



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 AM GMT

PDB ID : 2YHM  
Title : Structure of respiratory syncytial virus nucleocapsid protein, P212121 crystal form  
Authors : El Omari, K.; Dhaliwal, B.; Ren, J.; Abrescia, N.G.A.; Lockyer, M.; Powell, K.L.; Hawkins, A.R.; Stammers, D.K.  
Deposited on : 2011-05-04  
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

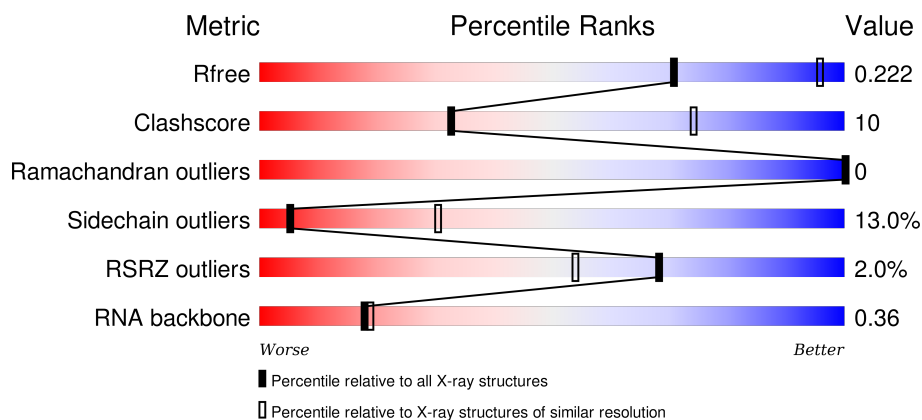
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	375	<div> <div></div> <div>72%</div> <div>25%</div> <div>•</div> </div>
1	B	375	<div> <div></div> <div>72%</div> <div>25%</div> <div>•</div> </div>
1	C	375	<div> <div>2%</div> <div>69%</div> <div>27%</div> <div>•</div> </div>
1	D	375	<div> <div></div> <div>69%</div> <div>27%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	375	<div><div></div><div>3%</div><div>70%</div><div>26%</div><div></div></div>
1	F	375	<div><div></div><div>%</div><div>68%</div><div>29%</div><div></div></div>
1	G	375	<div><div></div><div>2%</div><div>71%</div><div>26%</div><div></div></div>
1	H	375	<div><div></div><div>3%</div><div>72%</div><div>24%</div><div></div></div>
1	I	375	<div><div></div><div>3%</div><div>72%</div><div>24%</div><div></div></div>
1	J	375	<div><div></div><div>4%</div><div>69%</div><div>28%</div><div></div></div>
2	K	70	<div><div></div><div>30%</div><div>59%</div><div>11%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30600 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 NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	B	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	C	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	D	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	E	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	F	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	G	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	H	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	I	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	J	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			

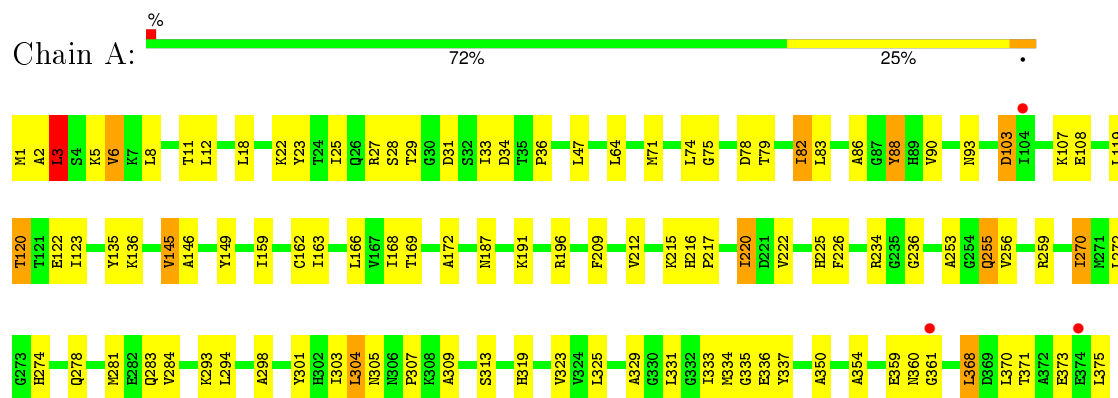
- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			

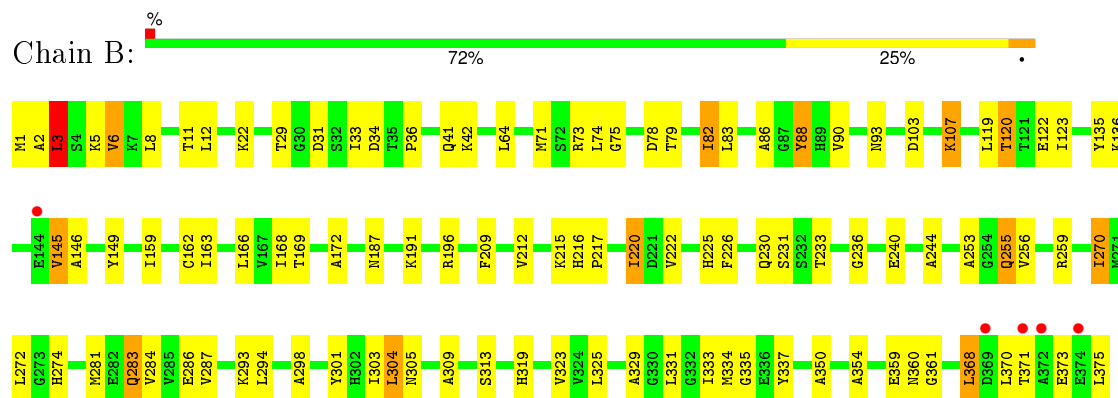
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

