



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:24 am GMT

PDB ID : 1IJG  
Title : Structure of the Bacteriophage phi29 Head-Tail Connector Protein  
Authors : Simpson, A.A.; Leiman, P.G.; Tao, Y.; He, Y.; Badasso, M.; Jardine, P.J.;  
Anderson, D.L.; Rossmann, M.G.  
Deposited on : 2001-04-26  
Resolution : 2.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

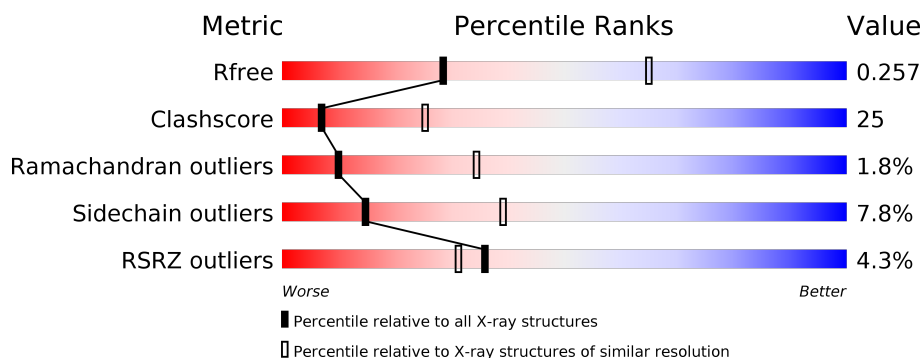
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	309	<div> <div>2%</div> <div> <div>50%</div> <div>28%</div> <div>6%</div> <div>17%</div> </div> </div>
1	B	309	<div> <div>5%</div> <div> <div>50%</div> <div>28%</div> <div>5%</div> <div>17%</div> </div> </div>
1	C	309	<div> <div>4%</div> <div> <div>48%</div> <div>29%</div> <div>6%</div> <div>17%</div> </div> </div>
1	D	309	<div> <div>2%</div> <div> <div>47%</div> <div>33%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	309	<div> <div>11%</div> <div> <div>47%</div> <div>31%</div> <div>5%</div> <div>17%</div> </div> </div>
1	F	309	<div> <div>5%</div> <div> <div>39%</div> <div>39%</div> <div>5%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	309	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>42%</div><div>37%</div><div>•</div><div>17%</div></div></div>
1	H	309	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>46%</div><div>33%</div><div>•</div><div>17%</div></div></div>
1	I	309	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>50%</div><div>28%</div><div>5%</div><div>17%</div></div></div>
1	J	309	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>50%</div><div>29%</div><div>•</div><div>17%</div></div></div>
1	K	309	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>43%</div><div>34%</div><div>5%</div><div>17%</div></div></div>
1	L	309	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>43%</div><div>35%</div><div>5%</div><div>17%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25977 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 UPPER COLLAR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	B	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	C	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	D	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	E	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	F	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	G	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	H	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	I	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	J	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	K	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			
1	L	257	Total	C	N	O	S	0	0	0
			2102	1349	347	399	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	55	Total	O	0	0
			55	55		

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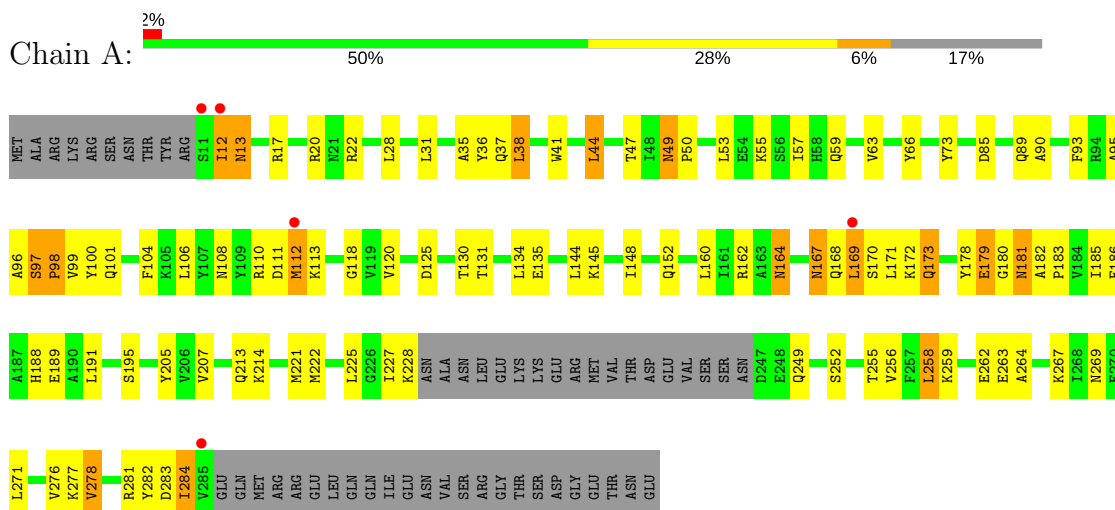
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	56	Total 56	O 56	0	0
2	D	67	Total 67	O 67	0	0
2	E	35	Total 35	O 35	0	0
2	F	69	Total 69	O 69	0	0
2	G	59	Total 59	O 59	0	0
2	H	65	Total 65	O 65	0	0
2	I	73	Total 73	O 73	0	0
2	J	67	Total 67	O 67	0	0
2	K	68	Total 68	O 68	0	0
2	L	71	Total 71	O 71	0	0

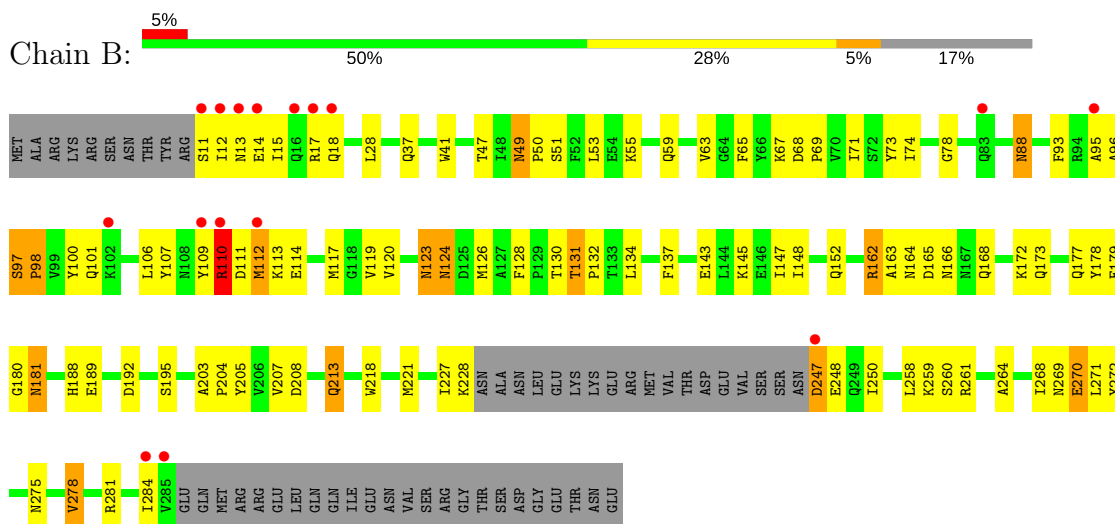
### 3 Residue-property plots

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

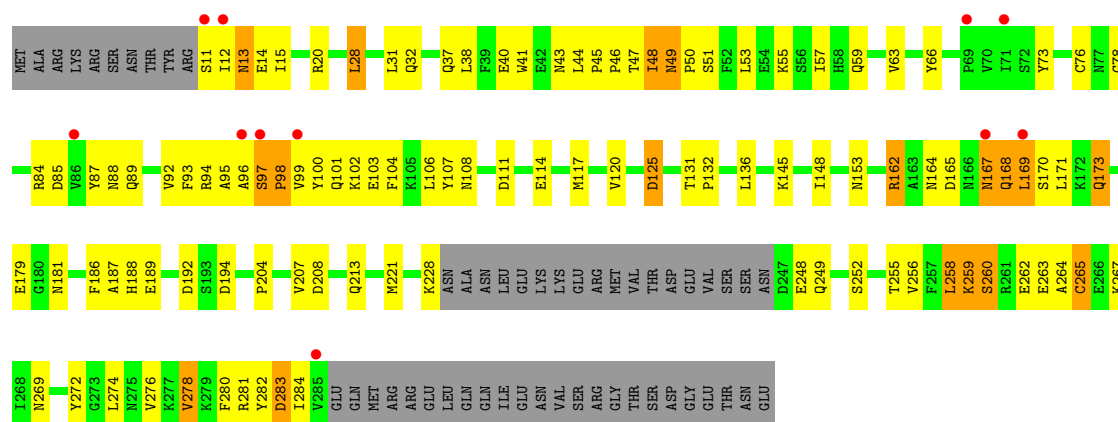


#### • Molecule 1: UPPER COLLAR PROTEIN

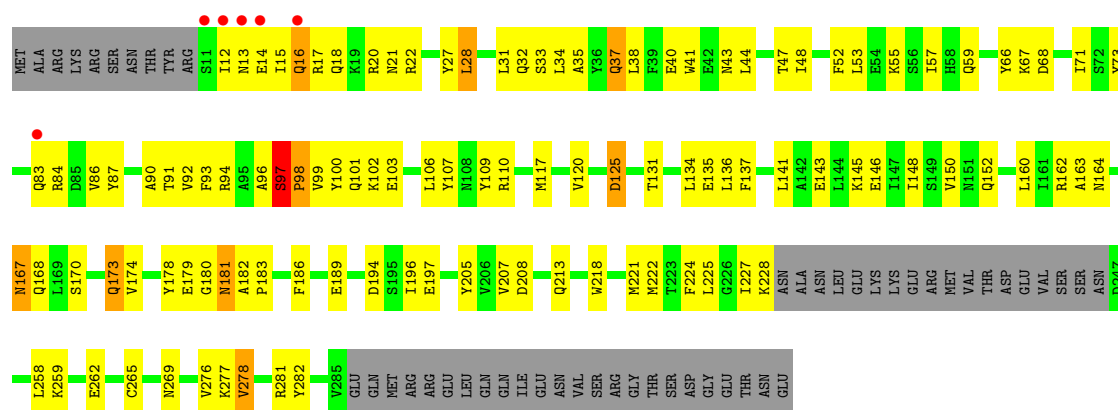


#### • Molecule 1: UPPER COLLAR PROTEIN

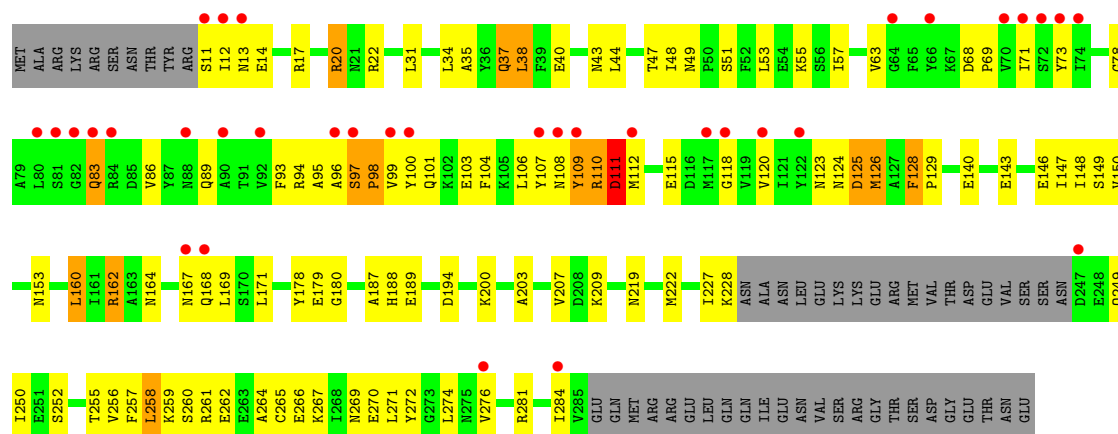




• Molecule 1: UPPER COLLAR PROTEIN

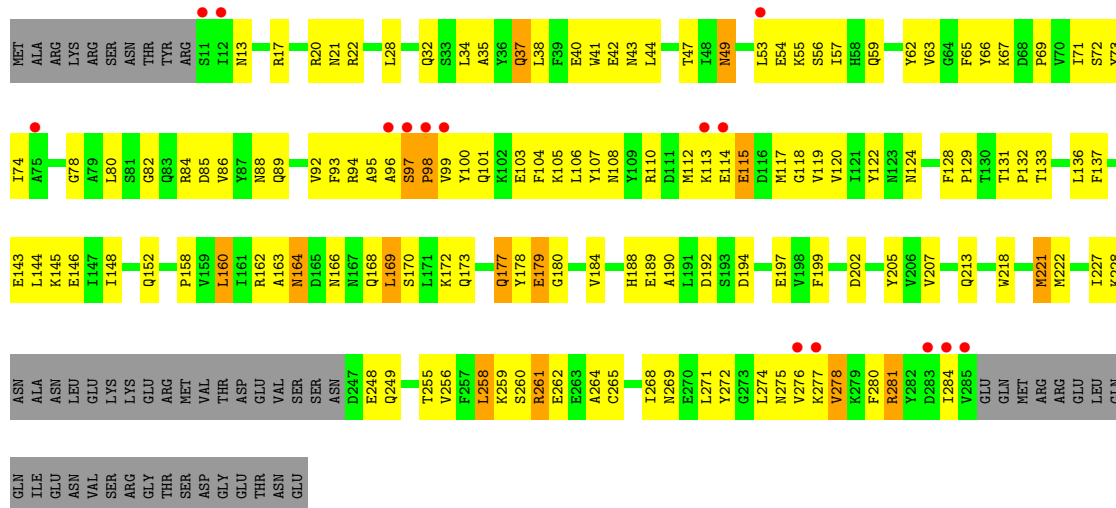


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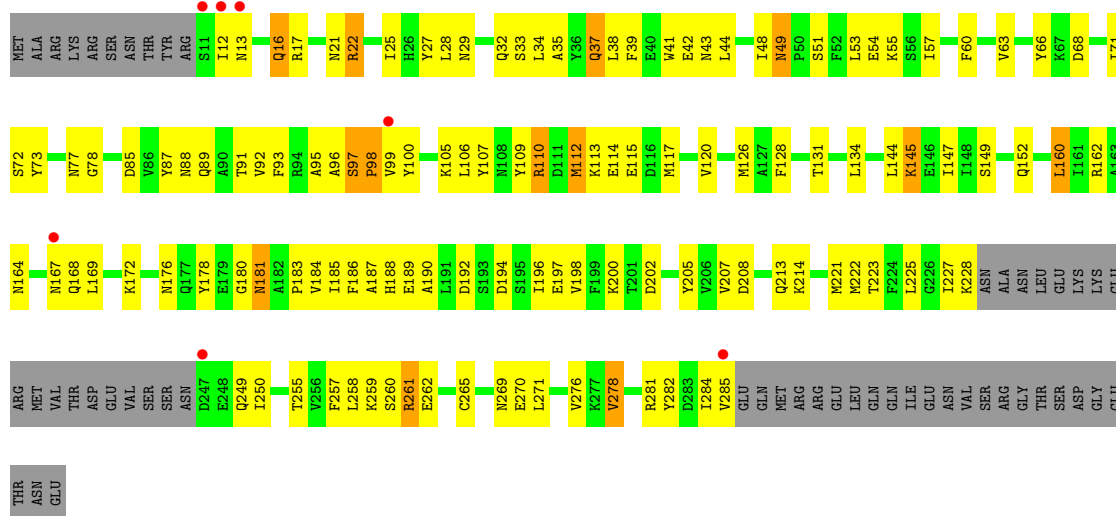
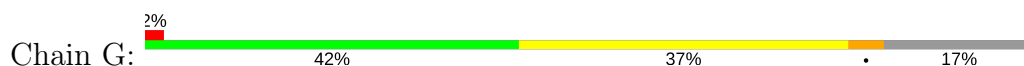


