



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2017 – 01:28 PM EST

PDB ID : 5HZZ  
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 Full wwPDB X-ray Structure Validation 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

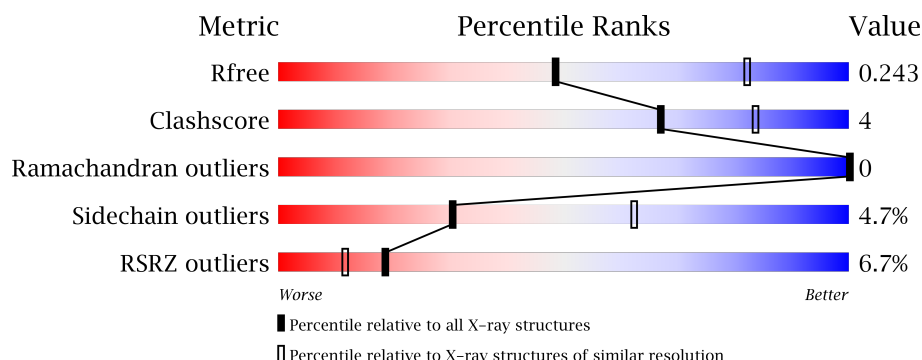
# 1 Overall quality at a glance

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></div><div>8%</div><div>85%</div><div>14%</div></div>
1	G	215	<div><div></div><div>10%</div><div>87%</div><div>13%</div></div>
1	H	215	<div><div></div><div>%</div><div>87%</div><div>13%</div></div>
1	I	215	<div><div></div><div>5%</div><div>88%</div><div>10%</div><div>..</div></div>
1	J	215	<div><div></div><div>10%</div><div>86%</div><div>12%</div><div>..</div></div>
1	K	215	<div><div></div><div>6%</div><div>77%</div><div>10%</div><div>•</div><div>12%</div></div>
1	L	215	<div><div></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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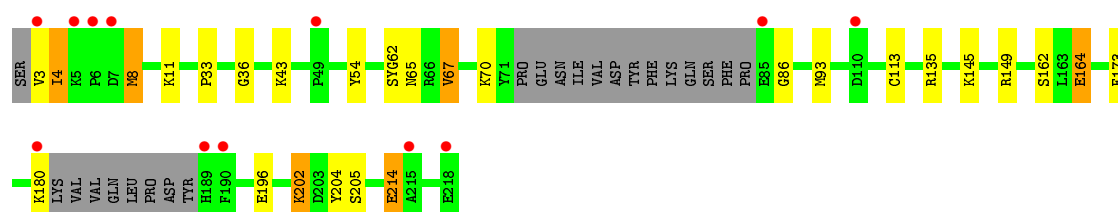
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	4	Total	O	0	0
			4	4		

### 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.

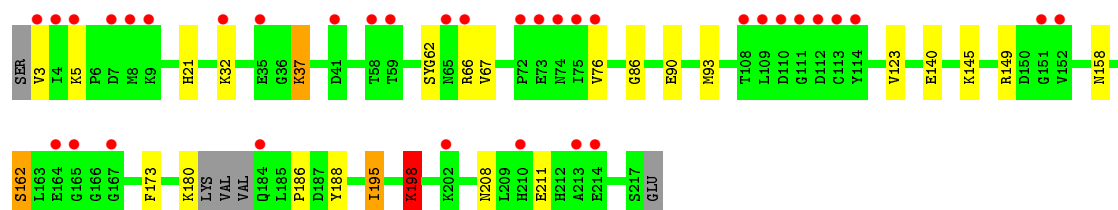
#### • Molecule 1: Fluorescent protein Dronpa

Chain A: 




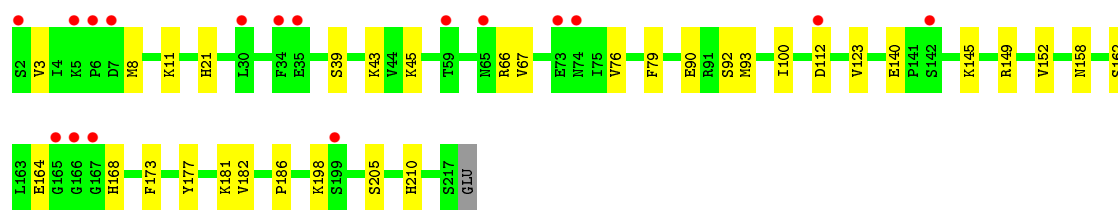
#### • Molecule 1: Fluorescent protein Dronpa

Chain B: 




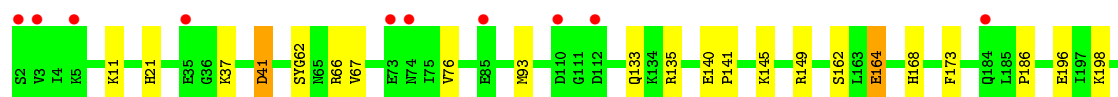
#### • Molecule 1: Fluorescent protein Dronpa

Chain C: 



#### • Molecule 1: Fluorescent protein Dronpa

Chain D: 







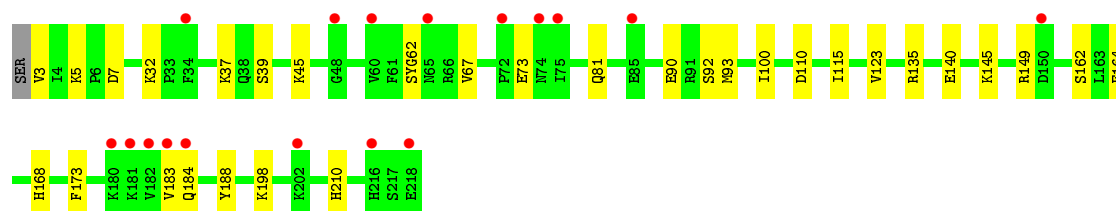
- Molecule 1: Fluorescent protein Dronpa

