



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 12:43 am BST

PDB ID : 2P1B  
Title : Crystal structure of human nucleophosmin-core  
Authors : Lee, H.H.; Kim, H.S.; Kang, J.Y.; Lee, B.I.; Ha, J.Y.; Yoon, H.J.; Lim, S.O.;  
Jung, G.; Suh, S.W.  
Deposited on : 2007-03-03  
Resolution : 2.75 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

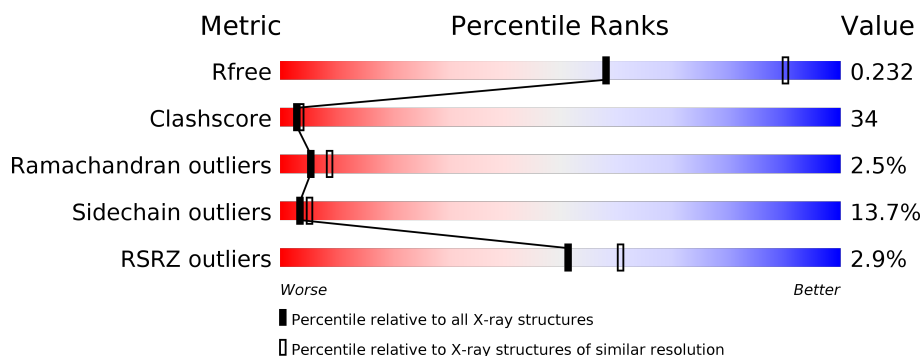
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	122	<div> <div>2%</div> <div> <div></div> <div>38%</div> <div>35%</div> <div>9%</div> <div>18%</div> </div> </div>
1	B	122	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>32%</div> <div>6%</div> <div>18%</div> </div> </div>
1	C	122	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>42%</div> <div>7%</div> <div>18%</div> </div> </div>
1	D	122	<div> <div>2%</div> <div> <div></div> <div>32%</div> <div>41%</div> <div>8%</div> <div>18%</div> </div> </div>
1	E	122	<div> <div>3%</div> <div> <div></div> <div>34%</div> <div>41%</div> <div>7%</div> <div>18%</div> </div> </div>
1	F	122	<div> <div>2%</div> <div> <div></div> <div>38%</div> <div>39%</div> <div>6%</div> <div>18%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	122	<div><div></div><div>2%</div><div>38%</div><div>33%</div><div>11%</div><div>18%</div></div>
1	H	122	<div><div></div><div>4%</div><div>41%</div><div>30%</div><div>11%</div><div>•</div><div>18%</div></div>
1	I	122	<div><div></div><div>3%</div><div>39%</div><div>38%</div><div>5%</div><div>18%</div></div>
1	J	122	<div><div></div><div>%</div><div>45%</div><div>33%</div><div>•</div><div>18%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7686 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 Nucleophosmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	B	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	C	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	D	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	E	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	F	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	G	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	H	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	I	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			
1	J	100	Total	C	N	O	S	0	0	0
			760	484	129	143	4			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	LEU	-	EXPRESSION TAG	UNP P06748
A	124	GLU	-	EXPRESSION TAG	UNP P06748
A	125	HIS	-	EXPRESSION TAG	UNP P06748
A	126	HIS	-	EXPRESSION TAG	UNP P06748
A	127	HIS	-	EXPRESSION TAG	UNP P06748
A	128	HIS	-	EXPRESSION TAG	UNP P06748
A	129	HIS	-	EXPRESSION TAG	UNP P06748
A	130	HIS	-	EXPRESSION TAG	UNP P06748
B	123	LEU	-	EXPRESSION TAG	UNP P06748

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	124	GLU	-	EXPRESSION TAG	UNP P06748
B	125	HIS	-	EXPRESSION TAG	UNP P06748
B	126	HIS	-	EXPRESSION TAG	UNP P06748
B	127	HIS	-	EXPRESSION TAG	UNP P06748
B	128	HIS	-	EXPRESSION TAG	UNP P06748
B	129	HIS	-	EXPRESSION TAG	UNP P06748
B	130	HIS	-	EXPRESSION TAG	UNP P06748
C	123	LEU	-	EXPRESSION TAG	UNP P06748
C	124	GLU	-	EXPRESSION TAG	UNP P06748
C	125	HIS	-	EXPRESSION TAG	UNP P06748
C	126	HIS	-	EXPRESSION TAG	UNP P06748
C	127	HIS	-	EXPRESSION TAG	UNP P06748
C	128	HIS	-	EXPRESSION TAG	UNP P06748
C	129	HIS	-	EXPRESSION TAG	UNP P06748
C	130	HIS	-	EXPRESSION TAG	UNP P06748
D	123	LEU	-	EXPRESSION TAG	UNP P06748
D	124	GLU	-	EXPRESSION TAG	UNP P06748
D	125	HIS	-	EXPRESSION TAG	UNP P06748
D	126	HIS	-	EXPRESSION TAG	UNP P06748
D	127	HIS	-	EXPRESSION TAG	UNP P06748
D	128	HIS	-	EXPRESSION TAG	UNP P06748
D	129	HIS	-	EXPRESSION TAG	UNP P06748
D	130	HIS	-	EXPRESSION TAG	UNP P06748
E	123	LEU	-	EXPRESSION TAG	UNP P06748
E	124	GLU	-	EXPRESSION TAG	UNP P06748
E	125	HIS	-	EXPRESSION TAG	UNP P06748
E	126	HIS	-	EXPRESSION TAG	UNP P06748
E	127	HIS	-	EXPRESSION TAG	UNP P06748
E	128	HIS	-	EXPRESSION TAG	UNP P06748
E	129	HIS	-	EXPRESSION TAG	UNP P06748
E	130	HIS	-	EXPRESSION TAG	UNP P06748
F	123	LEU	-	EXPRESSION TAG	UNP P06748
F	124	GLU	-	EXPRESSION TAG	UNP P06748
F	125	HIS	-	EXPRESSION TAG	UNP P06748
F	126	HIS	-	EXPRESSION TAG	UNP P06748
F	127	HIS	-	EXPRESSION TAG	UNP P06748
F	128	HIS	-	EXPRESSION TAG	UNP P06748
F	129	HIS	-	EXPRESSION TAG	UNP P06748
F	130	HIS	-	EXPRESSION TAG	UNP P06748
G	123	LEU	-	EXPRESSION TAG	UNP P06748
G	124	GLU	-	EXPRESSION TAG	UNP P06748
G	125	HIS	-	EXPRESSION TAG	UNP P06748

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	126	HIS	-	EXPRESSION TAG	UNP P06748
G	127	HIS	-	EXPRESSION TAG	UNP P06748
G	128	HIS	-	EXPRESSION TAG	UNP P06748
G	129	HIS	-	EXPRESSION TAG	UNP P06748
G	130	HIS	-	EXPRESSION TAG	UNP P06748
H	123	LEU	-	EXPRESSION TAG	UNP P06748
H	124	GLU	-	EXPRESSION TAG	UNP P06748
H	125	HIS	-	EXPRESSION TAG	UNP P06748
H	126	HIS	-	EXPRESSION TAG	UNP P06748
H	127	HIS	-	EXPRESSION TAG	UNP P06748
H	128	HIS	-	EXPRESSION TAG	UNP P06748
H	129	HIS	-	EXPRESSION TAG	UNP P06748
H	130	HIS	-	EXPRESSION TAG	UNP P06748
I	123	LEU	-	EXPRESSION TAG	UNP P06748
I	124	GLU	-	EXPRESSION TAG	UNP P06748
I	125	HIS	-	EXPRESSION TAG	UNP P06748
I	126	HIS	-	EXPRESSION TAG	UNP P06748
I	127	HIS	-	EXPRESSION TAG	UNP P06748
I	128	HIS	-	EXPRESSION TAG	UNP P06748
I	129	HIS	-	EXPRESSION TAG	UNP P06748
I	130	HIS	-	EXPRESSION TAG	UNP P06748
J	123	LEU	-	EXPRESSION TAG	UNP P06748
J	124	GLU	-	EXPRESSION TAG	UNP P06748
J	125	HIS	-	EXPRESSION TAG	UNP P06748
J	126	HIS	-	EXPRESSION TAG	UNP P06748
J	127	HIS	-	EXPRESSION TAG	UNP P06748
J	128	HIS	-	EXPRESSION TAG	UNP P06748
J	129	HIS	-	EXPRESSION TAG	UNP P06748
J	130	HIS	-	EXPRESSION TAG	UNP P06748

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	15	Total O 15 15	0	0
2	C	8	Total O 8 8	0	0
2	D	8	Total O 8 8	0	0
2	E	5	Total O 5 5	0	0

