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	211	GLU	Peptide
1	K	190	PHE	Peptide
1	K	61	PHE	Mainchain

## 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	1551	0	1482	16	0
1	B	1698	0	1618	32	0
1	C	1727	0	1655	15	1
1	D	1736	0	1662	8	1
1	E	1736	0	1662	20	0
1	F	1730	0	1657	22	0
1	G	1727	0	1655	12	0
1	H	1736	0	1662	13	2
1	I	1721	0	1651	18	1
1	J	1704	0	1624	16	0
1	K	1519	0	1454	8	1
1	L	1730	0	1657	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	12	0	0	1	0
3	B	3	0	0	4	0
3	C	3	0	0	2	0
3	D	3	0	0	3	0
3	E	6	0	0	4	0
3	F	2	0	0	3	0
3	G	3	0	0	1	0
3	H	7	0	0	6	0
3	I	5	0	0	4	0
3	J	3	0	0	4	0
3	K	10	0	0	3	0
3	L	4	0	0	6	0
All	All	20400	0	19439	179	3

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.

The worst 5 of 179 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:K:140:GLU:OE1	3:K:401:HOH:O	1.68	1.11
1:E:140:GLU:OE1	3:E:401:HOH:O	1.73	1.07
1:L:140:GLU:OE1	3:L:401:HOH:O	1.72	1.07
1:D:140:GLU:OE1	3:D:401:HOH:O	1.75	1.05
1:B:198:LYS:CE	1:B:208:ASN:OD1	2.05	1.04

All (3) 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:C:45:LYS:NZ	1:I:110:ASP:OD1[1_656]	1.64	0.56
1:D:135:ARG:NE	1:H:48:GLY:O[1_565]	1.95	0.25
1:H:32:LYS:NZ	1:K:35:GLU:OE2[1_455]	2.13	0.07

## 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	186/215 (86%)	181 (97%)	5 (3%)	0	100	100
1	B	205/215 (95%)	201 (98%)	4 (2%)	0	100	100
1	C	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
1	D	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
1	E	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
1	F	211/215 (98%)	207 (98%)	4 (2%)	0	100	100
1	G	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
1	H	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
1	I	210/215 (98%)	206 (98%)	4 (2%)	0	100	100
1	J	206/215 (96%)	203 (98%)	3 (2%)	0	100	100
1	K	182/215 (85%)	178 (98%)	4 (2%)	0	100	100
1	L	211/215 (98%)	207 (98%)	4 (2%)	0	100	100
All	All	2469/2580 (96%)	2428 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	163/185 (88%)	154 (94%)	9 (6%)	25	55
1	B	180/185 (97%)	171 (95%)	9 (5%)	28	59
1	C	184/185 (100%)	173 (94%)	11 (6%)	22	51
1	D	185/185 (100%)	175 (95%)	10 (5%)	26	56
1	E	185/185 (100%)	177 (96%)	8 (4%)	33	66
1	F	184/185 (100%)	179 (97%)	5 (3%)	50	81
1	G	184/185 (100%)	177 (96%)	7 (4%)	38	70
1	H	185/185 (100%)	177 (96%)	8 (4%)	33	66
1	I	183/185 (99%)	178 (97%)	5 (3%)	50	81
1	J	181/185 (98%)	175 (97%)	6 (3%)	43	75
1	K	160/185 (86%)	149 (93%)	11 (7%)	18	44
1	L	184/185 (100%)	172 (94%)	12 (6%)	20	47
All	All	2158/2220 (97%)	2057 (95%)	101 (5%)	30	62

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	162	SER
1	G	162	SER
1	L	149	ARG
1	F	3	VAL
1	F	162	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	212	HIS
1	I	158	ASN
1	L	81	GLN
1	G	158	ASN
1	K	158	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

