



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:33 pm GMT

PDB ID : 4H4L  
Title : Crystal Structure of ternary complex of HutP(HutP-L-His-Zn)  
Authors : Dhakshnamoorthy, B.; Misono, T.S.; Mizuno, H.; Kumar, P.K.R.  
Deposited on : 2012-09-17  
Resolution : 2.50 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

<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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

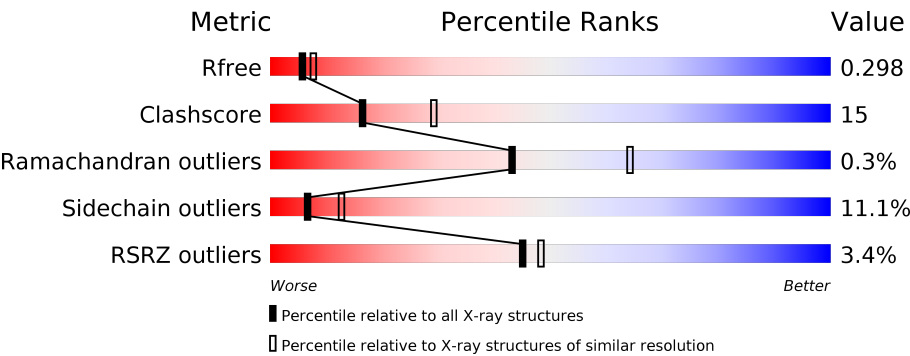
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	148	
1	B	148	
1	C	148	
1	D	148	
1	E	148	
1	F	148	

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Mol	Chain	Length	Quality of chain
1	G	148	
1	H	148	
1	I	148	
1	J	148	
1	K	148	
1	L	148	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HIS	A	201	-	-	X	-
2	HIS	B	201	-	-	X	-
2	HIS	F	201	-	-	X	-
2	HIS	J	201	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13047 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 Hut operon positive regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	1	0	0
			1072	676	192	200	4			
1	B	143	Total	C	N	O	S	1	0	0
			1057	668	189	196	4			
1	C	139	Total	C	N	O	S	9	0	0
			1062	669	191	198	4			
1	D	142	Total	C	N	O	S	1	0	0
			1065	672	191	198	4			
1	E	143	Total	C	N	O	S	1	0	0
			1061	670	189	198	4			
1	F	143	Total	C	N	O	S	9	0	0
			1088	685	196	203	4			
1	G	142	Total	C	N	O	S	1	0	0
			1065	672	191	198	4			
1	H	143	Total	C	N	O	S	1	0	0
			1065	672	189	200	4			
1	I	141	Total	C	N	O	S	9	0	0
			1078	679	193	202	4			
1	J	142	Total	C	N	O	S	0	0	0
			1065	672	191	198	4			
1	K	143	Total	C	N	O	S	1	0	0
			1061	670	189	198	4			
1	L	142	Total	C	N	O	S	9	0	0
			1083	682	195	202	4			

There are 12 discrepancies between the modelled and reference sequences:

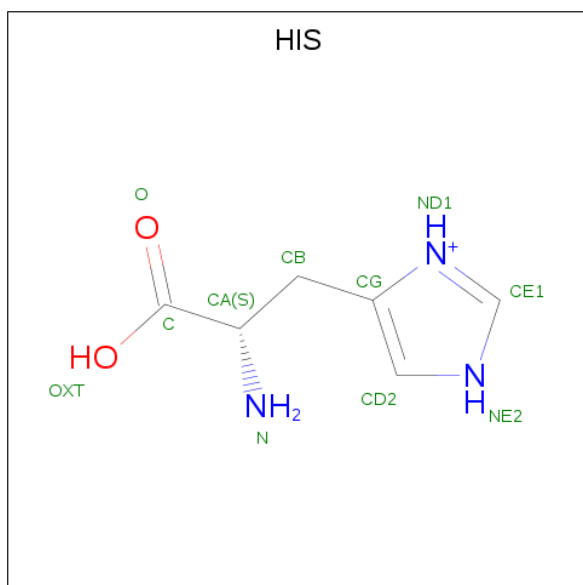
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
B	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
C	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
D	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
E	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943

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Chain	Residue	Modelled	Actual	Comment	Reference
F	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
G	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
H	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
I	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
J	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
K	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943
L	51	ILE	VAL	ENGINEERED MUTATION	UNP P10943

- Molecule 2 is HISTIDINE (three-letter code: HIS) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	3	2		
2	B	1	Total	C	N	O	0	0
			11	6	3	2		
2	C	1	Total	C	N	O	0	0
			11	6	3	2		
2	D	1	Total	C	N	O	0	0
			11	6	3	2		
2	D	1	Total	C	N	O	0	0
			11	6	3	2		
2	F	1	Total	C	N	O	0	0
			11	6	3	2		
2	G	1	Total	C	N	O	0	0
			11	6	3	2		
2	G	1	Total	C	N	O	0	0
			11	6	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			11	6	3	2		
2	J	1	Total	C	N	O	0	0
			11	6	3	2		
2	J	1	Total	C	N	O	0	0
			11	6	3	2		
2	L	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		

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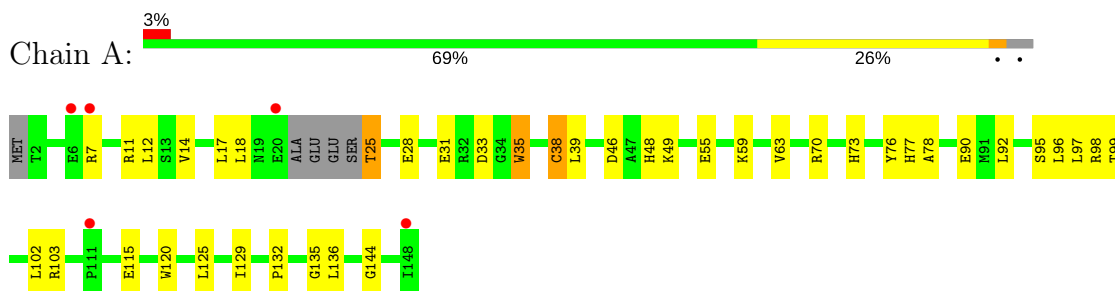
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total 8	O 8	0	0
4	C	10	Total 10	O 10	0	0
4	D	6	Total 6	O 6	0	0
4	E	6	Total 6	O 6	0	0
4	F	7	Total 7	O 7	0	0
4	G	6	Total 6	O 6	0	0
4	H	9	Total 9	O 9	0	0
4	I	5	Total 5	O 5	0	0
4	J	5	Total 5	O 5	0	0
4	K	3	Total 3	O 3	0	0
4	L	6	Total 6	O 6	0	0

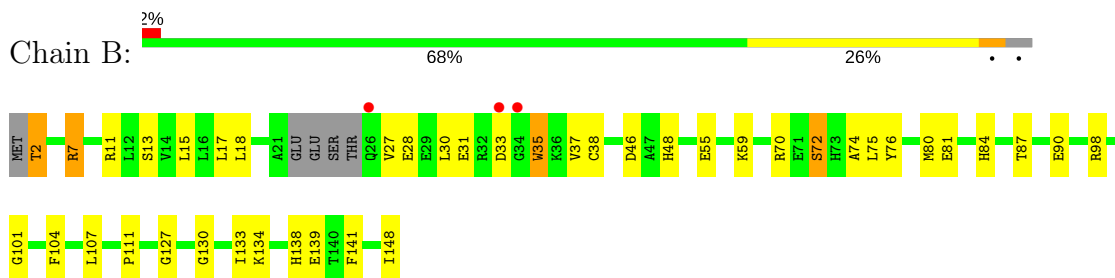
### 3 Residue-property plots [i](#)

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.