*Continued on next page...*

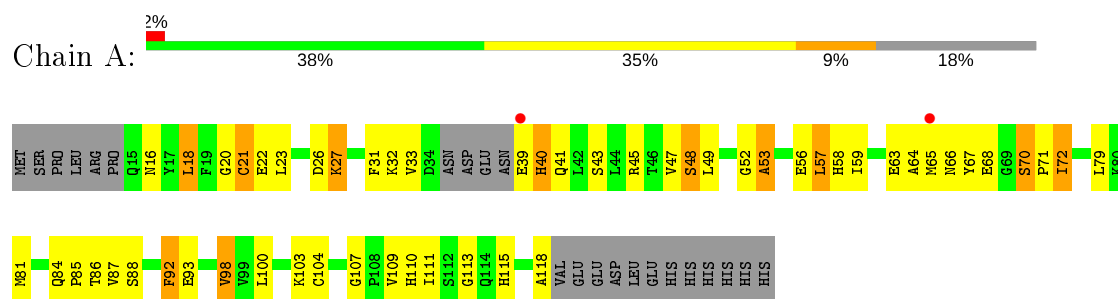
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	8	Total 8	O 8	0	0
2	G	5	Total 5	O 5	0	0
2	H	11	Total 11	O 11	0	0
2	I	5	Total 5	O 5	0	0
2	J	11	Total 11	O 11	0	0

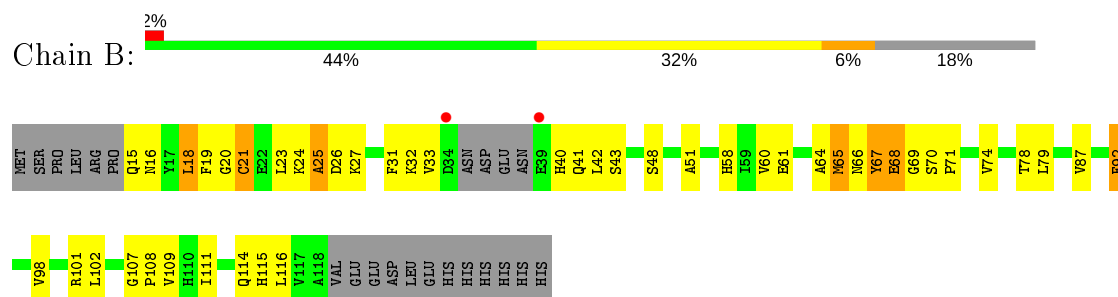
### 3 Residue-property plots [i](#)

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.

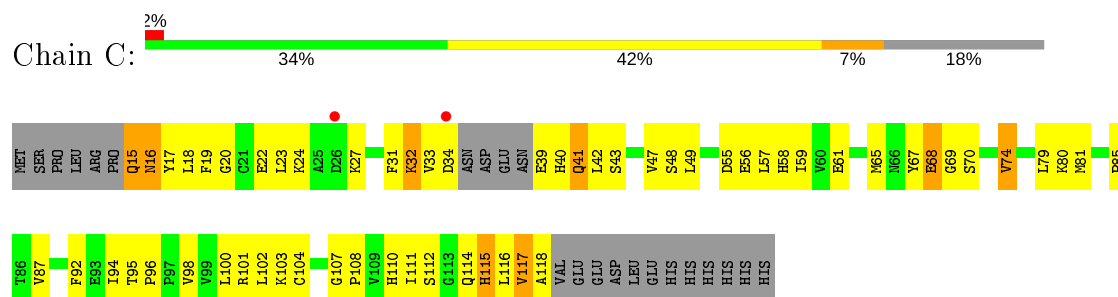
#### • Molecule 1: Nucleophosmin



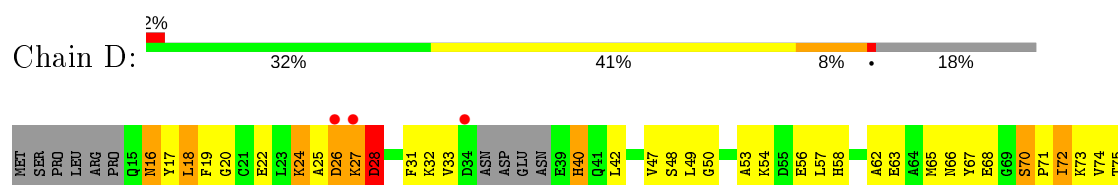
#### • Molecule 1: Nucleophosmin



#### • Molecule 1: Nucleophosmin



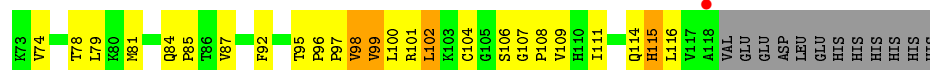
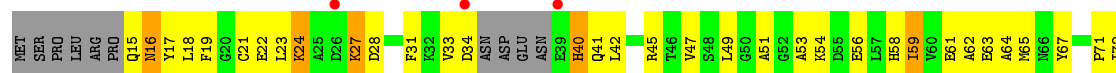
#### • Molecule 1: Nucleophosmin



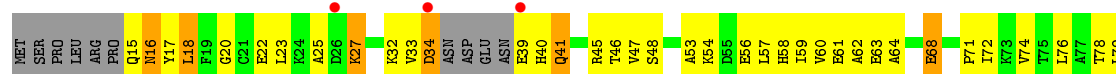




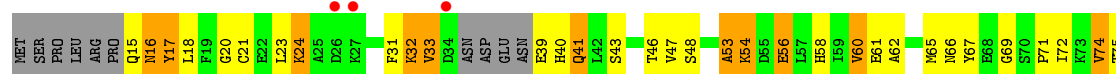
• Molecule 1: Nucleophosmin



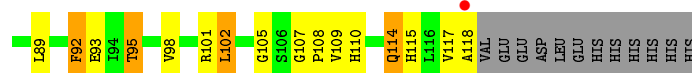
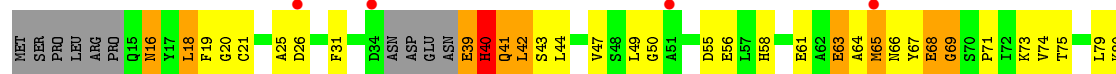
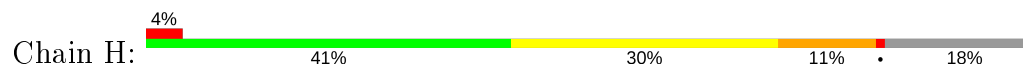
• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin

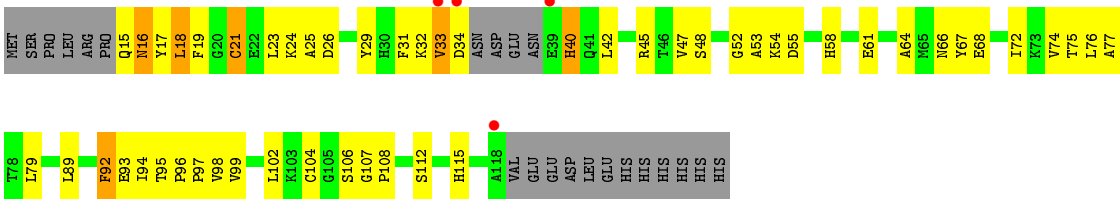


• Molecule 1: Nucleophosmin

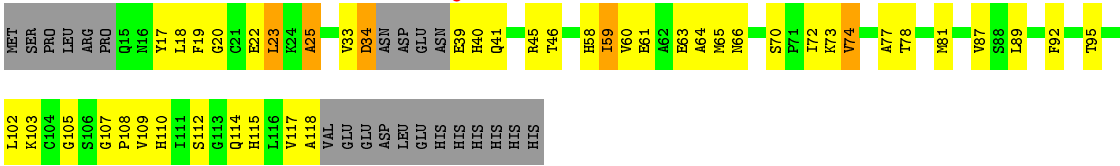


• Molecule 1: Nucleophosmin





● Molecule 1: Nucleophosmin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.26 Å 107.84 Å 108.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.75 19.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.91-2.75) 94.6 (19.91-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.75 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.232 0.211 , 0.232	Depositor DCC
$R_{free}$ test set	2915 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 38.05 % 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 3.9082e-04. 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 ⓘ

### 5.1 Standard geometry ⓘ

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	0.39	0/774	0.74	0/1046
1	B	0.44	0/774	0.75	0/1046
1	C	0.42	0/774	0.75	0/1046
1	D	0.42	0/774	0.76	0/1046
1	E	0.42	0/774	0.79	0/1046
1	F	0.39	0/774	0.72	0/1046
1	G	0.40	0/774	0.75	0/1046
1	H	0.44	0/774	0.88	2/1046 (0.2%)
1	I	0.40	0/774	0.75	0/1046
1	J	0.42	0/774	0.79	1/1046 (0.1%)
All	All	0.41	0/7740	0.77	3/10460 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	40	HIS	N-CA-C	8.06	132.76	111.00
1	J	25	ALA	N-CA-C	6.24	127.86	111.00
1	H	39	GLU	CB-CA-C	5.30	121.00	110.40

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	760	0	767	52	0
1	B	760	0	767	51	0
1	C	760	0	767	71	0
1	D	760	0	767	76	0
1	E	760	0	767	80	0
1	F	760	0	767	58	0
1	G	760	0	767	50	0
1	H	760	0	767	61	0
1	I	760	0	767	63	0
1	J	760	0	767	47	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
2	E	5	0	0	0	0
2	F	8	0	0	0	0
2	G	5	0	0	0	0
2	H	11	0	0	1	0
2	I	5	0	0	0	0
2	J	11	0	0	0	0
All	All	7686	0	7670	526	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 34.