Chain E: 87% 12%



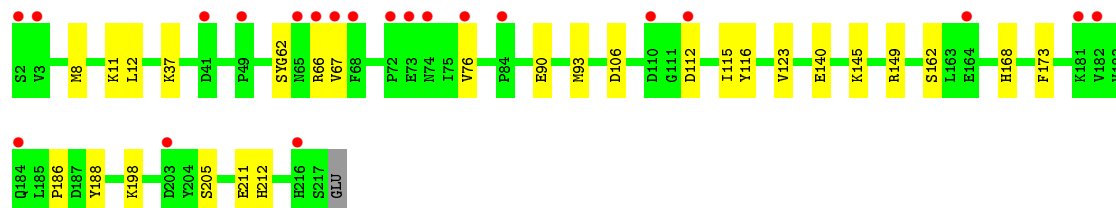
- Molecule 1: Fluorescent protein Dronpa

Chain F: 8% 85% 14%



- Molecule 1: Fluorescent protein Dronpa

Chain G: 10% 87% 13%



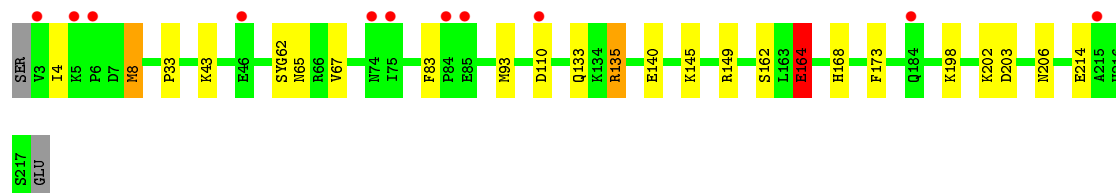
- Molecule 1: Fluorescent protein Dronpa

Chain H: 0% 87% 13%

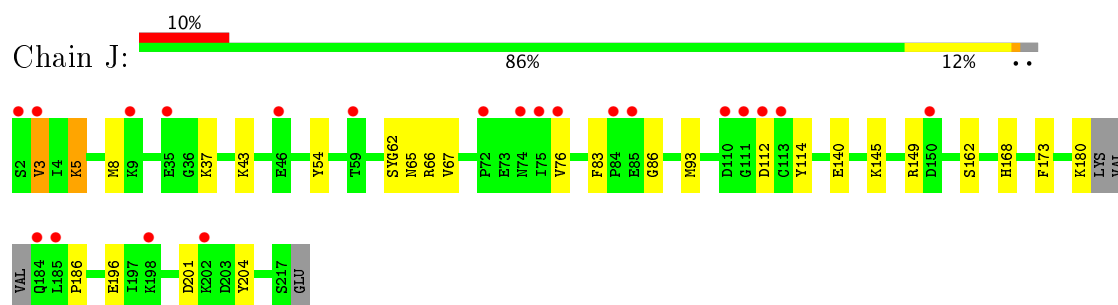


- Molecule 1: Fluorescent protein Dronpa

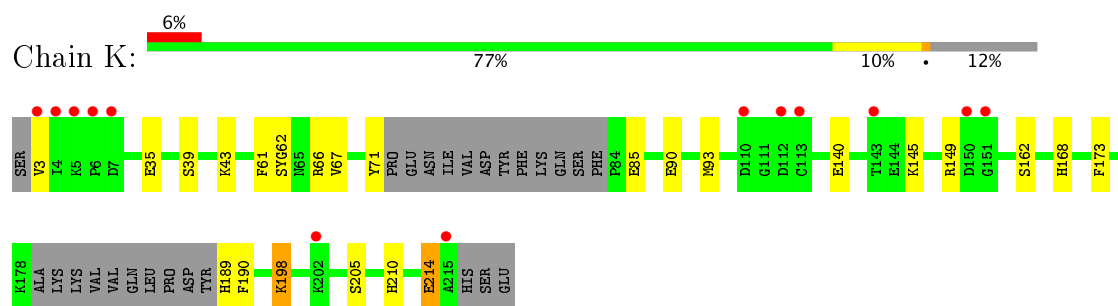
Chain I: 5% 88% 10%



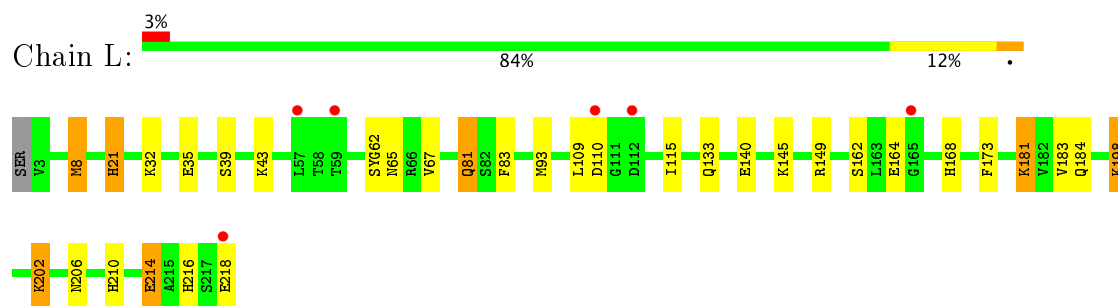
- Molecule 1: Fluorescent protein Dronpa