12 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	GYS	A	62	1	22,22,23	3.98	5 (22%)	27,30,32	3.75	11 (40%)
1	GYS	B	62	1	22,22,23	3.48	5 (22%)	27,30,32	3.97	9 (33%)
1	GYS	C	62	1	22,22,23	3.47	6 (27%)	27,30,32	4.03	6 (22%)
1	GYS	D	62	1	22,22,23	4.02	6 (27%)	27,30,32	4.24	10 (37%)
1	GYS	E	62	1	22,22,23	3.84	5 (22%)	27,30,32	5.36	8 (29%)
1	GYS	F	62	1	22,22,23	3.31	6 (27%)	27,30,32	4.62	7 (25%)
1	GYS	G	62	1	22,22,23	3.37	5 (22%)	27,30,32	4.35	7 (25%)
1	GYS	H	62	1	22,22,23	3.95	6 (27%)	27,30,32	4.65	10 (37%)
1	GYS	I	62	1	22,22,23	3.65	5 (22%)	27,30,32	3.86	9 (33%)
1	GYS	J	62	1	22,22,23	3.50	4 (18%)	27,30,32	4.52	7 (25%)
1	GYS	K	62	1	22,22,23	4.05	4 (18%)	27,30,32	4.44	7 (25%)
1	GYS	L	62	1	22,22,23	3.39	6 (27%)	27,30,32	4.10	8 (29%)

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	GYS	A	62	1	-	0/9/29/30	0/2/2/2
1	GYS	B	62	1	-	0/9/29/30	0/2/2/2
1	GYS	C	62	1	-	0/9/29/30	0/2/2/2
1	GYS	D	62	1	-	0/9/29/30	0/2/2/2
1	GYS	E	62	1	-	0/9/29/30	0/2/2/2
1	GYS	F	62	1	-	0/9/29/30	0/2/2/2
1	GYS	G	62	1	-	0/9/29/30	0/2/2/2
1	GYS	H	62	1	-	0/9/29/30	0/2/2/2
1	GYS	I	62	1	-	0/9/29/30	0/2/2/2
1	GYS	J	62	1	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYS	K	62	1	-	0/9/29/30	0/2/2/2
1	GYS	L	62	1	-	0/9/29/30	0/2/2/2

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	GYS	CA2-C2	-3.93	1.44	1.48
1	K	62	GYS	C2-N3	-3.76	1.30	1.39
1	I	62	GYS	CA1-C1	-3.66	1.46	1.51
1	A	62	GYS	C2-N3	-3.65	1.30	1.39
1	E	62	GYS	C2-N3	-3.64	1.30	1.39

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	GYS	O2-C2-CA2	-16.50	122.07	130.97
1	E	62	GYS	O2-C2-CA2	-14.84	122.97	130.97
1	L	62	GYS	O2-C2-CA2	-13.97	123.44	130.97
1	J	62	GYS	O2-C2-CA2	-13.74	123.56	130.97
1	G	62	GYS	O2-C2-CA2	-12.35	124.31	130.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	62	GYS	1	0
1	B	62	GYS	2	0
1	D	62	GYS	1	0
1	E	62	GYS	1	0
1	F	62	GYS	1	0
1	G	62	GYS	1	0
1	H	62	GYS	2	0
1	I	62	GYS	1	0
1	J	62	GYS	1	0
1	K	62	GYS	1	0
1	L	62	GYS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 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	192/215 (89%)	0.14	12 (6%) 21 13	22, 47, 94, 115	0
1	B	209/215 (97%)	0.87	35 (16%) 2 1	28, 72, 113, 135	0
1	C	213/215 (99%)	0.40	17 (7%) 13 7	35, 67, 95, 122	0
1	D	214/215 (99%)	0.07	11 (5%) 29 20	23, 48, 94, 132	0
1	E	214/215 (99%)	-0.19	1 (0%) 90 88	21, 39, 61, 85	0
1	F	213/215 (99%)	0.35	17 (7%) 13 7	35, 59, 94, 106	0
1	G	213/215 (99%)	0.42	21 (9%) 8 4	31, 64, 107, 146	0
1	H	214/215 (99%)	-0.27	3 (1%) 75 70	23, 38, 62, 77	0
1	I	212/215 (98%)	0.22	11 (5%) 28 20	27, 55, 90, 117	0
1	J	210/215 (97%)	0.46	21 (10%) 8 4	28, 63, 107, 120	0
1	K	188/215 (87%)	0.26	13 (6%) 18 11	26, 51, 89, 102	0
1	L	213/215 (99%)	-0.14	6 (2%) 53 44	19, 40, 63, 90	0
All	All	2505/2580 (97%)	0.21	168 (6%) 19 12	19, 53, 97, 146	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	SER	10.3
1	B	35	GLU	7.0
1	D	2	SER	6.1
1	G	74	ASN	6.0
1	K	3	VAL	5.7