• Molecule 1: UPPER COLLAR PROTEIN

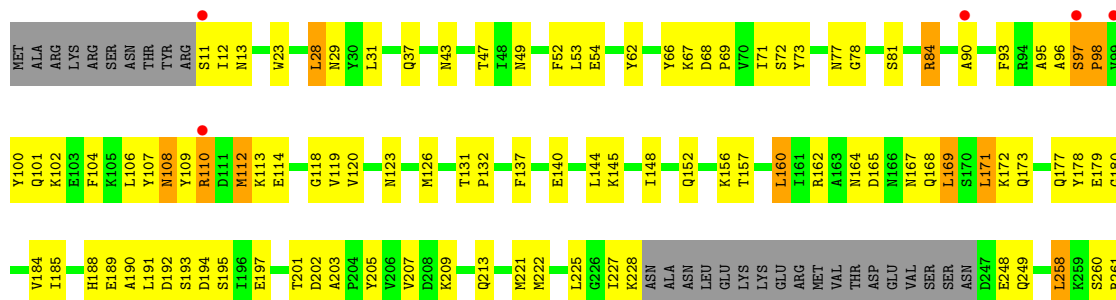




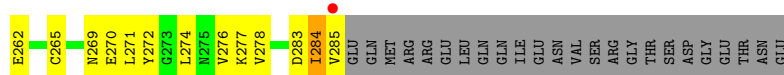
### • Molecule 1: UPPER COLLAR PROTEIN



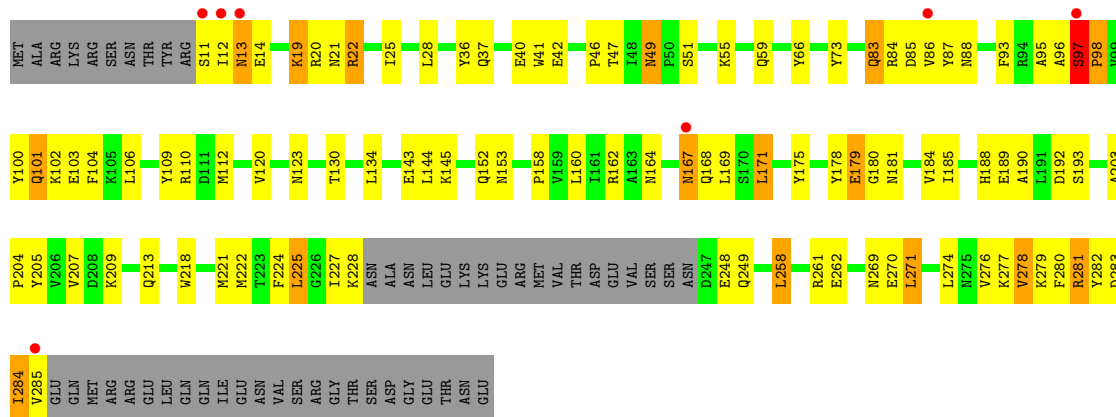
### • Molecule 1: UPPER COLLAR PROTEIN



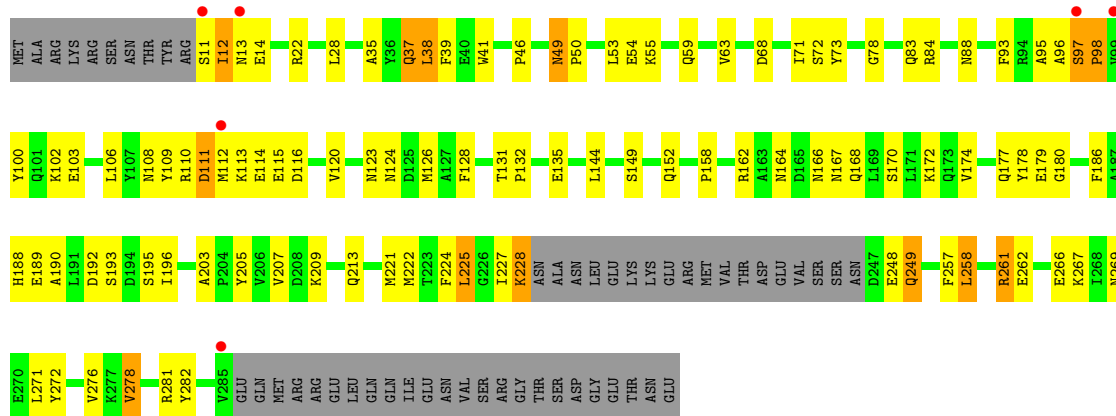




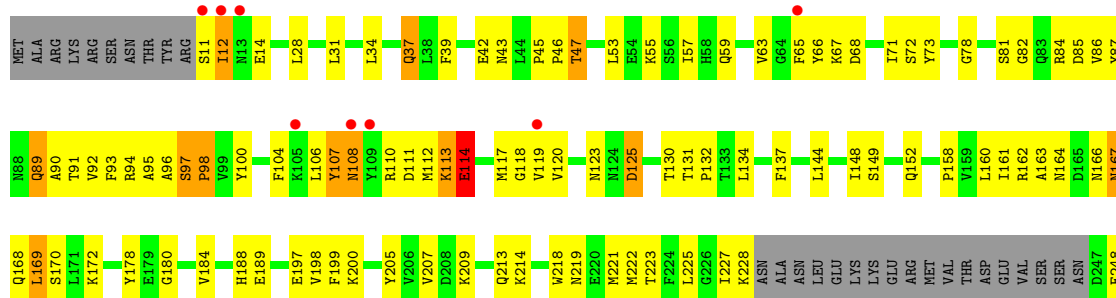
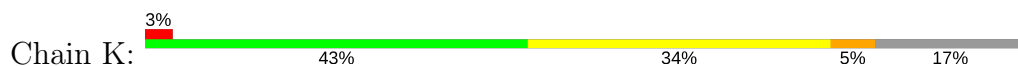
• Molecule 1: UPPER COLLAR PROTEIN

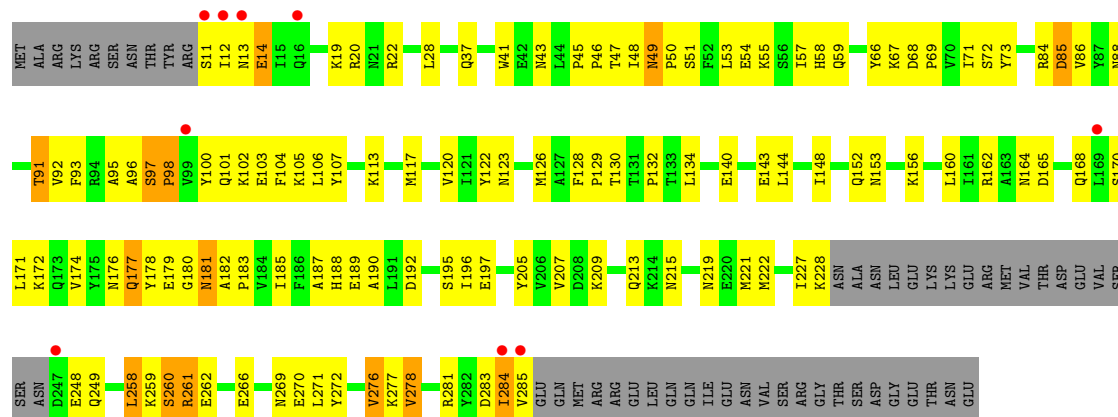


• Molecule 1: UPPER COLLAR PROTEIN



• Molecule 1: UPPER COLLAR PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.75Å 171.57Å 184.71Å 90.00° 112.21° 90.00°	Depositor
Resolution (Å)	500.00 – 2.90 48.46 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (500.00-2.90) 97.8 (48.46-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.09 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.224 , 0.264 0.221 , 0.257	Depositor DCC
$R_{free}$ test set	2500 reflections (2.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.43	0/2147	0.61	0/2909
1	B	0.41	0/2147	0.59	0/2909
1	C	0.43	0/2147	0.61	1/2909 (0.0%)
1	D	0.41	0/2147	0.60	0/2909
1	E	0.38	0/2147	0.57	0/2909
1	F	0.39	0/2147	0.59	0/2909
1	G	0.40	0/2147	0.61	0/2909
1	H	0.38	0/2147	0.58	0/2909
1	I	0.43	0/2147	0.61	0/2909
1	J	0.43	0/2147	0.62	0/2909
1	K	0.40	0/2147	0.57	0/2909
1	L	0.44	0/2147	0.61	0/2909
All	All	0.41	0/25764	0.60	1/34908 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	283	ASP	N-CA-C	-5.42	96.37	111.00

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	2102	0	2050	111	0
1	B	2102	0	2050	108	0
1	C	2102	0	2050	124	0
1	D	2102	0	2050	117	0
1	E	2102	0	2050	112	0
1	F	2102	0	2050	155	0
1	G	2102	0	2050	122	0
1	H	2102	0	2050	132	0
1	I	2102	0	2050	101	0
1	J	2102	0	2050	98	0
1	K	2102	0	2050	132	1
1	L	2102	0	2050	118	0
2	A	68	0	0	3	0
2	B	55	0	0	3	0
2	C	56	0	0	4	0
2	D	67	0	0	7	0
2	E	35	0	0	1	0
2	F	69	0	0	3	0
2	G	59	0	0	4	0
2	H	65	0	0	4	0
2	I	73	0	0	11	0
2	J	67	0	0	4	0
2	K	68	0	0	3	0
2	L	71	0	0	1	0
All	All	25977	0	24600	1268	1

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 25.