- 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

All (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
1	L	8	MET	CG-SD-CE	8.57	113.92	100.20
1	G	106	ASP	CB-CG-OD2	8.47	125.93	118.30
1	J	43	LYS	CD-CE-NZ	8.24	130.66	111.70
1	J	37	LYS	CD-CE-NZ	7.80	129.65	111.70
1	I	135	ARG	CA-CB-CG	7.42	129.72	113.40
1	J	201	ASP	N-CA-CB	-7.30	97.46	110.60
1	F	5	LYS	CA-CB-CG	7.25	129.35	113.40
1	D	41	ASP	CB-CG-OD1	7.02	124.62	118.30
1	D	37	LYS	CD-CE-NZ	6.90	127.57	111.70
1	F	37	LYS	CD-CE-NZ	6.87	127.50	111.70
1	G	37	LYS	CD-CE-NZ	6.82	127.39	111.70
1	J	201	ASP	CB-CA-C	-6.57	97.25	110.40
1	B	195	ILE	CG1-CB-CG2	6.42	125.53	111.40
1	H	184	GLN	N-CA-CB	6.22	121.79	110.60
1	D	41	ASP	OD1-CG-OD2	-5.71	112.45	123.30
1	L	32	LYS	CD-CE-NZ	5.71	124.83	111.70
1	K	198	LYS	CA-CB-CG	5.64	125.81	113.40
1	D	133	GLN	CA-CB-CG	-5.44	101.44	113.40
1	A	8	MET	CG-SD-CE	-5.42	91.53	100.20
1	L	198	LYS	CA-CB-CG	5.42	125.32	113.40
1	I	8	MET	CG-SD-CE	-5.40	91.55	100.20
1	K	214	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	L	133	GLN	CA-CB-CG	-5.30	101.75	113.40
1	I	214	GLU	CB-CA-C	-5.27	99.86	110.40
1	D	164	GLU	N-CA-C	-5.24	96.86	111.00
1	L	81	GLN	CB-CA-C	5.20	120.79	110.40
1	C	164	GLU	N-CA-C	-5.17	97.03	111.00
1	L	214	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	B	198	LYS	CD-CE-NZ	5.14	123.53	111.70
1	D	41	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	214	GLU	OE1-CD-OE2	-5.13	117.15	123.30
1	L	202	LYS	CD-CE-NZ	5.11	123.46	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	106	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	I	164	GLU	N-CA-C	-5.06	97.34	111.00
1	I	133	GLN	CA-CB-CG	-5.03	102.33	113.40
1	A	202	LYS	CD-CE-NZ	5.02	123.25	111.70
1	F	73	GLU	OE1-CD-OE2	-5.01	117.29	123.30