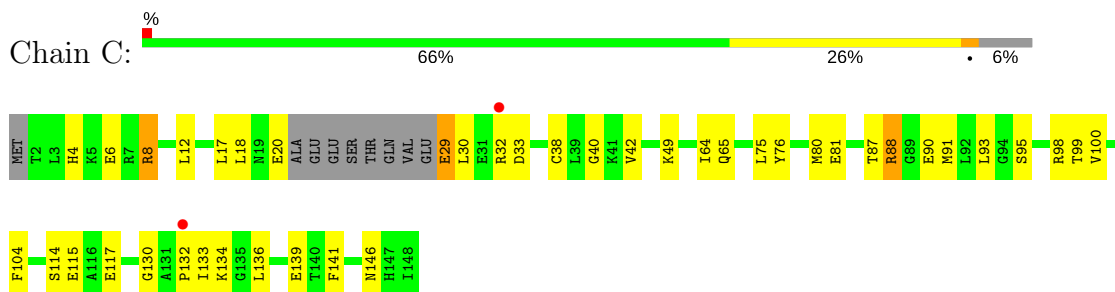
- Molecule 1: Hut operon positive regulatory protein



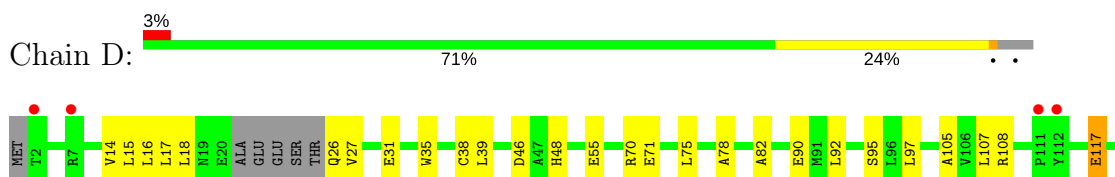
- Molecule 1: Hut operon positive regulatory protein



- Molecule 1: Hut operon positive regulatory protein



- Molecule 1: Hut operon positive regulatory protein



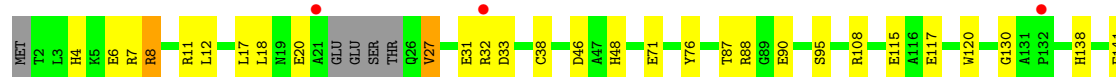
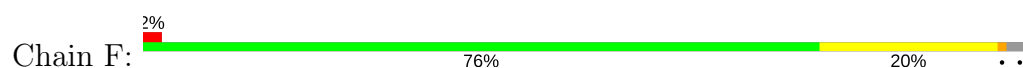




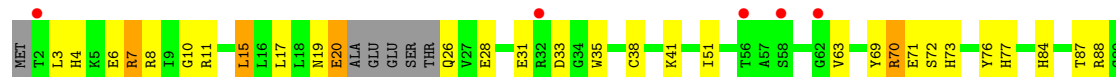
- Molecule 1: Hut operon positive regulatory protein



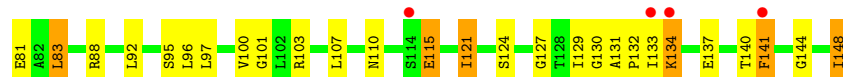
- Molecule 1: Hut operon positive regulatory protein



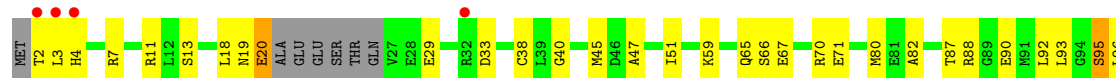
- Molecule 1: Hut operon positive regulatory protein

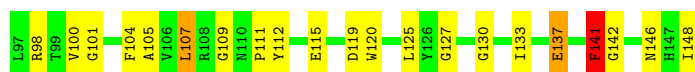


- Molecule 1: Hut operon positive regulatory protein

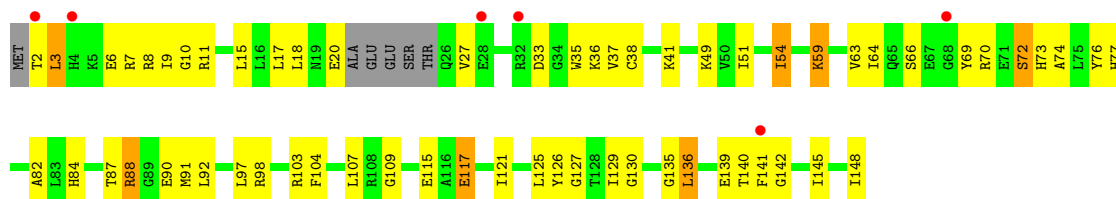


- Molecule 1: Hut operon positive regulatory protein

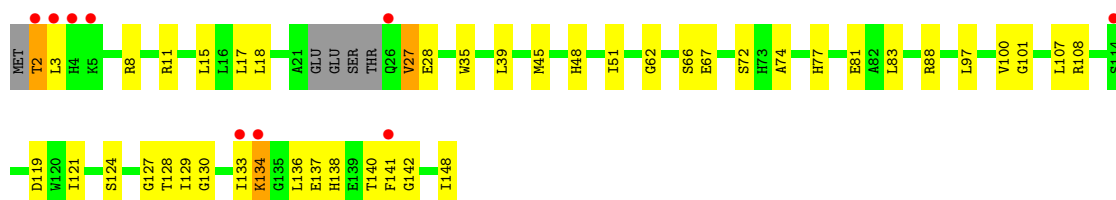




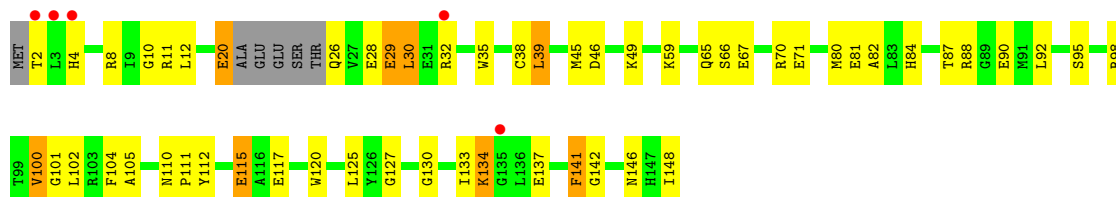
- Molecule 1: Hut operon positive regulatory protein



- Molecule 1: Hut operon positive regulatory protein



- Molecule 1: Hut operon positive regulatory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.53Å 129.53Å 76.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.28 – 2.50 32.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.28-2.50) 98.1 (32.99-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.219 , 0.298 0.220 , 0.298	Depositor DCC
$R_{free}$ test set	2507 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 24.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l 0.054 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0059e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN

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	0.68	2/1089 (0.2%)	0.79	0/1471
1	B	0.66	1/1073 (0.1%)	0.79	0/1450
1	C	0.73	1/1079 (0.1%)	0.80	0/1453
1	D	0.68	2/1082 (0.2%)	0.82	0/1461
1	E	0.64	0/1077	0.81	1/1455 (0.1%)
1	F	0.73	1/1105 (0.1%)	0.82	0/1489
1	G	0.67	0/1082	0.83	0/1461
1	H	0.64	1/1081 (0.1%)	0.85	0/1460
1	I	0.68	1/1095 (0.1%)	0.79	1/1475 (0.1%)
1	J	0.67	0/1082	0.82	0/1461
1	K	0.66	1/1077 (0.1%)	0.82	0/1455
1	L	0.75	1/1100 (0.1%)	0.89	3/1482 (0.2%)
All	All	0.68	11/13022 (0.1%)	0.82	5/17573 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	120	TRP	CD2-CE2	5.76	1.48	1.41
1	C	134	LYS	CB-CG	-5.65	1.37	1.52
1	K	35	TRP	CD2-CE2	5.26	1.47	1.41
1	F	120	TRP	CD2-CE2	5.20	1.47	1.41
1	D	120	TRP	CD2-CE2	5.20	1.47	1.41
1	I	120	TRP	CD2-CE2	5.20	1.47	1.41
1	D	35	TRP	CD2-CE2	5.18	1.47	1.41
1	H	35	TRP	CD2-CE2	5.17	1.47	1.41
1	B	35	TRP	CD2-CE2	5.14	1.47	1.41
1	A	120	TRP	CD2-CE2	5.05	1.47	1.41
1	A	35	TRP	CD2-CE2	5.02	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	141	PHE	CB-CA-C	-5.63	99.14	110.40
1	E	66	SER	CA-CB-OG	5.44	125.90	111.20
1	L	39	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	L	30	LEU	N-CA-C	-5.06	97.33	111.00
1	L	134	LYS	N-CA-CB	5.02	119.64	110.60

There are no chirality outliers.

There are no planarity outliers.