All (526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LYS:HG2	1:D:28:ASP:N	1.56	1.12
1:D:27:LYS:CG	1:D:28:ASP:H	1.68	1.04
1:D:27:LYS:HG2	1:D:28:ASP:H	0.87	1.02
1:E:16:ASN:HD22	1:E:16:ASN:H	1.10	0.97
1:I:58:HIS:HE1	1:I:107:GLY:H	0.97	0.97
1:D:50:GLY:HA3	1:D:108:PRO:HG2	1.46	0.95
1:H:74:VAL:HG21	1:I:18:LEU:HD22	1.48	0.94
1:J:58:HIS:HE1	1:J:107:GLY:H	1.16	0.94
1:I:58:HIS:CE1	1:I:107:GLY:H	1.85	0.93
1:D:16:ASN:H	1:D:16:ASN:HD22	1.09	0.92
1:E:59:ILE:HG13	1:E:104:CYS:SG	2.09	0.92
1:E:58:HIS:HE1	1:E:107:GLY:H	1.17	0.92
1:A:58:HIS:HE1	1:A:107:GLY:H	1.20	0.90
1:F:20:GLY:HA3	1:J:74:VAL:HG22	1.54	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:HA3	1:C:74:VAL:HG22	1.54	0.89
1:B:24:LYS:O	1:B:26:ASP:N	2.06	0.89
1:B:58:HIS:HE1	1:B:107:GLY:H	1.22	0.88
1:H:68:GLU:H	1:H:68:GLU:CD	1.74	0.87
1:F:18:LEU:HD12	1:J:64:ALA:HB3	1.58	0.86
1:I:89:LEU:HD23	1:J:46:THR:HG21	1.57	0.85
1:D:16:ASN:N	1:D:16:ASN:HD22	1.74	0.85
1:I:58:HIS:HE1	1:I:107:GLY:N	1.75	0.84
1:C:15:GLN:HE21	1:C:15:GLN:HA	1.45	0.82
1:H:41:GLN:NE2	1:H:95:THR:HG23	1.96	0.81
1:D:18:LEU:HD12	1:E:64:ALA:HB3	1.61	0.80
1:H:18:LEU:HD22	1:H:19:PHE:H	1.47	0.79
1:B:40:HIS:ND1	1:B:115:HIS:HE1	1.81	0.78
1:E:16:ASN:HD22	1:E:16:ASN:N	1.82	0.78
1:E:64:ALA:HB2	1:E:98:VAL:HG23	1.65	0.78
1:F:33:VAL:HG11	1:F:40:HIS:CE1	2.19	0.77
1:H:58:HIS:HE1	1:H:107:GLY:H	1.31	0.77
1:H:65:MET:HA	1:H:71:PRO:HA	1.65	0.77
1:B:23:LEU:HB3	1:B:102:LEU:HD13	1.66	0.77
1:B:23:LEU:HD11	1:B:111:ILE:HD11	1.65	0.77
1:E:22:GLU:O	1:E:27:LYS:HE2	1.84	0.77
1:C:58:HIS:CE1	1:C:107:GLY:H	2.03	0.76
1:F:16:ASN:HD22	1:F:16:ASN:H	1.32	0.76
1:B:114:GLN:NE2	1:B:116:LEU:HD21	2.01	0.76
1:F:20:GLY:HA2	1:F:111:ILE:O	1.86	0.75
1:C:58:HIS:HE1	1:C:107:GLY:H	1.32	0.75
1:H:42:LEU:O	1:H:93:GLU:HA	1.86	0.74
1:I:64:ALA:HB2	1:I:98:VAL:HG23	1.69	0.74
1:A:33:VAL:HG11	1:A:40:HIS:CG	2.22	0.74
1:F:33:VAL:HG12	1:F:34:ASP:H	1.53	0.74
1:I:47:VAL:HG12	1:I:79:LEU:HD11	1.69	0.74
1:D:58:HIS:HE1	1:D:107:GLY:H	1.35	0.73
1:G:47:VAL:HG11	1:G:60:VAL:HG21	1.68	0.73
1:G:74:VAL:CG2	1:H:20:GLY:HA3	2.19	0.72
1:H:64:ALA:HB3	1:I:18:LEU:HD12	1.70	0.72
1:C:40:HIS:ND1	1:C:115:HIS:HE1	1.87	0.72
1:C:31:PHE:CE2	1:C:96:PRO:HG3	2.25	0.72
1:D:33:VAL:HG11	1:D:40:HIS:NE2	2.05	0.72
1:F:74:VAL:CG1	1:G:112:SER:HB2	2.20	0.71
1:A:64:ALA:HB3	1:E:18:LEU:HD12	1.71	0.71
1:B:58:HIS:CE1	1:B:107:GLY:H	2.08	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASN:HB3	1:D:72:ILE:HG21	1.72	0.71
1:J:58:HIS:CE1	1:J:107:GLY:H	2.05	0.70
1:H:41:GLN:HE22	1:H:95:THR:HG23	1.56	0.70
1:J:41:GLN:HE22	1:J:95:THR:HA	1.55	0.70
1:A:103:LYS:O	1:A:103:LYS:HG2	1.89	0.70
1:E:16:ASN:HB3	1:E:116:LEU:HD23	1.72	0.70
1:E:62:ALA:HA	1:E:99:VAL:O	1.91	0.70
1:A:58:HIS:HE1	1:A:107:GLY:N	1.89	0.70
1:C:16:ASN:HB3	1:C:116:LEU:HD23	1.75	0.69
1:B:20:GLY:HA3	1:C:74:VAL:CG2	2.21	0.69
1:F:74:VAL:HG22	1:G:20:GLY:HA3	1.73	0.69
1:C:79:LEU:HD21	1:C:87:VAL:HG23	1.74	0.69
1:F:33:VAL:HG12	1:F:34:ASP:N	2.08	0.69
1:J:41:GLN:NE2	1:J:95:THR:HA	2.06	0.69
1:F:58:HIS:CE1	1:F:107:GLY:H	2.11	0.69
1:I:89:LEU:HD23	1:J:46:THR:CG2	2.21	0.68
1:J:41:GLN:HE22	1:J:95:THR:CA	2.05	0.68
1:D:33:VAL:HG11	1:D:40:HIS:CE1	2.29	0.68
1:C:15:GLN:NE2	1:C:15:GLN:HA	2.09	0.68
1:G:65:MET:HG2	1:G:69:GLY:O	1.95	0.67
1:H:16:ASN:H	1:H:16:ASN:HD22	1.43	0.67
1:E:58:HIS:C	1:E:59:ILE:HG12	2.14	0.67
1:B:24:LYS:HE3	1:B:27:LYS:HE3	1.77	0.67
1:D:19:PHE:O	1:E:74:VAL:HG21	1.95	0.67
1:I:23:LEU:HB2	1:I:102:LEU:HD11	1.77	0.67
1:C:16:ASN:HB3	1:C:116:LEU:CD2	2.25	0.66
1:H:63:GLU:HG3	1:H:73:LYS:HG2	1.75	0.66
1:B:24:LYS:O	1:B:27:LYS:N	2.28	0.66
1:A:20:GLY:HA3	1:B:74:VAL:HG22	1.76	0.66
1:E:63:GLU:O	1:E:99:VAL:HG23	1.95	0.66
1:H:67:TYR:HB3	1:H:68:GLU:OE2	1.95	0.66
1:G:40:HIS:ND1	1:G:115:HIS:HE1	1.93	0.66
1:J:40:HIS:CE1	1:J:115:HIS:HE1	2.13	0.66
1:D:22:GLU:O	1:D:27:LYS:NZ	2.28	0.65
1:D:112:SER:HB2	1:E:74:VAL:CG1	2.26	0.65
1:C:20:GLY:HA3	1:D:74:VAL:HG22	1.79	0.65
1:E:53:ALA:HB2	1:E:108:PRO:HD2	1.77	0.65
1:D:47:VAL:HG12	1:D:79:LEU:HD11	1.79	0.65
1:F:61:GLU:OE1	1:F:101:ARG:HD2	1.97	0.65
1:C:79:LEU:CD2	1:C:87:VAL:HG23	2.27	0.65
1:F:58:HIS:HE1	1:F:107:GLY:H	1.42	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:HIS:CE1	1:H:117:VAL:HG13	2.32	0.64
1:G:74:VAL:HG23	1:H:20:GLY:HA3	1.77	0.64
1:H:117:VAL:HG12	1:H:118:ALA:N	2.13	0.63
1:H:39:GLU:N	2:H:136:HOH:O	2.30	0.63
1:H:40:HIS:ND1	1:H:117:VAL:HG22	2.14	0.63
1:C:58:HIS:HE1	1:C:107:GLY:N	1.96	0.63
1:F:20:GLY:HA3	1:J:74:VAL:CG2	2.28	0.63
1:D:67:TYR:HD2	1:D:68:GLU:OE2	1.81	0.63
1:J:22:GLU:C	1:J:23:LEU:HD23	2.19	0.63
1:C:40:HIS:CE1	1:C:117:VAL:HG13	2.34	0.63
1:F:16:ASN:ND2	1:F:16:ASN:H	1.97	0.63
1:A:20:GLY:O	1:A:21:CYS:HB3	1.97	0.62
1:C:32:LYS:O	1:C:33:VAL:HG23	1.99	0.62
1:F:61:GLU:HG2	1:F:101:ARG:HG3	1.81	0.62
1:C:31:PHE:HE2	1:C:96:PRO:HG3	1.63	0.62
1:E:21:CYS:HB2	1:E:111:ILE:HB	1.80	0.62
1:G:33:VAL:HG21	1:G:40:HIS:ND1	2.14	0.62
1:D:20:GLY:HA3	1:E:74:VAL:HG22	1.80	0.62
1:C:59:ILE:HG21	1:C:103:LYS:HD3	1.82	0.62
1:J:63:GLU:HG3	1:J:73:LYS:HG3	1.81	0.62
1:A:65:MET:HA	1:A:71:PRO:HA	1.81	0.62
1:B:19:PHE:CZ	1:B:21:CYS:SG	2.94	0.61
1:F:79:LEU:HD23	1:F:87:VAL:HG23	1.83	0.61
1:C:23:LEU:O	1:C:108:PRO:HA	2.00	0.61
1:E:16:ASN:ND2	1:E:16:ASN:H	1.92	0.61
1:E:58:HIS:HE1	1:E:107:GLY:N	1.96	0.61
1:D:102:LEU:HD23	1:D:105:GLY:O	2.00	0.60
1:D:63:GLU:HB3	1:D:99:VAL:HG23	1.83	0.60
1:G:102:LEU:HD23	1:G:105:GLY:O	2.01	0.60
1:C:61:GLU:OE1	1:C:101:ARG:HD2	2.01	0.60
1:H:43:SER:HB3	1:H:114:GLN:HG3	1.82	0.60
1:G:103:LYS:NZ	1:H:110:HIS:NE2	2.48	0.60
1:D:54:LYS:HB2	1:D:56:GLU:HG2	1.83	0.60
1:F:41:GLN:HB3	1:F:116:LEU:HB2	1.84	0.60
1:A:39:GLU:HB2	1:A:118:ALA:HB2	1.84	0.60
1:D:25:ALA:O	1:D:26:ASP:HB2	2.00	0.60
1:E:19:PHE:CZ	1:E:21:CYS:SG	2.95	0.60
1:E:28:ASP:OD1	1:E:100:LEU:O	2.19	0.60
1:H:31:PHE:HB3	1:H:98:VAL:HG12	1.84	0.60
1:E:61:GLU:OE1	1:E:101:ARG:HD2	2.01	0.59
1:G:23:LEU:HB2	1:G:102:LEU:CD1	2.32	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:SER:HB3	1:J:78:THR:OG1	2.03	0.59
1:B:24:LYS:O	1:B:25:ALA:C	2.40	0.59
1:F:27:LYS:CG	1:F:27:LYS:O	2.50	0.59
1:A:115:HIS:HD2	1:B:67:TYR:HB2	1.67	0.59
1:C:22:GLU:HG3	1:C:110:HIS:CE1	2.37	0.59
1:F:17:TYR:HB2	1:F:115:HIS:HB3	1.85	0.59
1:C:31:PHE:CE2	1:C:42:LEU:HB2	2.37	0.59
1:I:33:VAL:HG11	1:I:40:HIS:CE1	2.36	0.59
1:I:40:HIS:ND1	1:I:115:HIS:HE1	2.01	0.58
1:F:46:THR:HG21	1:J:89:LEU:CD2	2.33	0.58
1:D:24:LYS:H	1:D:27:LYS:HD2	1.68	0.58
1:E:40:HIS:ND1	1:E:115:HIS:HE1	2.01	0.58
1:C:112:SER:HB3	1:D:75:THR:O	2.02	0.58
1:B:61:GLU:OE1	1:B:101:ARG:HD2	2.04	0.58
1:G:31:PHE:HB3	1:G:98:VAL:HG13	1.86	0.58
1:I:75:THR:O	1:J:112:SER:HB3	2.04	0.58
1:H:67:TYR:HD1	1:I:17:TYR:CE1	2.22	0.58
1:A:81:MET:O	1:A:85:PRO:HG3	2.04	0.57
1:C:16:ASN:HD22	1:C:16:ASN:N	2.02	0.57
1:B:23:LEU:O	1:B:108:PRO:HA	2.04	0.57
1:E:49:LEU:HD23	1:E:109:VAL:HG22	1.85	0.57
1:F:62:ALA:HB2	1:F:76:LEU:HD11	1.87	0.57
1:E:22:GLU:O	1:E:23:LEU:HD23	2.03	0.57
1:E:23:LEU:C	1:E:24:LYS:HG2	2.25	0.57
1:I:42:LEU:O	1:I:93:GLU:HA	2.05	0.57
1:G:16:ASN:HB3	1:G:116:LEU:HD23	1.87	0.56
1:I:21:CYS:HB2	1:I:29:TYR:CD1	2.39	0.56
1:I:72:ILE:HD11	1:J:18:LEU:C	2.26	0.56
1:A:58:HIS:CE1	1:A:107:GLY:H	2.11	0.56
1:D:66:ASN:HB3	1:D:72:ILE:CG2	2.34	0.56
1:H:58:HIS:HE1	1:H:107:GLY:N	2.02	0.56
1:D:40:HIS:ND1	1:D:115:HIS:HE1	2.03	0.56
1:D:49:LEU:HD12	1:D:85:PRO:HA	1.87	0.56
1:H:117:VAL:CG1	1:H:118:ALA:N	2.69	0.56
1:J:39:GLU:HB2	1:J:118:ALA:HB2	1.86	0.56
1:E:54:LYS:HB2	1:E:56:GLU:OE1	2.05	0.56
1:F:57:LEU:HD11	1:G:81:MET:SD	2.45	0.56
1:C:17:TYR:CE1	1:D:67:TYR:HD1	2.24	0.56
1:D:112:SER:HB2	1:E:74:VAL:HG11	1.86	0.56