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

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:B:198:LYS:HE2	1:B:208:ASN:OD1	1.59	1.03
1:H:140:GLU:OE1	3:H:401:HOH:O	1.75	1.03
1:B:195:ILE:HD12	1:B:211:GLU:CB	1.91	1.01
1:A:135:ARG:NE	1:E:48:GLY:O	1.95	0.99
1:B:195:ILE:HD12	1:B:211:GLU:HB2	1.44	0.99
1:B:195:ILE:CD1	1:B:211:GLU:HB2	1.93	0.97
1:I:203:ASP:OD2	3:I:401:HOH:O	1.83	0.96
1:G:140:GLU:OE1	3:G:401:HOH:O	1.83	0.95
1:I:140:GLU:OE1	3:I:402:HOH:O	1.95	0.85
1:C:140:GLU:OE1	3:C:401:HOH:O	1.95	0.84
1:J:140:GLU:OE1	3:J:401:HOH:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LYS:NZ	1:L:110:ASP:OD1	2.12	0.83
1:B:198:LYS:CG	1:B:208:ASN:OD1	2.27	0.82
1:F:168:HIS:NE2	3:F:401:HOH:O	1.91	0.81
1:I:168:HIS:NE2	3:I:402:HOH:O	1.93	0.80
1:E:216:HIS:NE2	3:E:402:HOH:O	2.15	0.80
1:F:140:GLU:OE1	3:F:401:HOH:O	2.01	0.79
1:E:168:HIS:NE2	3:E:401:HOH:O	1.84	0.79
1:H:168:HIS:NE2	3:H:401:HOH:O	1.98	0.77
1:K:168:HIS:NE2	3:K:401:HOH:O	1.76	0.77
1:F:7:ASP:OD1	1:F:32:LYS:HE3	1.85	0.76
1:B:195:ILE:CD1	1:B:211:GLU:HG3	2.17	0.74
1:B:195:ILE:HD12	1:B:211:GLU:CG	2.19	0.72
1:A:4:ILE:HG23	1:A:8:MET:HE1	1.73	0.71
1:B:198:LYS:HG3	1:B:208:ASN:OD1	1.90	0.71
1:L:168:HIS:NE2	3:L:401:HOH:O	1.98	0.70
1:C:168:HIS:NE2	3:C:401:HOH:O	2.03	0.70
1:H:75:ILE:HD11	1:H:217:SER:HB3	1.74	0.70
1:A:11:LYS:HE3	1:A:113:CYS:SG	2.32	0.70
1:B:198:LYS:HE3	1:B:208:ASN:OD1	1.89	0.69
1:B:195:ILE:HD12	1:B:211:GLU:HG3	1.74	0.68
1:E:39:SER:HB3	1:E:210:HIS:HD1	1.58	0.68
1:J:196:GLU:OE1	3:J:402:HOH:O	2.12	0.68
1:J:168:HIS:NE2	3:J:401:HOH:O	2.14	0.67
1:H:62:GYS:OG1	1:H:211:GLU:OE1	2.11	0.66
1:K:140:GLU:OE2	3:K:402:HOH:O	2.13	0.66
1:E:84:PRO:HB3	1:F:135:ARG:HD3	1.78	0.65
1:B:195:ILE:CD1	1:B:211:GLU:CG	2.75	0.65
1:B:195:ILE:CD1	1:B:211:GLU:CB	2.62	0.64
1:I:4:ILE:HG23	1:I:8:MET:HE1	1.79	0.64
1:A:65:ASN:OD1	1:A:67:VAL:HG22	1.98	0.64
1:L:216:HIS:NE2	3:L:402:HOH:O	2.24	0.64
1:E:2:SER:O	1:E:5:LYS:NZ	2.28	0.63
1:F:39:SER:HB3	1:F:210:HIS:HD1	1.64	0.63
1:B:21:HIS:CG	3:B:403:HOH:O	2.52	0.62
1:L:39:SER:HB3	1:L:210:HIS:HD1	1.65	0.62
1:L:21:HIS:CD2	3:L:403:HOH:O	2.54	0.61
1:I:43:LYS:HD2	1:I:206:ASN:HD21	1.67	0.60
1:C:39:SER:HB3	1:C:210:HIS:HD1	1.67	0.59
1:I:135:ARG:NH2	1:I:164:GLU:OE2	2.36	0.58
1:I:4:ILE:HG23	1:I:8:MET:CE	2.34	0.58
1:H:210:HIS:NE2	3:H:402:HOH:O	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:GLN:NE2	1:L:184:GLN:H	2.01	0.58
1:B:32:LYS:HD2	1:B:37:LYS:HD2	1.86	0.58
1:J:3:VAL:O	1:J:5:LYS:HD2	2.03	0.58
1:A:4:ILE:HG23	1:A:8:MET:CE	2.35	0.57
1:H:37:LYS:HD3	3:H:402:HOH:O	2.04	0.57
1:I:168:HIS:CE1	3:I:402:HOH:O	2.47	0.56
1:B:195:ILE:HD11	1:B:211:GLU:HB2	1.86	0.55
1:I:8:MET:HE2	1:I:33:PRO:HG2	1.88	0.55
1:B:195:ILE:HD13	1:B:211:GLU:HG3	1.87	0.55
1:A:36:GLY:HA3	1:A:70:LYS:HG3	1.88	0.55
1:I:43:LYS:HD2	1:I:206:ASN:ND2	2.21	0.55
1:F:168:HIS:CE1	3:F:401:HOH:O	2.49	0.55
1:J:83:PHE:CE2	1:J:114:TYR:HE1	2.25	0.54
1:D:168:HIS:NE2	3:D:401:HOH:O	2.04	0.54
1:K:62:GYS:HD1	1:K:62:GYS:N2	2.23	0.54
1:B:140:GLU:OE1	3:B:402:HOH:O	2.18	0.54
1:I:65:ASN:OD1	1:I:67:VAL:HG22	2.08	0.54
1:F:81:GLN:NE2	1:F:183:VAL:HG13	2.23	0.54
1:I:135:ARG:CZ	1:I:164:GLU:OE2	2.57	0.52
1:L:65:ASN:OD1	1:L:67:VAL:HG22	2.10	0.52
1:B:198:LYS:CD	1:B:208:ASN:OD1	2.57	0.52
1:D:141:PRO:HG2	1:E:218:GLU:C	2.29	0.52
1:J:65:ASN:OD1	1:J:67:VAL:HG22	2.09	0.52
1:A:54:TYR:CD2	1:A:204:TYR:HB3	2.45	0.51
1:C:79:PHE:HE1	1:C:177:TYR:CD2	2.29	0.51
1:L:81:GLN:HE21	1:L:183:VAL:HB	1.76	0.51
1:I:67:VAL:HG11	1:I:83:PHE:CE2	2.46	0.51
1:E:21:HIS:HD2	1:E:51:PRO:HG3	1.76	0.50
1:E:216:HIS:CE1	3:E:402:HOH:O	2.60	0.50
1:L:67:VAL:HG11	1:L:83:PHE:CE2	2.45	0.50
1:G:8:MET:HE3	1:G:112:ASP:HA	1.93	0.50
1:A:43:LYS:HA	1:A:205:SER:O	2.12	0.50
1:L:181:LYS:HD2	1:L:183:VAL:HG13	1.94	0.50
1:C:92:SER:OG	1:F:100:ILE:HG13	2.12	0.49
1:B:123:VAL:HB	1:G:90:GLU:HB3	1.94	0.49
1:D:62:GYS:HD1	1:D:62:GYS:N2	2.28	0.49