All (1268) 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:A:269:ASN:HD21	1:A:276:VAL:HG12	1.18	1.01
1:H:283:ASP:HB3	1:H:285:VAL:HG12	1.44	0.97
1:F:55:LYS:HG2	1:F:59:GLN:HE21	1.26	0.96
1:K:89:GLN:HB3	1:K:108:ASN:HD21	1.29	0.96
1:F:93:PHE:HB2	1:F:106:LEU:HD21	1.50	0.94
1:J:213:GLN:HE21	1:J:213:GLN:HA	1.30	0.93
1:F:255:THR:HG21	1:G:281:ARG:HD3	1.51	0.91
1:B:168:GLN:HG2	1:B:188:HIS:NE2	1.85	0.91
1:J:168:GLN:HG2	1:J:188:HIS:CE1	2.07	0.90
1:F:110:ARG:NH1	1:F:113:LYS:HG2	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:GLN:HG2	1:F:188:HIS:CE1	2.07	0.89
1:C:12:ILE:H	1:C:12:ILE:HD12	1.35	0.89
1:A:55:LYS:O	1:A:59:GLN:HG3	1.73	0.89
1:E:11:SER:HB2	1:E:12:ILE:HD12	1.53	0.89
1:K:119:VAL:HG21	1:K:268:ILE:HG12	1.55	0.88
1:E:93:PHE:HB2	1:E:106:LEU:HD21	1.56	0.87
1:G:105:LYS:HD2	1:G:105:LYS:N	1.89	0.87
1:J:168:GLN:HG2	1:J:188:HIS:NE2	1.89	0.87
1:I:19:LYS:HA	1:I:19:LYS:HE3	1.56	0.86
1:B:137:PHE:CD1	1:B:221:MET:HE2	2.11	0.86
1:E:123:ASN:HA	1:E:261:ARG:HH12	1.39	0.85
1:B:37:GLN:HG2	1:B:281:ARG:HD2	1.58	0.85
1:C:255:THR:HG21	1:D:281:ARG:HD3	1.58	0.85
1:E:269:ASN:HD21	1:E:276:VAL:HG22	1.40	0.85
1:L:55:LYS:O	1:L:59:GLN:HG3	1.75	0.85
1:F:55:LYS:HG2	1:F:59:GLN:NE2	1.92	0.84
1:A:49:ASN:C	1:A:49:ASN:HD22	1.79	0.84
1:A:269:ASN:HD21	1:A:276:VAL:CG1	1.91	0.83
1:A:269:ASN:ND2	1:A:276:VAL:HG12	1.93	0.83
1:H:188:HIS:CD2	1:H:190:ALA:H	1.96	0.83
1:K:91:THR:HG23	1:K:92:VAL:HG23	1.60	0.83
1:H:93:PHE:HB2	1:H:106:LEU:HD21	1.60	0.83
1:D:37:GLN:HG2	1:D:281:ARG:HD2	1.60	0.83
1:I:168:GLN:HG2	1:I:188:HIS:CD2	2.12	0.83
1:H:113:LYS:HZ2	1:H:270:GLU:HG3	1.41	0.82
1:I:188:HIS:CD2	1:I:190:ALA:H	1.97	0.81
1:F:168:GLN:HG2	1:F:188:HIS:NE2	1.95	0.81
1:G:257:PHE:O	1:G:261:ARG:HD2	1.81	0.81
1:F:40:GLU:HG3	1:F:281:ARG:NH2	1.96	0.81
1:C:162:ARG:HH11	1:C:162:ARG:HG3	1.46	0.80
1:J:213:GLN:NE2	1:J:213:GLN:HA	1.97	0.80
1:K:119:VAL:HG21	1:K:268:ILE:CG1	2.11	0.80
1:L:269:ASN:HD21	1:L:276:VAL:H	1.30	0.80
1:E:162:ARG:HG3	1:E:162:ARG:HH11	1.47	0.79
1:L:266:GLU:O	1:L:270:GLU:HG3	1.82	0.79
1:J:113:LYS:O	1:J:114:GLU:HG3	1.83	0.79
1:F:248:GLU:HB3	1:G:227:ILE:HG23	1.62	0.79
1:H:107:TYR:OH	1:H:110:ARG:HA	1.83	0.79
1:L:91:THR:HG22	1:L:92:VAL:HG23	1.65	0.79
1:L:258:LEU:HD22	1:L:262:GLU:HG3	1.62	0.79
1:C:93:PHE:HB2	1:C:106:LEU:HD21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ASN:ND2	1:D:168:GLN:HE21	1.80	0.79
1:I:168:GLN:HG2	1:I:188:HIS:CG	2.18	0.79
1:A:282:TYR:CE2	1:L:248:GLU:HA	2.18	0.79
1:A:93:PHE:HB2	1:A:106:LEU:HD21	1.64	0.78
1:J:249:GLN:NE2	1:K:218:TRP:HE1	1.81	0.78
1:A:188:HIS:HB3	1:A:191:LEU:HD13	1.66	0.78
1:J:258:LEU:HD22	1:J:262:GLU:HG3	1.66	0.78
1:G:114:GLU:H	1:G:117:MET:HE2	1.48	0.78
1:J:55:LYS:O	1:J:59:GLN:HG3	1.83	0.77
1:H:12:ILE:HD12	1:H:12:ILE:H	1.49	0.77
1:G:13:ASN:O	1:G:17:ARG:HG3	1.85	0.77
1:H:258:LEU:HD22	1:H:262:GLU:HG3	1.66	0.77
1:F:137:PHE:CG	1:F:221:MET:HG2	2.20	0.76
1:D:28:LEU:O	1:D:32:GLN:HG3	1.84	0.76
1:E:269:ASN:ND2	1:E:276:VAL:HG22	1.99	0.76
1:B:168:GLN:HG2	1:B:188:HIS:CE1	2.20	0.76
1:E:89:GLN:NE2	1:E:108:ASN:HD21	1.83	0.76
1:G:205:TYR:CE2	1:G:207:VAL:HB	2.21	0.76
1:G:126:MET:HG2	1:G:128:PHE:CZ	2.20	0.75
1:A:167:ASN:ND2	1:A:168:GLN:HG2	2.01	0.75
1:E:261:ARG:HH11	1:E:261:ARG:HG2	1.51	0.75
1:B:114:GLU:H	1:B:114:GLU:CD	1.90	0.75
1:H:201:THR:HG21	2:I:310:HOH:O	1.86	0.75
1:F:222:MET:HE3	1:F:227:ILE:HG21	1.69	0.75
1:G:85:ASP:OD1	1:G:89:GLN:HB2	1.85	0.74
1:K:55:LYS:HG2	1:K:59:GLN:HE21	1.51	0.74
1:K:55:LYS:HG2	1:K:59:GLN:NE2	2.02	0.74
1:B:213:GLN:HG3	1:C:207:VAL:HG11	1.69	0.74
1:A:249:GLN:NE2	1:B:218:TRP:HE1	1.85	0.74
1:B:55:LYS:O	1:B:59:GLN:HG3	1.88	0.74
1:C:269:ASN:HD21	1:C:276:VAL:HG22	1.53	0.74
1:H:13:ASN:ND2	1:J:179:GLU:HG2	2.03	0.74
1:D:167:ASN:HD22	1:D:168:GLN:NE2	1.85	0.74
1:C:248:GLU:HB3	1:D:227:ILE:HG23	1.70	0.74
1:L:102:LYS:HD3	1:L:103:GLU:H	1.52	0.74
1:E:51:SER:O	1:E:55:LYS:HG3	1.88	0.73
1:G:145:LYS:HD3	1:G:145:LYS:O	1.88	0.73
1:L:107:TYR:HA	1:L:117:MET:HE3	1.70	0.73
1:G:115:GLU:H	1:G:115:GLU:CD	1.91	0.73
1:I:168:GLN:HG3	1:I:169:LEU:N	2.04	0.73
1:F:96:ALA:HB1	1:F:101:GLN:HG2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLN:HE21	1:C:168:GLN:H	1.37	0.73
1:F:42:GLU:HG3	1:F:277:LYS:HB2	1.71	0.73
1:J:49:ASN:C	1:J:49:ASN:HD22	1.91	0.73
1:L:172:LYS:NZ	1:L:176:ASN:HD21	1.87	0.73
1:D:213:GLN:HA	1:D:213:GLN:HE21	1.54	0.72
1:A:106:LEU:HD22	1:A:120:VAL:HG23	1.69	0.72
1:A:167:ASN:HD22	1:A:168:GLN:H	1.36	0.72
1:C:264:ALA:HA	1:C:267:LYS:HE3	1.70	0.72
1:J:269:ASN:HD21	1:J:276:VAL:H	1.38	0.72
1:B:106:LEU:HD22	1:B:120:VAL:HG23	1.71	0.72
1:A:131:THR:O	1:A:135:GLU:HG3	1.90	0.71
1:D:93:PHE:HB2	1:D:106:LEU:HD21	1.70	0.71
1:J:188:HIS:CD2	1:J:190:ALA:H	2.08	0.71
1:B:114:GLU:HA	1:B:117:MET:SD	2.29	0.71
1:B:49:ASN:C	1:B:49:ASN:HD22	1.92	0.71
1:G:93:PHE:HB2	1:G:106:LEU:HD21	1.71	0.71
1:K:162:ARG:HH11	1:K:162:ARG:HG2	1.55	0.71
1:A:264:ALA:HA	1:A:267:LYS:NZ	2.04	0.71
1:H:171:LEU:HD13	1:I:185:ILE:HD13	1.73	0.71
1:B:162:ARG:HG3	1:B:162:ARG:HH11	1.55	0.70
1:K:14:GLU:H	1:K:14:GLU:CD	1.94	0.70
1:L:102:LYS:HD3	1:L:103:GLU:N	2.05	0.70
1:B:269:ASN:ND2	1:B:275:ASN:HA	2.06	0.70
1:D:107:TYR:OH	1:D:110:ARG:HA	1.92	0.70
1:D:17:ARG:HG2	1:D:20:ARG:NH2	2.05	0.70
1:F:106:LEU:HD22	1:F:120:VAL:HG22	1.73	0.70
1:B:148:ILE:HG23	1:B:207:VAL:HG13	1.72	0.70
1:F:28:LEU:O	1:F:32:GLN:HG3	1.91	0.70
1:G:44:LEU:HD22	1:G:48:ILE:HG21	1.73	0.70
1:B:96:ALA:O	1:B:97:SER:HB2	1.91	0.70
1:F:56:SER:HB2	1:F:63:VAL:HG11	1.72	0.70
1:I:258:LEU:HD22	1:I:262:GLU:HG3	1.72	0.70
1:A:181:ASN:ND2	1:A:181:ASN:H	1.90	0.70
1:F:265:CYS:SG	1:F:276:VAL:HG23	2.31	0.70
1:H:157:THR:O	1:H:201:THR:HG23	1.92	0.70
1:C:192:ASP:HB2	1:C:194:ASP:OD1	1.91	0.70
1:J:249:GLN:HB3	1:K:222:MET:HE2	1.73	0.70
1:H:107:TYR:CD2	1:H:271:LEU:HB2	2.27	0.70
1:H:269:ASN:HD21	1:H:276:VAL:HG22	1.55	0.70
1:H:269:ASN:HD21	1:H:276:VAL:H	1.39	0.70
1:B:111:ASP:O	1:B:112:MET:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:LEU:HD23	1:E:271:LEU:O	1.92	0.69
1:A:167:ASN:N	1:A:167:ASN:HD22	1.91	0.69
1:B:124:ASN:HD21	1:B:128:PHE:H	1.39	0.69
1:K:68:ASP:OD2	1:K:71:ILE:HG12	1.91	0.69
1:C:283:ASP:O	1:C:284:ILE:HG12	1.93	0.69
1:B:53:LEU:HD12	1:B:63:VAL:HG11	1.73	0.69
1:H:165:ASP:OD1	1:H:191:LEU:HD23	1.92	0.69
1:E:13:ASN:O	1:E:17:ARG:HG3	1.91	0.69
1:E:86:VAL:HG11	1:F:74:ILE:HD11	1.74	0.69
1:I:87:TYR:HD1	1:I:109:TYR:HH	1.41	0.68
1:B:93:PHE:HB2	1:B:106:LEU:HD21	1.75	0.68
1:H:123:ASN:OD1	1:H:261:ARG:NH2	2.27	0.68
1:J:144:LEU:HD21	1:K:152:GLN:NE2	2.08	0.68
1:D:227:ILE:O	1:D:228:LYS:HB3	1.94	0.68
1:E:269:ASN:HD21	1:E:276:VAL:H	1.41	0.68
1:D:40:GLU:HG3	1:D:281:ARG:HH21	1.59	0.68
1:E:148:ILE:HG23	1:E:207:VAL:HG13	1.76	0.68
1:I:98:PRO:HG2	1:I:100:TYR:H	1.59	0.68
1:B:166:ASN:ND2	1:C:187:ALA:HB1	2.08	0.68
1:I:167:ASN:HB2	1:J:189:GLU:OE2	1.94	0.68
1:G:105:LYS:H	1:G:105:LYS:HD2	1.58	0.67
1:B:65:PHE:CD2	1:B:268:ILE:HD12	2.30	0.67
1:K:107:TYR:HD2	1:K:271:LEU:HD13	1.58	0.67
1:G:167:ASN:HB3	1:G:168:GLN:NE2	2.09	0.67
1:A:44:LEU:H	1:A:44:LEU:HD12	1.60	0.67
1:G:145:LYS:HD3	1:G:145:LYS:C	2.15	0.67
1:H:84:ARG:NH1	1:H:84:ARG:HB3	2.09	0.67
1:I:123:ASN:OD1	1:I:261:ARG:NH2	2.28	0.67
1:G:221:MET:HE3	1:G:225:LEU:HG	1.75	0.67
1:D:164:ASN:O	1:E:189:GLU:HA	1.95	0.67
1:K:45:PRO:HG3	1:K:274:LEU:HD11	1.77	0.67
1:D:106:LEU:HD22	1:D:120:VAL:HG23	1.76	0.66
1:F:96:ALA:HB2	1:F:101:GLN:HE21	1.61	0.66
1:G:113:LYS:HE2	1:G:270:GLU:HG3	1.76	0.66
1:I:283:ASP:O	1:I:284:ILE:HB	1.96	0.66
1:G:205:TYR:CZ	1:G:207:VAL:HB	2.30	0.66
1:L:123:ASN:OD1	1:L:261:ARG:NH2	2.28	0.66
1:C:267:LYS:HG2	2:C:313:HOH:O	1.95	0.66
1:D:213:GLN:HA	1:D:213:GLN:NE2	2.10	0.66
1:I:93:PHE:HB2	1:I:106:LEU:HD21	1.77	0.66
1:H:248:GLU:HG3	1:I:282:TYR:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:PHE:O	1:D:141:LEU:HD22	1.95	0.66
1:D:167:ASN:HD22	1:D:168:GLN:HE21	1.39	0.66
1:G:51:SER:O	1:G:55:LYS:HG3	1.95	0.66
1:K:274:LEU:CD2	1:K:275:ASN:H	2.07	0.66
1:E:222:MET:HE3	1:E:227:ILE:HG21	1.78	0.65
1:H:73:TYR:HE2	1:H:272:TYR:CD1	2.14	0.65
1:I:106:LEU:HD22	1:I:120:VAL:HG23	1.77	0.65
1:A:179:GLU:CD	1:A:179:GLU:H	2.00	0.65
1:J:96:ALA:O	1:J:97:SER:HB2	1.94	0.65
1:H:168:GLN:CD	1:H:168:GLN:H	1.99	0.65
1:K:98:PRO:HG2	1:K:100:TYR:H	1.59	0.65
1:E:12:ILE:H	1:E:12:ILE:HD12	1.61	0.65
1:I:144:LEU:HD21	1:J:152:GLN:NE2	2.12	0.65
1:L:14:GLU:CD	1:L:14:GLU:H	1.99	0.65
1:D:16:GLN:O	1:D:20:ARG:HD3	1.95	0.65
1:D:21:ASN:HB2	2:D:322:HOH:O	1.96	0.65
1:F:213:GLN:HA	1:F:213:GLN:HE21	1.62	0.65
1:F:82:GLY:HA3	1:F:92:VAL:HG23	1.79	0.65
1:F:56:SER:HB2	1:F:63:VAL:CG1	2.26	0.65
1:K:107:TYR:CD2	1:K:271:LEU:HD13	2.32	0.65
1:F:213:GLN:HA	1:F:213:GLN:NE2	2.12	0.65
1:H:173:GLN:HG3	1:H:177:GLN:NE2	2.11	0.65
1:H:12:ILE:HD12	1:H:12:ILE:N	2.11	0.64
1:K:227:ILE:O	1:K:228:LYS:HB3	1.97	0.64
1:G:91:THR:HG23	1:G:92:VAL:HG23	1.79	0.64
1:H:269:ASN:ND2	1:H:276:VAL:HG22	2.13	0.64
1:I:269:ASN:HD21	1:I:276:VAL:HG13	1.63	0.64
1:K:47:THR:HG23	1:K:73:TYR:HB2	1.79	0.64
1:A:264:ALA:HA	1:A:267:LYS:HZ3	1.61	0.64
1:H:167:ASN:HB2	1:H:168:GLN:NE2	2.13	0.64
1:C:12:ILE:N	1:C:12:ILE:HD12	2.12	0.64
1:D:148:ILE:O	1:D:152:GLN:HG3	1.98	0.64
1:G:265:CYS:SG	1:G:276:VAL:HG23	2.38	0.64
1:E:160:LEU:HD23	1:F:184:VAL:HG12	1.79	0.64
1:F:86:VAL:HG12	1:G:100:TYR:HB2	1.80	0.64
1:J:35:ALA:O	1:J:38:LEU:HB2	1.98	0.64
1:C:168:GLN:NE2	1:C:168:GLN:H	1.95	0.64
1:I:98:PRO:HA	2:I:325:HOH:O	1.98	0.64
1:C:106:LEU:HD22	1:C:120:VAL:HG23	1.80	0.63
1:C:41:TRP:CE3	1:C:278:VAL:HG13	2.32	0.63
1:C:49:ASN:HD22	1:C:49:ASN:C	2.00	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:ILE:HG22	1:F:274:LEU:HD12	1.80	0.63
1:I:19:LYS:CE	1:I:19:LYS:HA	2.29	0.63
1:B:107:TYR:OH	1:B:270:GLU:HG2	1.98	0.63
1:J:68:ASP:OD2	1:J:71:ILE:HG12	1.99	0.63
1:L:68:ASP:OD2	1:L:71:ILE:HG12	1.99	0.63
1:H:160:LEU:HD23	1:I:184:VAL:HG12	1.80	0.63
1:D:17:ARG:HG2	1:D:20:ARG:HH22	1.64	0.63
1:H:98:PRO:HG2	1:H:100:TYR:H	1.62	0.63
1:I:21:ASN:O	1:I:25:ILE:HG12	1.97	0.63
1:J:106:LEU:HD22	1:J:120:VAL:HG23	1.80	0.63
1:F:144:LEU:HD21	1:G:152:GLN:NE2	2.13	0.63
1:C:12:ILE:H	1:C:12:ILE:CD1	2.10	0.63
1:D:84:ARG:NH1	1:D:90:ALA:HB2	2.14	0.63
1:F:164:ASN:O	1:G:189:GLU:HA	1.99	0.63
1:J:123:ASN:OD1	1:J:261:ARG:NH2	2.32	0.63
1:B:110:ARG:HG3	1:B:111:ASP:N	2.14	0.63
1:G:128:PHE:CZ	1:H:29:ASN:ND2	2.67	0.63
1:D:222:MET:HE3	1:D:227:ILE:HD12	1.80	0.63
1:K:213:GLN:HA	1:K:213:GLN:HE21	1.64	0.63
1:D:205:TYR:CE2	1:D:207:VAL:HB	2.34	0.62
1:C:269:ASN:ND2	1:C:276:VAL:HG22	2.14	0.62
1:D:173:GLN:HG2	2:D:365:HOH:O	1.98	0.62
1:K:104:PHE:CE2	1:K:118:GLY:HA3	2.35	0.62
1:C:265:CYS:SG	1:C:276:VAL:HG23	2.39	0.62
1:E:272:TYR:HB2	1:E:274:LEU:HD13	1.81	0.62
1:G:37:GLN:HG2	1:G:281:ARG:HD2	1.80	0.62
1:F:20:ARG:HD2	1:F:146:GLU:OE2	1.99	0.62
1:K:73:TYR:HE2	1:K:272:TYR:CD1	2.17	0.62
1:J:13:ASN:HD21	1:L:179:GLU:HG2	1.61	0.62
1:F:34:LEU:O	1:F:37:GLN:HG3	2.00	0.62
1:F:93:PHE:CE2	1:F:95:ALA:HB2	2.35	0.62
1:G:106:LEU:HD22	1:G:120:VAL:HG23	1.80	0.62
1:H:272:TYR:HB2	1:H:274:LEU:HD23	1.82	0.62
1:A:167:ASN:ND2	1:A:168:GLN:H	1.98	0.62
1:G:172:LYS:HG3	2:G:327:HOH:O	1.98	0.62
1:A:35:ALA:O	1:A:38:LEU:HB2	2.01	0.61
1:D:131:THR:O	1:D:135:GLU:HG3	2.00	0.61
1:B:88:ASN:CG	1:B:88:ASN:O	2.38	0.61
1:C:256:VAL:CG1	1:D:33:SER:HB2	2.31	0.61
1:E:94:ARG:HG2	1:E:103:GLU:OE2	2.00	0.61
1:A:181:ASN:HD22	1:A:181:ASN:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:TYR:CB	1:E:271:LEU:HD12	2.30	0.61
1:I:167:ASN:HB2	1:J:189:GLU:CD	2.21	0.61
1:A:162:ARG:HH11	1:A:162:ARG:HG3	1.66	0.61
1:A:222:MET:HE1	1:A:227:ILE:HG21	1.82	0.61
1:A:96:ALA:CB	1:A:101:GLN:HG3	2.30	0.61
1:C:259:LYS:O	1:C:263:GLU:HG3	2.00	0.61
1:G:131:THR:HA	1:G:134:LEU:HD12	1.81	0.61
1:F:20:ARG:NH2	1:F:143:GLU:HG3	2.16	0.61
1:J:110:ARG:O	1:J:112:MET:N	2.34	0.61
1:F:118:GLY:HA2	1:F:272:TYR:OH	2.01	0.61
1:G:188:HIS:CD2	1:G:190:ALA:H	2.19	0.61
1:H:272:TYR:CB	1:H:274:LEU:HD23	2.31	0.61
1:H:283:ASP:CB	1:H:285:VAL:HG12	2.27	0.61
1:I:213:GLN:HA	1:I:213:GLN:HE21	1.66	0.61
1:C:94:ARG:HG2	1:C:103:GLU:HG2	1.81	0.60
1:H:227:ILE:O	1:H:228:LYS:HB3	2.00	0.60
1:K:167:ASN:OD1	1:L:189:GLU:HB3	2.01	0.60
1:L:49:ASN:C	1:L:49:ASN:HD22	2.02	0.60
1:E:12:ILE:N	1:E:12:ILE:HD12	2.16	0.60
1:L:213:GLN:HA	1:L:213:GLN:HE21	1.66	0.60
1:B:113:LYS:O	1:B:113:LYS:HG3	2.02	0.60
1:D:13:ASN:O	1:D:17:ARG:HG3	2.00	0.60
1:A:258:LEU:HD13	1:A:262:GLU:OE1	2.01	0.60
1:F:41:TRP:CZ2	1:F:261:ARG:HG2	2.36	0.60
1:I:42:GLU:OE2	1:I:279:LYS:HD3	2.02	0.60
1:A:97:SER:OG	1:A:98:PRO:HD3	2.02	0.60
1:F:98:PRO:HG2	1:F:100:TYR:H	1.66	0.60
1:F:13:ASN:ND2	1:H:179:GLU:HG2	2.16	0.60
1:K:258:LEU:HD22	1:K:262:GLU:HG3	1.83	0.60
1:F:94:ARG:HG2	1:F:103:GLU:OE1	2.01	0.60
1:A:164:ASN:OD1	1:A:195:SER:HA	2.00	0.60
1:F:284:ILE:HD12	2:F:350:HOH:O	2.01	0.60
1:H:84:ARG:HB3	1:H:84:ARG:CZ	2.32	0.60
1:B:213:GLN:HG3	1:C:207:VAL:CG1	2.32	0.60
1:B:137:PHE:HB2	1:B:221:MET:HE2	1.83	0.59
1:F:107:TYR:CD1	1:F:271:LEU:HD13	2.37	0.59
1:G:113:LYS:HA	1:G:117:MET:HE1	1.82	0.59
1:H:188:HIS:HD2	1:H:190:ALA:H	1.44	0.59
1:E:128:PHE:HD2	1:E:129:PRO:CD	2.16	0.59
1:E:40:GLU:HB2	1:E:281:ARG:HE	1.67	0.59
1:I:285:VAL:HB	2:I:362:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:GLU:HB2	1:K:117:MET:SD	2.42	0.59
1:K:131:THR:HB	1:K:132:PRO:HD3	1.84	0.59
1:F:264:ALA:O	1:F:268:ILE:HG12	2.02	0.59
1:G:258:LEU:HD13	1:G:262:GLU:HG3	1.84	0.59
1:B:164:ASN:O	1:C:189:GLU:HA	2.02	0.59
1:K:213:GLN:HA	1:K:213:GLN:NE2	2.18	0.59
1:L:93:PHE:HB2	1:L:106:LEU:HD21	1.83	0.59
1:B:137:PHE:HB2	1:B:221:MET:CE	2.32	0.59
1:C:167:ASN:HB2	1:D:189:GLU:CD	2.23	0.59
1:G:202:ASP:HA	2:G:314:HOH:O	2.01	0.59
1:G:261:ARG:HG2	1:G:261:ARG:HH11	1.67	0.59
1:H:43:ASN:O	1:H:276:VAL:HG12	2.03	0.59
1:K:258:LEU:CD2	1:K:262:GLU:HG3	2.33	0.59
1:K:43:ASN:O	1:K:276:VAL:HG12	2.02	0.59
1:B:137:PHE:CG	1:B:221:MET:HE2	2.37	0.59
1:L:168:GLN:HA	1:L:168:GLN:NE2	2.18	0.59
1:B:284:ILE:HG23	1:B:284:ILE:O	2.03	0.59
1:F:42:GLU:CG	1:F:277:LYS:HB2	2.32	0.59
1:L:84:ARG:HG2	2:L:343:HOH:O	2.02	0.59
1:A:222:MET:CE	1:A:227:ILE:HG21	2.33	0.59
1:B:247:ASP:HB3	2:B:316:HOH:O	2.02	0.58
1:C:96:ALA:HB1	1:C:101:GLN:HG2	1.84	0.58
1:C:98:PRO:HG2	1:C:100:TYR:H	1.66	0.58
1:D:162:ARG:NH1	1:D:197:GLU:OE2	2.36	0.58
1:C:87:TYR:HA	1:D:52:PHE:CE1	2.38	0.58
1:H:265:CYS:SG	1:H:276:VAL:HG23	2.44	0.58
1:E:96:ALA:O	1:E:97:SER:HB2	2.04	0.58
1:F:55:LYS:O	1:F:59:GLN:HG3	2.02	0.58
1:I:55:LYS:O	1:I:59:GLN:HG3	2.03	0.58
1:L:162:ARG:NH1	1:L:197:GLU:OE1	2.36	0.58
1:L:97:SER:OG	1:L:98:PRO:HD3	2.03	0.58
1:J:84:ARG:HD2	1:J:88:ASN:O	2.04	0.58
1:C:47:THR:CG2	1:C:73:TYR:HB2	2.33	0.58
1:F:248:GLU:HB3	1:G:227:ILE:CG2	2.32	0.58
1:G:223:THR:HG23	1:G:250:ILE:HD13	1.84	0.58
1:I:168:GLN:HG2	1:I:188:HIS:CE1	2.38	0.58
1:L:105:LYS:N	1:L:105:LYS:HD2	2.18	0.58
1:E:167:ASN:OD1	1:E:168:GLN:HG2	2.03	0.58
1:F:133:THR:HG22	1:F:221:MET:HE3	1.84	0.58
1:G:213:GLN:OE1	1:G:213:GLN:HA	2.03	0.58
1:H:144:LEU:HD21	1:I:152:GLN:NE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:ASN:H	1:L:181:ASN:ND2	2.01	0.58
1:A:49:ASN:ND2	1:A:49:ASN:C	2.53	0.58
1:E:272:TYR:CB	1:E:274:LEU:HD13	2.33	0.58
1:B:71:ILE:HD11	1:B:74:ILE:HD12	1.85	0.58
1:D:143:GLU:OE2	1:E:153:ASN:ND2	2.26	0.58
1:F:249:GLN:HG2	1:G:222:MET:CE	2.34	0.58
1:F:96:ALA:CB	1:F:101:GLN:HG2	2.33	0.58
1:E:107:TYR:CD1	1:E:271:LEU:HB2	2.38	0.57
1:H:97:SER:OG	1:H:98:PRO:HD3	2.04	0.57
1:L:53:LEU:O	1:L:57:ILE:HG13	2.04	0.57
1:C:269:ASN:HD21	1:C:276:VAL:H	1.52	0.57
1:C:93:PHE:CE2	1:C:95:ALA:HB2	2.40	0.57
1:G:227:ILE:O	1:G:228:LYS:HB3	2.04	0.57
1:H:249:GLN:OE1	1:I:218:TRP:NE1	2.28	0.57
1:K:106:LEU:HD22	1:K:120:VAL:HG13	1.85	0.57
1:C:164:ASN:O	1:D:189:GLU:HA	2.04	0.57
1:B:208:ASP:N	1:B:208:ASP:OD2	2.37	0.57
1:D:182:ALA:HB1	1:D:183:PRO:HD2	1.86	0.57
1:A:145:LYS:HZ3	1:L:140:GLU:CD	2.08	0.57
1:C:148:ILE:HG23	1:C:207:VAL:HG13	1.86	0.57
1:C:47:THR:HG23	1:C:73:TYR:HB2	1.87	0.57
1:J:49:ASN:C	1:J:49:ASN:ND2	2.57	0.57
1:K:123:ASN:OD1	1:K:261:ARG:NH2	2.34	0.57
1:A:99:VAL:CG2	1:L:86:VAL:HG12	2.33	0.57
1:C:145:LYS:C	1:C:145:LYS:HD3	2.24	0.57
1:C:258:LEU:HD22	1:C:262:GLU:CG	2.34	0.57
1:H:164:ASN:O	1:I:189:GLU:HA	2.04	0.57
1:J:110:ARG:O	1:J:111:ASP:C	2.41	0.57
1:D:27:TYR:O	1:D:31:LEU:HG	2.03	0.57
1:G:71:ILE:O	1:G:72:SER:HB3	2.05	0.57
1:H:107:TYR:CZ	1:H:110:ARG:HA	2.39	0.57
1:J:49:ASN:HD22	1:J:50:PRO:N	2.03	0.57
1:B:259:LYS:HE2	2:B:361:HOH:O	2.04	0.57
1:C:44:LEU:HD13	1:C:48:ILE:HG21	1.86	0.57
1:I:37:GLN:O	1:I:281:ARG:HD2	2.04	0.57
1:K:164:ASN:O	1:L:189:GLU:HA	2.04	0.57
1:B:168:GLN:CG	1:B:188:HIS:NE2	2.64	0.57
1:D:162:ARG:NH2	1:D:194:ASP:O	2.37	0.57
1:E:261:ARG:HH11	1:E:261:ARG:CG	2.18	0.57
1:I:205:TYR:CZ	1:I:207:VAL:HB	2.40	0.57
1:C:258:LEU:HD22	1:C:262:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:LYS:O	1:G:176:ASN:ND2	2.38	0.57
1:J:123:ASN:HD22	1:J:124:ASN:ND2	2.03	0.56
1:J:168:GLN:HG2	1:J:188:HIS:CD2	2.40	0.56
1:C:283:ASP:O	1:C:284:ILE:CG1	2.53	0.56
1:F:66:TYR:HB2	1:F:104:PHE:CE2	2.40	0.56
1:I:47:THR:HG23	1:I:73:TYR:HB2	1.88	0.56
1:L:68:ASP:OD1	1:L:69:PRO:HD2	2.04	0.56
1:C:259:LYS:HD2	1:D:281:ARG:NH1	2.20	0.56
1:H:12:ILE:CD1	1:H:12:ILE:H	2.17	0.56
1:K:47:THR:CG2	1:K:73:TYR:HB2	2.35	0.56
1:A:249:GLN:HE21	1:B:218:TRP:HE1	1.52	0.56
1:E:107:TYR:HB2	1:E:271:LEU:HD12	1.87	0.56
1:E:128:PHE:HD2	1:E:129:PRO:HD2	1.71	0.56
1:E:250:ILE:N	1:E:250:ILE:HD12	2.20	0.56
1:F:177:GLN:NE2	1:F:178:TYR:HA	2.21	0.56
1:F:13:ASN:O	1:F:17:ARG:HG3	2.05	0.56
1:G:35:ALA:O	1:G:38:LEU:HB2	2.05	0.56
1:H:47:THR:HG23	1:H:73:TYR:HB2	1.87	0.56
1:K:89:GLN:HB3	1:K:108:ASN:ND2	2.09	0.56
1:L:98:PRO:HG2	1:L:100:TYR:H	1.69	0.56
1:F:188:HIS:CD2	1:F:190:ALA:H	2.24	0.56
1:G:113:LYS:CE	1:G:270:GLU:HG3	2.35	0.56
1:L:177:GLN:O	1:L:177:GLN:HG2	2.05	0.56
1:B:119:VAL:HB	1:B:268:ILE:CD1	2.36	0.56
1:F:53:LEU:HD22	1:F:63:VAL:HG21	1.88	0.56
1:H:213:GLN:NE2	1:H:213:GLN:HA	2.21	0.56
1:D:181:ASN:ND2	1:D:181:ASN:H	2.04	0.56
1:B:123:ASN:ND2	1:B:261:ARG:NH2	2.54	0.56
1:H:284:ILE:HD13	1:H:284:ILE:H	1.70	0.56
1:I:11:SER:O	1:I:12:ILE:HD13	2.05	0.56
1:A:17:ARG:HG3	1:A:20:ARG:HH12	1.71	0.56
1:C:258:LEU:O	1:C:262:GLU:HG3	2.06	0.56
1:E:259:LYS:HG3	1:E:260:SER:N	2.20	0.56
1:F:162:ARG:NH1	1:F:197:GLU:OE2	2.39	0.56
1:F:96:ALA:HB2	1:F:101:GLN:NE2	2.21	0.56
1:I:179:GLU:HB2	1:I:181:ASN:ND2	2.21	0.56
1:K:222:MET:HE1	1:K:227:ILE:HG21	1.88	0.56
1:K:274:LEU:HD22	1:K:275:ASN:H	1.70	0.56
1:H:284:ILE:HD13	1:H:284:ILE:N	2.21	0.55
1:H:71:ILE:HG13	1:H:71:ILE:O	2.06	0.55