1:G:23:LEU:HB2	1:G:102:LEU:HD11	1.87	0.56
1:H:74:VAL:HG21	1:I:18:LEU:CD2	2.28	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:HIS:CE1	1:J:115:HIS:CE1	2.94	0.56
1:E:16:ASN:HB3	1:E:116:LEU:CD2	2.36	0.56
1:H:61:GLU:OE1	1:H:101:ARG:HD2	2.06	0.56
1:I:33:VAL:HG11	1:I:40:HIS:NE2	2.20	0.56
1:B:24:LYS:HE3	1:B:27:LYS:CE	2.35	0.56
1:E:47:VAL:HG12	1:E:79:LEU:HD11	1.87	0.56
1:J:58:HIS:HE1	1:J:107:GLY:N	1.97	0.55
1:H:102:LEU:HD11	1:H:109:VAL:HG21	1.88	0.55
1:H:49:LEU:HD21	1:H:79:LEU:HB2	1.89	0.55
1:I:67:TYR:HA	1:J:17:TYR:CG	2.41	0.55
1:G:81:MET:O	1:G:85:PRO:HG3	2.06	0.55
1:C:79:LEU:HD21	1:C:87:VAL:CG2	2.36	0.55
1:J:39:GLU:HB2	1:J:118:ALA:CB	2.37	0.55
1:E:23:LEU:O	1:E:108:PRO:HA	2.07	0.55
1:I:66:ASN:HB3	1:I:72:ILE:HG12	1.89	0.55
1:B:58:HIS:HE1	1:B:107:GLY:N	1.98	0.55
1:E:21:CYS:SG	1:E:100:LEU:HD12	2.47	0.55
1:I:17:TYR:HB2	1:I:115:HIS:HB3	1.89	0.55
1:D:57:LEU:HD11	1:D:78:THR:CG2	2.36	0.55
1:F:25:ALA:HB2	1:F:106:SER:CB	2.37	0.55
1:F:74:VAL:HG13	1:G:112:SER:HB2	1.88	0.54
1:G:67:TYR:HB2	1:H:115:HIS:CD2	2.41	0.54
1:J:59:ILE:HG21	1:J:103:LYS:HD3	1.89	0.54
1:C:31:PHE:CD2	1:C:42:LEU:HD22	2.42	0.54
1:E:28:ASP:OD1	1:E:101:ARG:HA	2.07	0.54
1:A:22:GLU:HG3	1:A:110:HIS:CE1	2.42	0.54
1:C:41:GLN:HA	1:C:41:GLN:HE21	1.72	0.54
1:C:61:GLU:HG2	1:C:101:ARG:CG	2.37	0.54
1:D:42:LEU:HD23	1:D:98:VAL:HG11	1.89	0.54
1:C:41:GLN:HB3	1:C:116:LEU:HB2	1.90	0.54
1:G:67:TYR:HB2	1:H:115:HIS:HD2	1.72	0.54
1:B:31:PHE:HB3	1:B:98:VAL:HG13	1.89	0.54
1:C:42:LEU:HD23	1:C:98:VAL:HG11	1.90	0.54
1:H:18:LEU:HD22	1:H:19:PHE:N	2.21	0.54
1:I:74:VAL:HG22	1:J:20:GLY:HA3	1.89	0.54
1:D:18:LEU:HB3	1:E:72:ILE:HD11	1.90	0.53
1:H:31:PHE:CD2	1:H:42:LEU:HD13	2.42	0.53
1:I:72:ILE:HD11	1:J:18:LEU:HB3	1.91	0.53
1:A:33:VAL:HG11	1:A:40:HIS:ND1	2.22	0.53
1:C:81:MET:O	1:C:85:PRO:HG3	2.07	0.53
1:C:31:PHE:HB3	1:C:98:VAL:HG13	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:HG21	1:E:67:TYR:CE1	2.44	0.53
1:C:112:SER:HB2	1:D:74:VAL:CG1	2.39	0.53
1:F:27:LYS:O	1:F:27:LYS:HG2	2.08	0.53
1:A:66:ASN:OD1	1:A:68:GLU:N	2.39	0.53
1:C:41:GLN:HE21	1:C:41:GLN:CA	2.20	0.53
1:C:67:TYR:HB3	1:C:68:GLU:OE2	2.09	0.53
1:I:29:TYR:O	1:I:99:VAL:HG13	2.09	0.53
1:G:40:HIS:ND1	1:G:115:HIS:CE1	2.77	0.52
1:J:41:GLN:HE22	1:J:95:THR:CB	2.23	0.52
1:D:112:SER:CB	1:E:74:VAL:HG13	2.39	0.52
1:H:41:GLN:HE22	1:H:95:THR:CG2	2.23	0.52
1:E:95:THR:HG22	1:E:96:PRO:O	2.09	0.52
1:D:25:ALA:O	1:D:26:ASP:CB	2.57	0.52
1:F:54:LYS:HB2	1:F:56:GLU:HG2	1.91	0.52
1:G:105:GLY:O	1:G:106:SER:C	2.48	0.52
1:C:47:VAL:HG12	1:C:79:LEU:HD11	1.92	0.52
1:D:40:HIS:CE1	1:D:117:VAL:HG22	2.44	0.52
1:D:16:ASN:N	1:D:16:ASN:ND2	2.47	0.52
1:D:18:LEU:HD22	1:E:74:VAL:HG21	1.91	0.52
1:G:43:SER:HB2	1:G:93:GLU:HG2	1.91	0.52
1:D:49:LEU:HD13	1:D:81:MET:HE2	1.92	0.52
1:D:31:PHE:CD2	1:D:42:LEU:HD22	2.45	0.52
1:D:20:GLY:HA3	1:E:74:VAL:CG2	2.40	0.51
1:E:81:MET:O	1:E:85:PRO:HG3	2.10	0.51
1:G:41:GLN:HB3	1:G:116:LEU:HB2	1.91	0.51
1:I:16:ASN:O	1:I:16:ASN:ND2	2.43	0.51
1:H:92:PHE:CE1	1:I:45:ARG:HG3	2.46	0.51
1:B:67:TYR:HB3	1:B:68:GLU:OE2	2.10	0.51
1:H:63:GLU:O	1:H:98:VAL:HA	2.10	0.51
1:A:115:HIS:CD2	1:B:67:TYR:HB2	2.46	0.51
1:D:63:GLU:HG3	1:D:73:LYS:HG3	1.92	0.51
1:B:18:LEU:HD11	1:C:74:VAL:HB	1.93	0.51
1:C:23:LEU:C	1:C:24:LYS:HG2	2.31	0.51
1:E:58:HIS:CE1	1:E:107:GLY:H	2.09	0.51
1:C:24:LYS:HD3	1:C:108:PRO:HB3	1.93	0.51
1:F:16:ASN:N	1:F:16:ASN:HD22	1.96	0.51
1:C:55:ASP:OD2	1:C:80:LYS:NZ	2.44	0.50
1:G:17:TYR:CD1	1:G:17:TYR:N	2.79	0.50
1:G:39:GLU:HB2	1:G:118:ALA:HA	1.92	0.50
1:F:46:THR:HG21	1:J:89:LEU:HD22	1.92	0.50
1:E:61:GLU:HA	1:E:74:VAL:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:31:PHE:HD2	1:I:98:VAL:HG12	1.76	0.50
1:J:19:PHE:CG	1:J:20:GLY:N	2.79	0.50
1:C:15:GLN:O	1:C:116:LEU:HA	2.11	0.50
1:H:55:ASP:O	1:H:80:LYS:HE2	2.11	0.50
1:H:44:LEU:HB2	1:H:92:PHE:HB3	1.93	0.50
1:J:60:VAL:HG21	1:J:109:VAL:HG11	1.94	0.50
1:A:66:ASN:ND2	1:A:70:SER:O	2.44	0.50
1:E:56:GLU:O	1:E:58:HIS:HD2	1.95	0.50
1:G:61:GLU:HB2	1:G:74:VAL:O	2.12	0.50
1:A:52:GLY:O	1:A:53:ALA:C	2.50	0.50
1:B:15:GLN:O	1:B:116:LEU:HA	2.12	0.50
1:B:65:MET:HE1	1:B:69:GLY:O	2.11	0.50
1:E:100:LEU:HD13	1:E:111:ILE:HD12	1.93	0.50
1:A:92:PHE:CD1	1:E:45:ARG:HG3	2.47	0.50
1:E:64:ALA:HB2	1:E:98:VAL:CG2	2.40	0.50
1:G:39:GLU:O	1:G:118:ALA:N	2.45	0.50
1:G:47:VAL:CG1	1:G:60:VAL:HG21	2.39	0.50
1:E:61:GLU:HG2	1:E:101:ARG:CG	2.42	0.49
1:B:33:VAL:HG12	1:B:33:VAL:O	2.11	0.49
1:F:80:LYS:HD3	1:F:83:VAL:HG23	1.94	0.49
1:A:31:PHE:HB3	1:A:98:VAL:HG13	1.94	0.49
1:F:33:VAL:CG1	1:F:34:ASP:H	2.23	0.49
1:J:66:ASN:HD22	1:J:72:ILE:HG23	1.77	0.49
1:C:43:SER:HB3	1:C:114:GLN:HB2	1.94	0.49
1:F:59:ILE:HD13	1:F:78:THR:OG1	2.13	0.49
1:B:23:LEU:HD11	1:B:111:ILE:CD1	2.39	0.49
1:H:16:ASN:N	1:H:16:ASN:HD22	2.07	0.49
1:J:102:LEU:HD23	1:J:105:GLY:O	2.13	0.49
1:A:22:GLU:O	1:A:27:LYS:HE3	2.13	0.49
1:D:25:ALA:HB2	1:D:105:GLY:O	2.13	0.49
1:D:24:LYS:NZ	1:D:108:PRO:HB3	2.28	0.49
1:C:65:MET:HG2	1:C:69:GLY:O	2.13	0.49
1:D:85:PRO:HD2	1:E:84:GLN:OE1	2.12	0.49
1:A:33:VAL:O	1:A:33:VAL:HG12	2.12	0.49
1:A:22:GLU:O	1:A:27:LYS:NZ	2.45	0.49
1:C:61:GLU:HG2	1:C:101:ARG:HG3	1.95	0.49
1:G:21:CYS:SG	1:G:111:ILE:HB	2.52	0.49
1:G:33:VAL:HG21	1:G:40:HIS:CG	2.48	0.49
1:I:64:ALA:HB2	1:I:98:VAL:CG2	2.40	0.49
1:F:41:GLN:HA	1:F:41:GLN:HE21	1.78	0.48
1:B:24:LYS:HE3	1:B:27:LYS:NZ	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:HD13	1:D:111:ILE:HD12	1.96	0.48
1:D:112:SER:HB2	1:E:74:VAL:HG13	1.96	0.48
1:D:48:SER:HB3	1:E:78:THR:OG1	2.13	0.48
1:E:40:HIS:CE1	1:E:115:HIS:HE1	2.31	0.48
1:I:31:PHE:CD2	1:I:42:LEU:HD22	2.48	0.48
1:H:102:LEU:HD11	1:H:109:VAL:CG2	2.44	0.48
1:D:58:HIS:HA	1:D:104:CYS:O	2.12	0.48
1:A:92:PHE:CG	1:E:45:ARG:HG3	2.48	0.48
1:I:67:TYR:HD2	1:I:68:GLU:OE2	1.97	0.48
1:C:42:LEU:HD12	1:C:43:SER:N	2.28	0.48
1:F:107:GLY:HA2	1:F:109:VAL:HG23	1.96	0.48
1:F:79:LEU:CD2	1:F:87:VAL:HG23	2.44	0.48
1:B:68:GLU:H	1:B:68:GLU:CD	2.16	0.48
1:A:16:ASN:HD21	1:B:41:GLN:NE2	2.12	0.48
1:A:67:TYR:HB3	1:A:68:GLU:OE2	2.14	0.48
1:C:33:VAL:HG11	1:C:40:HIS:CE1	2.48	0.48
1:F:107:GLY:CA	1:F:109:VAL:HG23	2.44	0.48
1:G:47:VAL:HG12	1:G:79:LEU:HD11	1.95	0.48
1:I:21:CYS:SG	1:I:23:LEU:HG	2.54	0.48
1:D:80:LYS:NZ	1:I:55:ASP:OD2	2.42	0.48
1:C:112:SER:HB2	1:D:74:VAL:HG11	1.96	0.47
1:E:31:PHE:HB3	1:E:98:VAL:HG12	1.96	0.47
1:I:18:LEU:HD23	1:I:19:PHE:H	1.79	0.47
1:B:79:LEU:CD2	1:B:87:VAL:HG23	2.43	0.47
1:C:19:PHE:CG	1:C:20:GLY:N	2.81	0.47
1:J:23:LEU:HD12	1:J:102:LEU:CD1	2.44	0.47
1:A:67:TYR:HD2	1:A:68:GLU:OE2	1.97	0.47
1:F:102:LEU:HD11	1:F:109:VAL:HG21	1.95	0.47
1:B:40:HIS:O	1:B:41:GLN:OE1	2.33	0.47
1:D:67:TYR:CD2	1:D:68:GLU:OE2	2.66	0.47
1:F:40:HIS:ND1	1:F:117:VAL:HG22	2.29	0.47
1:F:61:GLU:HG2	1:F:101:ARG:CG	2.45	0.47
1:A:18:LEU:HD12	1:B:64:ALA:HB3	1.96	0.47
1:E:40:HIS:CE1	1:E:115:HIS:CE1	3.02	0.47
1:I:15:GLN:NE2	1:I:17:TYR:OH	2.47	0.47
1:A:47:VAL:HG12	1:A:79:LEU:HD11	1.96	0.47
1:F:41:GLN:HE21	1:F:41:GLN:CA	2.27	0.47
1:G:16:ASN:HB3	1:G:116:LEU:CD2	2.45	0.47
1:G:16:ASN:HD22	1:G:16:ASN:H	1.63	0.47
1:H:64:ALA:HB2	1:H:98:VAL:HG23	1.96	0.47
1:B:65:MET:HA	1:B:65:MET:HE3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:96:PRO:HA	1:I:97:PRO:C	2.35	0.47
1:H:67:TYR:O	1:H:69:GLY:N	2.37	0.47
1:I:18:LEU:HD23	1:I:19:PHE:N	2.29	0.47
1:H:41:GLN:NE2	1:H:95:THR:HA	2.30	0.46
1:C:114:GLN:HE21	1:C:116:LEU:HD21	1.81	0.46
1:B:51:ALA:HB2	1:C:59:ILE:CD1	2.46	0.46
1:D:54:LYS:C	1:D:56:GLU:H	2.17	0.46
1:F:33:VAL:CG1	1:F:34:ASP:N	2.77	0.46
1:H:75:THR:O	1:I:112:SER:HB3	2.16	0.46
1:A:59:ILE:HB	1:A:104:CYS:HB3	1.98	0.46
1:E:15:GLN:NE2	1:E:17:TYR:OH	2.48	0.46