1:J:62:GYS:N2	1:J:62:GYS:HD1	2.27	0.49
1:L:62:GYS:N2	1:L:62:GYS:HD1	2.29	0.48
1:L:65:ASN:CG	1:L:67:VAL:HG22	2.33	0.48
1:F:62:GYS:N2	1:F:62:GYS:HD1	2.29	0.47
1:F:81:GLN:NE2	1:F:183:VAL:CG1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:PRO:CB	1:F:135:ARG:HD3	2.42	0.47
1:I:8:MET:CE	1:I:33:PRO:HG2	2.45	0.47
1:J:3:VAL:O	1:J:3:VAL:HG13	2.15	0.47
1:K:39:SER:HB3	1:K:210:HIS:HD1	1.79	0.47
1:B:62:GYS:OG1	1:B:195:ILE:HD11	2.15	0.47
1:C:8:MET:HE3	1:C:112:ASP:HA	1.97	0.47
1:I:62:GYS:HD1	1:I:62:GYS:N2	2.29	0.47
1:E:62:GYS:HD1	1:E:62:GYS:N2	2.30	0.46
1:I:65:ASN:CG	1:I:67:VAL:HG22	2.35	0.46
1:E:217:SER:O	1:E:218:GLU:HB2	2.16	0.46
1:A:8:MET:CE	1:A:33:PRO:HG2	2.46	0.46
1:F:188:TYR:HB2	1:G:168:HIS:CE1	2.51	0.46
1:J:65:ASN:CG	1:J:67:VAL:HG22	2.35	0.46
1:B:21:HIS:ND1	3:B:403:HOH:O	2.36	0.46
1:E:37:LYS:HE3	1:E:212:HIS:CE1	2.51	0.46
1:B:86:GLY:C	1:B:180:LYS:HD2	2.36	0.46
1:L:93:MET:HG2	1:L:173:PHE:CE1	2.52	0.45
1:A:8:MET:HE2	1:A:33:PRO:HG2	1.97	0.45
1:B:62:GYS:OG1	1:B:195:ILE:CD1	2.65	0.45
1:C:100:ILE:HG13	1:F:92:SER:OG	2.16	0.45
1:C:90:GLU:HB3	1:F:123:VAL:HB	1.97	0.45
1:B:195:ILE:HD12	1:B:211:GLU:CA	2.46	0.45
1:L:43:LYS:HD2	1:L:206:ASN:OD1	2.16	0.45
1:F:168:HIS:CE1	1:G:188:TYR:HB2	2.52	0.45
1:E:93:MET:HG2	1:E:173:PHE:CE1	2.52	0.44
1:H:216:HIS:NE2	3:H:403:HOH:O	2.35	0.44
1:J:83:PHE:CE2	1:J:114:TYR:CE1	3.05	0.44
1:L:168:HIS:CE1	3:L:401:HOH:O	2.59	0.44
1:A:86:GLY:C	1:A:180:LYS:HD2	2.38	0.44
1:G:93:MET:HG2	1:G:173:PHE:CE1	2.53	0.44
1:B:198:LYS:HG2	1:B:208:ASN:OD1	2.15	0.43
1:A:164:GLU:OE1	1:E:21:HIS:CE1	2.71	0.43
1:B:90:GLU:HB3	1:G:123:VAL:HB	2.00	0.43
1:E:5:LYS:CE	1:F:164:GLU:OE1	2.66	0.43
1:F:110:ASP:HB3	1:F:115:ILE:HD11	1.99	0.43
1:B:21:HIS:NE2	3:B:401:HOH:O	1.97	0.43
1:E:5:LYS:HE3	1:F:164:GLU:OE1	2.19	0.43
1:J:86:GLY:C	1:J:180:LYS:HD2	2.39	0.43
1:H:210:HIS:CE1	3:H:402:HOH:O	2.68	0.43
1:A:62:GYS:N2	1:A:62:GYS:HD1	2.34	0.43
1:G:198:LYS:HD3	1:G:198:LYS:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:MET:HG2	1:I:173:PHE:CE1	2.53	0.43
1:A:93:MET:HG2	1:A:173:PHE:CE1	2.53	0.43
1:F:93:MET:HG2	1:F:173:PHE:CE1	2.54	0.43
1:J:54:TYR:CD2	1:J:204:TYR:HB3	2.53	0.43
1:I:135:ARG:NH1	1:I:164:GLU:OE2	2.52	0.43
1:L:81:GLN:NE2	1:L:183:VAL:HB	2.33	0.43
1:H:93:MET:HG2	1:H:173:PHE:CE1	2.54	0.42
1:C:43:LYS:HA	1:C:205:SER:O	2.19	0.42
1:G:62:GYS:HD1	1:G:62:GYS:N2	2.33	0.42
1:K:43:LYS:HA	1:K:205:SER:O	2.20	0.42
1:D:93:MET:HG2	1:D:173:PHE:CE1	2.54	0.42
1:H:123:VAL:HB	1:K:90:GLU:HB3	2.01	0.42
1:A:196:GLU:OE1	3:A:402:HOH:O	2.21	0.42
1:L:216:HIS:CE1	3:L:402:HOH:O	2.70	0.42
1:J:93:MET:HG2	1:J:173:PHE:CE1	2.54	0.42
1:C:8:MET:CE	1:C:112:ASP:HA	2.49	0.42
1:E:76:VAL:HB	1:E:186:PRO:HB3	2.02	0.42
1:G:12:LEU:HB2	1:G:116:TYR:HB2	2.02	0.42
1:H:3:VAL:HG21	1:H:84:PRO:HD3	2.02	0.41
1:B:188:TYR:HB2	1:C:168:HIS:CE1	2.55	0.41
1:B:76:VAL:HB	1:B:186:PRO:HB3	2.03	0.41
1:B:93:MET:HG2	1:B:173:PHE:CE1	2.56	0.41
1:D:196:GLU:OE1	3:D:402:HOH:O	2.21	0.41
1:F:183:VAL:HG12	1:F:184:GLN:N	2.34	0.41
1:C:123:VAL:HB	1:F:90:GLU:HB3	2.03	0.41
1:J:168:HIS:CE1	3:J:401:HOH:O	2.63	0.41
1:L:8:MET:HE1	1:L:109:LEU:HD11	2.01	0.41
1:C:76:VAL:HB	1:C:186:PRO:HB3	2.02	0.41
1:H:62:GYS:N2	1:H:62:GYS:HD1	2.36	0.41
1:G:76:VAL:HB	1:G:186:PRO:HB3	2.03	0.41
1:A:164:GLU:OE1	1:E:21:HIS:ND1	2.53	0.41
1:G:11:LYS:O	1:G:115:ILE:HA	2.20	0.41
1:J:76:VAL:HB	1:J:186:PRO:HB3	2.03	0.41
1:J:8:MET:HE3	1:J:112:ASP:HA	2.03	0.40
1:H:76:VAL:HB	1:H:186:PRO:HB3	2.03	0.40
1:K:93:MET:HG2	1:K:173:PHE:CE1	2.56	0.40
1:B:158:ASN:OD1	1:C:158:ASN:CG	2.59	0.40
1:C:93:MET:HG2	1:C:173:PHE:CE1	2.55	0.40
1:D:76:VAL:HB	1:D:186:PRO:HB3	2.03	0.40
1:D:198:LYS:HD3	1:D:198:LYS:HA	1.90	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	4	ILE
1	A	67	VAL
1	A	145	LYS
1	A	149	ARG
1	A	162	SER
1	A	164	GLU
1	A	202	LYS
1	A	214	GLU
1	B	3	VAL
1	B	5	LYS
1	B	37	LYS
1	B	66	ARG
1	B	67	VAL
1	B	145	LYS
1	B	149	ARG
1	B	162	SER
1	B	198	LYS