1:H:104:PHE:CE2	1:H:118:GLY:HA3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:HA	1:C:282:TYR:CE2	2.41	0.55
1:D:145:LYS:HD3	1:D:145:LYS:C	2.26	0.55
1:J:41:TRP:CD2	1:J:278:VAL:HG13	2.41	0.55
1:A:41:TRP:CE3	1:A:278:VAL:HG13	2.41	0.55
1:B:11:SER:C	1:B:13:ASN:H	2.09	0.55
1:C:41:TRP:CD2	1:C:278:VAL:HG13	2.41	0.55
1:G:259:LYS:HG3	1:G:260:SER:N	2.21	0.55
1:H:69:PRO:HD2	1:H:102:LYS:NZ	2.21	0.55
1:J:222:MET:HE3	1:J:227:ILE:HG21	1.86	0.55
1:A:90:ALA:O	1:A:108:ASN:ND2	2.32	0.55
1:D:17:ARG:HG2	1:D:20:ARG:CZ	2.37	0.55
1:L:215:ASN:O	1:L:219:ASN:ND2	2.40	0.55
1:H:106:LEU:HD22	1:H:120:VAL:CG2	2.36	0.55
1:A:41:TRP:CD2	1:A:278:VAL:HG13	2.42	0.55
1:H:69:PRO:HD2	1:H:102:LYS:HZ1	1.72	0.55
1:K:107:TYR:HB2	1:K:271:LEU:HD22	1.88	0.55
1:A:41:TRP:C	1:A:44:LEU:HD11	2.27	0.55
1:B:41:TRP:CD2	1:B:278:VAL:HG13	2.42	0.54
1:D:35:ALA:O	1:D:38:LEU:HB2	2.07	0.54
1:L:213:GLN:HA	1:L:213:GLN:NE2	2.21	0.54
1:D:55:LYS:O	1:D:59:GLN:HG3	2.07	0.54
1:F:84:ARG:O	1:G:99:VAL:HG21	2.08	0.54
1:G:41:TRP:CD2	1:G:278:VAL:HG13	2.42	0.54
1:G:53:LEU:HD12	1:G:63:VAL:HG11	1.87	0.54
1:C:162:ARG:HH11	1:C:162:ARG:CG	2.17	0.54
1:D:102:LYS:HG3	1:D:103:GLU:N	2.23	0.54
1:D:17:ARG:HA	1:D:20:ARG:CZ	2.36	0.54
1:F:107:TYR:CB	1:F:271:LEU:HD22	2.38	0.54
1:F:43:ASN:N	1:F:43:ASN:HD22	2.04	0.54
1:J:249:GLN:HE22	1:K:218:TRP:HE1	1.52	0.54
1:A:213:GLN:HA	1:A:213:GLN:NE2	2.22	0.54
1:B:113:LYS:CG	1:B:113:LYS:O	2.55	0.54
1:H:113:LYS:NZ	1:H:270:GLU:HG3	2.19	0.54
1:J:162:ARG:HH11	1:J:162:ARG:HG2	1.71	0.54
1:D:205:TYR:CZ	1:D:207:VAL:HB	2.42	0.54
1:F:119:VAL:HB	1:F:268:ILE:CD1	2.38	0.54
1:G:257:PHE:O	1:G:261:ARG:CD	2.53	0.54
1:A:181:ASN:HD22	1:A:181:ASN:N	2.04	0.54
1:B:205:TYR:CZ	1:B:207:VAL:HB	2.43	0.54
1:D:167:ASN:ND2	1:D:168:GLN:NE2	2.47	0.54
1:A:44:LEU:N	1:A:44:LEU:HD12	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:HD22	1:A:168:GLN:N	2.04	0.54
1:C:248:GLU:HB3	1:D:227:ILE:CG2	2.37	0.54
1:D:97:SER:OG	1:D:98:PRO:HD3	2.08	0.54
1:K:130:THR:HG22	1:K:134:LEU:HG	1.89	0.54
1:K:144:LEU:O	1:K:148:ILE:HG13	2.07	0.54
1:A:47:THR:HG23	1:A:73:TYR:HB2	1.88	0.54
1:A:164:ASN:O	1:B:189:GLU:HA	2.08	0.54
1:B:259:LYS:HG3	1:B:260:SER:N	2.23	0.54
1:I:49:ASN:C	1:I:49:ASN:HD22	2.11	0.54
1:K:249:GLN:HG2	1:L:222:MET:CE	2.38	0.54
1:C:170:SER:HB3	1:C:173:GLN:HB2	1.90	0.53
1:A:96:ALA:HB1	1:A:101:GLN:HG3	1.90	0.53
1:A:37:GLN:O	1:A:281:ARG:HD2	2.09	0.53
1:C:84:ARG:O	1:D:99:VAL:HG21	2.08	0.53
1:G:53:LEU:O	1:G:57:ILE:HG13	2.08	0.53
1:B:271:LEU:HD23	1:B:272:TYR:CE1	2.43	0.53
1:K:53:LEU:HD12	1:K:63:VAL:HG11	1.90	0.53
1:B:264:ALA:O	1:B:268:ILE:HG12	2.08	0.53
1:I:109:TYR:HB2	1:I:112:MET:HG2	1.90	0.53
1:K:67:LYS:HB2	1:K:272:TYR:CE1	2.43	0.53
1:F:112:MET:HG2	1:F:113:LYS:N	2.22	0.53
1:E:98:PRO:HG2	1:E:100:TYR:H	1.73	0.53
1:F:35:ALA:O	1:F:38:LEU:HB2	2.09	0.53
1:G:222:MET:HE1	1:G:227:ILE:CD1	2.39	0.53
1:K:162:ARG:NH1	1:K:162:ARG:HG2	2.22	0.53
1:I:110:ARG:HD3	1:I:270:GLU:OE2	2.09	0.53
1:I:203:ALA:HB1	1:J:158:PRO:HG3	1.91	0.53
1:K:53:LEU:O	1:K:57:ILE:HG13	2.08	0.53
1:L:168:GLN:HA	1:L:168:GLN:HE21	1.73	0.53
1:B:130:THR:C	1:B:132:PRO:HD2	2.29	0.53
1:E:35:ALA:O	1:E:38:LEU:HB2	2.09	0.53
1:F:269:ASN:OD1	1:F:276:VAL:HG22	2.08	0.53
1:E:89:GLN:NE2	1:E:108:ASN:ND2	2.56	0.53
1:F:178:TYR:CZ	1:F:180:GLY:HA2	2.43	0.53
1:F:96:ALA:O	1:F:97:SER:HB2	2.08	0.53
1:D:41:TRP:CZ3	1:D:278:VAL:HG22	2.43	0.53
1:C:256:VAL:HG11	1:D:33:SER:HB2	1.89	0.53
1:E:162:ARG:HG3	1:E:162:ARG:NH1	2.21	0.53
1:E:43:ASN:O	1:E:276:VAL:HG12	2.09	0.53
1:F:113:LYS:HG3	1:F:114:GLU:H	1.73	0.53
1:A:170:SER:HB3	1:A:173:GLN:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLN:NE2	1:C:213:GLN:HA	2.25	0.52
1:C:255:THR:O	1:C:259:LYS:HG2	2.09	0.52
1:K:214:LYS:HE3	2:K:315:HOH:O	2.09	0.52
1:A:41:TRP:HB2	1:A:44:LEU:HD21	1.91	0.52
1:B:227:ILE:O	1:B:228:LYS:HB3	2.09	0.52
1:D:148:ILE:HG23	1:D:207:VAL:HG13	1.91	0.52
1:D:259:LYS:HB3	1:D:259:LYS:NZ	2.24	0.52
1:I:271:LEU:O	1:I:271:LEU:HD22	2.08	0.52
1:J:131:THR:OG1	1:J:132:PRO:HD3	2.09	0.52
1:K:97:SER:OG	1:K:98:PRO:HD3	2.09	0.52
1:B:68:ASP:OD1	1:B:69:PRO:HD2	2.09	0.52
1:H:93:PHE:CE2	1:H:95:ALA:HB2	2.44	0.52
1:L:126:MET:HG2	1:L:128:PHE:CZ	2.44	0.52
1:B:49:ASN:C	1:B:49:ASN:ND2	2.63	0.52
1:D:107:TYR:HB2	1:D:117:MET:HG2	1.92	0.52
1:F:137:PHE:CD2	1:F:221:MET:HG2	2.44	0.52
1:G:265:CYS:O	1:G:269:ASN:ND2	2.43	0.52
1:G:49:ASN:C	1:G:49:ASN:HD22	2.12	0.52
2:I:356:HOH:O	1:J:22:ARG:HD3	2.09	0.52
1:B:124:ASN:HD22	1:B:126:MET:H	1.56	0.52
1:B:166:ASN:HD21	1:C:187:ALA:HB1	1.73	0.52
1:D:84:ARG:HH12	1:D:90:ALA:HB2	1.74	0.52
1:D:174:VAL:HG21	1:D:186:PHE:HD1	1.75	0.52
1:D:98:PRO:HA	2:D:326:HOH:O	2.10	0.52
1:I:213:GLN:HA	1:I:213:GLN:NE2	2.25	0.52
1:J:126:MET:HG2	1:J:128:PHE:CE1	2.45	0.52
1:L:41:TRP:CD2	1:L:278:VAL:HG13	2.44	0.52
1:L:51:SER:O	1:L:55:LYS:HG3	2.10	0.52
1:C:14:GLU:HG2	1:C:15:ILE:N	2.24	0.52
1:A:98:PRO:HG2	1:A:100:TYR:H	1.74	0.52
1:A:222:MET:CE	1:L:249:GLN:HG2	2.39	0.52
1:D:14:GLU:O	1:D:18:GLN:HG2	2.09	0.52
1:I:221:MET:CE	1:I:225:LEU:HD13	2.40	0.52
1:A:145:LYS:NZ	1:L:140:GLU:OE1	2.42	0.52
1:B:178:TYR:CZ	1:B:180:GLY:HA2	2.44	0.52
1:C:73:TYR:CE2	1:C:274:LEU:HD11	2.45	0.52
1:C:43:ASN:HB2	1:C:276:VAL:HA	1.90	0.52
1:D:163:ALA:HB3	1:E:187:ALA:HB2	1.92	0.52
1:D:87:TYR:OH	1:E:48:ILE:HA	2.10	0.52
1:E:53:LEU:HD12	1:E:63:VAL:HG11	1.91	0.52
1:F:47:THR:CG2	1:F:73:TYR:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:GLU:HB2	2:I:331:HOH:O	2.10	0.52
1:L:195:SER:O	1:L:196:ILE:HD13	2.10	0.52
1:A:167:ASN:ND2	1:A:167:ASN:N	2.53	0.52
1:B:248:GLU:HA	1:C:282:TYR:CZ	2.45	0.52
1:F:131:THR:HB	1:F:132:PRO:HD3	1.92	0.52
1:H:277:LYS:HE3	1:H:278:VAL:H	1.74	0.52
1:I:227:ILE:O	1:I:228:LYS:HB3	2.10	0.52
1:I:97:SER:OG	1:I:98:PRO:HD3	2.09	0.52
1:L:20:ARG:NH1	1:L:143:GLU:HG3	2.25	0.52
1:F:258:LEU:HD22	1:F:262:GLU:HG3	1.91	0.51
1:F:93:PHE:HE2	1:F:95:ALA:HB2	1.74	0.51
1:G:22:ARG:HD2	2:G:317:HOH:O	2.10	0.51
1:H:110:ARG:HG2	1:H:270:GLU:HG2	1.92	0.51
1:I:85:ASP:OD1	1:I:87:TYR:N	2.39	0.51
1:J:222:MET:CE	1:J:227:ILE:HG21	2.39	0.51
1:A:47:THR:CG2	1:A:73:TYR:HB2	2.40	0.51
1:D:125:ASP:OD2	1:D:259:LYS:HE2	2.11	0.51
1:F:160:LEU:HD23	1:G:184:VAL:HG12	1.90	0.51
1:B:112:MET:H	1:B:114:GLU:CD	2.12	0.51
1:E:107:TYR:OH	1:E:110:ARG:HA	2.08	0.51
1:H:209:LYS:HD3	1:I:205:TYR:CD2	2.45	0.51
1:L:205:TYR:CZ	1:L:207:VAL:HB	2.45	0.51
1:E:110:ARG:HG2	1:E:111:ASP:OD1	2.10	0.51
1:I:258:LEU:HD22	1:I:262:GLU:CG	2.38	0.51
1:J:13:ASN:ND2	1:L:179:GLU:HG2	2.25	0.51
1:C:114:GLU:HG2	1:C:117:MET:CE	2.39	0.51
1:D:146:GLU:O	1:D:150:VAL:HG23	2.10	0.51
1:F:222:MET:HE3	1:F:227:ILE:CG2	2.39	0.51
1:H:107:TYR:CD2	1:H:271:LEU:HD13	2.46	0.51
1:C:93:PHE:HE2	1:C:95:ALA:HB2	1.75	0.51
1:E:68:ASP:OD1	1:E:69:PRO:HD2	2.09	0.51
1:F:41:TRP:HB3	1:F:44:LEU:CD1	2.41	0.51
1:J:12:ILE:HD13	1:J:12:ILE:N	2.24	0.51
1:K:119:VAL:HG21	1:K:268:ILE:HG13	1.93	0.51
1:K:169:LEU:HD23	1:K:170:SER:H	1.76	0.51
1:A:188:HIS:HB3	1:A:191:LEU:CD1	2.37	0.51
1:C:100:TYR:CE1	1:C:102:LYS:HB2	2.45	0.51
1:C:11:SER:C	1:C:13:ASN:H	2.13	0.51
1:E:249:GLN:NE2	1:F:218:TRP:HE1	2.07	0.51
1:D:145:LYS:HG2	2:D:338:HOH:O	2.11	0.51
1:H:173:GLN:HG3	1:H:177:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:LYS:HB3	1:I:205:TYR:CE2	2.46	0.51
1:A:259:LYS:O	1:A:263:GLU:HG3	2.11	0.51
1:B:14:GLU:HG3	1:B:15:ILE:N	2.25	0.51
1:D:87:TYR:CD1	1:E:49:ASN:HB2	2.46	0.51
1:E:264:ALA:HA	1:E:267:LYS:HD3	1.92	0.51
1:F:202:ASP:HA	2:F:328:HOH:O	2.10	0.51
1:A:36:TYR:HD2	1:L:126:MET:HE1	1.76	0.51
1:B:164:ASN:OD1	1:B:195:SER:HA	2.10	0.51
1:H:131:THR:HB	1:H:132:PRO:HD3	1.93	0.51
1:I:178:TYR:CZ	1:I:180:GLY:HA2	2.46	0.51
1:J:54:GLU:OE1	1:J:261:ARG:NH1	2.43	0.51
1:K:106:LEU:CD2	1:K:120:VAL:HG13	2.41	0.51
1:K:222:MET:CE	1:K:227:ILE:HG21	2.40	0.51
1:K:94:ARG:HH21	1:K:94:ARG:HG3	1.75	0.51
1:L:165:ASP:HB2	1:L:195:SER:OG	2.10	0.51
1:L:67:LYS:HB2	1:L:73:TYR:CE2	2.46	0.51
1:B:96:ALA:HB1	1:B:101:GLN:HE21	1.76	0.50
1:B:114:GLU:N	1:B:114:GLU:CD	2.62	0.50
1:F:41:TRP:CD2	1:F:278:VAL:HG13	2.46	0.50
1:F:255:THR:CG2	1:G:281:ARG:HD3	2.32	0.50
1:H:168:GLN:CD	1:H:168:GLN:N	2.63	0.50
1:K:53:LEU:CD1	1:K:63:VAL:HG11	2.41	0.50
1:C:53:LEU:HD12	1:C:63:VAL:HG11	1.93	0.50
1:E:162:ARG:CG	1:E:162:ARG:HH11	2.22	0.50
1:H:106:LEU:HD22	1:H:120:VAL:HG23	1.92	0.50
1:I:168:GLN:HG2	1:I:188:HIS:NE2	2.26	0.50
1:K:93:PHE:HB2	1:K:106:LEU:HD21	1.93	0.50
1:H:145:LYS:C	1:H:145:LYS:HD3	2.31	0.50
1:K:104:PHE:CD2	1:K:118:GLY:HA3	2.46	0.50
1:K:260:SER:HA	1:K:263:GLU:OE2	2.11	0.50
1:F:258:LEU:HD12	1:F:280:PHE:CE1	2.47	0.50
1:G:54:GLU:CD	1:G:261:ARG:HH12	2.15	0.50
1:I:168:GLN:CG	1:I:169:LEU:N	2.65	0.50
1:J:106:LEU:CD2	1:J:120:VAL:HG23	2.41	0.50
1:D:178:TYR:CZ	1:D:180:GLY:HA2	2.46	0.50
1:D:218:TRP:O	1:D:222:MET:HG2	2.11	0.50
1:F:179:GLU:OE2	1:F:180:GLY:N	2.45	0.50
1:G:128:PHE:CE1	1:H:29:ASN:ND2	2.80	0.50
1:H:23:TRP:CD1	1:H:145:LYS:HD2	2.45	0.50
1:K:66:TYR:HB2	1:K:104:PHE:CE2	2.47	0.50
1:A:282:TYR:CE1	1:L:248:GLU:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:LYS:NZ	1:G:149:SER:OG	2.42	0.50
1:I:102:LYS:HD3	1:I:103:GLU:H	1.76	0.50
1:L:85:ASP:OD1	1:L:85:ASP:C	2.49	0.50
1:F:119:VAL:HB	1:F:268:ILE:HD13	1.93	0.50
1:I:168:GLN:HG3	1:I:169:LEU:H	1.75	0.50
1:E:227:ILE:O	1:E:228:LYS:HB3	2.12	0.50
1:F:148:ILE:HG23	1:F:207:VAL:HG13	1.94	0.50
1:H:47:THR:CG2	1:H:73:TYR:HB2	2.41	0.50
1:K:219:ASN:O	1:K:223:THR:HG23	2.12	0.50
1:B:181:ASN:HD22	1:B:181:ASN:C	2.15	0.50
1:J:209:LYS:HB3	1:K:205:TYR:CE2	2.47	0.50
1:C:168:GLN:NE2	1:C:168:GLN:N	2.59	0.49
1:D:222:MET:HE3	1:D:227:ILE:HB	1.94	0.49
1:D:68:ASP:OD2	1:D:71:ILE:HG12	2.11	0.49
1:F:56:SER:CB	1:F:63:VAL:HG12	2.42	0.49
1:K:209:LYS:HB3	1:L:205:TYR:CE2	2.47	0.49
1:L:54:GLU:OE1	1:L:261:ARG:NH1	2.44	0.49
1:B:163:ALA:O	1:B:166:ASN:ND2	2.41	0.49
1:C:169:LEU:HB3	1:C:186:PHE:HE1	1.77	0.49
1:A:99:VAL:HG22	1:L:86:VAL:HA	1.94	0.49
1:C:49:ASN:C	1:C:49:ASN:ND2	2.65	0.49
1:F:120:VAL:HB	1:F:122:TYR:CE1	2.48	0.49
1:F:41:TRP:HB3	1:F:44:LEU:HD13	1.94	0.49
1:G:12:ILE:HG22	1:G:12:ILE:O	2.11	0.49
1:G:222:MET:HE1	1:G:227:ILE:HD12	1.93	0.49
1:I:162:ARG:NH1	1:J:193:SER:HA	2.27	0.49
1:I:19:LYS:O	1:I:22:ARG:HB2	2.12	0.49
1:A:221:MET:HE2	1:A:221:MET:O	2.12	0.49
1:F:106:LEU:HD22	1:F:120:VAL:CG2	2.42	0.49
1:F:43:ASN:O	1:F:276:VAL:HG12	2.12	0.49
1:G:255:THR:O	1:G:259:LYS:HG2	2.12	0.49
1:H:165:ASP:OD1	1:H:195:SER:HB3	2.12	0.49
1:K:178:TYR:CE2	1:K:184:VAL:HG22	2.48	0.49
1:A:167:ASN:ND2	1:A:168:GLN:N	2.60	0.49
1:C:162:ARG:HG3	1:C:162:ARG:NH1	2.23	0.49
1:G:228:LYS:HB3	1:G:228:LYS:NZ	2.27	0.49
1:I:66:TYR:HB2	1:I:104:PHE:CZ	2.47	0.49
1:J:131:THR:O	1:J:135:GLU:HG3	2.13	0.49
1:K:197:GLU:HG2	1:K:199:PHE:CE1	2.47	0.49
1:C:51:SER:OG	1:C:55:LYS:HD2	2.13	0.49
1:F:115:GLU:N	1:F:115:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:SER:HB3	1:J:98:PRO:HD3	1.93	0.49
1:B:37:GLN:HG2	1:B:281:ARG:CD	2.37	0.49
1:C:28:LEU:O	1:C:32:GLN:HG3	2.11	0.49
1:D:12:ILE:HG23	1:D:15:ILE:HD12	1.94	0.49
1:E:34:LEU:O	1:E:37:GLN:NE2	2.46	0.49
1:F:169:LEU:HD23	1:F:170:SER:H	1.78	0.49
1:G:98:PRO:HG2	1:G:100:TYR:H	1.78	0.49
1:J:203:ALA:HB1	1:K:158:PRO:HG3	1.94	0.49
1:L:172:LYS:HZ2	1:L:176:ASN:HD21	1.61	0.49
1:C:258:LEU:HD12	1:C:280:PHE:CE1	2.48	0.49
1:C:55:LYS:HB3	1:C:59:GLN:NE2	2.27	0.49
1:D:16:GLN:HA	1:D:16:GLN:HE21	1.77	0.49
1:E:106:LEU:CD1	1:E:120:VAL:HG13	2.42	0.49
1:E:178:TYR:CZ	1:E:180:GLY:HA2	2.47	0.49
1:F:148:ILE:O	1:F:152:GLN:HG2	2.13	0.49
1:F:227:ILE:HG22	1:F:228:LYS:N	2.28	0.49
1:H:172:LYS:HD3	2:I:368:HOH:O	2.11	0.49
1:J:93:PHE:HB2	1:J:106:LEU:HD21	1.95	0.49
1:J:108:ASN:O	1:J:109:TYR:CD1	2.66	0.49
1:A:49:ASN:HD22	1:A:50:PRO:N	2.09	0.49
1:B:123:ASN:ND2	1:B:261:ARG:HH21	2.11	0.49
1:B:51:SER:O	1:B:55:LYS:HG3	2.13	0.49
1:B:53:LEU:CD1	1:B:63:VAL:HG11	2.42	0.49
1:C:136:LEU:HD13	1:D:22:ARG:HD2	1.95	0.49
1:F:66:TYR:HB2	1:F:104:PHE:CZ	2.47	0.49
1:L:168:GLN:HE21	1:L:168:GLN:CA	2.26	0.49
1:K:87:TYR:OH	1:L:48:ILE:HD13	2.13	0.49
1:C:73:TYR:HE2	1:C:272:TYR:CD1	2.31	0.48
1:F:124:ASN:HA	1:F:260:SER:OG	2.13	0.48
1:F:13:ASN:HD21	1:H:179:GLU:HG2	1.77	0.48
1:G:25:ILE:HG22	1:G:29:ASN:ND2	2.28	0.48
1:F:248:GLU:HG2	1:G:282:TYR:CE2	2.47	0.48
1:H:67:LYS:HD3	1:H:73:TYR:CZ	2.48	0.48
1:K:163:ALA:HB3	1:L:187:ALA:HB2	1.95	0.48
1:J:209:LYS:HD3	1:K:205:TYR:CD2	2.48	0.48
1:A:282:TYR:CZ	1:L:248:GLU:HA	2.47	0.48
1:C:256:VAL:HG13	1:D:33:SER:HB2	1.95	0.48
1:F:96:ALA:CB	1:F:101:GLN:HE21	2.24	0.48
1:K:137:PHE:CD2	1:K:221:MET:HB2	2.49	0.48
1:A:169:LEU:HD23	1:A:170:SER:H	1.78	0.48
1:D:31:LEU:HB3	1:D:134:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:LEU:O	1:E:258:LEU:HD22	2.13	0.48
1:G:192:ASP:HB2	1:G:194:ASP:OD1	2.13	0.48
1:J:167:ASN:HD21	1:K:189:GLU:HB3	1.77	0.48
1:G:160:LEU:HD23	1:H:184:VAL:HG12	1.94	0.48
1:K:113:LYS:HE2	1:K:271:LEU:HA	1.94	0.48
1:K:31:LEU:HB3	1:K:134:LEU:HD22	1.96	0.48
1:C:11:SER:HB3	1:C:12:ILE:HD12	1.95	0.48
1:F:168:GLN:HG2	1:F:188:HIS:CD2	2.48	0.48
1:J:222:MET:HE3	1:J:227:ILE:CG2	2.43	0.48
1:A:167:ASN:CG	1:A:168:GLN:HE21	2.16	0.48
1:B:145:LYS:HD3	1:B:145:LYS:C	2.34	0.48
1:A:255:THR:HG21	1:B:281:ARG:HD3	1.95	0.48
1:C:44:LEU:HD13	1:C:48:ILE:CG2	2.43	0.48
1:I:96:ALA:O	1:I:97:SER:CB	2.61	0.48
1:K:284:ILE:O	1:K:284:ILE:HG23	2.13	0.48
1:L:107:TYR:CA	1:L:117:MET:HE3	2.40	0.48
1:L:122:TYR:O	1:L:260:SER:OG	2.30	0.48
1:B:131:THR:N	1:B:132:PRO:HD2	2.28	0.48
1:G:164:ASN:O	1:H:189:GLU:HA	2.14	0.48
1:L:227:ILE:O	1:L:228:LYS:HB3	2.14	0.48
1:C:167:ASN:ND2	1:C:167:ASN:O	2.46	0.48
2:J:350:HOH:O	1:K:200:LYS:HE3	2.14	0.48
1:K:96:ALA:O	1:K:97:SER:CB	2.62	0.48
1:F:205:TYR:CZ	1:F:207:VAL:HB	2.48	0.48
1:G:162:ARG:NH1	1:G:197:GLU:OE1	2.46	0.48
1:H:107:TYR:CE2	1:H:271:LEU:HB2	2.48	0.48
1:K:259:LYS:O	1:K:263:GLU:HG2	2.13	0.48
1:C:255:THR:CG2	1:D:281:ARG:HD3	2.35	0.48
1:K:93:PHE:CE2	1:K:95:ALA:HB2	2.49	0.48
1:L:283:ASP:O	1:L:285:VAL:N	2.47	0.48
1:L:88:ASN:O	1:L:88:ASN:CG	2.52	0.48
1:C:131:THR:HB	1:C:132:PRO:HD3	1.95	0.47
1:C:145:LYS:O	1:C:145:LYS:HD3	2.14	0.47
1:C:252:SER:O	1:C:256:VAL:HG23	2.14	0.47
1:D:179:GLU:HB2	2:D:336:HOH:O	2.14	0.47
1:E:219:ASN:OD1	1:E:228:LYS:HE2	2.15	0.47
1:E:265:CYS:SG	1:E:276:VAL:HG23	2.54	0.47
1:L:178:TYR:CZ	1:L:180:GLY:HA2	2.49	0.47
1:L:221:MET:O	1:L:221:MET:HE2	2.15	0.47
1:A:93:PHE:CE2	1:A:95:ALA:HB2	2.48	0.47
1:H:107:TYR:CG	1:H:271:LEU:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:125:ASP:OD1	1:K:259:LYS:NZ	2.40	0.47
1:E:104:PHE:CE2	1:E:118:GLY:HA3	2.49	0.47
1:G:144:LEU:HD21	1:H:152:GLN:NE2	2.30	0.47
1:L:19:LYS:HA	1:L:22:ARG:NH1	2.30	0.47
1:A:189:GLU:HA	1:L:164:ASN:O	2.14	0.47
1:B:12:ILE:O	1:B:12:ILE:HG22	2.13	0.47
1:B:269:ASN:HD21	1:B:275:ASN:HA	1.76	0.47
1:C:125:ASP:OD2	1:C:259:LYS:HE3	2.14	0.47
1:C:213:GLN:HE21	1:C:213:GLN:HA	1.80	0.47
1:D:145:LYS:HD3	1:D:145:LYS:O	2.13	0.47
1:D:87:TYR:CE1	1:E:47:THR:O	2.68	0.47
1:E:222:MET:HE3	1:E:227:ILE:CG2	2.43	0.47
1:H:140:GLU:OE1	1:I:145:LYS:HE3	2.14	0.47
1:G:87:TYR:CD1	1:H:49:ASN:HB2	2.49	0.47
1:K:71:ILE:O	1:K:72:SER:HB3	2.14	0.47
1:L:12:ILE:O	1:L:12:ILE:HG22	2.13	0.47
1:D:91:THR:HG23	1:D:92:VAL:HG23	1.97	0.47
1:F:37:GLN:O	1:F:281:ARG:HD2	2.14	0.47
1:I:204:PRO:HD2	2:I:319:HOH:O	2.14	0.47
1:J:221:MET:CE	1:J:225:LEU:HD13	2.44	0.47
1:J:164:ASN:O	1:K:189:GLU:HA	2.14	0.47
1:L:222:MET:HE1	1:L:227:ILE:HG21	1.97	0.47
1:F:56:SER:CB	1:F:63:VAL:CG1	2.93	0.47
1:H:162:ARG:NH1	1:H:197:GLU:OE1	2.48	0.47
1:G:249:GLN:HG2	1:H:222:MET:CE	2.45	0.47
1:K:168:GLN:HG3	1:K:188:HIS:NE2	2.30	0.47
1:A:213:GLN:HA	1:A:213:GLN:HE21	1.78	0.47
1:C:14:GLU:HG2	1:C:15:ILE:H	1.80	0.47
1:E:200:LYS:HG2	2:E:335:HOH:O	2.13	0.47
1:K:42:GLU:HB2	1:K:277:LYS:HG3	1.97	0.47
1:K:84:ARG:NH1	1:K:90:ALA:HB2	2.30	0.47
1:L:172:LYS:NZ	1:L:176:ASN:ND2	2.59	0.47
1:B:119:VAL:HB	1:B:268:ILE:HD13	1.96	0.47
1:B:67:LYS:HB2	1:B:272:TYR:CE2	2.50	0.47
1:I:87:TYR:HD1	1:I:109:TYR:OH	1.97	0.47
1:K:65:PHE:HB3	1:K:119:VAL:HG23	1.97	0.47
1:B:112:MET:N	1:B:114:GLU:OE1	2.44	0.47
1:D:17:ARG:HG2	1:D:20:ARG:NH1	2.29	0.47
1:D:265:CYS:SG	1:D:276:VAL:HG22	2.55	0.47
1:F:113:LYS:HG3	1:F:114:GLU:N	2.30	0.47
1:H:178:TYR:CZ	1:H:180:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:TRP:O	1:I:222:MET:HG2	2.15	0.47
1:J:37:GLN:O	1:J:281:ARG:HD2	2.14	0.47
2:J:332:HOH:O	1:K:228:LYS:HD2	2.13	0.47
1:A:252:SER:O	1:A:256:VAL:HG23	2.15	0.47
1:B:97:SER:HB3	1:B:98:PRO:HD3	1.95	0.47
1:F:163:ALA:HB3	1:G:187:ALA:HB2	1.97	0.47
1:F:97:SER:HB3	1:F:98:PRO:HD3	1.97	0.47
1:H:284:ILE:CD1	1:H:284:ILE:H	2.27	0.47
1:H:96:ALA:O	1:H:97:SER:CB	2.62	0.47
1:K:12:ILE:HG22	1:K:12:ILE:O	2.15	0.47
1:A:178:TYR:CZ	1:A:180:GLY:HA2	2.50	0.47
1:C:87:TYR:HB3	1:D:52:PHE:CD1	2.51	0.47
1:D:83:GLN:HA	1:D:83:GLN:OE1	2.15	0.47
1:E:20:ARG:HG3	1:E:146:GLU:OE1	2.15	0.47
1:G:105:LYS:CD	1:G:105:LYS:N	2.71	0.47
1:G:147:ILE:HG12	1:H:156:LYS:HD2	1.97	0.47
1:B:166:ASN:CG	1:C:187:ALA:HB1	2.35	0.46
1:D:170:SER:HB3	1:D:173:GLN:HB2	1.97	0.46
1:D:98:PRO:HG2	1:D:100:TYR:H	1.78	0.46
1:E:203:ALA:HB1	1:F:158:PRO:HG3	1.97	0.46
1:F:72:SER:OG	1:F:73:TYR:N	2.49	0.46
1:J:195:SER:O	1:J:196:ILE:HD13	2.15	0.46
1:J:249:GLN:HB3	1:K:222:MET:CE	2.44	0.46
1:D:47:THR:CG2	1:D:73:TYR:HB2	2.44	0.46
1:D:53:LEU:O	1:D:57:ILE:HG13	2.14	0.46
1:D:94:ARG:NH1	2:D:361:HOH:O	2.48	0.46
1:F:67:LYS:HB2	1:F:272:TYR:CE2	2.50	0.46
1:L:283:ASP:O	1:L:285:VAL:HG12	2.15	0.46
1:A:12:ILE:N	1:A:12:ILE:HD13	2.30	0.46
1:B:49:ASN:HD21	1:B:51:SER:HB3	1.81	0.46
1:C:49:ASN:HD22	1:C:50:PRO:N	2.12	0.46
1:C:55:LYS:HB3	1:C:59:GLN:HE21	1.80	0.46
1:D:87:TYR:HE1	1:E:47:THR:O	1.99	0.46
1:D:96:ALA:O	1:D:97:SER:CB	2.62	0.46
1:G:167:ASN:HB3	1:G:168:GLN:HE21	1.79	0.46
1:J:227:ILE:HG22	1:J:228:LYS:N	2.29	0.46
1:K:73:TYR:CE2	1:K:272:TYR:CD1	3.01	0.46
1:L:71:ILE:O	1:L:72:SER:OG	2.25	0.46
1:C:265:CYS:SG	1:C:278:VAL:HG22	2.55	0.46
1:H:165:ASP:O	1:H:165:ASP:OD2	2.33	0.46
1:J:248:GLU:HG3	1:K:282:TYR:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:274:LEU:HA	2:K:332:HOH:O	2.15	0.46
1:A:17:ARG:HG3	1:A:20:ARG:NH1	2.31	0.46
1:C:99:VAL:O	1:C:99:VAL:HG12	2.15	0.46
1:D:47:THR:HG23	1:D:73:TYR:HB2	1.98	0.46
1:D:67:LYS:HB2	1:D:73:TYR:CE2	2.51	0.46
1:E:222:MET:CE	1:E:227:ILE:HG21	2.45	0.46
1:E:47:THR:CG2	1:E:73:TYR:HB2	2.46	0.46
1:H:162:ARG:NH1	1:I:193:SER:HA	2.30	0.46
1:L:183:PRO:O	1:L:185:ILE:HG13	2.15	0.46
1:A:214:LYS:HE3	2:A:329:HOH:O	2.16	0.46
1:D:137:PHE:O	1:D:141:LEU:CD2	2.63	0.46
1:E:143:GLU:O	1:E:147:ILE:HG13	2.16	0.46