## 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	1072	0	1058	30	0
1	B	1057	0	1041	38	0
1	C	1062	0	1062	29	0
1	D	1065	0	1051	27	0
1	E	1061	0	1045	36	0
1	F	1088	0	1086	26	0
1	G	1065	0	1051	55	0
1	H	1065	0	1049	44	0
1	I	1078	0	1077	36	0
1	J	1065	0	1051	56	0
1	K	1061	0	1045	32	0
1	L	1083	0	1081	36	0
2	A	11	0	6	8	0
2	B	11	0	6	9	0
2	C	11	0	6	4	0
2	D	22	0	12	5	0
2	F	11	0	6	6	0
2	G	22	0	12	5	0
2	I	11	0	6	4	0
2	J	22	0	12	12	0
2	L	11	0	6	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	10	0	0	1	0
4	B	8	0	0	0	0
4	C	10	0	0	0	0
4	D	6	0	0	0	0
4	E	6	0	0	2	0
4	F	7	0	0	0	0
4	G	6	0	0	3	0
4	H	9	0	0	1	0
4	I	5	0	0	0	0
4	J	5	0	0	2	0
4	K	3	0	0	0	0
4	L	6	0	0	2	0
All	All	13047	0	12769	393	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 15.

All (393) 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:I:130:GLY:HA3	1:I:137:GLU:HB3	1.21	1.14
1:C:29:GLU:HG2	1:C:30:LEU:H	0.97	1.10
1:J:63:VAL:HG12	1:J:64:ILE:HD12	1.25	1.09
1:G:98:ARG:HD2	1:G:129:ILE:HD11	1.36	1.06
1:D:26:GLN:HG3	1:D:27:VAL:H	1.19	1.00
1:C:29:GLU:HG2	1:C:30:LEU:N	1.81	0.96
1:I:7:ARG:O	1:I:7:ARG:HG3	1.65	0.96
1:K:74:ALA:HB3	1:K:148:ILE:HD12	1.48	0.93
1:K:74:ALA:CB	1:K:148:ILE:HD12	1.98	0.93
1:F:4:HIS:HB3	1:F:7:ARG:HG3	1.54	0.90
1:H:101:GLY:O	1:H:127:GLY:HA3	1.71	0.90
1:K:101:GLY:O	1:K:127:GLY:HA3	1.71	0.89
1:B:2:THR:CG2	1:J:135:GLY:HA2	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:ARG:HD2	1:J:129:ILE:HD11	1.56	0.88
1:G:129:ILE:HG22	1:G:140:THR:HB	1.56	0.86
1:G:4:HIS:HD2	1:G:6:GLU:H	1.24	0.85
1:G:38:CYS:HB2	1:G:63:VAL:HG21	1.61	0.83
1:G:4:HIS:CD2	1:G:6:GLU:H	1.98	0.82
1:F:130:GLY:HA2	2:F:201:HIS:HB3	1.61	0.81
1:D:135:GLY:HA2	1:H:2:THR:HG23	1.61	0.80
1:I:4:HIS:HB3	1:I:7:ARG:HG2	1.63	0.80
1:I:130:GLY:CA	1:I:137:GLU:HB3	2.08	0.80
1:B:2:THR:HG23	1:J:135:GLY:HA2	1.63	0.79
1:D:26:GLN:HG3	1:D:27:VAL:N	1.98	0.78
1:A:46:ASP:HB3	1:A:48:HIS:CD2	2.19	0.78
1:I:92:LEU:HB2	1:I:96:LEU:HD12	1.64	0.78
1:J:130:GLY:HA2	2:J:203:HIS:HB3	1.64	0.77
1:B:37:VAL:HG12	1:B:107:LEU:HD12	1.66	0.76
1:J:64:ILE:HD11	1:J:121:ILE:CD1	2.16	0.76
1:E:133:ILE:HG22	1:E:134:LYS:HG2	1.67	0.75
1:H:17:LEU:HD11	1:H:124:SER:HB2	1.69	0.74
1:G:20:GLU:HB2	1:G:26:GLN:HE22	1.52	0.73
1:A:135:GLY:HA2	1:K:2:THR:HG23	1.69	0.73
1:K:100:VAL:HG12	1:K:129:ILE:HG13	1.70	0.72
1:E:2:THR:CG2	1:G:135:GLY:HA2	2.19	0.72
1:I:92:LEU:HB2	1:I:96:LEU:CD1	2.20	0.71
1:D:26:GLN:CG	1:D:27:VAL:H	1.98	0.70
1:C:29:GLU:CG	1:C:30:LEU:H	1.86	0.69
1:I:130:GLY:HA3	1:I:137:GLU:CB	2.13	0.69
1:B:133:ILE:HG22	1:B:134:LYS:H	1.57	0.69
1:A:39:LEU:HD13	1:A:103:ARG:HH21	1.59	0.68
1:L:65:GLN:HB2	1:L:67:GLU:OE1	1.93	0.68
1:B:133:ILE:HG22	1:B:134:LYS:N	2.09	0.68
1:E:117:GLU:O	1:I:70:ARG:NH2	2.27	0.68
1:F:4:HIS:HB3	1:F:7:ARG:CG	2.24	0.67
1:J:17:LEU:HD22	1:J:126:TYR:HB3	1.74	0.67
1:G:4:HIS:O	1:G:8:ARG:HG3	1.94	0.67
1:L:67:GLU:HB3	4:L:302:HOH:O	1.93	0.67
1:A:7:ARG:HB2	1:A:35:TRP:HZ2	1.59	0.67
1:A:18:LEU:O	1:K:11:ARG:NH2	2.27	0.67
1:F:88:ARG:HH22	2:F:201:HIS:HE1	1.43	0.66
1:F:8:ARG:O	1:F:12:LEU:HG	1.95	0.66
1:I:98:ARG:HD2	2:I:201:HIS:HD1	1.60	0.66
1:A:38:CYS:HB2	1:A:63:VAL:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:28:GLU:O	1:L:30:LEU:N	2.29	0.66
1:F:88:ARG:HH22	2:F:201:HIS:CE1	2.14	0.65
1:J:64:ILE:HD11	1:J:121:ILE:HD12	1.77	0.65
1:L:130:GLY:HA2	2:L:201:HIS:HB3	1.78	0.64
1:H:37:VAL:HG23	1:H:38:CYS:N	2.12	0.64
1:D:70:ARG:NH2	1:G:148:ILE:O	2.32	0.63
1:E:37:VAL:HG12	1:E:107:LEU:HD12	1.80	0.63
1:D:70:ARG:NH1	1:G:117:GLU:O	2.32	0.63
2:G:201:HIS:HB2	1:H:130:GLY:HA2	1.81	0.63
1:B:134:LYS:HD3	1:H:42:VAL:HA	1.81	0.63
1:I:98:ARG:HB2	2:I:201:HIS:HB2	1.80	0.63
1:L:67:GLU:CB	4:L:302:HOH:O	2.47	0.63
1:J:98:ARG:HB3	2:J:203:HIS:N	2.13	0.62
1:E:133:ILE:HG22	1:E:134:LYS:H	1.65	0.62
1:E:133:ILE:HG22	1:E:134:LYS:N	2.15	0.61
1:G:17:LEU:HD23	1:G:17:LEU:O	2.00	0.61
1:B:74:ALA:HB3	1:B:148:ILE:HD12	1.82	0.60
1:G:130:GLY:HA2	2:G:203:HIS:HB3	1.82	0.60
1:I:65:GLN:HG2	1:I:71:GLU:OE1	2.01	0.60
1:J:63:VAL:HG12	1:J:64:ILE:CD1	2.16	0.60
2:J:201:HIS:CE1	1:K:88:ARG:HH22	2.19	0.60
1:I:65:GLN:HB2	1:I:67:GLU:OE1	2.01	0.60
1:L:59:LYS:HE2	1:L:66:SER:HA	1.83	0.60
1:H:27:VAL:HG23	1:H:28:GLU:OE1	2.01	0.60
1:H:133:ILE:CG2	1:H:134:LYS:H	2.14	0.60
2:B:201:HIS:HB3	1:C:130:GLY:HA2	1.84	0.59
1:L:20:GLU:HA	1:L:20:GLU:OE1	2.02	0.59
1:A:38:CYS:CB	1:A:63:VAL:HG21	2.32	0.59
1:B:133:ILE:CG2	1:B:134:LYS:H	2.15	0.59
1:H:133:ILE:HG22	1:H:134:LYS:N	2.18	0.59
1:J:104:PHE:HB3	1:J:125:LEU:HD23	1.83	0.59
1:H:50:VAL:O	1:H:54:ILE:HG13	2.02	0.58
1:H:100:VAL:HG12	1:H:129:ILE:HG13	1.85	0.58
1:I:130:GLY:HA2	2:I:201:HIS:HB3	1.84	0.58
2:A:201:HIS:HB2	1:B:98:ARG:HB2	1.84	0.58
1:E:133:ILE:CG2	1:E:134:LYS:H	2.16	0.58
1:L:90:GLU:HB3	1:L:92:LEU:HD12	1.84	0.58
2:A:201:HIS:HB3	1:B:130:GLY:HA2	1.85	0.58
1:L:65:GLN:HG2	1:L:71:GLU:OE1	2.04	0.58
1:F:148:ILE:C	1:H:70:ARG:HH12	2.07	0.58
1:K:119:ASP:HB3	1:K:148:ILE:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ASP:HB3	1:B:48:HIS:CD2	2.38	0.58
1:D:97:LEU:HD12	1:D:132:PRO:HG2	1.85	0.57
2:A:201:HIS:HB2	1:B:98:ARG:CB	2.34	0.57
1:C:18:LEU:HD22	1:L:11:ARG:HG3	1.86	0.57
1:G:107:LEU:O	1:G:121:ILE:HG13	2.04	0.57
1:H:133:ILE:CG2	1:H:134:LYS:N	2.68	0.57
1:D:38:CYS:O	1:D:39:LEU:HD23	2.03	0.57
1:K:133:ILE:H	1:K:133:ILE:HD12	1.68	0.57
1:G:17:LEU:HD22	1:G:126:TYR:HB3	1.87	0.57
1:J:76:TYR:CG	2:J:201:HIS:HA	2.40	0.57
1:G:76:TYR:CD2	2:G:201:HIS:HA	2.40	0.57
1:G:69:TYR:CE2	1:H:137:GLU:C	2.78	0.56
1:K:74:ALA:HB3	1:K:148:ILE:CD1	2.29	0.56
1:F:18:LEU:HD22	1:I:11:ARG:HG3	1.87	0.56
1:C:40:GLY:HA3	1:C:104:PHE:CZ	2.40	0.56
2:D:201:HIS:HB2	1:E:98:ARG:HB3	1.86	0.56
1:G:117:GLU:HA	1:G:117:GLU:OE2	2.05	0.56
1:A:25:THR:O	1:A:28:GLU:HB3	2.05	0.56
1:E:81:GLU:OE1	1:G:88:ARG:HD2	2.05	0.56
1:G:51:ILE:HG22	1:H:97:LEU:HD23	1.86	0.56
1:G:38:CYS:CB	1:G:63:VAL:HG21	2.34	0.56
1:G:87:THR:HB	1:G:90:GLU:O	2.05	0.55
1:G:130:GLY:HA3	1:G:136:LEU:O	2.05	0.55
1:G:87:THR:HG21	1:G:91:MET:HA	1.87	0.55
1:J:64:ILE:HD11	1:J:121:ILE:HD11	1.87	0.55
1:A:76:TYR:CE2	2:A:201:HIS:HA	2.42	0.55
1:I:59:LYS:HE2	1:I:66:SER:HA	1.89	0.55
1:E:30:LEU:O	1:E:35:TRP:HB2	2.07	0.55
1:K:74:ALA:HB1	1:K:148:ILE:HD12	1.82	0.55