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Mol	Chain	Res	Type
1	C	3	VAL
1	C	11	LYS
1	C	21	HIS
1	C	66	ARG
1	C	67	VAL
1	C	145	LYS
1	C	149	ARG
1	C	152	VAL
1	C	162	SER
1	C	181	LYS
1	C	182	VAL
1	D	11	LYS
1	D	21	HIS
1	D	41	ASP
1	D	66	ARG
1	D	67	VAL
1	D	145	LYS
1	D	149	ARG
1	D	162	SER
1	D	164	GLU
1	D	214	GLU
1	E	3	VAL
1	E	11	LYS
1	E	21	HIS
1	E	67	VAL
1	E	145	LYS
1	E	149	ARG
1	E	162	SER
1	E	218	GLU
1	F	3	VAL
1	F	67	VAL
1	F	145	LYS
1	F	149	ARG
1	F	162	SER
1	G	66	ARG
1	G	67	VAL
1	G	145	LYS
1	G	149	ARG
1	G	162	SER
1	G	205	SER
1	G	212	HIS
1	H	21	HIS

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Mol	Chain	Res	Type
1	H	66	ARG
1	H	67	VAL
1	H	73	GLU
1	H	145	LYS
1	H	149	ARG
1	H	162	SER
1	H	214	GLU
1	I	145	LYS
1	I	149	ARG
1	I	162	SER
1	I	164	GLU
1	I	202	LYS
1	J	3	VAL
1	J	5	LYS
1	J	66	ARG
1	J	145	LYS
1	J	149	ARG
1	J	162	SER
1	K	3	VAL
1	K	66	ARG
1	K	67	VAL
1	K	71	TYR
1	K	85	GLU
1	K	145	LYS
1	K	149	ARG
1	K	162	SER
1	K	189	HIS
1	K	198	LYS
1	K	214	GLU
1	L	21	HIS
1	L	35	GLU
1	L	115	ILE
1	L	145	LYS
1	L	149	ARG
1	L	162	SER
1	L	164	GLU
1	L	181	LYS
1	L	198	LYS
1	L	202	LYS
1	L	214	GLU
1	L	218	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	GLN
1	E	21	HIS
1	E	158	ASN
1	F	81	GLN
1	F	158	ASN
1	G	158	ASN
1	H	212	HIS
1	I	158	ASN
1	I	206	ASN
1	J	81	GLN
1	J	158	ASN
1	K	158	ASN
1	L	81	GLN
1	L	158	ASN
1	L	212	HIS

### 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%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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

All (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
1	C	62	GYS	C2-N3	-3.51	1.31	1.39
1	J	62	GYS	CA2-C2	-3.49	1.45	1.48
1	H	62	GYS	CA1-C1	-3.39	1.46	1.51
1	G	62	GYS	CA2-C2	-3.33	1.45	1.48
1	L	62	GYS	CA1-C1	-3.25	1.46	1.51
1	I	62	GYS	C2-N3	-3.25	1.31	1.39
1	D	62	GYS	CA1-C1	-3.20	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	62	GYS	C2-N3	-3.15	1.32	1.39
1	L	62	GYS	CA2-C2	-3.14	1.45	1.48
1	G	62	GYS	C2-N3	-3.12	1.32	1.39
1	A	62	GYS	CA1-C1	-3.10	1.46	1.51
1	C	62	GYS	CA2-C2	-3.06	1.45	1.48
1	J	62	GYS	C2-N3	-3.05	1.32	1.39
1	E	62	GYS	CA2-C2	-3.03	1.45	1.48
1	B	62	GYS	C2-N3	-2.78	1.33	1.39
1	L	62	GYS	C2-N3	-2.51	1.33	1.39
1	D	62	GYS	C2-N3	-2.45	1.33	1.39
1	K	62	GYS	CA2-C2	-2.45	1.46	1.48
1	D	62	GYS	CA2-C2	-2.32	1.46	1.48
1	F	62	GYS	C2-N3	-2.24	1.34	1.39
1	B	62	GYS	CA2-C2	-2.22	1.46	1.48
1	E	62	GYS	CA1-C1	-2.11	1.48	1.51
1	H	62	GYS	CA2-C2	-2.06	1.46	1.48
1	C	62	GYS	CA2-N2	-2.05	1.34	1.38
1	F	62	GYS	CA1-C1	-2.01	1.48	1.51
1	H	62	GYS	O2-C2	2.32	1.28	1.23
1	C	62	GYS	O2-C2	2.38	1.28	1.23
1	A	62	GYS	O2-C2	2.46	1.28	1.23
1	I	62	GYS	O2-C2	2.50	1.28	1.23
1	G	62	GYS	O2-C2	2.60	1.28	1.23
1	B	62	GYS	O2-C2	2.70	1.29	1.23
1	L	62	GYS	O2-C2	2.78	1.29	1.23
1	F	62	GYS	O2-C2	2.88	1.29	1.23
1	D	62	GYS	O2-C2	3.29	1.30	1.23
1	C	62	GYS	C1-N2	3.57	1.37	1.32
1	L	62	GYS	C1-N2	3.69	1.37	1.32
1	D	62	GYS	C1-N2	3.75	1.38	1.32
1	H	62	GYS	C1-N2	3.82	1.38	1.32
1	F	62	GYS	C1-N2	3.85	1.38	1.32
1	I	62	GYS	C1-N2	4.07	1.38	1.32
1	J	62	GYS	C1-N2	4.13	1.38	1.32
1	G	62	GYS	C1-N2	4.25	1.38	1.32
1	B	62	GYS	C1-N2	4.28	1.38	1.32
1	E	62	GYS	C1-N2	4.60	1.39	1.32
1	K	62	GYS	C1-N2	4.61	1.39	1.32
1	A	62	GYS	C1-N2	4.72	1.39	1.32
1	F	62	GYS	CB2-CA2	13.51	1.47	1.35
1	G	62	GYS	CB2-CA2	13.92	1.47	1.35
1	L	62	GYS	CB2-CA2	13.97	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	GYS	CB2-CA2	14.55	1.48	1.35
1	J	62	GYS	CB2-CA2	14.71	1.48	1.35
1	B	62	GYS	CB2-CA2	14.83	1.48	1.35
1	I	62	GYS	CB2-CA2	15.18	1.48	1.35
1	E	62	GYS	CB2-CA2	16.15	1.49	1.35
1	A	62	GYS	CB2-CA2	16.62	1.49	1.35
1	H	62	GYS	CB2-CA2	16.91	1.50	1.35
1	D	62	GYS	CB2-CA2	17.14	1.50	1.35
1	K	62	GYS	CB2-CA2	17.48	1.50	1.35