1:F:136:LEU:HD13	1:G:22:ARG:HD3	1.97	0.46
1:A:130:THR:HG22	1:A:134:LEU:HG	1.97	0.46
1:A:167:ASN:HD21	1:A:168:GLN:HG2	1.78	0.46
1:B:143:GLU:OE2	1:C:153:ASN:ND2	2.44	0.46
1:C:204:PRO:HG2	2:D:328:HOH:O	2.14	0.46
1:C:281:ARG:HG2	2:C:314:HOH:O	2.15	0.46
1:E:255:THR:O	1:E:259:LYS:HG2	2.15	0.46
1:G:28:LEU:O	1:G:32:GLN:HG3	2.15	0.46
1:I:83:GLN:OE1	1:I:83:GLN:HA	2.15	0.46
1:J:178:TYR:CZ	1:J:180:GLY:HA2	2.50	0.46
1:K:221:MET:HE2	1:K:225:LEU:HD13	1.97	0.46
1:K:82:GLY:HA3	1:K:92:VAL:HG23	1.96	0.46
1:L:277:LYS:HA	1:L:277:LYS:HD3	1.58	0.46
1:A:96:ALA:HB2	1:A:101:GLN:HG3	1.96	0.46
1:C:168:GLN:HG2	1:C:188:HIS:NE2	2.31	0.46
1:C:76:CYS:HA	2:C:326:HOH:O	2.16	0.46
1:D:125:ASP:OD2	1:D:259:LYS:CE	2.64	0.46
1:H:119:VAL:HA	2:H:318:HOH:O	2.16	0.46
1:A:104:PHE:CE2	1:A:118:GLY:HA3	2.51	0.46
1:F:222:MET:CE	1:F:227:ILE:HG21	2.43	0.46
1:J:249:GLN:H	1:J:249:GLN:HG2	1.61	0.46
1:K:104:PHE:HE2	1:K:118:GLY:HA3	1.81	0.46
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.81	0.46
1:C:107:TYR:O	1:C:108:ASN:C	2.55	0.46
1:C:55:LYS:O	1:C:59:GLN:HG3	2.16	0.46
1:E:104:PHE:CD2	1:E:118:GLY:HA3	2.51	0.46
1:F:67:LYS:HB3	1:F:272:TYR:HE2	1.80	0.46
1:H:165:ASP:OD1	1:H:191:LEU:CD2	2.63	0.46
1:H:213:GLN:HE21	1:H:213:GLN:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:LYS:HG3	1:J:103:GLU:N	2.30	0.46
1:J:258:LEU:HD22	1:J:258:LEU:O	2.15	0.46
1:L:222:MET:CE	1:L:227:ILE:HG21	2.46	0.46
1:A:13:ASN:ND2	1:C:179:GLU:HG2	2.30	0.45
1:A:282:TYR:O	1:A:283:ASP:HB2	2.16	0.45
1:B:67:LYS:HB2	1:B:73:TYR:CE2	2.50	0.45
1:E:258:LEU:HD22	1:E:262:GLU:HG3	1.98	0.45
1:F:69:PRO:HA	2:F:335:HOH:O	2.15	0.45
1:I:88:ASN:HA	2:I:373:HOH:O	2.16	0.45
1:J:98:PRO:HG2	1:J:100:TYR:H	1.81	0.45
1:K:221:MET:HE3	1:K:221:MET:HA	1.97	0.45
1:K:249:GLN:HG2	1:L:222:MET:HE2	1.97	0.45
1:A:22:ARG:NH1	2:A:336:HOH:O	2.48	0.45
1:J:227:ILE:O	1:J:228:LYS:HB3	2.16	0.45
1:K:222:MET:HE1	1:K:227:ILE:CD1	2.46	0.45
1:K:274:LEU:HD23	1:K:275:ASN:H	1.80	0.45
1:A:66:TYR:HB2	1:A:104:PHE:CZ	2.51	0.45
1:F:110:ARG:HH11	1:F:113:LYS:HG2	1.72	0.45
1:G:172:LYS:HG2	1:H:185:ILE:HD12	1.98	0.45
1:L:113:LYS:HA	1:L:117:MET:CE	2.46	0.45
1:F:54:GLU:OE2	1:F:261:ARG:HD3	2.17	0.45
1:G:37:GLN:HG2	1:G:281:ARG:CD	2.47	0.45
1:I:188:HIS:CD2	1:I:190:ALA:HB3	2.52	0.45
1:I:88:ASN:HB2	2:I:333:HOH:O	2.16	0.45
1:L:48:ILE:O	1:L:50:PRO:HD3	2.16	0.45
1:F:115:GLU:CD	1:F:115:GLU:H	2.19	0.45
1:F:249:GLN:HG2	1:G:222:MET:HE2	1.97	0.45
1:I:188:HIS:NE2	1:I:190:ALA:HB3	2.31	0.45
1:I:221:MET:HE3	1:I:224:PHE:HB3	1.99	0.45
1:A:144:LEU:HD21	1:B:152:GLN:NE2	2.31	0.45
1:B:258:LEU:HD13	1:B:258:LEU:C	2.36	0.45
1:E:271:LEU:HD22	1:E:272:TYR:CE1	2.52	0.45
1:E:47:THR:HG23	1:E:73:TYR:HB2	1.99	0.45
1:G:68:ASP:OD2	1:G:71:ILE:HG12	2.16	0.45
1:I:19:LYS:HE3	1:I:19:LYS:CA	2.35	0.45
2:H:341:HOH:O	1:I:36:TYR:HB3	2.16	0.45
1:J:126:MET:HE2	1:J:126:MET:HB2	1.73	0.45
1:J:93:PHE:CE2	1:J:95:ALA:HB2	2.51	0.45
1:C:84:ARG:N	1:C:84:ARG:HD2	2.32	0.45
1:E:44:LEU:HD13	1:E:48:ILE:CG2	2.46	0.45
1:F:162:ARG:NH2	1:F:194:ASP:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:LYS:CB	1:F:272:TYR:HE2	2.30	0.45
1:J:167:ASN:HD22	1:J:167:ASN:N	2.14	0.45
1:K:73:TYR:CE2	1:K:272:TYR:HD1	2.35	0.45
1:D:164:ASN:HA	1:E:188:HIS:O	2.17	0.45
1:F:249:GLN:HG2	1:G:222:MET:HE3	1.98	0.45
1:B:162:ARG:HG3	1:B:162:ARG:NH1	2.28	0.45
1:B:93:PHE:CE2	1:B:95:ALA:HB2	2.51	0.45
1:D:181:ASN:HD22	1:D:181:ASN:H	1.64	0.45
1:E:164:ASN:O	1:F:189:GLU:HA	2.16	0.45
1:F:199:PHE:HB3	1:G:198:VAL:HG21	1.98	0.45
1:I:40:GLU:OE1	1:I:279:LYS:HE3	2.17	0.45
1:I:49:ASN:ND2	1:I:49:ASN:C	2.71	0.45
1:J:39:PHE:HZ	1:J:257:PHE:HB2	1.82	0.45
1:K:255:THR:HG21	1:L:281:ARG:HD3	1.99	0.45
1:E:126:MET:HE1	1:F:55:LYS:HD3	1.99	0.45
1:I:164:ASN:O	1:J:189:GLU:HA	2.17	0.45
1:J:97:SER:HB3	1:J:98:PRO:CD	2.47	0.45
1:L:93:PHE:HB2	1:L:106:LEU:HD11	1.99	0.45
1:L:181:ASN:ND2	1:L:181:ASN:N	2.62	0.45
1:L:258:LEU:HD22	1:L:262:GLU:CG	2.40	0.45
1:A:96:ALA:O	1:A:97:SER:CB	2.65	0.44
1:C:162:ARG:CG	1:C:162:ARG:NH1	2.78	0.44
1:C:53:LEU:O	1:C:57:ILE:HG13	2.18	0.44
1:E:93:PHE:CB	1:E:106:LEU:HD21	2.36	0.44
1:E:257:PHE:O	1:E:261:ARG:HG3	2.17	0.44
1:C:259:LYS:HG3	1:C:260:SER:N	2.32	0.44
1:E:249:GLN:CD	1:F:218:TRP:HE1	2.21	0.44
1:J:174:VAL:HG21	1:J:186:PHE:HD1	1.83	0.44
1:L:66:TYR:HB2	1:L:104:PHE:CE2	2.52	0.44
1:C:13:ASN:OD1	1:E:179:GLU:HG2	2.17	0.44
1:F:256:VAL:CG1	1:G:33:SER:HB2	2.46	0.44
1:J:213:GLN:CA	1:J:213:GLN:NE2	2.69	0.44
1:A:36:TYR:CD2	1:L:126:MET:HE1	2.53	0.44
1:L:43:ASN:HB2	1:L:276:VAL:HA	1.98	0.44
1:B:137:PHE:CB	1:B:221:MET:HE2	2.45	0.44
1:B:248:GLU:HB2	1:C:282:TYR:CE1	2.52	0.44
1:E:271:LEU:HD23	1:E:271:LEU:C	2.37	0.44
1:E:83:GLN:HB2	1:E:83:GLN:HE21	1.58	0.44
1:G:96:ALA:O	1:G:97:SER:CB	2.66	0.44
1:H:43:ASN:HB2	1:H:276:VAL:HA	1.99	0.44
1:E:108:ASN:HA	1:E:267:LYS:HZ1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:GLU:C	1:F:117:MET:N	2.70	0.44
1:G:34:LEU:O	1:G:37:GLN:NE2	2.51	0.44
1:H:205:TYR:CZ	1:H:207:VAL:HB	2.52	0.44
1:K:85:ASP:OD1	1:K:89:GLN:N	2.50	0.44
1:L:96:ALA:O	1:L:97:SER:CB	2.65	0.44
1:C:11:SER:C	1:C:13:ASN:N	2.70	0.44
1:E:249:GLN:HG3	1:F:222:MET:HE1	1.98	0.44
1:F:107:TYR:HD1	1:F:271:LEU:HB2	1.83	0.44
1:F:41:TRP:CH2	1:F:261:ARG:HG2	2.52	0.44
1:A:205:TYR:CD2	1:L:209:LYS:HD3	2.53	0.44
1:B:250:ILE:HD12	1:B:250:ILE:N	2.33	0.44
1:C:167:ASN:CB	1:D:189:GLU:OE2	2.65	0.44
1:D:41:TRP:HB2	1:D:44:LEU:HD11	1.98	0.44
1:E:12:ILE:HG22	1:E:12:ILE:O	2.17	0.44
1:I:258:LEU:HD12	1:I:280:PHE:CE1	2.53	0.44
1:L:45:PRO:HA	1:L:46:PRO:HD3	1.90	0.44
1:L:85:ASP:OD1	1:L:86:VAL:N	2.51	0.44
1:D:208:ASP:OD2	1:D:208:ASP:N	2.51	0.44
1:F:96:ALA:O	1:F:97:SER:CB	2.66	0.44
1:J:164:ASN:OD1	1:J:195:SER:HA	2.18	0.44
1:L:113:LYS:HB2	1:L:113:LYS:NZ	2.32	0.44
1:A:284:ILE:O	1:A:284:ILE:HG22	2.17	0.44
1:C:85:ASP:OD1	1:C:89:GLN:N	2.47	0.44
1:H:28:LEU:HD23	1:H:28:LEU:O	2.18	0.44
1:I:93:PHE:CE2	1:I:95:ALA:HB2	2.52	0.44
1:J:248:GLU:HG3	1:K:282:TYR:CG	2.52	0.44
1:C:66:TYR:HB2	1:C:104:PHE:CZ	2.53	0.43
1:G:178:TYR:CZ	1:G:180:GLY:HA2	2.53	0.43
1:H:202:ASP:HA	2:H:340:HOH:O	2.18	0.43
1:I:222:MET:HE1	1:I:227:ILE:HG21	2.00	0.43
1:J:166:ASN:ND2	1:J:170:SER:HA	2.33	0.43
1:A:249:GLN:NE2	1:B:218:TRP:NE1	2.61	0.43
1:B:49:ASN:HD22	1:B:50:PRO:N	2.15	0.43
1:F:218:TRP:O	1:F:222:MET:HG2	2.18	0.43
1:G:160:LEU:HD23	1:H:184:VAL:CG1	2.48	0.43
1:H:249:GLN:HG2	1:I:222:MET:CE	2.48	0.43
1:J:11:SER:O	1:J:14:GLU:OE2	2.36	0.43
1:J:271:LEU:HD12	1:J:272:TYR:CZ	2.53	0.43
1:B:97:SER:HB3	1:B:98:PRO:CD	2.48	0.43
1:C:208:ASP:OD2	1:C:208:ASP:N	2.51	0.43
1:G:13:ASN:OD1	1:I:179:GLU:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:284:ILE:HD12	1:G:285:VAL:H	1.83	0.43
1:L:11:SER:O	1:L:12:ILE:HD13	2.18	0.43
1:D:66:TYR:CE2	1:D:68:ASP:HA	2.53	0.43
1:E:128:PHE:HD2	1:E:129:PRO:N	2.15	0.43
1:F:56:SER:HB3	1:F:63:VAL:HG12	2.00	0.43
1:J:71:ILE:O	1:J:72:SER:HB3	2.19	0.43
1:K:55:LYS:CG	1:K:59:GLN:NE2	2.76	0.43
2:J:342:HOH:O	1:L:182:ALA:HA	2.19	0.43
1:F:73:TYR:OH	1:F:274:LEU:HD21	2.19	0.43
1:H:66:TYR:CE2	1:H:68:ASP:HA	2.54	0.43
1:I:209:LYS:HB3	1:J:205:TYR:CE2	2.53	0.43
1:K:169:LEU:HD23	1:K:170:SER:N	2.33	0.43
1:K:144:LEU:HD21	1:L:152:GLN:NE2	2.33	0.43
1:L:181:ASN:H	1:L:181:ASN:HD22	1.66	0.43
1:L:93:PHE:CE2	1:L:95:ALA:HB2	2.53	0.43
1:A:205:TYR:CZ	1:A:207:VAL:HB	2.54	0.43
1:B:172:LYS:NZ	1:C:181:ASN:OD1	2.49	0.43
1:C:248:GLU:HG2	1:D:282:TYR:CD2	2.53	0.43
1:D:221:MET:HE3	1:D:224:PHE:HB3	2.00	0.43
1:D:41:TRP:CB	1:D:44:LEU:HD11	2.48	0.43
1:H:109:TYR:CG	1:H:112:MET:SD	3.11	0.43
1:I:168:GLN:HG2	1:I:188:HIS:ND1	2.32	0.43
1:I:283:ASP:CG	1:I:284:ILE:N	2.72	0.43
1:K:39:PHE:HE2	1:K:280:PHE:CE2	2.36	0.43
1:K:73:TYR:HE2	1:K:272:TYR:HD1	1.66	0.43
1:K:91:THR:HG21	2:K:346:HOH:O	2.18	0.43
1:A:169:LEU:HB3	1:A:186:PHE:CE1	2.54	0.43
1:A:258:LEU:O	1:A:258:LEU:HD22	2.18	0.43
1:B:11:SER:C	1:B:13:ASN:N	2.71	0.43
1:C:96:ALA:O	1:C:97:SER:CB	2.67	0.43
1:D:96:ALA:HB2	1:D:101:GLN:HG3	2.00	0.43
1:E:128:PHE:CD2	1:E:129:PRO:HD2	2.53	0.43
1:E:252:SER:O	1:E:256:VAL:HG23	2.19	0.43
1:G:249:GLN:HG2	1:H:222:MET:HE3	2.00	0.43
1:G:60:PHE:CD1	1:G:77:ASN:OD1	2.71	0.43
1:H:165:ASP:OD1	1:H:195:SER:CB	2.66	0.43
1:H:54:GLU:OE1	1:H:261:ARG:NH1	2.52	0.43
1:I:248:GLU:HB2	1:J:282:TYR:CE2	2.53	0.43
1:I:258:LEU:O	1:I:262:GLU:HG3	2.18	0.43
1:K:161:ILE:HG12	1:K:198:VAL:HG22	2.01	0.43
1:K:178:TYR:CD2	1:K:184:VAL:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLN:HG2	1:D:222:MET:HE2	2.00	0.43
1:E:125:ASP:O	1:E:126:MET:HE3	2.19	0.43
1:E:160:LEU:HD23	1:F:184:VAL:CG1	2.47	0.43
1:E:271:LEU:HD22	1:E:272:TYR:CD1	2.53	0.43
1:G:208:ASP:N	1:G:208:ASP:OD2	2.52	0.43
1:J:78:GLY:HA3	1:J:95:ALA:HA	2.01	0.43
1:A:148:ILE:HG23	1:A:207:VAL:HG13	2.01	0.43
1:A:152:GLN:NE2	1:L:144:LEU:HD21	2.33	0.43
1:C:167:ASN:ND2	1:C:167:ASN:C	2.72	0.43
1:C:92:VAL:HG11	1:C:94:ARG:NH1	2.34	0.43
1:D:227:ILE:O	1:D:228:LYS:CB	2.64	0.43
1:G:68:ASP:CG	1:G:71:ILE:HG12	2.39	0.43
1:J:167:ASN:OD1	1:K:189:GLU:OE2	2.37	0.43
1:J:168:GLN:CG	1:J:188:HIS:CE1	2.91	0.43
1:K:270:GLU:OE1	1:K:271:LEU:N	2.52	0.43
1:K:39:PHE:HZ	1:K:257:PHE:HB2	1.84	0.43
1:K:248:GLU:HG2	1:L:227:ILE:HG23	2.00	0.43
1:B:213:GLN:CG	1:C:207:VAL:CG1	2.97	0.43
1:C:40:GLU:HA	2:C:315:HOH:O	2.18	0.43
1:D:48:ILE:CD1	1:D:73:TYR:HB3	2.49	0.43
1:F:271:LEU:HD23	1:F:272:TYR:CE1	2.54	0.43
1:H:164:ASN:OD1	1:H:165:ASP:N	2.52	0.43
1:B:13:ASN:ND2	1:B:17:ARG:HH21	2.16	0.42
1:B:67:LYS:CB	1:B:272:TYR:CE2	3.02	0.42
1:B:78:GLY:HA3	1:B:95:ALA:HA	2.01	0.42
1:E:53:LEU:CD1	1:E:63:VAL:HG11	2.49	0.42
1:H:137:PHE:CD2	1:H:221:MET:HB2	2.54	0.42
1:K:81:SER:HB2	1:K:94:ARG:NH2	2.32	0.42
1:L:181:ASN:N	1:L:181:ASN:HD22	2.17	0.42
1:A:222:MET:HE2	1:L:249:GLN:HG2	2.01	0.42
1:C:45:PRO:HA	1:C:46:PRO:HD3	1.96	0.42
1:F:128:PHE:HA	1:F:129:PRO:HD3	1.87	0.42
1:G:107:TYR:OH	1:G:110:ARG:HA	2.20	0.42
1:G:66:TYR:CE2	1:G:68:ASP:HA	2.54	0.42
1:G:98:PRO:HB2	1:G:99:VAL:H	1.61	0.42
1:H:67:LYS:HD3	1:H:73:TYR:CE2	2.54	0.42
1:K:11:SER:O	1:K:12:ILE:HD13	2.19	0.42
1:B:143:GLU:O	1:B:147:ILE:HG13	2.19	0.42
1:C:167:ASN:HB3	1:D:189:GLU:OE2	2.19	0.42
1:C:43:ASN:ND2	1:C:43:ASN:N	2.66	0.42
1:F:272:TYR:N	1:F:272:TYR:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:LEU:HD13	1:F:53:LEU:C	2.40	0.42
1:G:107:TYR:HB2	1:G:117:MET:HE3	2.01	0.42
1:I:85:ASP:OD1	1:I:85:ASP:C	2.57	0.42
1:L:130:THR:HG22	1:L:134:LEU:HG	2.02	0.42
1:D:258:LEU:HD13	1:D:262:GLU:HG3	2.00	0.42
1:E:78:GLY:HA3	1:E:95:ALA:HA	2.01	0.42
1:E:203:ALA:CB	1:F:158:PRO:HG3	2.48	0.42
1:G:60:PHE:HD1	1:G:77:ASN:OD1	2.02	0.42
1:H:126:MET:HG3	2:I:346:HOH:O	2.20	0.42
1:H:148:ILE:O	1:H:152:GLN:HG2	2.20	0.42
1:K:271:LEU:HG	1:K:272:TYR:CE2	2.55	0.42
1:A:85:ASP:OD2	1:A:89:GLN:N	2.49	0.42
1:A:97:SER:OG	1:A:98:PRO:CD	2.68	0.42
1:B:134:LEU:HA	1:B:221:MET:HE1	2.02	0.42
1:D:43:ASN:HB2	1:D:276:VAL:HA	2.00	0.42
1:E:68:ASP:OD2	1:E:71:ILE:HG12	2.20	0.42
1:F:78:GLY:HA3	1:F:95:ALA:HA	2.01	0.42
1:J:205:TYR:CZ	1:J:207:VAL:HB	2.55	0.42
1:K:87:TYR:CD1	1:L:49:ASN:HB2	2.55	0.42
1:L:259:LYS:HG3	1:L:260:SER:N	2.34	0.42
1:L:49:ASN:C	1:L:49:ASN:ND2	2.69	0.42
1:A:179:GLU:OE1	1:A:179:GLU:N	2.50	0.42
1:A:205:TYR:CE2	1:L:209:LYS:HB3	2.54	0.42
1:C:11:SER:CB	1:C:12:ILE:HD12	2.50	0.42
1:F:71:ILE:O	1:F:72:SER:HB3	2.19	0.42
1:J:72:SER:OG	1:J:73:TYR:N	2.52	0.42
1:L:144:LEU:O	1:L:148:ILE:HG13	2.20	0.42
1:B:203:ALA:O	1:B:204:PRO:C	2.57	0.42
1:E:93:PHE:N	1:E:106:LEU:HD21	2.33	0.42
1:J:213:GLN:NE2	2:J:340:HOH:O	2.53	0.42
1:K:107:TYR:CD1	1:K:107:TYR:C	2.93	0.42
1:K:107:TYR:HD1	1:K:107:TYR:C	2.22	0.42
1:K:34:LEU:O	1:K:37:GLN:NE2	2.53	0.42
1:B:112:MET:HA	1:B:112:MET:HE2	2.02	0.42
1:B:179:GLU:HG2	1:L:13:ASN:CG	2.40	0.42
1:G:16:GLN:NE2	1:G:17:ARG:HA	2.34	0.42
1:G:183:PRO:O	1:G:185:ILE:HG13	2.19	0.42
1:I:249:GLN:HG2	1:J:222:MET:CE	2.50	0.42
1:I:269:ASN:ND2	1:I:276:VAL:HG13	2.33	0.42
1:L:284:ILE:HG23	1:L:284:ILE:O	2.20	0.42
1:A:144:LEU:O	1:A:148:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HE2	1:A:95:ALA:HB2	1.85	0.42
1:D:186:PHE:CE2	1:D:196:ILE:HD11	2.55	0.42
1:D:136:LEU:HD13	1:E:22:ARG:HG2	2.01	0.42
1:G:78:GLY:HA3	1:G:95:ALA:HA	2.01	0.42
1:H:73:TYR:OH	1:H:274:LEU:HD21	2.20	0.42
1:L:73:TYR:OH	1:L:272:TYR:HB3	2.19	0.42
1:A:277:LYS:NZ	1:A:278:VAL:H	2.18	0.42
1:H:283:ASP:C	1:H:285:VAL:N	2.73	0.42
1:J:162:ARG:NH1	1:J:162:ARG:HG2	2.33	0.42
1:L:107:TYR:HD2	1:L:117:MET:CE	2.32	0.42
1:L:113:LYS:HA	1:L:117:MET:HE1	2.01	0.42
1:L:170:SER:O	1:L:174:VAL:HG23	2.19	0.42
1:L:188:HIS:CD2	1:L:190:ALA:H	2.37	0.42
1:D:12:ILE:HG22	1:D:12:ILE:O	2.20	0.41
1:D:265:CYS:SG	1:D:276:VAL:O	2.78	0.41
1:F:65:PHE:CD1	1:F:268:ILE:HD12	2.55	0.41
1:I:249:GLN:NE2	2:I:338:HOH:O	2.50	0.41
1:I:84:ARG:HD3	1:I:84:ARG:HA	1.82	0.41
1:K:110:ARG:O	1:K:112:MET:N	2.46	0.41
1:L:58:HIS:HD2	1:L:130:THR:OG1	2.03	0.41
1:B:173:GLN:HE21	1:B:177:GLN:CG	2.33	0.41
1:E:124:ASN:HA	1:E:260:SER:HB2	2.01	0.41
1:E:93:PHE:CE1	1:E:95:ALA:HB2	2.55	0.41
1:G:43:ASN:O	1:G:276:VAL:HG12	2.20	0.41
1:H:104:PHE:CD2	1:H:118:GLY:HA3	2.55	0.41
1:H:165:ASP:CG	1:H:195:SER:HB3	2.41	0.41
1:J:113:LYS:O	1:J:114:GLU:CG	2.63	0.41
1:J:41:TRP:CE2	1:J:278:VAL:HG13	2.54	0.41
1:E:250:ILE:CD1	1:E:250:ILE:N	2.84	0.41
1:F:47:THR:HG23	1:F:73:TYR:HB2	2.01	0.41
1:G:160:LEU:HB2	2:H:327:HOH:O	2.21	0.41
1:G:28:LEU:HD21	1:G:32:GLN:OE1	2.20	0.41
1:H:109:TYR:HB3	1:H:110:ARG:H	1.71	0.41
1:H:192:ASP:HB2	1:H:194:ASP:OD2	2.20	0.41
1:H:227:ILE:HG22	1:H:228:LYS:N	2.35	0.41
1:H:67:LYS:HB2	1:H:272:TYR:CE1	2.55	0.41
1:H:283:ASP:C	1:H:285:VAL:H	2.23	0.41
1:H:62:TYR:C	1:H:62:TYR:CD2	2.93	0.41
1:I:130:THR:HG22	1:I:134:LEU:HG	2.02	0.41
1:H:248:GLU:HB3	1:I:227:ILE:CG2	2.51	0.41
1:K:113:LYS:HB3	1:K:114:GLU:H	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.34	0.41
1:D:109:TYR:N	1:D:109:TYR:CD2	2.86	0.41
1:F:105:LYS:O	1:F:117:MET:HG3	2.20	0.41
1:F:43:ASN:N	1:F:43:ASN:ND2	2.68	0.41
1:G:258:LEU:C	1:G:258:LEU:HD13	2.40	0.41
1:G:72:SER:OG	1:G:73:TYR:N	2.53	0.41
1:I:13:ASN:HA	1:I:13:ASN:HD22	1.56	0.41
1:J:224:PHE:HD2	1:J:225:LEU:CD1	2.33	0.41
1:K:227:ILE:HG22	1:K:228:LYS:N	2.35	0.41
1:A:189:GLU:HG2	2:A:342:HOH:O	2.21	0.41
1:E:261:ARG:CG	1:E:261:ARG:NH1	2.77	0.41
1:E:44:LEU:HD13	1:E:48:ILE:HG21	2.01	0.41
1:F:67:LYS:CB	1:F:272:TYR:CE2	3.04	0.41
1:H:222:MET:HE3	1:H:227:ILE:HG21	2.01	0.41
1:H:84:ARG:CB	1:H:84:ARG:NH1	2.83	0.41
1:H:90:ALA:O	1:H:108:ASN:OD1	2.38	0.41
1:A:112:MET:O	1:A:112:MET:SD	2.78	0.41
1:A:179:GLU:CD	1:A:179:GLU:N	2.71	0.41
1:C:78:GLY:HA3	1:C:95:ALA:HA	2.02	0.41
1:E:209:LYS:HB3	1:F:205:TYR:CZ	2.55	0.41
1:F:57:ILE:HG12	1:F:63:VAL:HG13	2.02	0.41
1:F:94:ARG:HB3	1:F:94:ARG:CZ	2.51	0.41
1:E:86:VAL:HG22	1:F:99:VAL:CG2	2.51	0.41
1:G:261:ARG:NH1	1:G:261:ARG:HG2	2.32	0.41
1:G:27:TYR:OH	1:G:214:LYS:NZ	2.44	0.41
1:I:106:LEU:CD2	1:I:120:VAL:HG23	2.49	0.41
1:I:51:SER:O	1:I:55:LYS:HG3	2.19	0.41
1:K:178:TYR:CZ	1:K:180:GLY:HA2	2.56	0.41
1:K:43:ASN:HB2	1:K:276:VAL:HA	2.03	0.41
1:B:119:VAL:HB	1:B:268:ILE:HD11	2.03	0.41
1:B:145:LYS:HD3	1:B:145:LYS:O	2.21	0.41
1:E:146:GLU:O	1:E:150:VAL:HG23	2.19	0.41
1:E:57:ILE:HG21	1:E:261:ARG:NH1	2.35	0.41
1:F:265:CYS:O	1:F:269:ASN:ND2	2.53	0.41
1:G:21:ASN:O	1:G:25:ILE:HG12	2.21	0.41
1:G:285:VAL:HG12	1:G:285:VAL:O	2.21	0.41
1:K:172:LYS:HA	1:K:172:LYS:HD2	1.81	0.41
1:K:205:TYR:CZ	1:K:207:VAL:HB	2.55	0.41
1:L:153:ASN:HD21	1:L:156:LYS:HZ2	1.69	0.41
1:L:41:TRP:CE2	1:L:278:VAL:HG13	2.56	0.41
1:E:31:LEU:HD23	1:E:31:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LEU:O	1:E:57:ILE:HG13	2.20	0.41
1:G:109:TYR:HB2	1:G:112:MET:HB2	2.02	0.41
1:E:111:ASP:O	1:E:112:MET:HB3	2.21	0.41
1:E:98:PRO:HB2	1:E:99:VAL:H	1.66	0.41
1:G:39:PHE:HZ	1:G:257:PHE:HB2	1.86	0.41
1:B:123:ASN:HD21	1:B:261:ARG:HH21	1.69	0.41
1:E:249:GLN:NE2	1:F:218:TRP:NE1	2.69	0.41
1:E:97:SER:HB3	1:E:98:PRO:HD3	2.02	0.41
1:F:85:ASP:OD2	1:F:89:GLN:HB3	2.21	0.41
1:H:168:GLN:HB2	1:H:169:LEU:H	1.66	0.41
1:H:178:TYR:CD1	1:H:184:VAL:HG22	2.56	0.41
1:K:200:LYS:HA	1:K:200:LYS:HD3	1.80	0.41
1:K:55:LYS:HE2	1:K:59:GLN:NE2	2.36	0.41
1:L:113:LYS:HG3	1:L:271:LEU:HD12	2.03	0.41
1:A:98:PRO:HB2	1:A:99:VAL:H	1.70	0.41
1:C:38:LEU:O	1:C:281:ARG:HB3	2.21	0.41
1:C:43:ASN:HD22	1:C:43:ASN:N	2.19	0.41
1:D:269:ASN:OD1	1:D:276:VAL:HG13	2.21	0.41
1:F:62:TYR:CZ	1:F:80:LEU:HG	2.56	0.41
1:G:181:ASN:HD22	1:G:181:ASN:C	2.25	0.41
1:G:54:GLU:OE2	1:G:261:ARG:NH1	2.52	0.41
1:H:31:LEU:HA	1:H:31:LEU:HD23	1.82	0.41
1:I:171:LEU:HD22	1:I:175:TYR:CE1	2.56	0.41
1:H:110:ARG:HB3	1:I:46:PRO:HB2	2.02	0.41
1:I:98:PRO:HG2	1:I:100:TYR:N	2.32	0.41
1:J:188:HIS:CD2	1:J:190:ALA:HB3	2.56	0.41
1:K:221:MET:CE	1:K:225:LEU:HD13	2.51	0.41
1:L:106:LEU:HD22	1:L:120:VAL:HG23	2.03	0.41
1:L:129:PRO:O	1:L:132:PRO:HD2	2.21	0.41
1:A:181:ASN:HD22	1:A:182:ALA:N	2.20	0.40
1:A:183:PRO:O	1:A:185:ILE:HG13	2.22	0.40
1:B:178:TYR:CE2	1:B:180:GLY:HA2	2.55	0.40
1:B:98:PRO:HG2	1:B:100:TYR:H	1.85	0.40
1:E:140:GLU:OE1	1:F:145:LYS:NZ	2.48	0.40
1:H:11:SER:C	1:H:13:ASN:N	2.74	0.40
1:H:71:ILE:O	1:H:72:SER:HB3	2.20	0.40
1:H:78:GLY:HA3	1:H:95:ALA:HA	2.04	0.40
1:H:203:ALA:HB1	1:I:158:PRO:HG3	2.03	0.40
1:I:41:TRP:CZ3	1:I:278:VAL:HG22	2.56	0.40
1:L:227:ILE:HG22	1:L:228:LYS:N	2.35	0.40
1:G:186:PHE:CE2	1:G:196:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:PRO:CD	1:H:102:LYS:HZ1	2.34	0.40
1:I:14:GLU:HA	1:I:14:GLU:OE1	2.21	0.40
1:J:109:TYR:HE1	1:J:267:LYS:HG2	1.86	0.40
1:J:115:GLU:O	1:J:116:ASP:CB	2.69	0.40
1:J:53:LEU:HD12	1:J:63:VAL:HG11	2.02	0.40
1:K:65:PHE:HB3	1:K:119:VAL:CG2	2.50	0.40
1:D:277:LYS:HB3	1:D:277:LYS:HE2	1.83	0.40
1:F:170:SER:HB3	1:F:173:GLN:HB2	2.04	0.40
1:G:162:ARG:NH1	1:H:193:SER:HA	2.36	0.40
1:G:167:ASN:HB2	1:H:189:GLU:OE2	2.21	0.40
1:D:37:GLN:O	1:D:37:GLN:HG2	2.22	0.40
1:F:172:LYS:HA	1:F:172:LYS:HD2	1.94	0.40
1:F:49:ASN:ND2	1:F:49:ASN:C	2.74	0.40
1:G:98:PRO:HA	2:G:312:HOH:O	2.22	0.40
1:I:101:GLN:HB3	1:I:101:GLN:HE21	1.58	0.40
1:J:109:TYR:HD2	1:K:46:PRO:O	2.03	0.40
1:K:72:SER:OG	1:K:73:TYR:N	2.53	0.40
1:K:78:GLY:HA3	1:K:95:ALA:HA	2.03	0.40
1:A:168:GLN:HB2	1:A:169:LEU:H	1.69	0.40
1:A:53:LEU:HD12	1:A:63:VAL:HG11	2.02	0.40
1:A:53:LEU:O	1:A:57:ILE:HG13	2.21	0.40
1:B:119:VAL:HA	2:B:357:HOH:O	2.20	0.40
1:C:31:LEU:HD21	1:C:221:MET:HG2	2.03	0.40
1:F:20:ARG:HH22	1:F:143:GLU:HG3	1.82	0.40
1:F:248:GLU:HG2	1:G:282:TYR:CD2	2.56	0.40
1:F:258:LEU:HD12	1:F:280:PHE:CZ	2.56	0.40
1:H:52:PHE:CZ	1:H:77:ASN:ND2	2.89	0.40
1:H:52:PHE:HZ	1:H:77:ASN:ND2	2.20	0.40