1:H:47:VAL:HG12	1:H:79:LEU:HD11	1.96	0.46
1:I:61:GLU:HA	1:I:74:VAL:O	2.16	0.46
1:D:16:ASN:HB3	1:D:116:LEU:HD22	1.97	0.46
1:A:115:HIS:HE2	1:B:67:TYR:HD2	1.63	0.46
1:F:68:GLU:N	1:F:68:GLU:CD	2.69	0.46
1:H:49:LEU:CD2	1:H:79:LEU:HD12	2.45	0.46
1:I:95:THR:HA	1:I:96:PRO:HD3	1.74	0.46
1:I:42:LEU:HD23	1:I:98:VAL:HG11	1.97	0.46
1:J:77:ALA:HB1	1:J:87:VAL:HG21	1.98	0.46
1:D:42:LEU:O	1:D:93:GLU:HA	2.15	0.46
1:A:72:ILE:HD11	1:E:18:LEU:O	2.16	0.46
1:B:31:PHE:HB3	1:B:98:VAL:CG1	2.46	0.46
1:C:32:LYS:O	1:C:33:VAL:CG2	2.62	0.46
1:I:23:LEU:HB2	1:I:102:LEU:CD1	2.45	0.46
1:J:33:VAL:HG12	1:J:34:ASP:N	2.31	0.46
1:B:65:MET:HE1	1:B:71:PRO:HD3	1.98	0.46
1:C:16:ASN:ND2	1:C:16:ASN:N	2.63	0.46
1:E:56:GLU:OE2	1:E:106:SER:N	2.47	0.46
1:F:25:ALA:HB2	1:F:106:SER:HA	1.98	0.46
1:G:65:MET:HA	1:G:71:PRO:HA	1.97	0.46
1:B:60:VAL:HG21	1:B:109:VAL:HG11	1.98	0.45
1:E:102:LEU:HD11	1:E:109:VAL:HG21	1.98	0.45
1:F:96:PRO:HA	1:F:97:PRO:C	2.35	0.45
1:I:92:PHE:CD1	1:J:45:ARG:HG3	2.52	0.45
1:B:19:PHE:CE2	1:B:42:LEU:HD11	2.52	0.45
1:G:16:ASN:H	1:G:16:ASN:ND2	2.14	0.45
1:B:114:GLN:HE21	1:B:116:LEU:HD21	1.80	0.45
1:B:51:ALA:HA	1:C:57:LEU:CD2	2.47	0.45
1:I:74:VAL:HG21	1:J:19:PHE:O	2.17	0.45
1:I:67:TYR:HA	1:J:17:TYR:CD2	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:TYR:CD2	1:E:67:TYR:HA	2.51	0.45
1:C:114:GLN:NE2	1:C:116:LEU:HD21	2.32	0.45
1:D:117:VAL:O	1:D:118:ALA:C	2.55	0.45
1:H:40:HIS:CD2	1:H:40:HIS:H	2.28	0.45
1:J:61:GLU:HB2	1:J:74:VAL:O	2.16	0.45
1:A:23:LEU:HD11	1:A:111:ILE:HD11	1.98	0.45
1:F:58:HIS:HE1	1:F:107:GLY:N	2.12	0.45
1:H:56:GLU:OE1	1:H:105:GLY:HA2	2.17	0.45
1:E:28:ASP:OD1	1:E:101:ARG:CB	2.64	0.45
1:G:103:LYS:O	1:G:104:CYS:HB3	2.16	0.45
1:G:117:VAL:HG12	1:G:118:ALA:N	2.32	0.45
1:H:61:GLU:CD	1:H:73:LYS:HB3	2.37	0.45
1:I:34:ASP:OD1	1:I:34:ASP:N	2.50	0.45
1:D:27:LYS:CG	1:D:28:ASP:N	2.37	0.45
1:G:53:ALA:H	1:G:108:PRO:HD2	1.82	0.45
1:E:107:GLY:HA2	1:E:109:VAL:HG23	1.99	0.45
1:D:62:ALA:HB2	1:D:76:LEU:HD11	1.99	0.44
1:D:63:GLU:HB3	1:D:99:VAL:CG2	2.47	0.44
1:D:78:THR:C	1:D:79:LEU:HD23	2.36	0.44
1:E:33:VAL:HG11	1:E:40:HIS:CE1	2.51	0.44
1:F:34:ASP:N	1:F:34:ASP:OD1	2.50	0.44
1:B:65:MET:HE3	1:B:71:PRO:CA	2.47	0.44
1:A:63:GLU:HG3	1:A:72:ILE:O	2.18	0.44
1:I:58:HIS:CE1	1:I:106:SER:H	2.36	0.44
1:G:67:TYR:CE2	1:H:40:HIS:CE1	3.06	0.44
1:I:33:VAL:HG11	1:I:40:HIS:CD2	2.52	0.44
1:C:100:LEU:HD13	1:C:111:ILE:HD13	1.99	0.44
1:C:41:GLN:HA	1:C:41:GLN:NE2	2.33	0.44
1:I:72:ILE:HD11	1:J:18:LEU:CB	2.47	0.44
1:I:89:LEU:CD2	1:J:46:THR:HG21	2.37	0.44
1:A:57:LEU:HD11	1:E:81:MET:SD	2.58	0.44
1:F:45:ARG:HD3	1:F:45:ARG:HA	1.77	0.44
1:I:40:HIS:CE1	1:I:115:HIS:CE1	3.06	0.44
1:A:43:SER:HB2	1:A:93:GLU:HG2	1.99	0.44
1:C:23:LEU:O	1:C:24:LYS:HG2	2.17	0.44
1:F:47:VAL:HG11	1:F:60:VAL:HG21	2.00	0.44
1:D:78:THR:O	1:D:79:LEU:HD23	2.17	0.43
1:D:112:SER:HB3	1:E:74:VAL:HG13	2.00	0.43
1:D:33:VAL:HG21	1:D:115:HIS:CE1	2.53	0.43
1:E:79:LEU:CD2	1:E:87:VAL:HG23	2.48	0.43
1:C:61:GLU:HG2	1:C:101:ARG:HG2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ALA:HA	1:D:107:GLY:O	2.18	0.43
1:E:15:GLN:HG2	1:E:17:TYR:OH	2.19	0.43
1:D:117:VAL:HG12	1:D:118:ALA:N	2.34	0.43
1:G:66:ASN:HD22	1:G:72:ILE:CG2	2.31	0.43
1:I:94:ILE:HD13	1:J:18:LEU:HD21	1.99	0.43
1:F:25:ALA:HB2	1:F:106:SER:HB3	2.00	0.43
1:H:66:ASN:CG	1:H:68:GLU:OE1	2.57	0.43
1:C:16:ASN:HD22	1:C:16:ASN:H	1.64	0.43
1:A:67:TYR:HB2	1:E:115:HIS:CD2	2.53	0.43
1:H:68:GLU:N	1:H:68:GLU:CD	2.54	0.43
1:I:24:LYS:O	1:I:26:ASP:N	2.51	0.43
1:E:100:LEU:HD13	1:E:111:ILE:CD1	2.48	0.43
1:G:54:LYS:HG3	1:G:56:GLU:OE1	2.17	0.43
1:C:67:TYR:C	1:C:69:GLY:N	2.72	0.43
1:E:28:ASP:OD1	1:E:101:ARG:CA	2.66	0.43
1:A:86:THR:HG22	1:A:87:VAL:N	2.34	0.43
1:C:95:THR:HA	1:C:96:PRO:HD3	1.91	0.43
1:E:23:LEU:HB2	1:E:102:LEU:HD13	2.00	0.43
1:C:22:GLU:HG3	1:C:110:HIS:ND1	2.34	0.43
1:E:61:GLU:HG2	1:E:101:ARG:HG3	2.00	0.43
1:E:31:PHE:CG	1:E:42:LEU:HD22	2.54	0.43
1:F:56:GLU:O	1:F:58:HIS:CD2	2.72	0.43
1:J:40:HIS:CE1	1:J:117:VAL:HG22	2.54	0.43
1:H:18:LEU:CD2	1:H:19:PHE:H	2.26	0.42
1:I:76:LEU:O	1:I:77:ALA:HB2	2.18	0.42
1:E:45:ARG:HD3	1:E:45:ARG:HA	1.80	0.42
1:I:107:GLY:HA3	1:I:108:PRO:C	2.38	0.42
1:J:23:LEU:O	1:J:108:PRO:HA	2.19	0.42
1:A:84:GLN:OE1	1:E:85:PRO:HD2	2.18	0.42
1:C:39:GLU:HB3	1:C:118:ALA:HB2	2.02	0.42
1:G:24:LYS:HA	1:G:102:LEU:CD2	2.49	0.42
1:F:64:ALA:O	1:F:71:PRO:HA	2.20	0.42
1:H:44:LEU:N	1:H:92:PHE:O	2.33	0.42
1:D:24:LYS:HZ1	1:D:108:PRO:HB3	1.84	0.42
1:F:40:HIS:CE1	1:F:117:VAL:HG22	2.55	0.42
1:I:31:PHE:HB3	1:I:98:VAL:CG1	2.49	0.42
1:J:41:GLN:NE2	1:J:95:THR:OG1	2.52	0.42
1:A:27:LYS:O	1:A:27:LYS:HG2	2.19	0.42
1:D:102:LEU:HD11	1:D:109:VAL:HG21	2.01	0.42
1:D:33:VAL:HG21	1:D:115:HIS:NE2	2.34	0.42
1:A:103:LYS:O	1:A:103:LYS:CG	2.64	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLU:O	1:A:27:LYS:CE	2.68	0.42
1:G:56:GLU:O	1:G:58:HIS:HD2	2.03	0.42
1:I:67:TYR:CD2	1:I:68:GLU:OE2	2.72	0.42
1:A:45:ARG:HG2	1:A:113:GLY:HA2	2.02	0.42
1:I:75:THR:HB	1:J:110:HIS:HB3	2.02	0.42
1:C:67:TYR:O	1:C:69:GLY:N	2.53	0.42
1:D:117:VAL:CG1	1:D:118:ALA:N	2.83	0.42
1:E:28:ASP:OD1	1:E:101:ARG:HB3	2.20	0.42
1:F:41:GLN:HA	1:F:41:GLN:NE2	2.34	0.42
1:B:65:MET:CE	1:B:71:PRO:N	2.83	0.42
1:C:49:LEU:HD12	1:C:81:MET:HA	2.02	0.42
1:B:79:LEU:HD23	1:B:87:VAL:HG23	2.01	0.41
1:E:65:MET:HA	1:E:71:PRO:HA	2.02	0.41
1:I:93:GLU:O	1:J:114:GLN:OE1	2.38	0.41
1:B:92:PHE:CD2	1:B:92:PHE:C	2.93	0.41
1:C:58:HIS:CE1	1:C:107:GLY:N	2.78	0.41
1:F:22:GLU:C	1:F:23:LEU:HD23	2.41	0.41
1:F:46:THR:CG2	1:J:89:LEU:HD22	2.50	0.41
1:G:32:LYS:HB3	1:G:32:LYS:HE3	1.77	0.41
1:G:41:GLN:HE21	1:G:41:GLN:CA	2.33	0.41
1:A:48:SER:HB2	1:B:78:THR:OG1	2.19	0.41
1:C:59:ILE:CG2	1:C:103:LYS:HD3	2.49	0.41
1:C:94:ILE:HG22	1:C:95:THR:N	2.36	0.41
1:F:39:GLU:O	1:F:118:ALA:N	2.53	0.41
1:I:32:LYS:HB3	1:I:32:LYS:HE2	1.90	0.41
1:A:39:GLU:CG	1:A:118:ALA:HB2	2.50	0.41
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.84	0.41
1:B:23:LEU:CB	1:B:102:LEU:HD13	2.43	0.41
1:D:70:SER:HA	1:D:71:PRO:HD3	1.92	0.41
1:G:62:ALA:HA	1:G:99:VAL:O	2.20	0.41
1:H:65:MET:CA	1:H:71:PRO:HA	2.45	0.41
1:A:20:GLY:O	1:A:21:CYS:CB	2.68	0.41
1:G:74:VAL:HG11	1:H:18:LEU:HD21	2.01	0.41
1:C:68:GLU:H	1:C:68:GLU:CD	2.19	0.41
1:D:16:ASN:ND2	1:D:16:ASN:H	1.92	0.41
1:H:44:LEU:HB3	1:H:89:LEU:HD12	2.01	0.41
1:B:66:ASN:OD1	1:B:70:SER:O	2.38	0.41
1:C:117:VAL:O	1:C:118:ALA:C	2.59	0.41
1:G:79:LEU:CD2	1:G:87:VAL:HG23	2.50	0.41
1:A:100:LEU:HD13	1:A:111:ILE:HD13	2.03	0.41
1:A:66:ASN:HB3	1:A:72:ILE:CD1	2.50	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:HG21	1:E:67:TYR:CD1	2.56	0.41
1:E:58:HIS:O	1:E:59:ILE:HG12	2.21	0.41
1:F:63:GLU:HA	1:F:72:ILE:O	2.21	0.41
1:H:25:ALA:O	1:H:26:ASP:HB2	2.20	0.41
1:E:33:VAL:HG12	1:E:34:ASP:N	2.35	0.41
1:E:31:PHE:O	1:E:97:PRO:HA	2.20	0.41
1:A:49:LEU:HD23	1:A:109:VAL:HG22	2.02	0.41
1:A:67:TYR:CD2	1:A:68:GLU:OE2	2.74	0.41
1:D:33:VAL:HG11	1:D:40:HIS:CD2	2.55	0.41
1:H:50:GLY:HA3	1:H:108:PRO:HG2	2.03	0.41
1:I:23:LEU:CB	1:I:102:LEU:CD1	2.98	0.41
1:F:74:VAL:HG11	1:G:112:SER:HB2	1.98	0.40
1:G:75:THR:HB	1:H:110:HIS:HB3	2.04	0.40
1:H:92:PHE:CD1	1:I:45:ARG:HG3	2.56	0.40
1:A:49:LEU:CD2	1:A:109:VAL:HG22	2.52	0.40
1:B:43:SER:HB3	1:B:114:GLN:HB2	2.02	0.40
1:D:17:TYR:CD1	1:D:17:TYR:N	2.89	0.40
1:I:68:GLU:CD	1:I:68:GLU:N	2.75	0.40
1:B:64:ALA:O	1:B:71:PRO:HA	2.22	0.40
1:H:41:GLN:NE2	1:H:95:THR:CG2	2.76	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	96/122 (79%)	80 (83%)	12 (12%)	4 (4%)	3	3
1	B	96/122 (79%)	85 (88%)	9 (9%)	2 (2%)	7	12
1	C	96/122 (79%)	84 (88%)	11 (12%)	1 (1%)	15	27
1	D	96/122 (79%)	86 (90%)	7 (7%)	3 (3%)	4	6