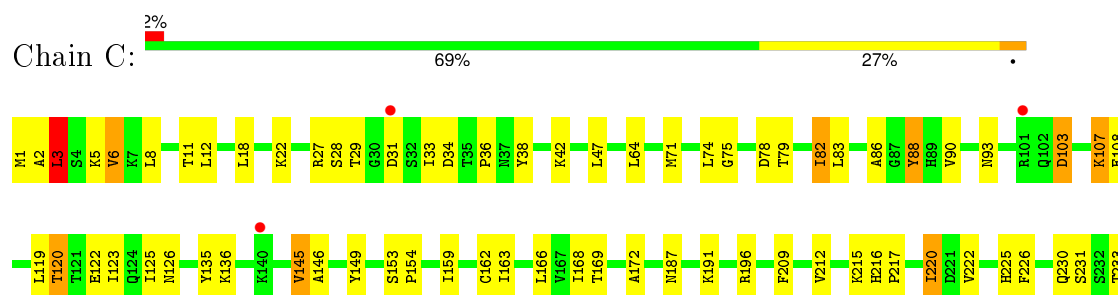
#### • Molecule 1: NUCLEOPROTEIN

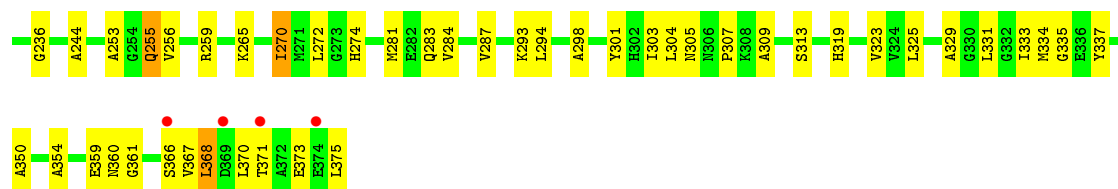


#### • Molecule 1: NUCLEOPROTEIN

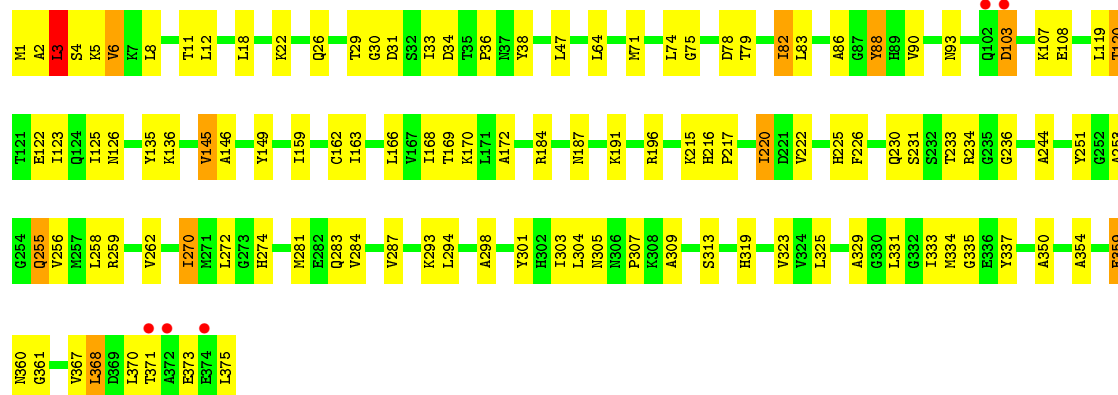


#### • Molecule 1: NUCLEOPROTEIN

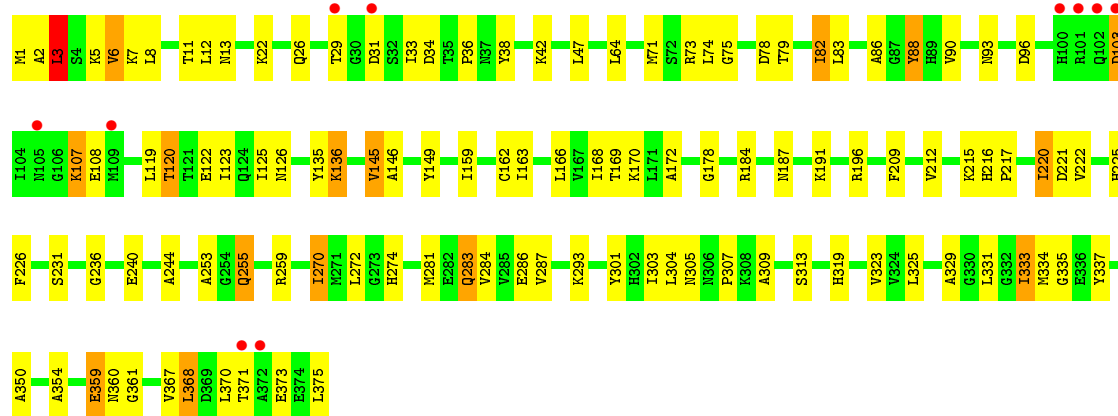




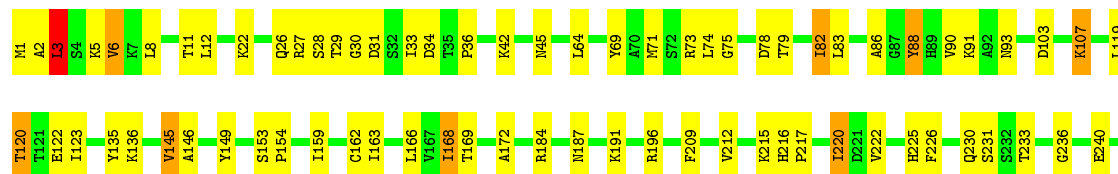
• Molecule 1: NUCLEOPROTEIN



• Molecule 1: NUCLEOPROTEIN

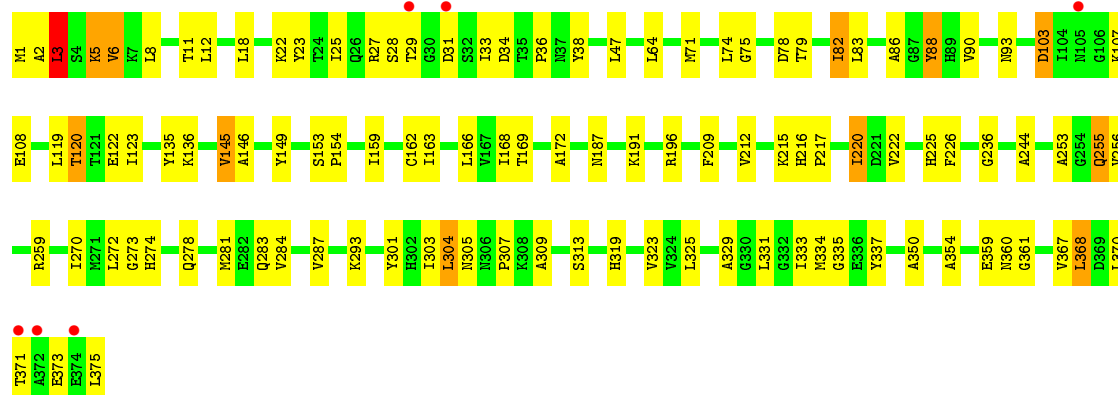


• Molecule 1: NUCLEOPROTEIN

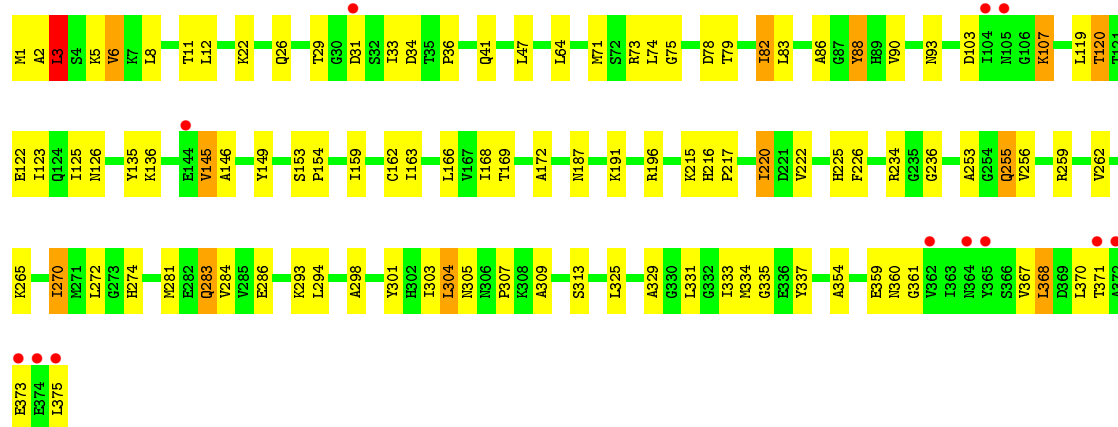




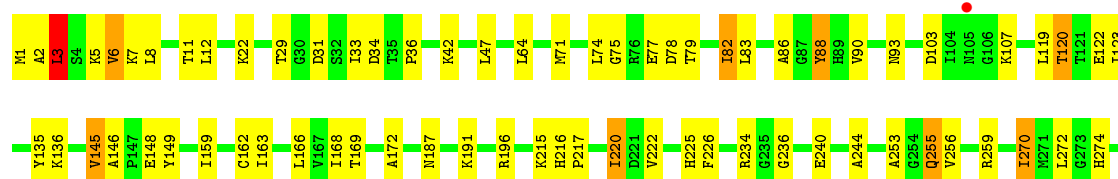
• Molecule 1: NUCLEOPROTEIN

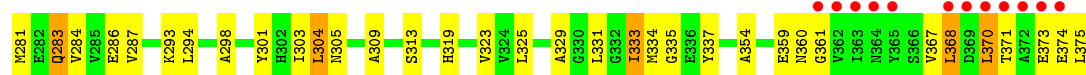


• Molecule 1: NUCLEOPROTEIN

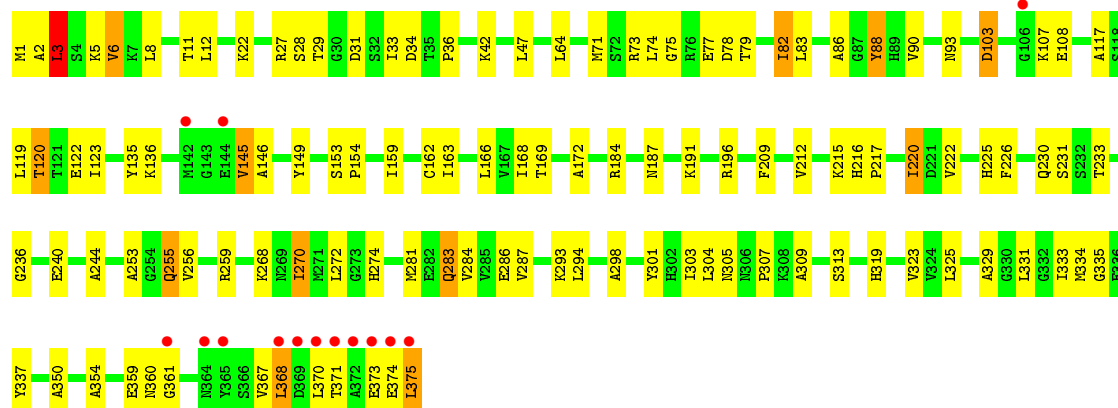


• Molecule 1: NUCLEOPROTEIN

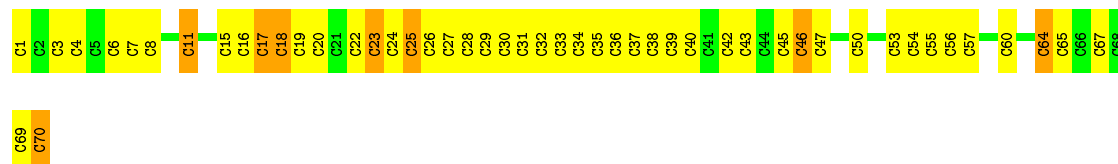
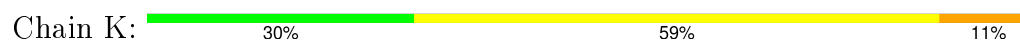




• Molecule 1: NUCLEOPROTEIN



• Molecule 2: RNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.61Å 149.91Å 255.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 29.35 – 3.49	Depositor EDS
% Data completeness (in resolution range)	83.4 (50.00-3.60) 80.3 (29.35-3.49)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.6.0077	Depositor
R, $R_{free}$	0.196 , 0.224 0.196 , 0.222	Depositor DCC
$R_{free}$ test set	2560 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.1	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 33.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 52965 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/2968	0.54	1/3998 (0.0%)
1	B	0.34	0/2968	0.54	1/3998 (0.0%)
1	C	0.35	0/2968	0.54	1/3998 (0.0%)
1	D	0.35	0/2968	0.55	1/3998 (0.0%)
1	E	0.36	0/2968	0.55	1/3998 (0.0%)
1	F	0.37	0/2968	0.55	1/3998 (0.0%)
1	G	0.36	0/2968	0.55	1/3998 (0.0%)
1	H	0.36	0/2968	0.55	1/3998 (0.0%)
1	I	0.36	0/2968	0.55	1/3998 (0.0%)
1	J	0.36	0/2968	0.55	1/3998 (0.0%)
2	K	0.27	0/1539	0.80	0/2376
All	All	0.35	0/31219	0.56	10/42356 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	H	3	LEU	CA-CB-CG	5.53	128.02	115.30
1	F	3	LEU	CA-CB-CG	5.46	127.85	115.30
1	C	3	LEU	CA-CB-CG	5.44	127.82	115.30
1	I	3	LEU	CA-CB-CG	5.43	127.79	115.30
1	E	3	LEU	CA-CB-CG	5.39	127.70	115.30
1	J	3	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	3	LEU	CA-CB-CG	5.29	127.45	115.30
1	B	3	LEU	CA-CB-CG	5.21	127.29	115.30
1	G	3	LEU	CA-CB-CG	5.19	127.25	115.30
1	A	3	LEU	CA-CB-CG	5.05	126.91	115.30

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	2920	0	2955	68	0
1	B	2920	0	2955	67	0
1	C	2920	0	2955	81	0
1	D	2920	0	2955	71	1
1	E	2920	0	2955	91	13
1	F	2920	0	2955	87	4
1	G	2920	0	2955	69	0
1	H	2920	0	2955	64	0
1	I	2920	0	2955	70	8
1	J	2920	0	2955	77	10
2	K	1400	0	771	28	0
All	All	30600	0	30321	635	18

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 10.