All (1) 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:K:189:GLU:OE1	1:K:189:GLU:OE1[2_556]	2.14	0.06

## 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	253/309 (82%)	234 (92%)	13 (5%)	6 (2%)	7	27
1	B	253/309 (82%)	235 (93%)	13 (5%)	5 (2%)	9	31
1	C	253/309 (82%)	237 (94%)	13 (5%)	3 (1%)	15	46
1	D	253/309 (82%)	242 (96%)	8 (3%)	3 (1%)	15	46
1	E	253/309 (82%)	236 (93%)	10 (4%)	7 (3%)	6	22
1	F	253/309 (82%)	235 (93%)	14 (6%)	4 (2%)	11	37
1	G	253/309 (82%)	241 (95%)	9 (4%)	3 (1%)	15	46
1	H	253/309 (82%)	233 (92%)	16 (6%)	4 (2%)	11	37
1	I	253/309 (82%)	236 (93%)	13 (5%)	4 (2%)	11	37
1	J	253/309 (82%)	236 (93%)	13 (5%)	4 (2%)	11	37
1	K	253/309 (82%)	235 (93%)	10 (4%)	8 (3%)	5	19
1	L	253/309 (82%)	238 (94%)	11 (4%)	4 (2%)	11	37
All	All	3036/3708 (82%)	2838 (94%)	143 (5%)	55 (2%)	10	34