1:A:98:ARG:HB3	2:C:201:HIS:HB2	1.89	0.55
1:F:148:ILE:OXT	1:H:70:ARG:NH1	2.40	0.54
1:L:26:GLN:N	1:L:26:GLN:CD	2.60	0.54
1:G:129:ILE:CG2	1:G:140:THR:HB	2.33	0.54
1:G:38:CYS:HB2	1:G:63:VAL:CG2	2.35	0.54
1:H:144:GLY:HA2	4:H:307:HOH:O	2.06	0.54
1:A:102:LEU:HD13	1:A:125:LEU:HD22	1.90	0.54
1:G:92:LEU:HD21	1:I:92:LEU:HD21	1.90	0.54
1:C:114:SER:HB3	1:C:117:GLU:HG2	1.90	0.54
1:G:35:TRP:CZ3	1:G:109:GLY:HA3	2.43	0.54
1:J:129:ILE:HG22	1:J:140:THR:HB	1.90	0.54
1:J:87:THR:HB	1:J:90:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ARG:HG3	1:B:111:PRO:HA	1.89	0.54
1:E:46:ASP:HB3	1:E:48:HIS:CD2	2.42	0.54
1:H:92:LEU:HB3	1:H:95:SER:HB3	1.89	0.54
1:I:82:ALA:O	1:I:142:GLY:HA3	2.08	0.54
1:D:16:LEU:HD21	1:D:39:LEU:HD21	1.89	0.53
1:H:110:ASN:ND2	1:H:115:GLU:HA	2.23	0.53
1:H:121:ILE:HD13	1:H:148:ILE:HD13	1.90	0.53
1:L:110:ASN:ND2	1:L:115:GLU:HA	2.23	0.53
1:A:14:VAL:HG21	1:K:141:PHE:CZ	2.43	0.53
1:J:84:HIS:HD2	4:J:304:HOH:O	1.90	0.53
1:A:92:LEU:HD22	1:A:95:SER:OG	2.09	0.53
1:A:98:ARG:CB	2:C:201:HIS:HB2	2.39	0.53
2:D:201:HIS:CD2	2:D:201:HIS:OXT	2.62	0.53
1:F:117:GLU:HA	1:F:117:GLU:OE1	2.09	0.53
1:K:48:HIS:HA	1:K:51:ILE:HD12	1.90	0.52
1:I:7:ARG:CG	1:I:7:ARG:O	2.43	0.52
1:F:4:HIS:CD2	1:F:6:GLU:HB2	2.44	0.52
1:L:46:ASP:HB2	1:L:49:LYS:HG3	1.90	0.52
1:C:18:LEU:HD21	1:C:141:PHE:HZ	1.73	0.52
1:E:35:TRP:CZ3	1:E:109:GLY:HA3	2.45	0.52
1:B:11:ARG:NH2	1:J:18:LEU:O	2.43	0.52
1:H:77:HIS:O	1:H:81:GLU:HG3	2.09	0.52
1:B:101:GLY:O	1:B:127:GLY:HA3	2.09	0.52
1:C:93:LEU:HD13	1:C:100:VAL:HG22	1.92	0.52
1:F:4:HIS:CD2	1:F:7:ARG:HG2	2.44	0.52
1:L:82:ALA:O	1:L:142:GLY:HA3	2.09	0.52
1:A:76:TYR:CZ	2:A:201:HIS:HA	2.45	0.52
1:G:84:HIS:CD2	4:G:305:HOH:O	2.63	0.52
1:E:8:ARG:HG3	4:E:302:HOH:O	2.10	0.51
1:D:97:LEU:CD1	1:D:132:PRO:HG2	2.40	0.51
1:E:18:LEU:O	1:G:11:ARG:NH2	2.43	0.51
1:E:101:GLY:O	1:E:127:GLY:HA3	2.11	0.51
1:A:97:LEU:HD12	1:A:132:PRO:HG2	1.93	0.51
1:B:133:ILE:CG2	1:B:134:LYS:N	2.73	0.51
1:D:78:ALA:O	1:D:144:GLY:HA3	2.11	0.51
1:E:133:ILE:CG2	1:E:134:LYS:N	2.74	0.51
1:C:133:ILE:HB	1:C:136:LEU:HD12	1.91	0.51
2:D:203:HIS:HA	1:F:76:TYR:CD1	2.46	0.51
1:F:11:ARG:HG3	1:I:18:LEU:HD22	1.92	0.50
1:H:74:ALA:HB3	1:H:148:ILE:HD12	1.93	0.50
1:I:40:GLY:HA3	1:I:104:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:ILE:HG21	1:K:148:ILE:HD13	1.94	0.50
1:G:76:TYR:CG	2:G:201:HIS:HA	2.47	0.50
1:A:70:ARG:NH2	1:J:148:ILE:O	2.45	0.50
1:E:40:GLY:HA3	1:E:104:PHE:CZ	2.47	0.49
1:G:73:HIS:O	1:G:77:HIS:HD2	1.94	0.49
1:B:81:GLU:O	1:B:84:HIS:HB2	2.12	0.49
1:D:90:GLU:HB3	1:D:92:LEU:HD12	1.94	0.49
1:I:119:ASP:HB3	1:I:148:ILE:HG23	1.93	0.49
1:J:126:TYR:CG	1:J:127:GLY:N	2.80	0.49
1:J:98:ARG:CB	2:J:203:HIS:N	2.76	0.49
1:J:84:HIS:CD2	4:J:304:HOH:O	2.64	0.49
1:J:87:THR:HG21	1:J:91:MET:HA	1.94	0.49
1:J:117:GLU:HA	1:J:117:GLU:OE2	2.12	0.49
1:D:130:GLY:HA2	2:D:203:HIS:HB3	1.95	0.49
4:A:307:HOH:O	1:K:142:GLY:HA2	2.13	0.49
1:K:77:HIS:O	1:K:81:GLU:HG3	2.13	0.49
1:J:51:ILE:HG22	1:K:97:LEU:CD2	2.43	0.49
1:E:33:ASP:OD2	1:E:33:ASP:N	2.46	0.49
1:C:4:HIS:HD2	1:C:6:GLU:H	1.61	0.48
1:B:81:GLU:OE1	1:J:88:ARG:HD2	2.12	0.48
1:E:2:THR:HG21	1:G:135:GLY:HA2	1.93	0.48
1:G:84:HIS:HD2	4:G:305:HOH:O	1.93	0.48
1:J:69:TYR:CE2	1:K:137:GLU:C	2.87	0.48
1:B:11:ARG:HG2	1:J:18:LEU:HD13	1.94	0.48
1:J:130:GLY:HA3	1:J:136:LEU:O	2.14	0.48
2:J:201:HIS:HE1	1:K:88:ARG:HH12	1.61	0.48
1:F:18:LEU:HD21	1:F:141:PHE:HZ	1.78	0.48
1:B:141:PHE:HE1	1:J:141:PHE:CD2	2.31	0.48
1:B:55:GLU:HA	1:B:75:LEU:HD21	1.94	0.48
1:D:14:VAL:HG21	1:H:141:PHE:CZ	2.48	0.48
1:D:18:LEU:HB3	1:H:11:ARG:HD2	1.96	0.48
1:K:108:ARG:HB2	1:K:121:ILE:HD12	1.95	0.48
1:G:17:LEU:HD21	1:G:103:ARG:HB3	1.94	0.48
1:J:88:ARG:HH12	2:J:203:HIS:CE1	2.31	0.48
1:G:11:ARG:HD3	4:G:302:HOH:O	2.14	0.47
1:A:11:ARG:NH2	1:K:18:LEU:O	2.28	0.47
1:H:40:GLY:O	1:H:103:ARG:HA	2.13	0.47
1:J:17:LEU:CD2	1:J:126:TYR:HB3	2.44	0.47
2:J:201:HIS:HE1	1:K:88:ARG:HH22	1.59	0.47
1:D:117:GLU:O	1:G:70:ARG:HD2	2.14	0.47
1:I:109:GLY:O	1:I:111:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:ARG:HD2	2:L:201:HIS:HD1	1.79	0.47
1:C:99:THR:HG22	1:C:130:GLY:O	2.14	0.47
1:E:141:PHE:HE1	1:G:141:PHE:CD2	2.32	0.47
1:J:35:TRP:CZ3	1:J:109:GLY:HA3	2.50	0.47
1:F:4:HIS:CG	1:F:7:ARG:HG2	2.50	0.47
1:J:27:VAL:HG13	1:J:37:VAL:HG11	1.97	0.47
2:B:201:HIS:HB2	1:C:98:ARG:HB3	1.96	0.47
1:E:92:LEU:HD22	1:E:95:SER:OG	2.14	0.47
1:H:74:ALA:CB	1:H:148:ILE:HD12	2.44	0.47
1:B:59:LYS:HZ1	1:B:72:SER:HG	1.59	0.47
2:B:201:HIS:CE1	1:C:88:ARG:HH22	2.33	0.47
1:E:17:LEU:HD21	1:E:104:PHE:C	2.35	0.47
1:F:27:VAL:O	1:F:31:GLU:HG3	2.14	0.47
1:I:87:THR:HB	1:I:90:GLU:O	2.15	0.47
1:L:100:VAL:HB	1:L:102:LEU:HG	1.96	0.47
1:I:101:GLY:O	1:I:127:GLY:HA3	2.14	0.47
1:E:69:TYR:OH	1:F:138:HIS:HD2	1.98	0.47
1:G:35:TRP:HB3	1:G:107:LEU:HD22	1.96	0.47
1:J:73:HIS:O	1:J:77:HIS:HD2	1.98	0.47
1:D:46:ASP:HB3	1:D:48:HIS:CD2	2.49	0.47
1:G:15:LEU:O	1:G:19:ASN:ND2	2.43	0.47
1:A:78:ALA:O	1:A:144:GLY:HA3	2.15	0.46
1:B:17:LEU:HD21	1:B:104:PHE:C	2.34	0.46
1:H:6:GLU:O	1:H:12:LEU:HD11	2.16	0.46
1:A:55:GLU:HG2	1:A:59:LYS:HD2	1.97	0.46
1:C:8:ARG:O	1:C:12:LEU:HG	2.15	0.46
1:K:130:GLY:HA3	1:K:136:LEU:O	2.16	0.46
1:D:92:LEU:HD22	1:D:95:SER:OG	2.16	0.46
1:I:104:PHE:HB3	1:I:125:LEU:HD23	1.98	0.46
1:E:87:THR:HB	1:E:90:GLU:O	2.16	0.46
1:J:8:ARG:O	1:J:11:ARG:HG2	2.15	0.46
1:L:38:CYS:O	1:L:105:ALA:HA	2.16	0.46
1:A:90:GLU:HB3	1:A:92:LEU:HD12	1.97	0.46
1:C:76:TYR:CD1	2:C:201:HIS:HA	2.50	0.46
1:B:28:GLU:HA	1:B:31:GLU:OE1	2.16	0.46
2:D:201:HIS:HB3	1:E:130:GLY:HA2	1.97	0.46
1:I:38:CYS:O	1:I:105:ALA:HA	2.16	0.46
1:K:133:ILE:CG2	1:K:134:LYS:N	2.79	0.46
1:H:37:VAL:CG2	1:H:38:CYS:N	2.78	0.46
1:H:92:LEU:HD21	1:I:92:LEU:HD21	1.97	0.46
1:K:8:ARG:HH11	1:K:11:ARG:CZ	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:ILE:HG22	1:K:134:LYS:N	2.30	0.46
1:A:76:TYR:CD2	2:A:201:HIS:HA	2.51	0.46
1:C:42:VAL:HG13	1:C:42:VAL:O	2.16	0.46
1:F:71:GLU:CD	1:F:108:ARG:HH12	2.19	0.46
1:J:88:ARG:HH12	2:J:203:HIS:HE1	1.62	0.46
1:B:148:ILE:OXT	1:L:70:ARG:NH1	2.48	0.46
1:F:87:THR:HB	1:F:90:GLU:O	2.17	0.45
1:J:2:THR:HB	1:J:3:LEU:H	1.58	0.45
1:F:148:ILE:C	1:H:70:ARG:NH1	2.69	0.45
1:C:117:GLU:HA	1:C:117:GLU:OE1	2.16	0.45