All (635) 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:F:82:ILE:HD11	1:F:222:VAL:HA	1.32	1.10
1:J:82:ILE:HD11	1:J:222:VAL:HA	1.34	1.10
1:H:82:ILE:HD11	1:H:222:VAL:HA	1.34	1.09
1:G:82:ILE:HD11	1:G:222:VAL:HA	1.32	1.09
1:A:82:ILE:HD11	1:A:222:VAL:HA	1.34	1.08
1:C:367:VAL:HG13	1:E:1:MET:HG3	1.29	1.08
1:E:82:ILE:HD11	1:E:222:VAL:HA	1.36	1.06
1:B:82:ILE:HD11	1:B:222:VAL:HA	1.35	1.05
1:C:82:ILE:HD11	1:C:222:VAL:HA	1.37	1.05
1:D:82:ILE:HD11	1:D:222:VAL:HA	1.35	1.02
1:I:361:GLY:HA3	1:J:274:HIS:NE2	1.75	1.01
1:I:82:ILE:HD11	1:I:222:VAL:HA	1.37	1.01
1:F:42:LYS:HD2	1:G:28:SER:HB3	1.40	1.00
1:C:367:VAL:O	1:E:1:MET:N	1.96	0.98
2:K:1:C:P	2:K:70:C:H3'	2.04	0.97
1:C:367:VAL:HA	1:E:1:MET:HG2	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:VAL:CG1	1:E:1:MET:HG3	1.99	0.93
1:H:75:GLY:O	1:H:79:THR:HG22	1.71	0.90
1:E:361:GLY:HA3	1:F:274:HIS:NE2	1.88	0.88
1:H:256:VAL:HG12	2:K:53:C:OP1	1.72	0.88
1:B:361:GLY:HA3	1:C:274:HIS:NE2	1.90	0.87
1:C:236:GLY:O	1:D:305:ASN:HB2	1.76	0.86
1:F:42:LYS:HD2	1:G:28:SER:CB	2.05	0.86
1:F:75:GLY:O	1:F:79:THR:HG22	1.76	0.85
1:G:75:GLY:O	1:G:79:THR:HG22	1.77	0.85
1:I:75:GLY:O	1:I:79:THR:HG22	1.76	0.85
1:E:75:GLY:O	1:E:79:THR:HG22	1.77	0.84
1:D:75:GLY:O	1:D:79:THR:HG22	1.77	0.84
1:A:75:GLY:O	1:A:79:THR:HG22	1.77	0.84
1:J:75:GLY:O	1:J:79:THR:HG22	1.78	0.83
1:F:361:GLY:HA3	1:G:274:HIS:NE2	1.93	0.83
1:A:28:SER:HB3	1:J:42:LYS:HD2	1.62	0.81
1:C:75:GLY:O	1:C:79:THR:HG22	1.80	0.81
1:D:256:VAL:HG12	2:K:25:C:OP1	1.81	0.80
1:C:367:VAL:HG13	1:E:1:MET:CG	2.11	0.80
1:B:75:GLY:O	1:B:79:THR:HG22	1.81	0.79
1:H:3:LEU:O	1:H:6:VAL:HG13	1.83	0.79
1:I:3:LEU:O	1:I:6:VAL:HG13	1.85	0.77
1:G:368:LEU:HG	1:I:3:LEU:HD11	1.67	0.77
1:C:3:LEU:O	1:C:6:VAL:HG13	1.85	0.76
1:B:3:LEU:O	1:B:6:VAL:HG13	1.86	0.76
1:D:3:LEU:O	1:D:6:VAL:HG13	1.85	0.76
1:J:3:LEU:O	1:J:6:VAL:HG13	1.86	0.76
1:D:367:VAL:HG12	1:F:3:LEU:HD13	1.68	0.75
1:F:3:LEU:O	1:F:6:VAL:HG13	1.86	0.75
1:I:256:VAL:HG12	2:K:60:C:OP1	1.87	0.74
1:A:3:LEU:O	1:A:6:VAL:HG13	1.87	0.74
1:H:331:LEU:HD13	1:H:354:ALA:HB1	1.70	0.74
1:A:28:SER:CB	1:J:42:LYS:HD2	2.18	0.73
1:I:331:LEU:HD13	1:I:354:ALA:HB1	1.69	0.73
1:D:331:LEU:HD13	1:D:354:ALA:HB1	1.69	0.72
1:C:331:LEU:HD13	1:C:354:ALA:HB1	1.70	0.72
1:E:3:LEU:O	1:E:6:VAL:HG13	1.88	0.72
1:A:331:LEU:HD13	1:A:354:ALA:HB1	1.72	0.72
1:G:3:LEU:O	1:G:6:VAL:HG13	1.88	0.71
1:H:253:ALA:HB3	1:H:303:ILE:HD11	1.72	0.71
1:B:253:ALA:HB3	1:B:303:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:LEU:HD13	1:E:354:ALA:HB1	1.73	0.71
1:B:331:LEU:HD13	1:B:354:ALA:HB1	1.72	0.71
1:E:42:LYS:NZ	1:F:30:GLY:C	2.45	0.71
1:F:253:ALA:HB3	1:F:303:ILE:HD11	1.72	0.70
1:F:331:LEU:HD13	1:F:354:ALA:HB1	1.71	0.70
1:G:331:LEU:HD13	1:G:354:ALA:HB1	1.73	0.70
1:D:236:GLY:O	1:E:305:ASN:HB2	1.90	0.70
1:I:253:ALA:HB3	1:I:303:ILE:HD11	1.74	0.70
1:E:29:THR:CG2	1:E:88:TYR:HB3	2.22	0.70
1:E:42:LYS:HZ2	1:F:30:GLY:C	1.96	0.69
1:E:361:GLY:HA3	1:F:274:HIS:HE2	1.55	0.69
1:H:236:GLY:O	1:I:305:ASN:HB2	1.92	0.69
1:F:29:THR:CG2	1:F:88:TYR:HB3	2.22	0.69
1:G:253:ALA:HB3	1:G:303:ILE:HD11	1.74	0.69
1:J:29:THR:CG2	1:J:88:TYR:HB3	2.23	0.69
1:A:29:THR:CG2	1:A:88:TYR:HB3	2.23	0.69
1:G:256:VAL:HG12	2:K:46:C:OP1	1.93	0.69
1:D:29:THR:CG2	1:D:88:TYR:HB3	2.23	0.69
1:C:29:THR:CG2	1:C:88:TYR:HB3	2.22	0.69
1:C:367:VAL:HA	1:E:1:MET:CG	2.22	0.68
1:I:29:THR:CG2	1:I:88:TYR:HB3	2.23	0.68
1:J:331:LEU:HD13	1:J:354:ALA:HB1	1.74	0.68
1:F:240:GLU:OE2	1:G:27:ARG:HD3	1.94	0.68
1:B:29:THR:CG2	1:B:88:TYR:HB3	2.24	0.67
1:J:253:ALA:HB3	1:J:303:ILE:HD11	1.76	0.67
1:H:29:THR:CG2	1:H:88:TYR:HB3	2.23	0.67
1:A:361:GLY:HA3	1:B:274:HIS:NE2	2.10	0.67
1:G:367:VAL:CG1	1:I:2:ALA:HB3	2.25	0.67
1:G:236:GLY:O	1:H:305:ASN:HB2	1.95	0.66
1:D:253:ALA:HB3	1:D:303:ILE:HD11	1.77	0.66
1:G:29:THR:CG2	1:G:88:TYR:HB3	2.25	0.66
1:G:361:GLY:HA3	1:H:274:HIS:NE2	2.11	0.66
1:G:146:ALA:HB3	1:G:149:TYR:HD2	1.60	0.66
1:I:361:GLY:HA3	1:J:274:HIS:HE2	1.59	0.65
1:B:236:GLY:O	1:C:305:ASN:HB2	1.96	0.65
1:E:253:ALA:HB3	1:E:303:ILE:HD11	1.79	0.65
1:A:146:ALA:HB3	1:A:149:TYR:HD2	1.61	0.65
1:A:253:ALA:HB3	1:A:303:ILE:HD11	1.78	0.64
1:D:367:VAL:HG12	1:F:3:LEU:CD1	2.26	0.64
1:C:146:ALA:HB3	1:C:149:TYR:HD2	1.62	0.64
1:J:146:ALA:HB3	1:J:149:TYR:HD2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ALA:HB3	1:E:149:TYR:HD2	1.63	0.63
1:A:274:HIS:NE2	1:J:361:GLY:HA3	2.13	0.63
1:F:256:VAL:HG12	2:K:39:C:OP1	1.98	0.63
1:B:146:ALA:HB3	1:B:149:TYR:HD2	1.63	0.63
1:C:368:LEU:H	1:C:368:LEU:HD12	1.64	0.63
1:D:146:ALA:HB3	1:D:149:TYR:HD2	1.63	0.62
1:H:146:ALA:HB3	1:H:149:TYR:HD2	1.64	0.62
1:C:1:MET:HG3	1:C:2:ALA:H	1.65	0.62
1:F:146:ALA:HB3	1:F:149:TYR:HD2	1.65	0.62
1:B:1:MET:HG3	1:B:2:ALA:H	1.65	0.62
1:E:42:LYS:NZ	1:F:30:GLY:O	2.33	0.61
1:A:236:GLY:O	1:B:305:ASN:HB2	2.00	0.61
1:I:146:ALA:HB3	1:I:149:TYR:HD2	1.64	0.61
1:H:234:ARG:NH2	1:I:86:ALA:HB2	2.14	0.61
1:D:368:LEU:H	1:D:368:LEU:HD12	1.65	0.61
1:F:1:MET:HG3	1:F:2:ALA:H	1.66	0.61
1:D:215:LYS:HE3	1:D:216:HIS:HE1	1.66	0.61
1:E:1:MET:HG3	1:E:2:ALA:H	1.67	0.60
1:I:1:MET:HG3	1:I:2:ALA:H	1.66	0.60
1:J:301:TYR:HB3	1:J:309:ALA:HB2	1.83	0.60
1:C:253:ALA:HB3	1:C:303:ILE:HD11	1.83	0.60
1:J:368:LEU:HD12	1:J:368:LEU:H	1.67	0.60
1:E:215:LYS:HE3	1:E:216:HIS:HE1	1.67	0.60
1:G:1:MET:HG3	1:G:2:ALA:H	1.66	0.60
1:A:368:LEU:HD12	1:A:368:LEU:H	1.67	0.60
1:C:301:TYR:HB3	1:C:309:ALA:HB2	1.83	0.59
1:A:274:HIS:HE2	1:J:361:GLY:HA3	1.67	0.59
1:E:301:TYR:HB3	1:E:309:ALA:HB2	1.82	0.59
1:J:29:THR:HG22	1:J:88:TYR:HB3	1.84	0.59
1:A:215:LYS:HE3	1:A:216:HIS:HE1	1.67	0.59
1:D:361:GLY:HA3	1:E:274:HIS:NE2	2.18	0.59
1:E:361:GLY:HA3	1:F:274:HIS:CE1	2.37	0.59
1:A:301:TYR:HB3	1:A:309:ALA:HB2	1.85	0.59
1:B:368:LEU:HG	1:D:3:LEU:HD11	1.85	0.59
1:D:367:VAL:CG1	1:F:3:LEU:CD1	2.81	0.59
1:J:256:VAL:HG12	2:K:67:C:OP1	2.03	0.59
1:F:29:THR:HG22	1:F:88:TYR:HB3	1.85	0.59
1:C:335:GLY:CA	1:C:337:TYR:H	2.16	0.59
1:C:29:THR:HG22	1:C:88:TYR:HB3	1.84	0.58
1:F:231:SER:HB2	1:G:18:LEU:HD22	1.85	0.58
1:E:29:THR:HG22	1:E:88:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:PRO:O	1:C:220:ILE:HG23	2.02	0.58
1:D:29:THR:HG22	1:D:88:TYR:HB3	1.85	0.58
1:A:256:VAL:HG12	2:K:4:C:OP1	2.04	0.58
1:B:368:LEU:HD12	1:B:368:LEU:H	1.67	0.58
1:D:1:MET:HG3	1:D:2:ALA:H	1.69	0.58
1:D:335:GLY:CA	1:D:337:TYR:H	2.17	0.58
1:F:301:TYR:HB3	1:F:309:ALA:HB2	1.86	0.58
1:F:335:GLY:CA	1:F:337:TYR:H	2.17	0.58
1:H:234:ARG:HH21	1:I:86:ALA:HB2	1.68	0.58
1:C:256:VAL:HG12	2:K:18:C:OP1	2.04	0.58
1:F:368:LEU:HD12	1:F:368:LEU:H	1.67	0.58
1:J:1:MET:HG3	1:J:2:ALA:H	1.68	0.58
1:H:335:GLY:CA	1:H:337:TYR:H	2.17	0.58
1:E:335:GLY:CA	1:E:337:TYR:H	2.16	0.58
1:B:335:GLY:CA	1:B:337:TYR:H	2.17	0.58
1:H:1:MET:HG3	1:H:2:ALA:H	1.67	0.58
1:G:368:LEU:HD12	1:G:368:LEU:H	1.67	0.57
1:D:301:TYR:HB3	1:D:309:ALA:HB2	1.86	0.57
1:E:368:LEU:H	1:E:368:LEU:HD12	1.68	0.57
1:E:217:PRO:O	1:E:220:ILE:HG23	2.04	0.57
1:J:335:GLY:CA	1:J:337:TYR:H	2.18	0.57
1:I:335:GLY:CA	1:I:337:TYR:H	2.17	0.57
1:F:289:GLU:OE2	1:G:5:LYS:HD2	2.04	0.57
1:A:1:MET:HG3	1:A:2:ALA:H	1.67	0.57
2:K:69:C:H2'	2:K:70:C:O4'	2.04	0.57
1:G:301:TYR:HB3	1:G:309:ALA:HB2	1.87	0.57
1:I:29:THR:HG22	1:I:88:TYR:HB3	1.85	0.57
1:H:29:THR:HG22	1:H:88:TYR:HB3	1.85	0.57
1:C:244:ALA:HB1	1:D:307:PRO:HB3	1.86	0.57
1:A:27:ARG:HD3	1:J:240:GLU:OE2	2.04	0.57
1:H:217:PRO:O	1:H:220:ILE:HG23	2.04	0.57
1:B:301:TYR:HB3	1:B:309:ALA:HB2	1.87	0.57
1:H:368:LEU:H	1:H:368:LEU:HD12	1.70	0.57
1:J:217:PRO:O	1:J:220:ILE:HG23	2.04	0.57
1:C:367:VAL:CG1	1:E:2:ALA:H	2.18	0.56
1:G:335:GLY:CA	1:G:337:TYR:H	2.17	0.56
1:A:29:THR:HG22	1:A:88:TYR:HB3	1.86	0.56
1:B:29:THR:HG22	1:B:88:TYR:HB3	1.86	0.56
1:I:301:TYR:HB3	1:I:309:ALA:HB2	1.87	0.56
1:H:367:VAL:O	1:J:1:MET:N	2.39	0.56
1:I:361:GLY:HA3	1:J:274:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:THR:HG22	1:G:88:TYR:HB3	1.88	0.56
1:B:217:PRO:O	1:B:220:ILE:HG23	2.06	0.56
1:I:215:LYS:HE3	1:I:216:HIS:HE1	1.70	0.56
1:B:244:ALA:HB1	1:C:307:PRO:HB3	1.88	0.56
1:I:236:GLY:O	1:J:305:ASN:HB2	2.05	0.56
1:C:335:GLY:HA2	1:C:337:TYR:H	1.70	0.56
1:I:368:LEU:H	1:I:368:LEU:HD12	1.69	0.56
1:E:244:ALA:HB1	1:F:307:PRO:HB3	1.87	0.55
1:F:82:ILE:HD12	1:F:225:HIS:HB2	1.88	0.55
1:A:82:ILE:HD12	1:A:225:HIS:HB2	1.89	0.55
1:A:335:GLY:CA	1:A:337:TYR:H	2.19	0.55
1:F:184:ARG:NH1	2:K:42:C:OP2	2.38	0.55
1:G:215:LYS:HE3	1:G:216:HIS:HE1	1.70	0.55
2:K:16:C:H2'	2:K:17:C:O4'	2.07	0.55
1:C:368:LEU:HD12	1:C:368:LEU:N	2.21	0.55
1:A:217:PRO:O	1:A:220:ILE:HG23	2.07	0.55
1:H:215:LYS:HE3	1:H:216:HIS:HE1	1.71	0.55
1:D:82:ILE:HD12	1:D:225:HIS:HB2	1.89	0.55
1:G:146:ALA:HB3	1:G:149:TYR:CD2	2.41	0.55
1:I:335:GLY:HA2	1:I:337:TYR:H	1.72	0.55
1:C:215:LYS:HE3	1:C:216:HIS:HE1	1.71	0.55
1:G:335:GLY:HA2	1:G:337:TYR:H	1.72	0.55
1:E:82:ILE:HD12	1:E:225:HIS:HB2	1.89	0.54
1:D:335:GLY:HA2	1:D:337:TYR:H	1.72	0.54
1:B:335:GLY:HA2	1:B:337:TYR:H	1.73	0.54
1:A:18:LEU:HD22	1:J:231:SER:HB2	1.89	0.54
1:G:368:LEU:HD12	1:G:368:LEU:N	2.23	0.54
1:F:236:GLY:O	1:G:305:ASN:HB2	2.07	0.54
1:F:335:GLY:HA2	1:F:337:TYR:H	1.72	0.54
1:I:82:ILE:HD12	1:I:225:HIS:HB2	1.90	0.54
1:C:368:LEU:HG	1:E:3:LEU:HD11	1.90	0.54
1:D:368:LEU:N	1:D:368:LEU:HD12	2.22	0.54