All (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
1	D	62	GYS	O2-C2-CA2	-12.12	124.44	130.97
1	H	62	GYS	O2-C2-CA2	-11.36	124.84	130.97
1	I	62	GYS	O2-C2-CA2	-10.24	125.45	130.97
1	C	62	GYS	O2-C2-CA2	-9.96	125.60	130.97
1	B	62	GYS	O2-C2-CA2	-9.84	125.67	130.97
1	K	62	GYS	O2-C2-CA2	-9.01	126.11	130.97
1	E	62	GYS	C2-CA2-N2	-7.61	103.36	108.93
1	H	62	GYS	C2-CA2-N2	-5.79	104.70	108.93
1	K	62	GYS	C2-CA2-N2	-5.63	104.81	108.93
1	B	62	GYS	C2-CA2-N2	-5.53	104.88	108.93
1	D	62	GYS	C2-CA2-N2	-5.50	104.91	108.93
1	G	62	GYS	C2-CA2-N2	-5.26	105.08	108.93
1	A	62	GYS	CA1-C1-N3	-5.19	118.53	124.75
1	E	62	GYS	O-C-CA3	-4.91	110.14	126.38
1	K	62	GYS	CG2-CB2-CA2	-4.89	124.51	130.19
1	D	62	GYS	CG2-CB2-CA2	-4.81	124.60	130.19
1	J	62	GYS	CG2-CB2-CA2	-4.76	124.66	130.19
1	A	62	GYS	O2-C2-CA2	-4.70	128.44	130.97
1	F	62	GYS	CG2-CB2-CA2	-4.63	124.82	130.19
1	L	62	GYS	O-C-CA3	-4.56	111.30	126.38
1	L	62	GYS	CG2-CB2-CA2	-4.53	124.93	130.19
1	C	62	GYS	C2-CA2-N2	-4.50	105.64	108.93
1	I	62	GYS	CG2-CB2-CA2	-4.44	125.03	130.19
1	C	62	GYS	CG2-CB2-CA2	-4.41	125.07	130.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GYS	C2-CA2-N2	-4.38	105.72	108.93
1	J	62	GYS	C2-CA2-N2	-4.29	105.79	108.93
1	F	62	GYS	C2-CA2-N2	-4.27	105.80	108.93
1	G	62	GYS	O-C-CA3	-3.98	113.23	126.38
1	C	62	GYS	O-C-CA3	-3.97	113.25	126.38
1	E	62	GYS	CG2-CB2-CA2	-3.92	125.63	130.19
1	A	62	GYS	CG2-CB2-CA2	-3.80	125.78	130.19
1	B	62	GYS	CA1-C1-N3	-3.80	120.20	124.75
1	H	62	GYS	O-C-CA3	-3.78	113.87	126.38
1	G	62	GYS	CG2-CB2-CA2	-3.62	125.98	130.19
1	K	62	GYS	O-C-CA3	-3.60	114.49	126.38
1	A	62	GYS	O-C-CA3	-3.58	114.55	126.38
1	I	62	GYS	O-C-CA3	-3.55	114.65	126.38
1	H	62	GYS	CG2-CB2-CA2	-3.52	126.11	130.19
1	D	62	GYS	O-C-CA3	-3.45	114.97	126.38
1	I	62	GYS	C2-CA2-N2	-3.44	106.41	108.93
1	A	62	GYS	OG1-CB1-CA1	-3.41	102.71	111.10
1	L	62	GYS	CA1-C1-N3	-3.40	120.67	124.75
1	B	62	GYS	O-C-CA3	-3.33	115.36	126.38
1	L	62	GYS	C2-CA2-N2	-3.22	106.57	108.93
1	H	62	GYS	OG1-CB1-CA1	-3.02	103.67	111.10
1	I	62	GYS	CA1-C1-N3	-2.99	121.17	124.75
1	J	62	GYS	O-C-CA3	-2.90	116.78	126.38
1	H	62	GYS	CA1-C1-N3	-2.63	121.59	124.75
1	F	62	GYS	O-C-CA3	-2.43	118.34	126.38
1	I	62	GYS	OG1-CB1-CA1	-2.42	105.14	111.10
1	J	62	GYS	CA1-C1-N3	-2.37	121.90	124.75
1	K	62	GYS	CA1-C1-N3	-2.36	121.92	124.75
1	D	62	GYS	CA1-C1-N3	-2.35	121.93	124.75
1	D	62	GYS	OG1-CB1-CA1	-2.30	105.43	111.10
1	D	62	GYS	CA2-N2-C1	2.00	107.32	105.75
1	E	62	GYS	CA2-N2-C1	2.00	107.32	105.75
1	L	62	GYS	CD1-CG2-CD2	2.07	120.73	117.63
1	G	62	GYS	CA2-N2-C1	2.14	107.43	105.75
1	A	62	GYS	CA1-C1-N2	2.15	127.89	123.56
1	H	62	GYS	CD1-CE1-CZ	2.19	122.36	119.88
1	F	62	GYS	CA2-N2-C1	2.20	107.48	105.75
1	D	62	GYS	CD1-CE1-CZ	2.33	122.52	119.88
1	B	62	GYS	CA2-N2-C1	2.38	107.62	105.75
1	B	62	GYS	CB1-CA1-C1	2.42	116.36	110.23
1	B	62	GYS	CA1-C1-N2	2.45	128.49	123.56
1	A	62	GYS	CD1-CE1-CZ	2.63	122.86	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	62	GYS	CB2-CA2-C2	2.69	125.70	122.32
1	I	62	GYS	N3-C1-N2	2.83	113.41	111.45
1	E	62	GYS	CD1-CE1-CZ	2.94	123.21	119.88
1	A	62	GYS	N3-C1-N2	3.08	113.59	111.45
1	I	62	GYS	CB2-CA2-C2	3.17	126.31	122.32
1	J	62	GYS	CB2-CA2-C2	3.76	127.05	122.32
1	H	62	GYS	N3-C1-N2	3.79	114.08	111.45
1	F	62	GYS	CB2-CA2-C2	3.94	127.27	122.32
1	G	62	GYS	CB2-CA2-C2	4.06	127.42	122.32
1	A	62	GYS	CB2-CA2-C2	4.21	127.62	122.32
1	B	62	GYS	CB2-CA2-C2	4.21	127.62	122.32
1	C	62	GYS	CB2-CA2-C2	4.66	128.19	122.32
1	K	62	GYS	CB2-CA2-C2	5.02	128.63	122.32
1	H	62	GYS	CB2-CA2-C2	5.25	128.93	122.32
1	D	62	GYS	CB2-CA2-C2	5.47	129.20	122.32
1	E	62	GYS	CB2-CA2-C2	5.58	129.34	122.32
1	L	62	GYS	CA2-C2-N3	12.74	108.98	103.30
1	I	62	GYS	CA2-C2-N3	14.27	109.67	103.30
1	D	62	GYS	CA2-C2-N3	14.34	109.70	103.30
1	A	62	GYS	CA2-C2-N3	14.79	109.90	103.30
1	F	62	GYS	CA2-C2-N3	14.93	109.96	103.30
1	B	62	GYS	CA2-C2-N3	15.01	110.00	103.30
1	C	62	GYS	CA2-C2-N3	15.35	110.15	103.30
1	G	62	GYS	CA2-C2-N3	16.27	110.56	103.30
1	J	62	GYS	CA2-C2-N3	16.67	110.74	103.30
1	H	62	GYS	CA2-C2-N3	17.79	111.24	103.30
1	K	62	GYS	CA2-C2-N3	18.33	111.48	103.30
1	E	62	GYS	CA2-C2-N3	20.01	112.23	103.30