1:I:111:PRO:HD2	1:I:112:TYR:HD1	1.81	0.45
1:A:96:LEU:HD21	1:C:91:MET:HG2	1.99	0.45
2:B:201:HIS:HE1	1:C:88:ARG:HH22	1.65	0.45
1:D:16:LEU:HD11	1:D:39:LEU:HD11	1.99	0.45
1:I:90:GLU:HB3	1:I:92:LEU:HD12	1.98	0.45
1:H:37:VAL:HG23	1:H:38:CYS:H	1.79	0.45
1:I:148:ILE:HG12	1:I:148:ILE:O	2.16	0.45
1:H:110:ASN:HD21	1:H:115:GLU:HA	1.82	0.45
1:H:131:ALA:HB1	1:H:132:PRO:HD2	1.98	0.45
1:A:97:LEU:CD1	1:A:132:PRO:HG2	2.47	0.45
1:G:17:LEU:CD2	1:G:126:TYR:HB3	2.47	0.45
1:H:9:ILE:HG23	1:H:10:GLY:N	2.31	0.45
2:A:201:HIS:HB3	1:B:130:GLY:CA	2.47	0.45
1:B:13:SER:HB3	1:B:107:LEU:HD22	1.99	0.44
1:H:133:ILE:HG22	1:H:134:LYS:H	1.80	0.44
1:C:139:GLU:OE1	1:L:10:GLY:N	2.42	0.44
1:H:11:ARG:HG2	1:H:15:LEU:HD22	1.99	0.44
1:I:125:LEU:O	1:I:141:PHE:HA	2.18	0.44
1:J:104:PHE:CB	1:J:125:LEU:HD23	2.46	0.44
1:J:17:LEU:HD21	1:J:103:ARG:HB3	1.98	0.44
1:F:88:ARG:HH12	2:F:201:HIS:HE1	1.66	0.44
1:A:73:HIS:CE1	1:A:77:HIS:CD2	3.06	0.44
1:D:55:GLU:HA	1:D:75:LEU:HD21	1.99	0.44
1:L:87:THR:HB	1:L:90:GLU:O	2.18	0.44
1:D:14:VAL:HG13	1:D:141:PHE:HZ	1.82	0.44
1:F:46:ASP:HB3	1:F:48:HIS:CD2	2.53	0.44
1:B:70:ARG:HD2	1:L:117:GLU:O	2.18	0.44
1:G:98:ARG:HB3	2:G:203:HIS:N	2.33	0.44
1:G:35:TRP:CE3	1:G:109:GLY:HA3	2.53	0.44
1:J:59:LYS:HB3	1:J:66:SER:OG	2.17	0.44
1:A:99:THR:O	1:A:129:ILE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:TYR:O	1:J:72:SER:HB2	2.18	0.43
1:G:26:GLN:C	1:G:28:GLU:N	2.69	0.43
1:G:4:HIS:HB3	1:G:7:ARG:HG2	2.01	0.43
1:J:76:TYR:CD1	2:J:201:HIS:N	2.86	0.43
1:L:148:ILE:HG12	1:L:148:ILE:O	2.18	0.43
1:D:48:HIS:HB2	1:E:97:LEU:HD13	2.00	0.43
1:I:19:ASN:O	1:I:20:GLU:OE1	2.36	0.43
1:J:74:ALA:HB3	1:J:148:ILE:HD12	2.01	0.43
1:J:90:GLU:HB3	1:J:92:LEU:HD12	2.00	0.43
1:L:101:GLY:O	1:L:127:GLY:HA3	2.18	0.43
1:E:7:ARG:HG3	1:E:111:PRO:HA	2.01	0.43
1:H:79:THR:O	1:H:83:LEU:HD12	2.19	0.43
2:B:201:HIS:HE1	1:C:88:ARG:HH12	1.67	0.43
1:L:8:ARG:HB2	1:L:11:ARG:HB3	2.00	0.43
1:G:69:TYR:HE2	1:H:137:GLU:C	2.22	0.43
1:L:81:GLU:O	1:L:84:HIS:HB2	2.19	0.43
1:H:48:HIS:HA	1:H:51:ILE:HD12	1.99	0.43
1:L:88:ARG:HH22	2:L:201:HIS:CE1	2.36	0.42
1:B:76:TYR:CE1	2:B:201:HIS:N	2.87	0.42
1:E:64:ILE:HB	1:E:71:GLU:HB3	2.00	0.42
1:G:126:TYR:CG	1:G:127:GLY:N	2.87	0.42
1:H:17:LEU:HD11	1:H:124:SER:CB	2.42	0.42
1:K:17:LEU:HD11	1:K:124:SER:CB	2.49	0.42
1:L:29:GLU:HA	1:L:32:ARG:HB2	2.00	0.42
1:G:4:HIS:HD2	1:G:6:GLU:N	2.04	0.42
1:J:107:LEU:HA	1:J:107:LEU:HD23	1.80	0.42
1:K:17:LEU:HD11	1:K:124:SER:HB2	2.00	0.42
1:L:39:LEU:HA	1:L:104:PHE:O	2.19	0.42
1:L:111:PRO:HD2	1:L:112:TYR:HD1	1.83	0.42
2:B:201:HIS:HB2	1:C:98:ARG:CB	2.49	0.42
1:E:18:LEU:HA	1:E:18:LEU:HD23	1.83	0.42
1:E:141:PHE:HB2	4:E:306:HOH:O	2.20	0.42
1:A:115:GLU:OE1	1:A:115:GLU:N	2.53	0.42
1:D:127:GLY:O	1:D:140:THR:N	2.53	0.42
1:F:88:ARG:HH12	2:F:201:HIS:CE1	2.38	0.42
1:G:71:GLU:HB3	1:G:148:ILE:HD11	2.02	0.42
1:J:9:ILE:HG23	1:J:10:GLY:N	2.34	0.42
1:D:26:GLN:CG	1:D:27:VAL:N	2.69	0.42
1:F:18:LEU:HD21	1:F:141:PHE:CZ	2.55	0.42
1:E:2:THR:HG23	1:G:135:GLY:HA2	2.00	0.42
1:H:27:VAL:O	1:H:31:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:LEU:HD13	1:I:100:VAL:HG22	2.02	0.41
1:J:82:ALA:O	1:J:142:GLY:HA3	2.20	0.41
2:A:201:HIS:OXT	2:A:201:HIS:CD2	2.73	0.41
1:D:71:GLU:CD	1:D:108:ARG:HH12	2.23	0.41
1:E:141:PHE:CE1	1:G:141:PHE:CD2	3.08	0.41
1:J:38:CYS:HB2	1:J:63:VAL:HG21	2.01	0.41
1:B:28:GLU:H	1:B:28:GLU:CD	2.23	0.41
1:C:4:HIS:CD2	1:C:6:GLU:HB2	2.55	0.41
1:B:141:PHE:CE1	1:J:141:PHE:CD2	3.08	0.41
1:A:46:ASP:HB3	1:A:48:HIS:HD2	1.79	0.41
1:F:88:ARG:NH2	2:F:201:HIS:HE1	2.13	0.41
1:G:26:GLN:C	1:G:28:GLU:H	2.23	0.41
1:B:138:HIS:HB2	1:J:145:ILE:HG21	2.03	0.41
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.94	0.41
1:B:33:ASP:OD2	1:B:33:ASP:N	2.54	0.41
1:E:139:GLU:OE1	1:G:10:GLY:N	2.50	0.41
1:E:28:GLU:HA	1:E:31:GLU:OE1	2.20	0.41
1:B:139:GLU:OE1	1:J:10:GLY:N	2.47	0.41
1:C:87:THR:HB	1:C:90:GLU:O	2.20	0.41
1:A:39:LEU:HD13	1:A:103:ARG:NH2	2.31	0.41
2:B:201:HIS:HD1	1:C:98:ARG:HD2	1.86	0.41
1:J:76:TYR:CD2	2:J:201:HIS:HA	2.56	0.41
1:E:35:TRP:CE3	1:E:109:GLY:HA3	2.56	0.41
1:G:51:ILE:CG2	1:H:97:LEU:HD23	2.50	0.41
1:J:17:LEU:O	1:J:17:LEU:HD23	2.21	0.41
1:J:73:HIS:CD2	1:K:138:HIS:HD2	2.39	0.41
1:C:76:TYR:CE1	2:C:201:HIS:HA	2.56	0.41
1:L:12:LEU:HD22	1:L:30:LEU:HD21	2.03	0.41
1:B:76:TYR:CD2	2:B:201:HIS:HA	2.56	0.41
1:I:88:ARG:HH22	2:I:201:HIS:CE1	2.38	0.41
1:J:54:ILE:HD11	1:J:125:LEU:HD21	2.03	0.41
2:J:201:HIS:OXT	1:K:130:GLY:HA2	2.21	0.41
1:D:82:ALA:O	1:D:142:GLY:HA3	2.21	0.41
1:G:4:HIS:HB3	1:G:7:ARG:CG	2.51	0.41
1:K:108:ARG:HG3	1:K:148:ILE:HG21	2.02	0.41
1:G:51:ILE:HD11	1:H:96:LEU:CD2	2.52	0.40
1:L:133:ILE:H	1:L:133:ILE:HG13	1.77	0.40
1:L:125:LEU:O	1:L:141:PHE:HA	2.20	0.40
1:L:30:LEU:O	1:L:35:TRP:HB2	2.21	0.40
1:D:39:LEU:HD23	1:D:105:ALA:HA	2.02	0.40
1:I:47:ALA:O	1:I:51:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:TYR:N	1:L:112:TYR:CD1	2.89	0.40
1:B:18:LEU:HD22	1:J:11:ARG:HB2	2.03	0.40
1:B:30:LEU:O	1:B:35:TRP:HB2	2.21	0.40
1:B:87:THR:HB	1:B:90:GLU:O	2.21	0.40
1:C:64:ILE:HD13	1:C:75:LEU:HD22	2.03	0.40
1:H:56:THR:HG23	1:H:60:LYS:HD2	2.03	0.40
1:L:98:ARG:HB3	2:L:201:HIS:N	2.36	0.40
1:E:100:VAL:HB	1:E:102:LEU:HG	2.04	0.40
1:K:27:VAL:HG23	1:K:28:GLU:OE1	2.22	0.40
1:I:13:SER:HB3	1:I:107:LEU:HD13	2.04	0.40
1:C:81:GLU:HB3	1:L:88:ARG:HD2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/148 (94%)	129 (93%)	10 (7%)	0	100	100
1	B	139/148 (94%)	128 (92%)	11 (8%)	0	100	100
1	C	135/148 (91%)	123 (91%)	11 (8%)	1 (1%)	24	42
1	D	138/148 (93%)	127 (92%)	11 (8%)	0	100	100
1	E	139/148 (94%)	128 (92%)	11 (8%)	0	100	100
1	F	139/148 (94%)	130 (94%)	9 (6%)	0	100	100
1	G	138/148 (93%)	123 (89%)	15 (11%)	0	100	100
1	H	139/148 (94%)	127 (91%)	12 (9%)	0	100	100
1	I	137/148 (93%)	123 (90%)	12 (9%)	2 (2%)	11	20
1	J	138/148 (93%)	125 (91%)	13 (9%)	0	100	100
1	K	139/148 (94%)	125 (90%)	13 (9%)	1 (1%)	24	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	138/148 (93%)	126 (91%)	11 (8%)	1 (1%)	24	42
All	All	1658/1776 (93%)	1514 (91%)	139 (8%)	5 (0%)	43	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	29	GLU
1	L	29	GLU
1	I	95	SER
1	C	132	PRO
1	K	62	GLY