1:D:217:PRO:O	1:D:220:ILE:HG23	2.08	0.54
1:F:215:LYS:HE3	1:F:216:HIS:HE1	1.72	0.54
1:H:301:TYR:HB3	1:H:309:ALA:HB2	1.90	0.54
1:A:278:GLN:OE1	1:J:367:VAL:HG11	2.08	0.54
1:E:335:GLY:HA2	1:E:337:TYR:H	1.71	0.54
1:B:368:LEU:HD12	1:B:368:LEU:N	2.23	0.54
1:E:38:TYR:CE1	1:F:26:GLN:HB2	2.43	0.54
1:B:215:LYS:HE3	1:B:216:HIS:HE1	1.73	0.54
1:D:172:ALA:HB2	1:D:253:ALA:HB1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:N	1:A:368:LEU:HD12	2.23	0.53
1:E:240:GLU:OE2	1:F:27:ARG:HD3	2.08	0.53
1:H:86:ALA:HB1	1:H:88:TYR:HE1	1.73	0.53
1:F:244:ALA:HB1	1:G:307:PRO:HB3	1.89	0.53
1:G:281:MET:HA	1:G:284:VAL:HG22	1.90	0.53
1:B:82:ILE:HD12	1:B:225:HIS:HB2	1.89	0.53
1:J:368:LEU:HD12	1:J:368:LEU:N	2.24	0.53
1:H:335:GLY:HA2	1:H:337:TYR:H	1.74	0.53
1:G:38:TYR:CE1	1:H:26:GLN:HB2	2.43	0.53
1:F:329:ALA:HA	1:F:334:MET:HG2	1.91	0.53
1:J:82:ILE:HD12	1:J:225:HIS:HB2	1.89	0.53
1:J:86:ALA:HB1	1:J:88:TYR:HE1	1.74	0.53
1:J:335:GLY:HA2	1:J:337:TYR:H	1.74	0.53
1:H:281:MET:HA	1:H:284:VAL:HG22	1.91	0.53
1:C:172:ALA:HB2	1:C:253:ALA:HB1	1.91	0.53
1:E:172:ALA:HB2	1:E:253:ALA:HB1	1.91	0.53
1:F:368:LEU:HD12	1:F:368:LEU:N	2.24	0.53
1:E:86:ALA:HB1	1:E:88:TYR:HE1	1.73	0.52
1:B:86:ALA:HB1	1:B:88:TYR:HE1	1.74	0.52
1:F:367:VAL:HG11	1:G:278:GLN:OE1	2.09	0.52
1:D:281:MET:HA	1:D:284:VAL:HG22	1.91	0.52
1:E:78:ASP:O	1:E:82:ILE:HG23	2.10	0.52
1:E:146:ALA:HB3	1:E:149:TYR:CD2	2.45	0.52
1:I:172:ALA:HB2	1:I:253:ALA:HB1	1.92	0.52
1:J:215:LYS:HE3	1:J:216:HIS:HE1	1.74	0.52
1:J:172:ALA:HB2	1:J:253:ALA:HB1	1.91	0.52
1:D:146:ALA:HB3	1:D:149:TYR:CD2	2.44	0.52
1:G:217:PRO:O	1:G:220:ILE:HG23	2.09	0.52
1:I:86:ALA:HB1	1:I:88:TYR:HE1	1.73	0.52
1:G:367:VAL:HG11	1:I:2:ALA:HB3	1.91	0.52
1:I:74:LEU:HD21	1:I:226:PHE:HA	1.90	0.52
1:G:86:ALA:HB1	1:G:88:TYR:HE1	1.73	0.52
1:I:368:LEU:N	1:I:368:LEU:HD12	2.25	0.52
1:F:217:PRO:O	1:F:220:ILE:HG23	2.09	0.52
1:C:366:SER:O	1:E:1:MET:CE	2.57	0.52
1:H:82:ILE:HD12	1:H:225:HIS:HB2	1.92	0.52
1:G:74:LEU:HD21	1:G:226:PHE:HA	1.92	0.52
1:G:303:ILE:HD12	1:G:303:ILE:H	1.75	0.51
1:I:217:PRO:O	1:I:220:ILE:HG23	2.11	0.51
1:D:244:ALA:HB1	1:E:307:PRO:HB3	1.92	0.51
1:C:82:ILE:HD12	1:C:225:HIS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:368:LEU:HG	1:J:3:LEU:HD11	1.92	0.51
1:F:86:ALA:HB1	1:F:88:TYR:HE1	1.75	0.51
1:J:146:ALA:HB3	1:J:149:TYR:CD2	2.45	0.51
1:B:172:ALA:HB2	1:B:253:ALA:HB1	1.92	0.51
1:E:236:GLY:O	1:F:305:ASN:HB2	2.09	0.51
1:E:368:LEU:N	1:E:368:LEU:HD12	2.24	0.51
1:G:82:ILE:HD12	1:G:225:HIS:HB2	1.91	0.51
1:A:305:ASN:HB2	1:J:236:GLY:O	2.09	0.51
1:G:329:ALA:HA	1:G:334:MET:HG2	1.93	0.51
1:C:86:ALA:HB1	1:C:88:TYR:HE1	1.76	0.51
1:A:329:ALA:HA	1:A:334:MET:HG2	1.93	0.51
1:E:367:VAL:HG12	1:G:3:LEU:CD1	2.39	0.51
1:G:172:ALA:HB2	1:G:253:ALA:HB1	1.91	0.51
1:A:86:ALA:HB1	1:A:88:TYR:HE1	1.75	0.51
1:B:329:ALA:HA	1:B:334:MET:HG2	1.93	0.51
1:D:329:ALA:HA	1:D:334:MET:HG2	1.92	0.51
1:C:367:VAL:HG11	1:E:2:ALA:HB3	1.92	0.51
1:C:146:ALA:HB3	1:C:149:TYR:CD2	2.45	0.51
1:F:146:ALA:HB3	1:F:149:TYR:CD2	2.46	0.51
1:C:329:ALA:HA	1:C:334:MET:HG2	1.93	0.51
2:K:3:C:H6	2:K:3:C:O5'	1.93	0.51
1:B:281:MET:HA	1:B:284:VAL:HG22	1.93	0.51
1:H:172:ALA:HB2	1:H:253:ALA:HB1	1.93	0.50
1:H:368:LEU:HD12	1:H:368:LEU:N	2.26	0.50
1:D:367:VAL:CG1	1:F:3:LEU:HD12	2.41	0.50
1:D:74:LEU:HD21	1:D:226:PHE:HA	1.93	0.50
1:C:361:GLY:HA3	1:D:274:HIS:NE2	2.27	0.50
1:H:78:ASP:O	1:H:82:ILE:HG23	2.11	0.50
1:H:303:ILE:HD12	1:H:303:ILE:H	1.76	0.50
1:D:303:ILE:H	1:D:303:ILE:HD12	1.75	0.50
2:K:64:C:H2'	2:K:65:C:O4'	2.11	0.50
1:A:172:ALA:HB2	1:A:253:ALA:HB1	1.92	0.50
1:A:74:LEU:HD21	1:A:226:PHE:HA	1.94	0.50
1:F:367:VAL:HG12	1:H:3:LEU:CD1	2.40	0.50
1:A:146:ALA:HB3	1:A:149:TYR:CD2	2.43	0.50
1:C:281:MET:HA	1:C:284:VAL:HG22	1.94	0.50
1:F:82:ILE:HG22	1:G:23:TYR:CE1	2.46	0.50
1:D:86:ALA:HB1	1:D:88:TYR:HE1	1.75	0.50
1:H:159:ILE:O	1:H:162:CYS:HB2	2.12	0.50
1:F:281:MET:HA	1:F:284:VAL:HG22	1.94	0.50
1:J:74:LEU:HD21	1:J:226:PHE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:O	1:C:169:THR:HB	2.11	0.50
1:I:146:ALA:HB3	1:I:149:TYR:CD2	2.45	0.50
1:C:303:ILE:HD12	1:C:303:ILE:H	1.76	0.50
1:A:166:LEU:O	1:A:169:THR:HB	2.12	0.50
1:H:329:ALA:HA	1:H:334:MET:HG2	1.93	0.50
1:E:329:ALA:HA	1:E:334:MET:HG2	1.94	0.49
1:J:281:MET:HA	1:J:284:VAL:HG22	1.94	0.49
1:F:240:GLU:CD	1:G:27:ARG:HH11	2.16	0.49
1:I:329:ALA:HA	1:I:334:MET:HG2	1.93	0.49
1:J:166:LEU:O	1:J:169:THR:HB	2.13	0.49
1:F:74:LEU:HD21	1:F:226:PHE:HA	1.94	0.49
1:F:78:ASP:O	1:F:82:ILE:HG23	2.13	0.49
1:A:335:GLY:HA2	1:A:337:TYR:H	1.75	0.49
1:E:166:LEU:O	1:E:169:THR:HB	2.13	0.49
1:E:36:PRO:HD2	1:E:71:MET:HB3	1.95	0.49
1:A:281:MET:HA	1:A:284:VAL:HG22	1.95	0.49
1:B:146:ALA:HB3	1:B:149:TYR:CD2	2.44	0.49
1:F:64:LEU:HD12	1:F:119:LEU:HD13	1.95	0.48
1:I:64:LEU:HD12	1:I:119:LEU:HD13	1.94	0.48
1:H:262:VAL:HG13	1:I:7:LYS:HA	1.95	0.48
1:B:166:LEU:O	1:B:169:THR:HB	2.13	0.48
1:D:38:TYR:CE1	1:E:26:GLN:HB2	2.48	0.48
1:E:78:ASP:O	1:E:82:ILE:CG2	2.62	0.48
1:F:172:ALA:HB2	1:F:253:ALA:HB1	1.95	0.48
1:H:74:LEU:HD21	1:H:226:PHE:HA	1.94	0.48
1:A:361:GLY:HA3	1:B:274:HIS:HE2	1.76	0.48
1:B:361:GLY:HA3	1:C:274:HIS:HE2	1.74	0.48
1:E:255:GLN:HB2	1:E:259:ARG:NH1	2.29	0.48
1:E:281:MET:HA	1:E:284:VAL:HG22	1.94	0.48
1:B:74:LEU:HD21	1:B:226:PHE:HA	1.95	0.48
1:G:78:ASP:O	1:G:82:ILE:HG23	2.14	0.48
1:C:88:TYR:CD1	1:C:88:TYR:N	2.82	0.48
1:C:366:SER:O	1:E:1:MET:HE3	2.14	0.48
1:H:166:LEU:O	1:H:169:THR:HB	2.14	0.48
1:G:34:ASP:HA	1:G:93:ASN:HB3	1.96	0.48
1:A:23:TYR:CE1	1:J:82:ILE:HG22	2.49	0.47
1:A:78:ASP:O	1:A:82:ILE:HG23	2.13	0.47
1:C:74:LEU:HD21	1:C:226:PHE:HA	1.95	0.47
1:J:329:ALA:HA	1:J:334:MET:HG2	1.95	0.47
1:D:64:LEU:HD12	1:D:119:LEU:HD13	1.95	0.47
1:A:23:TYR:CZ	1:J:82:ILE:HB	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ASP:O	1:D:82:ILE:HG23	2.15	0.47
1:E:303:ILE:HD12	1:E:303:ILE:H	1.80	0.47
1:I:88:TYR:N	1:I:88:TYR:CD1	2.82	0.47
2:K:30:C:H2'	2:K:31:C:O4'	2.15	0.47
1:H:78:ASP:O	1:H:82:ILE:CG2	2.62	0.47
1:B:34:ASP:HA	1:B:93:ASN:HB3	1.96	0.47
1:B:3:LEU:CD1	1:J:367:VAL:HG12	2.44	0.47
1:E:42:LYS:HD2	1:F:28:SER:HB3	1.97	0.47
1:I:234:ARG:HH21	1:J:86:ALA:HB2	1.79	0.47
1:H:88:TYR:CD1	1:H:88:TYR:N	2.83	0.47
1:B:64:LEU:HD12	1:B:119:LEU:HD13	1.96	0.47
1:F:78:ASP:O	1:F:82:ILE:CG2	2.63	0.47
1:I:303:ILE:HD12	1:I:303:ILE:H	1.80	0.47
1:J:64:LEU:HD12	1:J:119:LEU:HD13	1.96	0.47
1:J:34:ASP:HA	1:J:93:ASN:HB3	1.97	0.47
1:I:281:MET:HA	1:I:284:VAL:HG22	1.96	0.47
1:H:34:ASP:HA	1:H:93:ASN:HB3	1.96	0.47
1:I:187:ASN:O	1:I:191:LYS:HB3	2.15	0.47
1:F:107:LYS:HG3	1:F:107:LYS:H	1.58	0.47
1:E:34:ASP:HA	1:E:93:ASN:HB3	1.97	0.47
1:G:166:LEU:O	1:G:169:THR:HB	2.15	0.47
1:E:74:LEU:HD21	1:E:226:PHE:HA	1.97	0.47
1:C:367:VAL:CG1	1:E:1:MET:CG	2.80	0.47
1:B:361:GLY:HA3	1:C:274:HIS:CE1	2.50	0.47
1:E:337:TYR:CE1	2:K:32:C:H2'	2.50	0.47
1:B:303:ILE:H	1:B:303:ILE:HD12	1.80	0.46
1:E:135:TYR:OH	1:E:145:VAL:HG21	2.16	0.46
1:E:88:TYR:CD1	1:E:88:TYR:N	2.83	0.46
1:A:303:ILE:HD12	1:A:303:ILE:H	1.80	0.46
1:I:34:ASP:HA	1:I:93:ASN:HB3	1.96	0.46
1:A:34:ASP:HA	1:A:93:ASN:HB3	1.96	0.46
1:B:256:VAL:HG12	2:K:11:C:OP1	2.14	0.46
1:C:34:ASP:HA	1:C:93:ASN:HB3	1.96	0.46
1:G:64:LEU:HD12	1:G:119:LEU:HD13	1.96	0.46
1:A:78:ASP:O	1:A:82:ILE:CG2	2.64	0.46
1:A:28:SER:HB2	1:J:42:LYS:HD2	1.96	0.46
1:B:88:TYR:CD1	1:B:88:TYR:N	2.83	0.46
1:H:146:ALA:HB3	1:H:149:TYR:CD2	2.46	0.46
1:C:107:LYS:HG3	1:C:107:LYS:H	1.53	0.46
1:F:34:ASP:HA	1:F:93:ASN:HB3	1.97	0.46
1:I:78:ASP:O	1:I:82:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:TYR:CD1	1:J:88:TYR:N	2.83	0.46
1:B:231:SER:HB2	1:C:18:LEU:HD22	1.97	0.46
1:A:135:TYR:OH	1:A:145:VAL:HG21	2.16	0.46
1:F:303:ILE:HD12	1:F:303:ILE:H	1.80	0.46
1:B:78:ASP:O	1:B:82:ILE:HG23	2.15	0.46
1:D:88:TYR:CD1	1:D:88:TYR:N	2.83	0.46
2:K:54:C:N4	2:K:55:C:N4	2.63	0.46
1:D:215:LYS:HE3	1:D:216:HIS:CE1	2.50	0.46
1:C:64:LEU:HD12	1:C:119:LEU:HD13	1.97	0.46
1:I:166:LEU:O	1:I:169:THR:HB	2.16	0.46
1:D:255:GLN:HB2	1:D:259:ARG:NH1	2.31	0.46
1:G:78:ASP:O	1:G:82:ILE:CG2	2.64	0.46
1:C:265:LYS:HE3	1:D:4:SER:HA	1.97	0.46
1:I:120:THR:CG2	1:I:122:GLU:HG2	2.46	0.46
1:H:361:GLY:HA3	1:I:274:HIS:NE2	2.31	0.46
1:C:255:GLN:HB2	1:C:259:ARG:NH1	2.31	0.46
1:D:166:LEU:O	1:D:169:THR:HB	2.17	0.46
1:J:36:PRO:HD2	1:J:71:MET:HB3	1.98	0.46
1:F:42:LYS:CD	1:G:28:SER:HB3	2.28	0.45
1:G:361:GLY:HA3	1:H:274:HIS:HE2	1.79	0.45
1:B:187:ASN:O	1:B:191:LYS:HB3	2.16	0.45
1:E:231:SER:HA	1:F:307:PRO:HG2	1.97	0.45
1:H:64:LEU:HD12	1:H:119:LEU:HD13	1.96	0.45
1:C:78:ASP:O	1:C:82:ILE:HG23	2.16	0.45
1:H:120:THR:CG2	1:H:122:GLU:HG2	2.47	0.45
1:F:88:TYR:CD1	1:F:88:TYR:N	2.85	0.45
1:D:319:HIS:O	1:D:323:VAL:HG12	2.17	0.45
1:H:107:LYS:HG3	1:H:107:LYS:H	1.56	0.45
1:H:303:ILE:HD12	1:H:303:ILE:N	2.31	0.45
1:F:166:LEU:O	1:F:169:THR:HB	2.16	0.45
1:I:36:PRO:HD2	1:I:71:MET:HB3	1.99	0.45
1:H:187:ASN:O	1:H:191:LYS:HB3	2.16	0.45
1:D:34:ASP:HA	1:D:93:ASN:HB3	1.98	0.45
1:E:187:ASN:O	1:E:191:LYS:HB3	2.16	0.45
1:J:78:ASP:O	1:J:82:ILE:CG2	2.65	0.45
2:K:54:C:H2'	2:K:55:C:O4'	2.17	0.45
1:J:255:GLN:HB2	1:J:259:ARG:NH1	2.32	0.45
1:A:323:VAL:HG23	1:A:350:ALA:HB2	1.98	0.45
1:I:42:LYS:HD2	1:J:28:SER:HB3	1.99	0.45