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	B	97	SER
1	C	97	SER
1	D	97	SER
1	E	97	SER
1	E	284	ILE
1	F	97	SER
1	G	97	SER
1	H	97	SER
1	I	97	SER
1	I	98	PRO
1	I	284	ILE

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Mol	Chain	Res	Type
1	J	97	SER
1	J	111	ASP
1	K	97	SER
1	K	111	ASP
1	K	113	LYS
1	L	97	SER
1	A	98	PRO
1	B	98	PRO
1	B	110	ARG
1	C	98	PRO
1	D	98	PRO
1	E	98	PRO
1	E	109	TYR
1	E	111	ASP
1	F	98	PRO
1	F	108	ASN
1	G	98	PRO
1	H	98	PRO
1	J	98	PRO
1	K	98	PRO
1	K	108	ASN
1	L	98	PRO
1	L	284	ILE
1	A	111	ASP
1	A	113	LYS
1	A	284	ILE
1	H	114	GLU
1	B	112	MET
1	B	192	ASP
1	E	110	ARG
1	K	114	GLU
1	L	192	ASP
1	A	125	ASP
1	C	125	ASP
1	D	125	ASP
1	F	192	ASP
1	G	110	ARG
1	H	108	ASN
1	I	192	ASP
1	J	192	ASP
1	K	12	ILE
1	E	125	ASP