### 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	108/119 (91%)	101 (94%)	7 (6%)	19	35
1	B	104/119 (87%)	97 (93%)	7 (7%)	18	34
1	C	109/119 (92%)	95 (87%)	14 (13%)	5	9
1	D	107/119 (90%)	101 (94%)	6 (6%)	23	43
1	E	105/119 (88%)	95 (90%)	10 (10%)	9	18
1	F	111/119 (93%)	101 (91%)	10 (9%)	10	20
1	G	107/119 (90%)	94 (88%)	13 (12%)	5	10
1	H	106/119 (89%)	91 (86%)	15 (14%)	3	7
1	I	111/119 (93%)	98 (88%)	13 (12%)	6	11
1	J	107/119 (90%)	88 (82%)	19 (18%)	2	3
1	K	105/119 (88%)	91 (87%)	14 (13%)	4	8
1	L	111/119 (93%)	99 (89%)	12 (11%)	7	13
All	All	1291/1428 (90%)	1151 (89%)	140 (11%)	7	13

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	25	THR
1	A	31	GLU
1	A	33	ASP
1	A	38	CYS
1	A	49	LYS
1	A	136	LEU
1	B	2	THR
1	B	7	ARG
1	B	15	LEU
1	B	27	VAL
1	B	38	CYS
1	B	72	SER
1	B	80	MET
1	C	8	ARG
1	C	17	LEU
1	C	20	GLU
1	C	29	GLU
1	C	32	ARG
1	C	33	ASP
1	C	38	CYS
1	C	49	LYS
1	C	65	GLN
1	C	80	MET
1	C	88	ARG
1	C	95	SER
1	C	115	GLU
1	C	146	ASN
1	D	15	LEU
1	D	17	LEU
1	D	31	GLU
1	D	107	LEU
1	D	117	GLU
1	D	136	LEU
1	E	2	THR
1	E	8	ARG
1	E	15	LEU
1	E	27	VAL
1	E	33	ASP
1	E	38	CYS
1	E	66	SER
1	E	72	SER
1	E	80	MET