1:B:159:ILE:O	1:B:162:CYS:HB2	2.17	0.45
1:A:64:LEU:HD12	1:A:119:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:23:C:H2'	2:K:24:C:O4'	2.17	0.45
1:A:88:TYR:N	1:A:88:TYR:CD1	2.84	0.45
1:A:3:LEU:CD1	1:I:367:VAL:HG12	2.47	0.44
1:E:42:LYS:HZ1	1:F:30:GLY:C	2.18	0.44
1:G:120:THR:CG2	1:G:122:GLU:HG2	2.47	0.44
1:C:135:TYR:OH	1:C:145:VAL:HG21	2.17	0.44
1:J:323:VAL:HG23	1:J:350:ALA:HB2	1.99	0.44
1:F:159:ILE:O	1:F:162:CYS:HB2	2.17	0.44
1:D:303:ILE:N	1:D:303:ILE:HD12	2.31	0.44
1:F:135:TYR:OH	1:F:145:VAL:HG21	2.18	0.44
1:F:120:THR:CG2	1:F:122:GLU:HG2	2.47	0.44
1:D:78:ASP:O	1:D:82:ILE:CG2	2.66	0.44
1:I:240:GLU:OE2	1:J:27:ARG:HD3	2.16	0.44
1:G:88:TYR:N	1:G:88:TYR:CD1	2.85	0.44
1:G:153:SER:HA	1:G:154:PRO:HD2	1.82	0.44
1:G:159:ILE:O	1:G:162:CYS:HB2	2.18	0.44
1:C:230:GLN:O	1:C:233:THR:HG22	2.18	0.44
1:D:135:TYR:OH	1:D:145:VAL:HG21	2.17	0.44
1:J:270:ILE:HD13	1:J:270:ILE:HA	1.76	0.44
1:F:255:GLN:HB2	1:F:259:ARG:NH1	2.33	0.44
1:G:303:ILE:HD12	1:G:303:ILE:N	2.33	0.44
1:E:73:ARG:CZ	1:F:27:ARG:HG2	2.48	0.44
1:C:36:PRO:HD2	1:C:71:MET:HB3	1.99	0.44
1:C:187:ASN:O	1:C:191:LYS:HB3	2.17	0.44
1:D:251:TYR:OH	1:E:13:ASN:HB3	2.18	0.44
1:I:78:ASP:O	1:I:82:ILE:CG2	2.66	0.44
1:F:323:VAL:HG23	1:F:350:ALA:HB2	1.99	0.44
1:I:159:ILE:O	1:I:162:CYS:HB2	2.18	0.44
1:B:78:ASP:O	1:B:82:ILE:CG2	2.66	0.44
1:E:184:ARG:NH1	2:K:35:C:OP2	2.50	0.44
1:A:120:THR:CG2	1:A:122:GLU:HG2	2.47	0.44
1:G:255:GLN:HB2	1:G:259:ARG:NH1	2.33	0.43
1:E:120:THR:CG2	1:E:122:GLU:HG2	2.47	0.43
1:J:187:ASN:O	1:J:191:LYS:HB3	2.18	0.43
1:C:367:VAL:CA	1:E:1:MET:HG2	2.32	0.43
1:A:234:ARG:HH21	1:B:86:ALA:HB2	1.83	0.43
1:B:255:GLN:HB2	1:B:259:ARG:NH1	2.33	0.43
1:F:29:THR:HG22	1:F:88:TYR:HD2	1.83	0.43
1:H:135:TYR:OH	1:H:145:VAL:HG21	2.18	0.43
1:A:159:ILE:O	1:A:162:CYS:HB2	2.18	0.43
1:D:120:THR:CG2	1:D:122:GLU:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:PRO:HD2	1:H:71:MET:HB3	2.00	0.43
1:A:270:ILE:HA	1:A:270:ILE:HD13	1.78	0.43
1:B:303:ILE:HD12	1:B:303:ILE:N	2.34	0.43
1:J:319:HIS:O	1:J:323:VAL:HG12	2.18	0.43
1:H:255:GLN:HB2	1:H:259:ARG:NH1	2.33	0.43
1:A:187:ASN:O	1:A:191:LYS:HB3	2.18	0.43
1:D:230:GLN:O	1:D:233:THR:HG22	2.18	0.43
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.78	0.43
1:G:135:TYR:OH	1:G:145:VAL:HG21	2.18	0.43
1:H:6:VAL:O	1:H:6:VAL:HG22	2.18	0.43
1:B:120:THR:CG2	1:B:122:GLU:HG2	2.49	0.43
1:H:265:LYS:HG3	1:I:3:LEU:O	2.18	0.43
1:G:6:VAL:HG22	1:G:6:VAL:O	2.17	0.43
1:F:187:ASN:O	1:F:191:LYS:HB3	2.19	0.43
1:F:230:GLN:O	1:F:233:THR:HG22	2.19	0.43
1:E:159:ILE:O	1:E:162:CYS:HB2	2.18	0.43
1:I:333:ILE:HG13	1:I:333:ILE:H	1.68	0.43
1:F:319:HIS:O	1:F:323:VAL:HG12	2.19	0.43
1:I:319:HIS:O	1:I:323:VAL:HG12	2.19	0.43
1:A:294:LEU:HB3	1:A:298:ALA:HB2	2.01	0.43
1:C:38:TYR:CE1	1:D:26:GLN:HB2	2.53	0.43
1:D:270:ILE:HD13	1:D:270:ILE:HA	1.79	0.43
1:C:366:SER:O	1:E:1:MET:HE2	2.19	0.43
1:G:319:HIS:O	1:G:323:VAL:HG12	2.18	0.43
1:G:29:THR:HG22	1:G:88:TYR:HD2	1.84	0.43
1:J:135:TYR:OH	1:J:145:VAL:HG21	2.19	0.43
1:A:36:PRO:HD2	1:A:71:MET:HB3	2.01	0.43
1:F:36:PRO:HD2	1:F:71:MET:HB3	2.00	0.43
1:E:303:ILE:HD12	1:E:303:ILE:N	2.34	0.42
1:I:244:ALA:HB1	1:J:307:PRO:HB3	2.01	0.42
1:F:294:LEU:HB3	1:F:298:ALA:HB2	2.01	0.42
1:I:215:LYS:HE3	1:I:216:HIS:CE1	2.54	0.42
1:H:301:TYR:O	1:H:304:LEU:O	2.37	0.42
1:E:103:ASP:HA	1:E:108:GLU:HA	2.01	0.42
1:I:370:LEU:HG	1:J:268:LYS:HD3	2.01	0.42
1:I:29:THR:HG22	1:I:88:TYR:HD2	1.83	0.42
1:I:270:ILE:HA	1:I:270:ILE:HD13	1.80	0.42
1:B:36:PRO:HD2	1:B:71:MET:HB3	2.00	0.42
1:J:303:ILE:H	1:J:303:ILE:HD12	1.84	0.42
1:A:319:HIS:O	1:A:323:VAL:HG12	2.19	0.42
1:C:120:THR:CG2	1:C:122:GLU:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:230:GLN:O	1:J:233:THR:HG22	2.19	0.42
1:A:3:LEU:HD13	1:I:367:VAL:HG12	2.01	0.42
1:A:335:GLY:HA2	1:A:336:GLU:HA	1.87	0.42
1:G:323:VAL:HG23	1:G:350:ALA:HB2	2.01	0.42
1:A:25:ILE:HA	1:J:73:ARG:O	2.19	0.42
1:G:187:ASN:O	1:G:191:LYS:HB3	2.19	0.42
1:D:258:LEU:HA	1:D:258:LEU:HD12	1.93	0.42
1:D:187:ASN:O	1:D:191:LYS:HB3	2.19	0.42
1:C:294:LEU:HB3	1:C:298:ALA:HB2	2.02	0.42
1:D:184:ARG:NH1	2:K:28:C:OP2	2.52	0.42
1:I:361:GLY:HA3	1:J:274:HIS:CD2	2.51	0.42
1:J:34:ASP:OD2	1:J:117:ALA:N	2.46	0.42
2:K:6:C:H2'	2:K:7:C:O4'	2.20	0.42
1:B:240:GLU:OE2	1:C:27:ARG:HD3	2.18	0.42
1:F:73:ARG:O	1:G:25:ILE:HA	2.20	0.42
1:A:209:PHE:HA	1:A:212:VAL:HG12	2.00	0.42
1:C:6:VAL:O	1:C:6:VAL:HG22	2.20	0.42
1:A:234:ARG:NH2	1:B:86:ALA:HB2	2.35	0.42
1:E:335:GLY:HA2	1:E:337:TYR:N	2.35	0.42
1:I:283:GLN:O	1:I:286:GLU:HB2	2.19	0.42
1:D:262:VAL:HG13	1:E:7:LYS:HA	2.02	0.42
1:F:364:ASN:HB3	1:G:273:GLY:O	2.19	0.42
1:I:255:GLN:HB2	1:I:259:ARG:NH1	2.34	0.42
1:F:153:SER:HA	1:F:154:PRO:HD2	1.80	0.42
2:K:19:C:H2'	2:K:20:C:O4'	2.20	0.42
1:A:29:THR:HG22	1:A:88:TYR:HD2	1.85	0.42
1:A:255:GLN:HB2	1:A:259:ARG:NH1	2.35	0.42
1:J:209:PHE:HA	1:J:212:VAL:HG12	2.01	0.42
1:E:64:LEU:HD12	1:E:119:LEU:HD13	2.00	0.42
1:G:36:PRO:HD2	1:G:71:MET:HB3	2.00	0.42
1:C:159:ILE:O	1:C:162:CYS:HB2	2.20	0.42
1:H:270:ILE:HA	1:H:270:ILE:HD13	1.78	0.42
1:B:209:PHE:HA	1:B:212:VAL:HG12	2.01	0.42
1:D:234:ARG:NH2	1:E:86:ALA:HB2	2.34	0.42
1:D:36:PRO:HD2	1:D:71:MET:HB3	2.01	0.42
1:B:42:LYS:HD2	1:C:28:SER:HB3	2.00	0.42
1:J:78:ASP:O	1:J:82:ILE:HG23	2.19	0.42
1:H:29:THR:HG22	1:H:88:TYR:HD2	1.84	0.42
1:C:303:ILE:N	1:C:303:ILE:HD12	2.33	0.42
1:I:301:TYR:O	1:I:304:LEU:O	2.38	0.42
1:D:323:VAL:HG23	1:D:350:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LYS:NZ	1:D:30:GLY:C	2.74	0.42
1:D:159:ILE:O	1:D:162:CYS:HB2	2.19	0.42
1:E:333:ILE:H	1:E:333:ILE:HG13	1.69	0.42
1:G:244:ALA:HB1	1:H:307:PRO:HB3	2.01	0.42
1:C:78:ASP:O	1:C:82:ILE:CG2	2.68	0.41
1:C:29:THR:HG22	1:C:88:TYR:HD2	1.84	0.41
1:J:294:LEU:HB3	1:J:298:ALA:HB2	2.02	0.41
1:B:135:TYR:OH	1:B:145:VAL:HG21	2.20	0.41
1:H:153:SER:HA	1:H:154:PRO:HD2	1.80	0.41
1:C:323:VAL:HG23	1:C:350:ALA:HB2	2.00	0.41
1:C:153:SER:HA	1:C:154:PRO:HD2	1.81	0.41
1:J:153:SER:HA	1:J:154:PRO:HD2	1.83	0.41
1:D:234:ARG:NH2	1:E:221:ASP:OD1	2.52	0.41
1:H:294:LEU:HB3	1:H:298:ALA:HB2	2.03	0.41
1:E:107:LYS:HG3	1:E:107:LYS:H	1.56	0.41
1:H:215:LYS:HE3	1:H:216:HIS:CE1	2.54	0.41
1:J:120:THR:CG2	1:J:122:GLU:HG2	2.50	0.41
1:I:294:LEU:HB3	1:I:298:ALA:HB2	2.03	0.41
1:C:103:ASP:HA	1:C:108:GLU:HA	2.02	0.41
1:F:166:LEU:HD21	1:F:246:LEU:HD22	2.02	0.41
1:D:125:ILE:HG13	1:D:126:ASN:N	2.36	0.41
1:C:231:SER:HB2	1:D:18:LEU:HD22	2.03	0.41
1:J:159:ILE:O	1:J:162:CYS:HB2	2.19	0.41
1:J:184:ARG:NH2	2:K:69:C:OP1	2.50	0.41
1:B:6:VAL:O	1:B:6:VAL:HG22	2.20	0.41
1:J:29:THR:HG22	1:J:88:TYR:HD2	1.85	0.41
1:B:323:VAL:HG23	1:B:350:ALA:HB2	2.03	0.41
1:G:103:ASP:HA	1:G:108:GLU:HA	2.02	0.41
1:I:303:ILE:HD12	1:I:303:ILE:N	2.35	0.41
1:C:335:GLY:HA2	1:C:337:TYR:N	2.35	0.41
1:E:319:HIS:O	1:E:323:VAL:HG12	2.19	0.41
2:K:26:C:H2'	2:K:27:C:O4'	2.21	0.41
1:I:88:TYR:HD1	1:I:88:TYR:H	1.69	0.41
1:B:301:TYR:O	1:B:304:LEU:O	2.39	0.41
1:B:319:HIS:O	1:B:323:VAL:HG12	2.20	0.41
1:I:29:THR:HG22	1:I:88:TYR:CD2	2.56	0.41
1:F:283:GLN:O	1:F:286:GLU:HB2	2.21	0.41
1:E:125:ILE:HG13	1:E:126:ASN:N	2.35	0.41
1:A:307:PRO:HB3	1:J:244:ALA:HB1	2.01	0.41
1:A:23:TYR:CD1	1:J:82:ILE:HG22	2.56	0.41
1:D:6:VAL:HG22	1:D:6:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:THR:HG22	1:F:88:TYR:CD2	2.56	0.41
1:H:29:THR:HG22	1:H:88:TYR:CD2	2.56	0.41
1:F:335:GLY:HA2	1:F:336:GLU:HA	1.88	0.41
1:E:323:VAL:HG23	1:E:350:ALA:HB2	2.03	0.41
1:C:209:PHE:HA	1:C:212:VAL:HG12	2.02	0.41
1:G:209:PHE:HA	1:G:212:VAL:HG12	2.02	0.41
2:K:33:C:H2'	2:K:34:C:O4'	2.20	0.41
1:E:283:GLN:O	1:E:286:GLU:HB2	2.21	0.41
1:F:45:ASN:HB2	1:F:69:TYR:CE1	2.56	0.41
1:E:270:ILE:HA	1:E:270:ILE:HD13	1.77	0.41
1:F:303:ILE:HD12	1:F:303:ILE:N	2.35	0.41
1:A:303:ILE:HD12	1:A:303:ILE:N	2.36	0.41
1:I:42:LYS:HD2	1:J:28:SER:CB	2.50	0.41
1:E:209:PHE:HA	1:E:212:VAL:HG12	2.02	0.41
1:A:103:ASP:HA	1:A:108:GLU:HA	2.03	0.41
1:B:283:GLN:O	1:B:286:GLU:HB2	2.21	0.41
1:E:29:THR:HG22	1:E:88:TYR:HD2	1.84	0.40
1:A:301:TYR:O	1:A:304:LEU:O	2.39	0.40
2:K:37:C:H2'	2:K:38:C:O4'	2.21	0.40
1:B:294:LEU:HB3	1:B:298:ALA:HB2	2.02	0.40
1:H:125:ILE:HG13	1:H:126:ASN:N	2.36	0.40
1:E:367:VAL:HG21	1:F:278:GLN:CD	2.41	0.40
1:D:29:THR:HG22	1:D:88:TYR:HD2	1.85	0.40
1:B:335:GLY:HA2	1:B:337:TYR:N	2.37	0.40
1:D:231:SER:HA	1:E:307:PRO:HG2	2.03	0.40
1:C:319:HIS:O	1:C:323:VAL:HG12	2.21	0.40
1:I:135:TYR:OH	1:I:145:VAL:HG21	2.20	0.40
1:B:29:THR:HG22	1:B:88:TYR:HD2	1.86	0.40
1:D:294:LEU:HB3	1:D:298:ALA:HB2	2.03	0.40
1:B:230:GLN:O	1:B:233:THR:HG22	2.21	0.40
1:B:41:GLN:NE2	1:B:73:ARG:HA	2.37	0.40
1:J:283:GLN:O	1:J:286:GLU:HB2	2.22	0.40
1:G:301:TYR:O	1:G:304:LEU:O	2.40	0.40
1:B:42:LYS:HD2	1:C:28:SER:CB	2.51	0.40
1:J:103:ASP:HA	1:J:108:GLU:HA	2.02	0.40
1:C:125:ILE:HG13	1:C:126:ASN:N	2.37	0.40
1:F:209:PHE:HA	1:F:212:VAL:HG12	2.03	0.40
1:B:107:LYS:H	1:B:107:LYS:HG3	1.51	0.40
1:E:6:VAL:HG22	1:E:6:VAL:O	2.22	0.40
1:F:168:ILE:HG22	1:F:250:ALA:CB	2.52	0.40
1:D:103:ASP:HA	1:D:108:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:GLN:O	1:H:286:GLU:HB2	2.21	0.40
1:C:270:ILE:HA	1:C:270:ILE:HD13	1.78	0.40
1:H:41:GLN:NE2	1:H:73:ARG:HA	2.37	0.40
1:E:170:LYS:HB3	1:E:178:GLY:HA3	2.03	0.40