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Mol	Chain	Res	Type
1	K	125	ASP

### 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	228/277 (82%)	206 (90%)	22 (10%)	10	29
1	B	228/277 (82%)	211 (92%)	17 (8%)	16	42
1	C	228/277 (82%)	207 (91%)	21 (9%)	11	32
1	D	228/277 (82%)	216 (95%)	12 (5%)	26	60
1	E	228/277 (82%)	208 (91%)	20 (9%)	12	34
1	F	228/277 (82%)	209 (92%)	19 (8%)	13	36
1	G	228/277 (82%)	213 (93%)	15 (7%)	19	49
1	H	228/277 (82%)	213 (93%)	15 (7%)	19	49
1	I	228/277 (82%)	206 (90%)	22 (10%)	10	29
1	J	228/277 (82%)	211 (92%)	17 (8%)	16	42
1	K	228/277 (82%)	211 (92%)	17 (8%)	16	42
1	L	228/277 (82%)	211 (92%)	17 (8%)	16	42
All	All	2736/3324 (82%)	2522 (92%)	214 (8%)	15	39

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	ASN
1	A	28	LEU
1	A	38	LEU
1	A	44	LEU
1	A	49	ASN
1	A	110	ARG
1	A	112	MET
1	A	160	LEU

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	167	ASN
1	A	169	LEU
1	A	171	LEU
1	A	172	LYS
1	A	173	GLN
1	A	179	GLU
1	A	181	ASN
1	A	225	LEU
1	A	228	LYS
1	A	258	LEU
1	A	271	LEU
1	A	278	VAL
1	B	18	GLN
1	B	28	LEU
1	B	47	THR
1	B	49	ASN
1	B	88	ASN
1	B	109	TYR
1	B	110	ARG
1	B	123	ASN
1	B	124	ASN
1	B	131	THR
1	B	162	ARG
1	B	165	ASP
1	B	181	ASN
1	B	213	GLN
1	B	247	ASP
1	B	270	GLU
1	B	278	VAL
1	C	13	ASN
1	C	20	ARG
1	C	28	LEU
1	C	37	GLN
1	C	48	ILE
1	C	49	ASN
1	C	88	ASN
1	C	111	ASP
1	C	162	ARG
1	C	165	ASP
1	C	167	ASN
1	C	168	GLN

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Mol	Chain	Res	Type
1	C	169	LEU
1	C	171	LEU
1	C	173	GLN
1	C	228	LYS
1	C	258	LEU
1	C	259	LYS
1	C	260	SER
1	C	265	CYS
1	C	278	VAL
1	D	16	GLN
1	D	28	LEU
1	D	34	LEU
1	D	37	GLN
1	D	86	VAL
1	D	97	SER
1	D	160	LEU
1	D	167	ASN
1	D	173	GLN
1	D	181	ASN
1	D	225	LEU
1	D	278	VAL
1	E	14	GLU
1	E	20	ARG
1	E	37	GLN
1	E	38	LEU
1	E	83	GLN
1	E	101	GLN
1	E	109	TYR
1	E	111	ASP
1	E	115	GLU
1	E	126	MET
1	E	128	PHE
1	E	149	SER
1	E	160	LEU
1	E	162	ARG
1	E	169	LEU
1	E	171	LEU
1	E	194	ASP
1	E	258	LEU
1	E	266	GLU
1	E	270	GLU
1	F	21	ASN

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Mol	Chain	Res	Type
1	F	22	ARG
1	F	37	GLN
1	F	49	ASN
1	F	88	ASN
1	F	115	GLU
1	F	160	LEU
1	F	164	ASN
1	F	166	ASN
1	F	169	LEU
1	F	177	GLN
1	F	179	GLU
1	F	221	MET
1	F	258	LEU
1	F	259	LYS
1	F	261	ARG
1	F	275	ASN
1	F	278	VAL
1	F	281	ARG
1	G	16	GLN
1	G	22	ARG
1	G	37	GLN
1	G	42	GLU
1	G	49	ASN
1	G	88	ASN
1	G	112	MET
1	G	145	LYS
1	G	160	LEU
1	G	169	LEU
1	G	181	ASN
1	G	200	LYS
1	G	261	ARG
1	G	271	LEU
1	G	278	VAL
1	H	28	LEU
1	H	37	GLN
1	H	53	LEU
1	H	81	SER
1	H	84	ARG
1	H	101	GLN
1	H	110	ARG
1	H	112	MET
1	H	160	LEU

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Mol	Chain	Res	Type
1	H	169	LEU
1	H	171	LEU
1	H	225	LEU
1	H	258	LEU
1	H	260	SER
1	H	284	ILE
1	I	13	ASN
1	I	19	LYS
1	I	20	ARG
1	I	22	ARG
1	I	28	LEU
1	I	49	ASN
1	I	83	GLN
1	I	86	VAL
1	I	97	SER
1	I	101	GLN
1	I	153	ASN
1	I	160	LEU
1	I	167	ASN
1	I	171	LEU
1	I	179	GLU
1	I	225	LEU
1	I	258	LEU
1	I	271	LEU
1	I	274	LEU
1	I	277	LYS
1	I	278	VAL
1	I	281	ARG
1	J	12	ILE
1	J	28	LEU
1	J	37	GLN
1	J	38	LEU
1	J	46	PRO
1	J	49	ASN
1	J	83	GLN
1	J	149	SER
1	J	172	LYS
1	J	177	GLN
1	J	225	LEU
1	J	228	LYS
1	J	249	GLN
1	J	258	LEU

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Mol	Chain	Res	Type
1	J	261	ARG
1	J	266	GLU
1	J	278	VAL
1	K	28	LEU
1	K	37	GLN
1	K	47	THR
1	K	86	VAL
1	K	89	GLN
1	K	107	TYR
1	K	114	GLU
1	K	149	SER
1	K	160	LEU
1	K	166	ASN
1	K	167	ASN
1	K	169	LEU
1	K	258	LEU
1	K	261	ARG
1	K	270	GLU
1	K	274	LEU
1	K	278	VAL
1	L	14	GLU
1	L	28	LEU
1	L	37	GLN
1	L	47	THR
1	L	49	ASN
1	L	85	ASP
1	L	91	THR
1	L	101	GLN
1	L	160	LEU
1	L	171	LEU
1	L	177	GLN
1	L	181	ASN
1	L	258	LEU
1	L	260	SER
1	L	261	ARG
1	L	276	VAL
1	L	278	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN

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Mol	Chain	Res	Type
1	A	18	GLN
1	A	32	GLN
1	A	43	ASN
1	A	49	ASN
1	A	101	GLN
1	A	152	GLN
1	A	166	ASN
1	A	167	ASN
1	A	168	GLN
1	A	177	GLN
1	A	181	ASN
1	A	213	GLN
1	A	215	ASN
1	A	249	GLN
1	A	269	ASN
1	B	13	ASN
1	B	32	GLN
1	B	43	ASN
1	B	49	ASN
1	B	59	GLN
1	B	101	GLN
1	B	108	ASN
1	B	123	ASN
1	B	124	ASN
1	B	152	GLN
1	B	168	GLN
1	B	173	GLN
1	B	181	ASN
1	B	213	GLN
1	C	37	GLN
1	C	43	ASN
1	C	49	ASN
1	C	59	GLN
1	C	83	GLN
1	C	152	GLN
1	C	167	ASN
1	C	168	GLN
1	C	213	GLN
1	C	219	ASN
1	C	269	ASN
1	D	16	GLN
1	D	29	ASN

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Mol	Chain	Res	Type
1	D	37	GLN
1	D	59	GLN
1	D	88	ASN
1	D	89	GLN
1	D	101	GLN
1	D	168	GLN
1	D	177	GLN
1	D	181	ASN
1	D	213	GLN
1	D	275	ASN
1	E	29	ASN
1	E	37	GLN
1	E	43	ASN
1	E	59	GLN
1	E	83	GLN
1	E	89	GLN
1	E	152	GLN
1	E	269	ASN
1	E	275	ASN
1	F	13	ASN
1	F	29	ASN
1	F	37	GLN
1	F	43	ASN
1	F	49	ASN
1	F	59	GLN
1	F	88	ASN
1	F	101	GLN
1	F	108	ASN
1	F	176	ASN
1	F	188	HIS
1	F	213	GLN
1	F	275	ASN
1	G	29	ASN
1	G	37	GLN
1	G	49	ASN
1	G	59	GLN
1	G	88	ASN
1	G	152	GLN
1	G	168	GLN
1	G	177	GLN
1	G	181	ASN
1	G	188	HIS

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Mol	Chain	Res	Type
1	H	13	ASN
1	H	29	ASN
1	H	32	GLN
1	H	83	GLN
1	H	101	GLN
1	H	108	ASN
1	H	152	GLN
1	H	167	ASN
1	H	176	ASN
1	H	177	GLN
1	H	188	HIS
1	H	213	GLN
1	H	269	ASN
1	I	13	ASN
1	I	18	GLN
1	I	32	GLN
1	I	49	ASN
1	I	89	GLN
1	I	101	GLN
1	I	108	ASN
1	I	152	GLN
1	I	167	ASN
1	I	168	GLN
1	I	173	GLN
1	I	181	ASN
1	I	188	HIS
1	I	213	GLN
1	I	215	ASN
1	I	269	ASN
1	I	275	ASN
1	J	13	ASN
1	J	16	GLN
1	J	32	GLN
1	J	37	GLN
1	J	49	ASN
1	J	89	GLN
1	J	101	GLN
1	J	108	ASN
1	J	152	GLN
1	J	153	ASN
1	J	166	ASN
1	J	167	ASN

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Mol	Chain	Res	Type
1	J	177	GLN
1	J	188	HIS
1	J	213	GLN
1	J	215	ASN
1	J	249	GLN
1	J	269	ASN
1	J	275	ASN
1	K	18	GLN
1	K	21	ASN
1	K	32	GLN
1	K	37	GLN
1	K	59	GLN
1	K	88	ASN
1	K	101	GLN
1	K	108	ASN
1	K	152	GLN
1	K	177	GLN
1	K	213	GLN
1	K	215	ASN
1	K	275	ASN
1	L	32	GLN
1	L	37	GLN
1	L	49	ASN
1	L	58	HIS
1	L	59	GLN
1	L	89	GLN
1	L	101	GLN
1	L	152	GLN
1	L	168	GLN
1	L	176	ASN
1	L	181	ASN
1	L	188	HIS
1	L	213	GLN
1	L	269	ASN
1	L	275	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 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	257/309 (83%)	-0.25	5 (1%) 67 64	21, 42, 78, 92	0
1	B	257/309 (83%)	0.05	16 (6%) 21 16	22, 56, 97, 122	0
1	C	257/309 (83%)	-0.07	11 (4%) 36 31	24, 51, 84, 103	0
1	D	257/309 (83%)	-0.16	6 (2%) 61 57	22, 51, 99, 129	0
1	E	257/309 (83%)	0.44	35 (13%) 3 2	22, 68, 106, 115	0
1	F	257/309 (83%)	0.06	15 (5%) 24 19	24, 59, 99, 108	0
1	G	257/309 (83%)	-0.16	7 (2%) 55 50	23, 50, 86, 120	0
1	H	257/309 (83%)	-0.03	6 (2%) 61 57	24, 51, 90, 103	0
1	I	257/309 (83%)	-0.17	7 (2%) 55 50	21, 45, 85, 125	0
1	J	257/309 (83%)	-0.26	6 (2%) 61 57	21, 42, 82, 92	0
1	K	257/309 (83%)	0.07	10 (3%) 40 35	22, 52, 96, 112	0
1	L	257/309 (83%)	-0.18	9 (3%) 44 38	17, 44, 81, 125	0
All	All	3084/3708 (83%)	-0.05	133 (4%) 36 31	17, 50, 95, 129	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	285	VAL	10.8
1	D	11	SER	8.8
1	A	285	VAL	7.9
1	G	11	SER	6.9
1	K	11	SER	6.5
1	B	11	SER	6.1
1	L	11	SER	6.0
1	A	11	SER	5.5
1	I	11	SER	5.3
1	L	12	ILE	5.3
1	B	13	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	H	11	SER	4.9
1	J	11	SER	4.7
1	E	11	SER	4.7
1	E	81	SER	4.5
1	G	12	ILE	4.4
1	E	109	TYR	4.3
1	L	13	ASN	4.2
1	K	13	ASN	4.2
1	F	97	SER	4.2
1	C	11	SER	4.0
1	B	17	ARG	4.0
1	L	99	VAL	3.9
1	B	247	ASP	3.8
1	E	96	ALA	3.7
1	G	247	ASP	3.7
1	E	80	LEU	3.7
1	G	13	ASN	3.6
1	H	99	VAL	3.6
1	E	72	SER	3.5
1	E	120	VAL	3.4
1	E	118	GLY	3.3
1	F	99	VAL	3.3
1	B	18	GLN	3.3
1	B	12	ILE	3.3
1	E	97	SER	3.3
1	E	73	TYR	3.3
1	C	97	SER	3.2
1	E	90	ALA	3.2
1	B	95	ALA	3.2
1	J	97	SER	3.1
1	E	276	VAL	3.1
1	D	16	GLN	3.1
1	A	169	LEU	3.0
1	E	74	ILE	3.0
1	L	169	LEU	3.0
1	E	112	MET	3.0
1	B	284	ILE	3.0
1	E	117	MET	2.9
1	H	90	ALA	2.9
1	L	247	ASP	2.9
1	B	110	ARG	2.9
1	J	112	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	12	ILE	2.9
1	I	13	ASN	2.9
1	B	112	MET	2.9
1	E	71	ILE	2.9
1	E	108	ASN	2.9
1	F	98	PRO	2.8
1	K	109	TYR	2.8
1	B	14	GLU	2.8
1	C	285	VAL	2.7
1	E	83	GLN	2.7
1	H	97	SER	2.7
1	H	285	VAL	2.7
1	F	11	SER	2.7
1	D	13	ASN	2.7
1	I	12	ILE	2.7
1	K	285	VAL	2.6
1	D	83	GLN	2.6
1	C	169	LEU	2.5
1	F	96	ALA	2.5
1	E	84	ARG	2.5
1	C	167	ASN	2.5
1	J	13	ASN	2.5
1	G	285	VAL	2.4
1	C	96	ALA	2.4
1	B	109	TYR	2.4
1	I	97	SER	2.4
1	K	12	ILE	2.4
1	F	53	LEU	2.4
1	F	277	LYS	2.4
1	I	86	VAL	2.4
1	E	70	VAL	2.4
1	G	167	ASN	2.4
1	F	12	ILE	2.3
1	F	276	VAL	2.3
1	C	71	ILE	2.3
1	B	16	GLN	2.3
1	C	69	PRO	2.3
1	K	119	VAL	2.3
1	E	284	ILE	2.3
1	F	113	LYS	2.3
1	A	12	ILE	2.3
1	E	82	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	107	TYR	2.3
1	D	14	GLU	2.2
1	E	66	TYR	2.2
1	E	13	ASN	2.2
1	K	105	LYS	2.2
1	E	92	VAL	2.2
1	J	285	VAL	2.2
1	I	167	ASN	2.2
1	F	114	GLU	2.2
1	D	12	ILE	2.2
1	F	75	ALA	2.2
1	K	284	ILE	2.2
1	E	64	GLY	2.1
1	E	100	TYR	2.2
1	F	283	ASP	2.1
1	E	88	ASN	2.1
1	B	102	LYS	2.1
1	C	99	VAL	2.1
1	E	99	VAL	2.1
1	A	112	MET	2.1
1	B	285	VAL	2.1
1	G	99	VAL	2.1
1	K	108	ASN	2.1
1	I	285	VAL	2.1
1	H	110	ARG	2.1
1	B	83	GLN	2.1
1	C	12	ILE	2.1
1	E	247	ASP	2.1
1	L	285	VAL	2.1
1	L	16	GLN	2.0
1	F	284	ILE	2.0
1	C	86	VAL	2.0
1	J	99	VAL	2.0
1	E	168	GLN	2.0
1	L	284	ILE	2.0
1	E	122	TYR	2.0
1	K	65	PHE	2.0
1	E	167	ASN	2.0

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

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.