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Mol	Chain	Res	Type
1	E	113	GLU
1	F	8	ARG
1	F	17	LEU
1	F	20	GLU
1	F	27	VAL
1	F	32	ARG
1	F	33	ASP
1	F	38	CYS
1	F	95	SER
1	F	115	GLU
1	F	146	ASN
1	G	3	LEU
1	G	7	ARG
1	G	15	LEU
1	G	20	GLU
1	G	31	GLU
1	G	33	ASP
1	G	41	LYS
1	G	70	ARG
1	G	72	SER
1	G	97	LEU
1	G	115	GLU
1	G	117	GLU
1	G	136	LEU
1	H	2	THR
1	H	15	LEU
1	H	45	MET
1	H	65	GLN
1	H	66	SER
1	H	80	MET
1	H	83	LEU
1	H	88	ARG
1	H	107	LEU
1	H	115	GLU
1	H	121	ILE
1	H	134	LYS
1	H	140	THR
1	H	141	PHE
1	H	148	ILE
1	I	2	THR
1	I	3	LEU
1	I	20	GLU

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Mol	Chain	Res	Type
1	I	33	ASP
1	I	45	MET
1	I	80	MET
1	I	95	SER
1	I	107	LEU
1	I	115	GLU
1	I	133	ILE
1	I	137	GLU
1	I	141	PHE
1	I	146	ASN
1	J	3	LEU
1	J	6	GLU
1	J	7	ARG
1	J	15	LEU
1	J	20	GLU
1	J	33	ASP
1	J	36	LYS
1	J	41	LYS
1	J	49	LYS
1	J	54	ILE
1	J	59	LYS
1	J	70	ARG
1	J	72	SER
1	J	88	ARG
1	J	97	LEU
1	J	115	GLU
1	J	117	GLU
1	J	136	LEU
1	J	139	GLU
1	K	2	THR
1	K	3	LEU
1	K	15	LEU
1	K	27	VAL
1	K	39	LEU
1	K	45	MET
1	K	66	SER
1	K	67	GLU
1	K	72	SER
1	K	83	LEU
1	K	107	LEU
1	K	128	THR
1	K	134	LYS

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Mol	Chain	Res	Type
1	K	140	THR
1	L	2	THR
1	L	4	HIS
1	L	20	GLU
1	L	45	MET
1	L	80	MET
1	L	95	SER
1	L	100	VAL
1	L	115	GLU
1	L	134	LYS
1	L	137	GLU
1	L	141	PHE
1	L	146	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	B	84	HIS
1	C	4	HIS
1	C	19	ASN
1	C	65	GLN
1	C	146	ASN
1	D	48	HIS
1	D	84	HIS
1	E	48	HIS
1	E	84	HIS
1	F	4	HIS
1	F	48	HIS
1	F	65	GLN
1	F	146	ASN
1	G	4	HIS
1	G	26	GLN
1	G	48	HIS
1	G	65	GLN
1	G	84	HIS
1	H	84	HIS
1	I	48	HIS
1	I	65	GLN
1	I	146	ASN
1	J	4	HIS
1	J	84	HIS