All (18) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ASP:OD2	1:I:374:GLU:CA[4_555]	1.20	1.00
1:E:359:GLU:CG	1:J:77:GLU:OE1[4_455]	1.36	0.84
1:E:96:ASP:OD2	1:I:374:GLU:CB[4_555]	1.42	0.78
1:E:359:GLU:CD	1:J:77:GLU:OE1[4_455]	1.46	0.74
1:E:96:ASP:CG	1:I:374:GLU:CG[4_555]	1.49	0.71
1:F:91:LYS:CE	1:J:374:GLU:O[4_555]	1.53	0.67
1:E:96:ASP:CB	1:I:374:GLU:CG[4_555]	1.65	0.55
1:E:96:ASP:OD2	1:I:374:GLU:CG[4_555]	1.77	0.43
1:F:91:LYS:NZ	1:J:375:LEU:C[4_555]	1.84	0.36
1:D:359:GLU:O	1:I:77:GLU:OE2[4_455]	1.86	0.34
1:E:136:LYS:NZ	1:I:148:GLU:OE1[1_565]	1.91	0.29
1:F:91:LYS:NZ	1:J:374:GLU:O[4_555]	2.05	0.15
1:F:91:LYS:NZ	1:J:375:LEU:CA[4_555]	2.06	0.14
1:E:359:GLU:CD	1:J:77:GLU:CD[4_455]	2.13	0.07
1:E:359:GLU:OE2	1:J:77:GLU:OE1[4_455]	2.14	0.06
1:E:359:GLU:OE1	1:J:77:GLU:CD[4_455]	2.18	0.02
1:E:96:ASP:CG	1:I:374:GLU:CB[4_555]	2.19	0.01
1:E:359:GLU:OE1	1:J:77:GLU:OE1[4_455]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/375 (100%)	370 (99%)	3 (1%)	0	100	100
1	B	373/375 (100%)	370 (99%)	3 (1%)	0	100	100
1	C	373/375 (100%)	369 (99%)	4 (1%)	0	100	100
1	D	373/375 (100%)	368 (99%)	5 (1%)	0	100	100
1	E	373/375 (100%)	369 (99%)	4 (1%)	0	100	100
1	F	373/375 (100%)	370 (99%)	3 (1%)	0	100	100
1	G	373/375 (100%)	368 (99%)	5 (1%)	0	100	100
1	H	373/375 (100%)	369 (99%)	4 (1%)	0	100	100
1	I	373/375 (100%)	370 (99%)	3 (1%)	0	100	100
1	J	373/375 (100%)	369 (99%)	4 (1%)	0	100	100
All	All	3730/3750 (100%)	3692 (99%)	38 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	313/313 (100%)	273 (87%)	40 (13%)	5	31
1	B	313/313 (100%)	273 (87%)	40 (13%)	5	31
1	C	313/313 (100%)	272 (87%)	41 (13%)	5	30
1	D	313/313 (100%)	271 (87%)	42 (13%)	5	29
1	E	313/313 (100%)	272 (87%)	41 (13%)	5	30
1	F	313/313 (100%)	274 (88%)	39 (12%)	6	32
1	G	313/313 (100%)	272 (87%)	41 (13%)	5	30
1	H	313/313 (100%)	273 (87%)	40 (13%)	5	31
1	I	313/313 (100%)	272 (87%)	41 (13%)	5	30
1	J	313/313 (100%)	272 (87%)	41 (13%)	5	30
All	All	3130/3130 (100%)	2724 (87%)	406 (13%)	5	30