### 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	GYS	J	62	21/22	0.95	0.29	-	49,53,61,74	0
1	GYS	F	62	21/22	0.91	0.31	-	41,43,47,51	0
1	GYS	L	62	21/22	0.93	0.29	-	30,33,39,41	0
1	GYS	B	62	21/22	0.88	0.35	-	53,70,81,90	0
1	GYS	D	62	21/22	0.93	0.22	-	29,31,39,45	0
1	GYS	K	62	21/22	0.93	0.24	-	38,45,50,66	0
1	GYS	I	62	21/22	0.91	0.26	-	45,47,55,58	0
1	GYS	G	62	21/22	0.94	0.29	-	46,49,57,59	0
1	GYS	E	62	21/22	0.95	0.29	-	26,29,33,39	0
1	GYS	C	62	21/22	0.90	0.33	-	55,60,65,68	0
1	GYS	A	62	21/22	0.93	0.29	-	26,34,43,44	0
1	GYS	H	62	21/22	0.96	0.22	-	22,28,36,38	0

### 6.3 Carbohydrates

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	H	302	1/1	0.98	0.09	-	68,68,68,68	0
2	CU	D	301	1/1	0.97	0.04	-	83,83,83,83	0
2	CU	K	302	1/1	0.95	0.05	-	84,84,84,84	0
2	CU	E	301	1/1	0.95	0.05	-	81,81,81,81	0
2	CU	A	301	1/1	0.95	0.05	-	81,81,81,81	0
2	CU	D	302	1/1	0.96	0.17	-	79,79,79,79	0
2	CU	I	302	1/1	0.97	0.08	-	78,78,78,78	0
2	CU	J	301	1/1	0.91	0.06	-	113,113,113,113	0
2	CU	G	301	1/1	0.88	0.08	-	113,113,113,113	0
2	CU	C	302	1/1	0.97	0.03	-	90,90,90,90	0
2	CU	B	301	1/1	0.81	0.09	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	F	302	1/1	0.93	0.07	-	94,94,94,94	0
2	CU	G	302	1/1	0.98	0.02	-	78,78,78,78	0
2	CU	I	301	1/1	0.68	0.06	-	102,102,102,102	0
2	CU	L	302	1/1	0.94	0.10	-	73,73,73,73	0
2	CU	H	301	1/1	0.92	0.05	-	80,80,80,80	0
2	CU	F	301	1/1	0.87	0.06	-	115,115,115,115	0
2	CU	C	301	1/1	0.79	0.16	-	124,124,124,124	0
2	CU	J	302	1/1	0.85	0.08	-	93,93,93,93	0
2	CU	B	302	1/1	0.86	0.06	-	108,108,108,108	0
2	CU	E	302	1/1	0.98	0.03	-	76,76,76,76	0
2	CU	K	301	1/1	0.85	0.05	-	92,92,92,92	0
2	CU	L	301	1/1	0.94	0.02	-	82,82,82,82	0
2	CU	A	302	1/1	0.96	0.06	-	82,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.