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Mol	Chain	Res	Type
1	L	65	GLN
1	L	146	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	HIS	A	201	3	3,11,11	0.37	0	3,14,14	1.73	1 (33%)
2	HIS	B	201	3	3,11,11	0.49	0	3,14,14	1.60	1 (33%)
2	HIS	C	201	3	3,11,11	0.38	0	3,14,14	1.83	1 (33%)
2	HIS	D	201	3	3,11,11	0.62	0	3,14,14	1.72	1 (33%)
2	HIS	D	203	3	3,11,11	0.37	0	3,14,14	1.73	1 (33%)
2	HIS	F	201	3	3,11,11	0.54	0	3,14,14	1.70	1 (33%)
2	HIS	G	201	3	3,11,11	0.22	0	3,14,14	1.24	0
2	HIS	G	203	3	3,11,11	0.46	0	3,14,14	1.50	1 (33%)
2	HIS	I	201	3	3,11,11	0.51	0	3,14,14	1.47	1 (33%)
2	HIS	J	201	3	3,11,11	0.30	0	3,14,14	1.30	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HIS	J	203	3	3,11,11	0.25	0	3,14,14	1.49	1 (33%)
2	HIS	L	201	3	3,11,11	0.59	0	3,14,14	1.36	1 (33%)

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
2	HIS	A	201	3	-	0/4/8/8	0/1/1/1
2	HIS	B	201	3	-	0/4/8/8	0/1/1/1
2	HIS	C	201	3	-	0/4/8/8	0/1/1/1
2	HIS	D	201	3	-	0/4/8/8	0/1/1/1
2	HIS	D	203	3	-	0/4/8/8	0/1/1/1
2	HIS	F	201	3	-	0/4/8/8	0/1/1/1
2	HIS	G	201	3	-	0/4/8/8	0/1/1/1
2	HIS	G	203	3	-	0/4/8/8	0/1/1/1
2	HIS	I	201	3	-	0/4/8/8	0/1/1/1
2	HIS	J	201	3	-	0/4/8/8	0/1/1/1
2	HIS	J	203	3	-	0/4/8/8	0/1/1/1
2	HIS	L	201	3	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	201	HIS	CD2-NE2-CE1	2.10	109.06	105.78
2	L	201	HIS	CD2-NE2-CE1	2.15	109.14	105.78
2	I	201	HIS	CD2-NE2-CE1	2.26	109.31	105.78
2	J	203	HIS	CD2-NE2-CE1	2.33	109.42	105.78
2	G	203	HIS	CD2-NE2-CE1	2.37	109.48	105.78
2	B	201	HIS	CD2-NE2-CE1	2.48	109.65	105.78
2	F	201	HIS	CD2-NE2-CE1	2.64	109.91	105.78
2	D	203	HIS	CD2-NE2-CE1	2.71	110.00	105.78
2	A	201	HIS	CD2-NE2-CE1	2.83	110.20	105.78
2	D	201	HIS	CD2-NE2-CE1	2.86	110.25	105.78
2	C	201	HIS	CD2-NE2-CE1	2.95	110.38	105.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	HIS	8	0
2	B	201	HIS	9	0
2	C	201	HIS	4	0
2	D	201	HIS	3	0
2	D	203	HIS	2	0
2	F	201	HIS	6	0
2	G	201	HIS	3	0
2	G	203	HIS	2	0
2	I	201	HIS	4	0
2	J	201	HIS	7	0
2	J	203	HIS	5	0
2	L	201	HIS	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	143/148 (96%)	-0.20	5 (3%)	44	47	32, 53, 97, 135	1 (0%)
1	B	143/148 (96%)	-0.23	3 (2%)	63	66	33, 54, 89, 110	1 (0%)
1	C	139/148 (93%)	-0.40	2 (1%)	75	77	30, 44, 74, 108	2 (1%)
1	D	142/148 (95%)	-0.20	4 (2%)	53	56	31, 54, 93, 130	1 (0%)
1	E	143/148 (96%)	-0.23	1 (0%)	87	88	33, 56, 90, 108	1 (0%)
1	F	143/148 (96%)	-0.37	3 (2%)	63	66	26, 44, 76, 105	2 (1%)
1	G	142/148 (95%)	0.08	7 (4%)	29	32	39, 63, 95, 118	1 (0%)
1	H	143/148 (96%)	0.13	9 (6%)	20	21	39, 59, 101, 145	1 (0%)
1	I	141/148 (95%)	-0.15	4 (2%)	53	56	34, 51, 95, 133	2 (1%)
1	J	142/148 (95%)	0.20	6 (4%)	36	39	35, 63, 93, 120	0
1	K	143/148 (96%)	0.33	9 (6%)	20	21	37, 59, 101, 157	1 (0%)
1	L	142/148 (95%)	-0.12	5 (3%)	44	47	29, 51, 100, 123	2 (1%)
All	All	1706/1776 (96%)	-0.10	58 (3%)	45	48	26, 55, 96, 157	15 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	4	HIS	19.2
1	K	2	THR	11.0
1	G	2	THR	8.1
1	H	4	HIS	8.1
1	L	2	THR	7.7
1	H	2	THR	6.0
1	I	2	THR	5.2
1	K	5	LYS	5.2
1	L	32	ARG	4.8
1	K	114	SER	4.7
1	H	114	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	4	HIS	4.6
1	C	32	ARG	4.4
1	J	68	GLY	4.3
1	J	2	THR	4.0
1	K	3	LEU	3.9
1	D	7	ARG	3.9
1	I	3	LEU	3.9
1	A	111	PRO	3.8
1	H	3	LEU	3.7
1	A	6	GLU	3.6
1	L	4	HIS	3.4
1	H	134	LYS	3.3
1	L	3	LEU	3.2
1	D	111	PRO	3.1
1	L	135	GLY	3.1
1	G	141	PHE	3.1
1	B	34	GLY	3.0
1	H	141	PHE	3.0
1	H	5	LYS	3.0
1	I	32	ARG	2.9
1	B	26	GLN	2.9
1	F	32	ARG	2.8
1	G	32	ARG	2.7
1	J	32	ARG	2.6
1	K	133	ILE	2.6
1	K	141	PHE	2.6
1	E	2	THR	2.5
1	A	7	ARG	2.5
1	K	134	LYS	2.5
1	G	148	ILE	2.4
1	J	141	PHE	2.4
1	H	133	ILE	2.4
1	G	62	GLY	2.3
1	J	4	HIS	2.3
1	F	21	ALA	2.2
1	B	33	ASP	2.2
1	J	28	GLU	2.2
1	A	20	GLU	2.1
1	G	56	THR	2.1
1	D	112	TYR	2.1
1	A	148	ILE	2.1
1	H	17	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	132	PRO	2.1
1	D	2	THR	2.1
1	G	58	SER	2.0
1	K	26	GLN	2.0
1	C	132	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no 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. 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	HIS	I	201	11/11	0.90	0.23	42,55,60,62	0
2	HIS	J	203	11/11	0.90	0.23	43,46,52,52	0
2	HIS	F	201	11/11	0.91	0.17	38,39,44,50	0
2	HIS	A	201	11/11	0.91	0.20	41,46,51,52	0
2	HIS	D	203	11/11	0.92	0.18	41,45,49,49	0
2	HIS	D	201	11/11	0.92	0.17	41,47,59,63	0
2	HIS	C	201	11/11	0.92	0.20	41,48,51,51	0
2	HIS	J	201	11/11	0.93	0.16	68,72,84,88	0
2	HIS	G	203	11/11	0.93	0.18	42,44,48,53	0
2	HIS	B	201	11/11	0.94	0.15	36,39,47,50	0
2	HIS	L	201	11/11	0.94	0.17	43,54,60,62	0
2	HIS	G	201	11/11	0.95	0.14	76,80,85,92	0
3	ZN	C	202	1/1	0.95	0.12	48,48,48,48	0
3	ZN	I	202	1/1	0.96	0.15	56,56,56,56	0
3	ZN	A	202	1/1	0.96	0.15	47,47,47,47	0
3	ZN	D	202	1/1	0.97	0.12	46,46,46,46	0
3	ZN	B	202	1/1	0.97	0.14	50,50,50,50	0
3	ZN	E	201	1/1	0.98	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	F	202	1/1	0.98	0.12	43,43,43,43	0
3	ZN	L	202	1/1	0.98	0.14	54,54,54,54	0
3	ZN	H	201	1/1	0.99	0.14	46,46,46,46	0
3	ZN	K	201	1/1	0.99	0.12	46,46,46,46	0
3	ZN	J	202	1/1	0.99	0.11	60,60,60,60	0
3	ZN	G	202	1/1	1.00	0.12	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.