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	96/122 (79%)	86 (90%)	9 (9%)	1 (1%)	15	27
1	F	96/122 (79%)	86 (90%)	8 (8%)	2 (2%)	7	12
1	G	96/122 (79%)	83 (86%)	11 (12%)	2 (2%)	7	12
1	H	96/122 (79%)	82 (85%)	11 (12%)	3 (3%)	4	6
1	I	96/122 (79%)	83 (86%)	9 (9%)	4 (4%)	3	3
1	J	96/122 (79%)	83 (86%)	11 (12%)	2 (2%)	7	12
All	All	960/1220 (79%)	838 (87%)	98 (10%)	24 (2%)	5	9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	CYS
1	B	25	ALA
1	D	26	ASP
1	D	40	HIS
1	E	51	ALA
1	F	27	LYS
1	F	53	ALA
1	G	53	ALA
1	H	40	HIS
1	I	25	ALA
1	I	53	ALA
1	J	25	ALA
1	A	40	HIS
1	D	28	ASP
1	H	68	GLU
1	H	69	GLY
1	I	40	HIS
1	I	52	GLY
1	B	68	GLU
1	A	27	LYS
1	C	68	GLU
1	G	104	CYS
1	J	81	MET
1	A	53	ALA

### 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	84/106 (79%)	72 (86%)	12 (14%)	3	4
1	B	84/106 (79%)	76 (90%)	8 (10%)	8	15
1	C	84/106 (79%)	68 (81%)	16 (19%)	1	2
1	D	84/106 (79%)	71 (84%)	13 (16%)	2	3
1	E	84/106 (79%)	72 (86%)	12 (14%)	3	4
1	F	84/106 (79%)	74 (88%)	10 (12%)	5	8
1	G	84/106 (79%)	66 (79%)	18 (21%)	1	1
1	H	84/106 (79%)	73 (87%)	11 (13%)	4	6
1	I	84/106 (79%)	76 (90%)	8 (10%)	8	15
1	J	84/106 (79%)	77 (92%)	7 (8%)	11	20
All	All	840/1060 (79%)	725 (86%)	115 (14%)	3	5