All (406) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	5	LYS
1	A	6	VAL
1	A	8	LEU
1	A	11	THR
1	A	12	LEU
1	A	22	LYS
1	A	31	ASP
1	A	33	ILE
1	A	47	LEU
1	A	82	ILE
1	A	83	LEU
1	A	88	TYR
1	A	90	VAL
1	A	103	ASP
1	A	107	LYS
1	A	120	THR
1	A	123	ILE
1	A	136	LYS
1	A	145	VAL
1	A	163	ILE
1	A	168	ILE
1	A	196	ARG
1	A	220	ILE
1	A	255	GLN
1	A	270	ILE
1	A	272	LEU
1	A	283	GLN
1	A	293	LYS
1	A	304	LEU
1	A	313	SER
1	A	325	LEU
1	A	333	ILE
1	A	359	GLU
1	A	360	ASN
1	A	368	LEU
1	A	370	LEU
1	A	371	THR
1	A	373	GLU
1	A	375	LEU
1	B	3	LEU
1	B	5	LYS

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Mol	Chain	Res	Type
1	B	6	VAL
1	B	8	LEU
1	B	11	THR
1	B	12	LEU
1	B	22	LYS
1	B	31	ASP
1	B	33	ILE
1	B	82	ILE
1	B	83	LEU
1	B	88	TYR
1	B	90	VAL
1	B	103	ASP
1	B	107	LYS
1	B	120	THR
1	B	123	ILE
1	B	136	LYS
1	B	145	VAL
1	B	163	ILE
1	B	168	ILE
1	B	196	ARG
1	B	220	ILE
1	B	255	GLN
1	B	270	ILE
1	B	272	LEU
1	B	283	GLN
1	B	287	VAL
1	B	293	LYS
1	B	304	LEU
1	B	313	SER
1	B	325	LEU
1	B	333	ILE
1	B	359	GLU
1	B	360	ASN
1	B	368	LEU
1	B	370	LEU
1	B	371	THR
1	B	373	GLU
1	B	375	LEU
1	C	3	LEU
1	C	5	LYS
1	C	6	VAL
1	C	8	LEU