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

### 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, 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

All (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
1	K	4	ILE	5.3
1	B	114	TYR	5.0
1	B	113	CYS	4.9
1	I	6	PRO	4.8
1	K	150	ASP	4.8
1	A	85	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	3	VAL	4.6
1	D	112	ASP	4.6
1	B	110	ASP	4.6
1	B	73	GLU	4.6
1	I	3	VAL	4.5
1	I	215	ALA	4.5
1	B	4	ILE	4.4
1	J	2	SER	4.3
1	B	41	ASP	4.2
1	B	112	ASP	4.1
1	B	184	GLN	4.0
1	C	112	ASP	4.0
1	J	112	ASP	3.9
1	D	3	VAL	3.9
1	A	6	PRO	3.8
1	D	218	GLU	3.7
1	K	113	CYS	3.7
1	K	215	ALA	3.7
1	J	85	GLU	3.7
1	B	213	ALA	3.7
1	A	180	LYS	3.6
1	B	164	GLU	3.6
1	J	184	GLN	3.6
1	B	9	LYS	3.6
1	G	66	ARG	3.6
1	B	3	VAL	3.6
1	I	74	ASN	3.6
1	C	5	LYS	3.5
1	J	9	LYS	3.5
1	G	84	PRO	3.5
1	F	74	ASN	3.5
1	K	202	LYS	3.5
1	G	181	LYS	3.4
1	F	180	LYS	3.4
1	C	7	ASP	3.4
1	B	111	GLY	3.3
1	B	7	ASP	3.3
1	J	110	ASP	3.3
1	A	5	LYS	3.3
1	J	72	PRO	3.3
1	B	5	LYS	3.3
1	G	65	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	202	LYS	3.2
1	B	109	LEU	3.2
1	G	164	GLU	3.2
1	B	167	GLY	3.2
1	G	182	VAL	3.1
1	F	34	PHE	3.1
1	K	5	LYS	3.1
1	G	49	PRO	3.1
1	I	5	LYS	3.1
1	J	150	ASP	3.1
1	K	6	PRO	3.1
1	B	32	LYS	3.1
1	C	165	GLY	3.1
1	G	73	GLU	3.0
1	J	75	ILE	3.0
1	F	202	LYS	3.0
1	B	59	THR	3.0
1	J	76	VAL	3.0
1	C	142	SER	3.0
1	A	7	ASP	3.0
1	B	214	GLU	3.0
1	F	85	GLU	3.0
1	B	151	GLY	2.9
1	C	74	ASN	2.9
1	D	74	ASN	2.9
1	F	216	HIS	2.9
1	G	184	GLN	2.9
1	I	84	PRO	2.8
1	J	84	PRO	2.8
1	G	3	VAL	2.8
1	G	76	VAL	2.8
1	I	184	GLN	2.8
1	L	59	THR	2.8
1	B	152	VAL	2.8
1	B	210	HIS	2.8
1	D	5	LYS	2.8
1	F	48	GLY	2.7
1	K	110	ASP	2.7
1	C	30	LEU	2.7
1	G	72	PRO	2.7
1	G	112	ASP	2.7
1	B	66	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	165	GLY	2.7
1	B	8	MET	2.6
1	B	74	ASN	2.6
1	C	73	GLU	2.6
1	D	184	GLN	2.6
1	A	189	HIS	2.6
1	L	110	ASP	2.6
1	C	166	GLY	2.5
1	F	181	LYS	2.5
1	J	198	LYS	2.5
1	C	65	ASN	2.5
1	B	72	PRO	2.5
1	C	2	SER	2.5
1	J	46	GLU	2.5
1	K	143	THR	2.5
1	B	65	ASN	2.4
1	A	215	ALA	2.4
1	B	58	THR	2.4
1	C	59	THR	2.4
1	C	35	GLU	2.4
1	J	35	GLU	2.4
1	G	68	PHE	2.4
1	B	76	VAL	2.4
1	I	110	ASP	2.4
1	J	113	CYS	2.4
1	D	35	GLU	2.4
1	J	59	THR	2.4
1	G	110	ASP	2.4
1	J	74	ASN	2.4
1	J	111	GLY	2.4
1	F	182	VAL	2.3
1	F	150	ASP	2.3
1	L	218	GLU	2.3
1	A	110	ASP	2.3
1	C	6	PRO	2.3
1	F	72	PRO	2.3
1	K	112	ASP	2.3
1	I	75	ILE	2.3
1	F	183	VAL	2.3
1	F	218	GLU	2.2
1	C	199	SER	2.2
1	B	165	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	216	HIS	2.2
1	K	7	ASP	2.2
1	G	67	VAL	2.2
1	K	151	GLY	2.2
1	F	184	GLN	2.2
1	D	73	GLU	2.2
1	H	73	GLU	2.2
1	A	49	PRO	2.2
1	H	72	PRO	2.2
1	H	2	SER	2.1
1	D	110	ASP	2.1
1	J	185	LEU	2.1
1	A	3	VAL	2.1
1	F	65	ASN	2.1
1	B	75	ILE	2.1
1	I	46	GLU	2.1
1	I	85	GLU	2.1
1	F	60	VAL	2.1
1	C	34	PHE	2.1
1	E	59	THR	2.1
1	C	167	GLY	2.1
1	G	203	ASP	2.1
1	B	202	LYS	2.1
1	L	57	LEU	2.0
1	G	41	ASP	2.0
1	A	218	GLU	2.0
1	L	112	ASP	2.0
1	B	108	THR	2.0
1	D	85	GLU	2.0
1	F	75	ILE	2.0
1	A	190	PHE	2.0

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

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( $\text{\AA}^2$ )	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 [i](#)

There are no carbohydrates 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. 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( $\text{\AA}^2$ )	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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.