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	26	ASP
1	A	32	LYS
1	A	41	GLN
1	A	48	SER
1	A	56	GLU
1	A	57	LEU
1	A	70	SER
1	A	72	ILE
1	A	88	SER
1	A	92	PHE
1	A	98	VAL
1	B	16	ASN
1	B	18	LEU
1	B	21	CYS
1	B	32	LYS
1	B	48	SER
1	B	65	MET
1	B	67	TYR
1	B	92	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	15	GLN
1	C	16	ASN
1	C	18	LEU
1	C	27	LYS
1	C	32	LYS
1	C	34	ASP
1	C	41	GLN
1	C	48	SER
1	C	56	GLU
1	C	70	SER
1	C	74	VAL
1	C	92	PHE
1	C	102	LEU
1	C	104	CYS
1	C	115	HIS
1	C	117	VAL
1	D	16	ASN
1	D	18	LEU
1	D	24	LYS
1	D	27	LYS
1	D	28	ASP
1	D	32	LYS
1	D	65	MET
1	D	70	SER
1	D	72	ILE
1	D	92	PHE
1	D	99	VAL
1	D	103	LYS
1	D	115	HIS
1	E	16	ASN
1	E	24	LYS
1	E	27	LYS
1	E	40	HIS
1	E	41	GLN
1	E	59	ILE
1	E	92	PHE
1	E	98	VAL
1	E	99	VAL
1	E	102	LEU
1	E	114	GLN
1	E	115	HIS
1	F	15	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	16	ASN
1	F	18	LEU
1	F	32	LYS
1	F	34	ASP
1	F	41	GLN
1	F	68	GLU
1	F	92	PHE
1	F	98	VAL
1	F	117	VAL
1	G	15	GLN
1	G	16	ASN
1	G	17	TYR
1	G	18	LEU
1	G	24	LYS
1	G	32	LYS
1	G	33	VAL
1	G	41	GLN
1	G	46	THR
1	G	48	SER
1	G	54	LYS
1	G	56	GLU
1	G	60	VAL
1	G	74	VAL
1	G	92	PHE
1	G	100	LEU
1	G	112	SER
1	G	115	HIS
1	H	16	ASN
1	H	18	LEU
1	H	21	CYS
1	H	41	GLN
1	H	42	LEU
1	H	63	GLU
1	H	65	MET
1	H	92	PHE
1	H	95	THR
1	H	102	LEU
1	H	114	GLN
1	I	16	ASN
1	I	18	LEU
1	I	21	CYS
1	I	33	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	48	SER
1	I	54	LYS
1	I	92	PHE
1	I	104	CYS
1	J	23	LEU
1	J	34	ASP
1	J	59	ILE
1	J	65	MET
1	J	70	SER
1	J	74	VAL
1	J	92	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	41	GLN
1	A	58	HIS
1	A	110	HIS
1	B	16	ASN
1	B	58	HIS
1	B	114	GLN
1	B	115	HIS
1	C	15	GLN
1	C	16	ASN
1	C	41	GLN
1	C	58	HIS
1	C	114	GLN
1	C	115	HIS
1	D	16	ASN
1	D	58	HIS
1	D	110	HIS
1	D	115	HIS
1	E	16	ASN
1	E	41	GLN
1	E	58	HIS
1	E	114	GLN
1	E	115	HIS
1	F	15	GLN
1	F	16	ASN
1	F	41	GLN
1	F	58	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	114	GLN
1	G	16	ASN
1	G	41	GLN
1	G	58	HIS
1	G	110	HIS
1	G	114	GLN
1	G	115	HIS
1	H	16	ASN
1	H	41	GLN
1	H	58	HIS
1	H	114	GLN
1	H	115	HIS
1	I	15	GLN
1	I	16	ASN
1	I	58	HIS
1	I	114	GLN
1	I	115	HIS
1	J	40	HIS
1	J	58	HIS
1	J	115	HIS