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Mol	Chain	Res	Type
1	C	11	THR
1	C	12	LEU
1	C	22	LYS
1	C	31	ASP
1	C	33	ILE
1	C	47	LEU
1	C	82	ILE
1	C	83	LEU
1	C	88	TYR
1	C	90	VAL
1	C	103	ASP
1	C	107	LYS
1	C	120	THR
1	C	123	ILE
1	C	136	LYS
1	C	145	VAL
1	C	163	ILE
1	C	168	ILE
1	C	196	ARG
1	C	220	ILE
1	C	255	GLN
1	C	270	ILE
1	C	272	LEU
1	C	283	GLN
1	C	287	VAL
1	C	293	LYS
1	C	304	LEU
1	C	313	SER
1	C	325	LEU
1	C	333	ILE
1	C	359	GLU
1	C	360	ASN
1	C	368	LEU
1	C	370	LEU
1	C	371	THR
1	C	373	GLU
1	C	375	LEU
1	D	3	LEU
1	D	5	LYS
1	D	6	VAL
1	D	8	LEU
1	D	11	THR

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Mol	Chain	Res	Type
1	D	12	LEU
1	D	22	LYS
1	D	31	ASP
1	D	33	ILE
1	D	47	LEU
1	D	82	ILE
1	D	83	LEU
1	D	88	TYR
1	D	90	VAL
1	D	103	ASP
1	D	107	LYS
1	D	120	THR
1	D	123	ILE
1	D	136	LYS
1	D	145	VAL
1	D	163	ILE
1	D	168	ILE
1	D	170	LYS
1	D	196	ARG
1	D	220	ILE
1	D	255	GLN
1	D	270	ILE
1	D	272	LEU
1	D	283	GLN
1	D	287	VAL
1	D	293	LYS
1	D	304	LEU
1	D	313	SER
1	D	325	LEU
1	D	333	ILE
1	D	359	GLU
1	D	360	ASN
1	D	368	LEU
1	D	370	LEU
1	D	371	THR
1	D	373	GLU
1	D	375	LEU
1	E	3	LEU
1	E	5	LYS
1	E	6	VAL
1	E	8	LEU
1	E	11	THR

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Mol	Chain	Res	Type
1	E	12	LEU
1	E	22	LYS
1	E	31	ASP
1	E	33	ILE
1	E	47	LEU
1	E	82	ILE
1	E	83	LEU
1	E	88	TYR
1	E	90	VAL
1	E	103	ASP
1	E	107	LYS
1	E	120	THR
1	E	123	ILE
1	E	136	LYS
1	E	145	VAL
1	E	163	ILE
1	E	168	ILE
1	E	196	ARG
1	E	220	ILE
1	E	255	GLN
1	E	270	ILE
1	E	272	LEU
1	E	283	GLN
1	E	287	VAL
1	E	293	LYS
1	E	304	LEU
1	E	313	SER
1	E	325	LEU
1	E	333	ILE
1	E	359	GLU
1	E	360	ASN
1	E	368	LEU
1	E	370	LEU
1	E	371	THR
1	E	373	GLU
1	E	375	LEU
1	F	3	LEU
1	F	5	LYS
1	F	6	VAL
1	F	8	LEU
1	F	11	THR
1	F	12	LEU

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Mol	Chain	Res	Type
1	F	22	LYS
1	F	31	ASP
1	F	33	ILE
1	F	82	ILE
1	F	83	LEU
1	F	88	TYR
1	F	90	VAL
1	F	103	ASP
1	F	107	LYS
1	F	120	THR
1	F	123	ILE
1	F	136	LYS
1	F	145	VAL
1	F	163	ILE
1	F	168	ILE
1	F	196	ARG
1	F	220	ILE
1	F	255	GLN
1	F	270	ILE
1	F	272	LEU
1	F	283	GLN
1	F	293	LYS
1	F	304	LEU
1	F	313	SER
1	F	325	LEU
1	F	333	ILE
1	F	359	GLU
1	F	360	ASN
1	F	368	LEU
1	F	370	LEU
1	F	371	THR
1	F	373	GLU
1	F	375	LEU
1	G	3	LEU
1	G	5	LYS
1	G	6	VAL
1	G	8	LEU
1	G	11	THR
1	G	12	LEU
1	G	22	LYS
1	G	31	ASP
1	G	33	ILE

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Mol	Chain	Res	Type
1	G	47	LEU
1	G	82	ILE
1	G	83	LEU
1	G	88	TYR
1	G	90	VAL
1	G	103	ASP
1	G	107	LYS
1	G	120	THR
1	G	123	ILE
1	G	136	LYS
1	G	145	VAL
1	G	163	ILE
1	G	168	ILE
1	G	196	ARG
1	G	220	ILE
1	G	255	GLN
1	G	270	ILE
1	G	272	LEU
1	G	283	GLN
1	G	287	VAL
1	G	293	LYS
1	G	304	LEU
1	G	313	SER
1	G	325	LEU
1	G	333	ILE
1	G	359	GLU
1	G	360	ASN
1	G	368	LEU
1	G	370	LEU
1	G	371	THR
1	G	373	GLU
1	G	375	LEU
1	H	3	LEU
1	H	5	LYS
1	H	6	VAL
1	H	8	LEU
1	H	11	THR
1	H	12	LEU
1	H	22	LYS
1	H	31	ASP
1	H	33	ILE
1	H	47	LEU

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Mol	Chain	Res	Type
1	H	82	ILE
1	H	83	LEU
1	H	88	TYR
1	H	90	VAL
1	H	103	ASP
1	H	107	LYS
1	H	120	THR
1	H	123	ILE
1	H	136	LYS
1	H	145	VAL
1	H	163	ILE
1	H	168	ILE
1	H	196	ARG
1	H	220	ILE
1	H	255	GLN
1	H	270	ILE
1	H	272	LEU
1	H	283	GLN
1	H	293	LYS
1	H	304	LEU
1	H	313	SER
1	H	325	LEU
1	H	333	ILE
1	H	359	GLU
1	H	360	ASN
1	H	368	LEU
1	H	370	LEU
1	H	371	THR
1	H	373	GLU
1	H	375	LEU
1	I	3	LEU
1	I	5	LYS
1	I	6	VAL
1	I	8	LEU
1	I	11	THR
1	I	12	LEU
1	I	22	LYS
1	I	31	ASP
1	I	33	ILE
1	I	47	LEU
1	I	82	ILE
1	I	83	LEU

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Mol	Chain	Res	Type
1	I	88	TYR
1	I	90	VAL
1	I	103	ASP
1	I	107	LYS
1	I	120	THR
1	I	123	ILE
1	I	136	LYS
1	I	145	VAL
1	I	163	ILE
1	I	168	ILE
1	I	196	ARG
1	I	220	ILE
1	I	255	GLN
1	I	270	ILE
1	I	272	LEU
1	I	283	GLN
1	I	287	VAL
1	I	293	LYS
1	I	304	LEU
1	I	313	SER
1	I	325	LEU
1	I	333	ILE
1	I	359	GLU
1	I	360	ASN
1	I	368	LEU
1	I	370	LEU
1	I	371	THR
1	I	373	GLU
1	I	375	LEU
1	J	3	LEU
1	J	5	LYS
1	J	6	VAL
1	J	8	LEU
1	J	11	THR
1	J	12	LEU
1	J	22	LYS
1	J	31	ASP
1	J	33	ILE
1	J	47	LEU
1	J	82	ILE
1	J	83	LEU
1	J	88	TYR

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Mol	Chain	Res	Type
1	J	90	VAL
1	J	103	ASP
1	J	107	LYS
1	J	120	THR
1	J	123	ILE
1	J	136	LYS
1	J	145	VAL
1	J	163	ILE
1	J	168	ILE
1	J	196	ARG
1	J	220	ILE
1	J	255	GLN
1	J	270	ILE
1	J	272	LEU
1	J	283	GLN
1	J	287	VAL
1	J	293	LYS
1	J	304	LEU
1	J	313	SER
1	J	325	LEU
1	J	333	ILE
1	J	359	GLU
1	J	360	ASN
1	J	368	LEU
1	J	370	LEU
1	J	371	THR
1	J	373	GLU
1	J	375	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	187	ASN
1	B	151	HIS
1	B	187	ASN
1	C	151	HIS
1	C	187	ASN
1	D	41	GLN
1	D	151	HIS
1	D	187	ASN
1	E	151	HIS

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Mol	Chain	Res	Type
1	E	187	ASN
1	F	151	HIS
1	F	187	ASN
1	G	151	HIS
1	G	187	ASN
1	H	41	GLN
1	H	151	HIS
1	H	187	ASN
1	I	41	GLN
1	I	151	HIS
1	I	187	ASN
1	J	151	HIS
1	J	187	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	K	69/70 (98%)	16 (23%)	4 (5%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	K	8	C
2	K	15	C
2	K	17	C
2	K	22	C
2	K	23	C
2	K	29	C
2	K	36	C
2	K	40	C
2	K	43	C
2	K	45	C
2	K	47	C
2	K	50	C
2	K	56	C
2	K	57	C
2	K	64	C
2	K	70	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	K	11	C
2	K	18	C
2	K	25	C
2	K	46	C

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	375/375 (100%)	-0.34	3 (0%) 87 78	63, 100, 171, 212	0
1	B	375/375 (100%)	-0.32	5 (1%) 79 66	68, 106, 183, 272	0
1	C	375/375 (100%)	-0.39	7 (1%) 70 56	63, 98, 182, 269	0
1	D	375/375 (100%)	-0.35	5 (1%) 79 66	64, 94, 165, 260	0
1	E	375/375 (100%)	-0.37	10 (2%) 58 43	46, 91, 182, 251	0
1	F	375/375 (100%)	-0.44	3 (0%) 87 78	50, 86, 173, 231	0
1	G	375/375 (100%)	-0.45	6 (1%) 74 61	50, 90, 171, 273	0
1	H	375/375 (100%)	-0.33	12 (3%) 51 37	55, 89, 171, 291	0
1	I	375/375 (100%)	-0.33	13 (3%) 48 34	56, 90, 181, 334	0
1	J	375/375 (100%)	-0.26	14 (3%) 45 32	57, 95, 182, 337	0
2	K	70/70 (100%)	-0.53	0 100 100	71, 85, 96, 107	0
All	All	3820/3820 (100%)	-0.36	78 (2%) 68 54	46, 93, 178, 337	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	374	GLU	10.0
1	B	371	THR	8.2
1	J	371	THR	5.8
1	D	371	THR	5.7
1	H	375	LEU	4.9
1	I	371	THR	4.7
1	H	364	ASN	4.5
1	G	374	GLU	4.5
1	I	363	ILE	4.5
1	J	374	GLU	4.5
1	J	372	ALA	4.2
1	I	365	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	374	GLU	4.2
1	H	362	VAL	4.1
1	H	372	ALA	4.0
1	B	372	ALA	3.9
1	C	369	ASP	3.8
1	E	31	ASP	3.8
1	I	362	VAL	3.8
1	I	374	GLU	3.7
1	H	373	GLU	3.7
1	H	371	THR	3.7
1	C	371	THR	3.4
1	B	369	ASP	3.3
1	D	372	ALA	3.3
1	J	144	GLU	3.3
1	C	366	SER	3.1
1	I	364	ASN	3.1
1	I	361	GLY	3.0
1	J	373	GLU	3.0
1	I	105	ASN	2.9
1	E	371	THR	2.9
1	G	31	ASP	2.9
1	C	140	LYS	2.9
1	I	369	ASP	2.8
1	F	371	THR	2.8
1	E	105	ASN	2.7
1	I	370	LEU	2.7
1	G	371	THR	2.7
1	I	373	GLU	2.7
1	J	106	GLY	2.7
1	J	142	MET	2.6
1	E	29	THR	2.6
1	J	364	ASN	2.6
1	J	365	TYR	2.6
1	E	103	ASP	2.6
1	I	372	ALA	2.6
1	H	144	GLU	2.6
1	B	374	GLU	2.5
1	F	374	GLU	2.5
1	J	368	LEU	2.5
1	J	370	LEU	2.5
1	E	109	MET	2.4
1	E	100	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	374	GLU	2.4
1	B	144	GLU	2.3
1	C	31	ASP	2.3
1	E	372	ALA	2.3
1	J	369	ASP	2.3
1	C	101	ARG	2.3
1	A	104	ILE	2.2
1	H	365	TYR	2.2
1	G	372	ALA	2.2
1	E	101	ARG	2.2
1	A	374	GLU	2.2
1	F	364	ASN	2.2
1	H	104	ILE	2.2
1	J	361	GLY	2.2
1	E	102	GLN	2.2
1	H	105	ASN	2.2
1	D	102	GLN	2.1
1	G	105	ASN	2.1
1	D	103	ASP	2.1
1	H	31	ASP	2.1
1	I	368	LEU	2.0
1	J	375	LEU	2.0
1	G	29	THR	2.0
1	A	361	GLY	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.