### 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 ⓘ

There are no ligands in this entry.



## 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	100/122 (81%)	-0.34	2 (2%) 65 73	7, 29, 65, 70	0
1	B	100/122 (81%)	-0.38	2 (2%) 65 73	3, 20, 57, 81	0
1	C	100/122 (81%)	-0.55	2 (2%) 65 73	3, 20, 54, 73	0
1	D	100/122 (81%)	-0.26	3 (3%) 50 59	6, 27, 63, 87	0
1	E	100/122 (81%)	-0.11	4 (4%) 38 45	9, 32, 73, 99	0
1	F	100/122 (81%)	-0.32	3 (3%) 50 59	6, 25, 64, 95	0
1	G	100/122 (81%)	-0.43	3 (3%) 50 59	6, 23, 55, 91	0
1	H	100/122 (81%)	-0.10	5 (5%) 28 35	8, 36, 71, 85	0
1	I	100/122 (81%)	-0.08	4 (4%) 38 45	11, 34, 67, 95	0
1	J	100/122 (81%)	-0.30	1 (1%) 82 87	8, 30, 61, 83	0
All	All	1000/1220 (81%)	-0.29	29 (2%) 51 61	3, 28, 65, 99	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	39	GLU	7.4
1	I	39	GLU	4.9
1	F	39	GLU	4.6
1	J	39	GLU	4.5
1	E	26	ASP	4.4
1	G	34	ASP	3.9
1	H	34	ASP	3.7
1	H	26	ASP	3.5
1	F	34	ASP	3.5
1	E	34	ASP	3.5
1	H	65	MET	3.3
1	F	26	ASP	3.2
1	I	34	ASP	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	34	ASP	3.1
1	B	34	ASP	3.0
1	G	26	ASP	2.9
1	D	26	ASP	2.9
1	A	39	GLU	2.7
1	C	34	ASP	2.5
1	E	118	ALA	2.5
1	G	27	LYS	2.4
1	H	118	ALA	2.3
1	B	39	GLU	2.2
1	C	26	ASP	2.2
1	I	33	VAL	2.2
1	I	118	ALA	2.2
1	H	51	ALA	2.1
1	A	65	MET	2.1
1	D	27	LYS	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.