



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:46 pm BST

PDB ID : 5CDI  
Title : Chloroplast chaperonin 60b1 of Chlamydomonas  
Authors : Zhang, S.; Zhou, H.; Yu, F.; Gao, F.; He, J.; Liu, C.  
Deposited on : 2015-07-04  
Resolution : 3.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

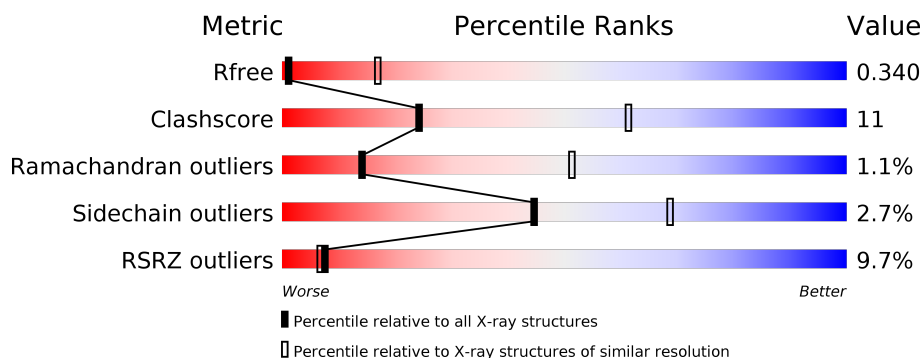
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	552	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• •</div> </div> </div>
1	B	552	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	552	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	D	552	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	E	552	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>• •</div> </div> </div>
1	F	552	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	552	<div><div>9%</div><div><div></div><div>74%</div><div>21%</div><div></div></div><div></div></div>
1	H	552	<div><div>9%</div><div><div></div><div>75%</div><div>20%</div><div></div></div><div></div></div>
1	I	552	<div><div>11%</div><div><div></div><div>74%</div><div>21%</div><div></div></div><div></div></div>
1	J	552	<div><div>10%</div><div><div></div><div>74%</div><div>21%</div><div></div></div><div></div></div>
1	K	552	<div><div>12%</div><div><div></div><div>76%</div><div>19%</div><div></div></div><div></div></div>
1	L	552	<div><div>14%</div><div><div></div><div>75%</div><div>20%</div><div></div></div><div></div></div>
1	M	552	<div><div>14%</div><div><div></div><div>75%</div><div>20%</div><div></div></div><div></div></div>
1	N	552	<div><div>11%</div><div><div></div><div>78%</div><div>17%</div><div></div></div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 55706 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 Chaperonin 60B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	N	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	B	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	C	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	D	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	E	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	F	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	G	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	H	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	I	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	J	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	K	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	L	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			
1	M	528	Total	C	N	O	S	0	0	0
			3979	2471	696	788	24			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A8JE91

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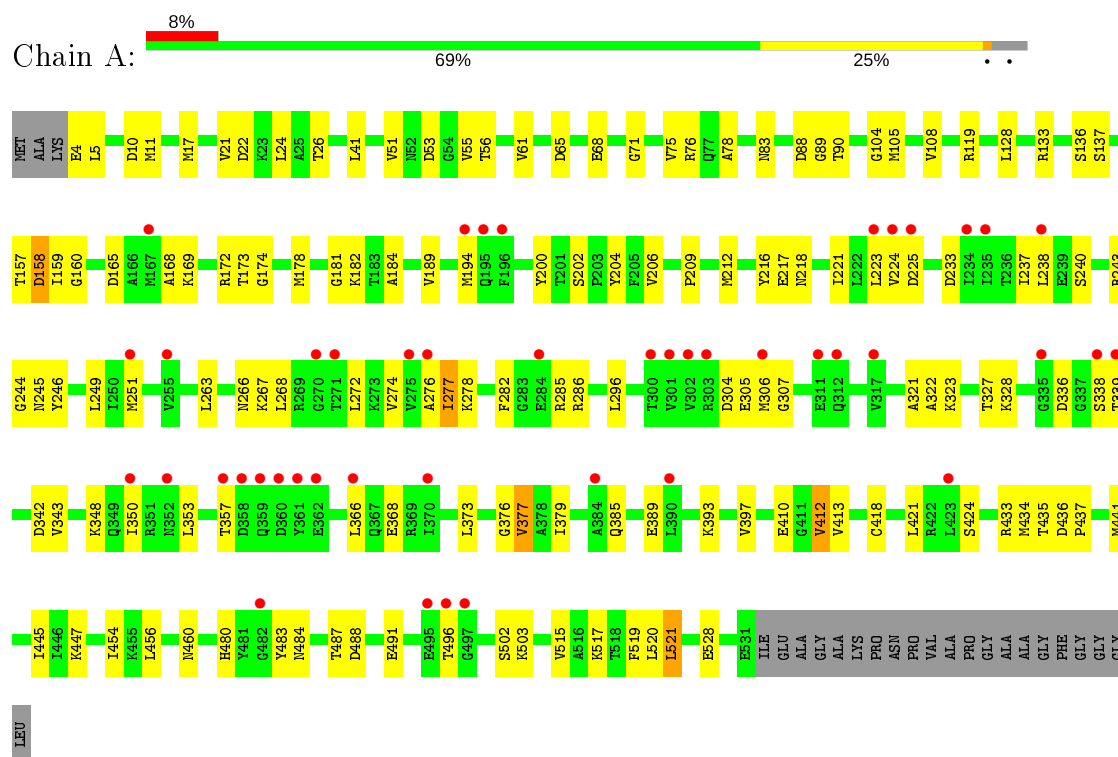
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Chain	Residue	Modelled	Actual	Comment	Reference
A	138	VAL	-	see sequence details	UNP A8JE91
N	1	MET	-	expression tag	UNP A8JE91
N	138	VAL	-	see sequence details	UNP A8JE91
B	1	MET	-	expression tag	UNP A8JE91
B	138	VAL	-	see sequence details	UNP A8JE91
C	1	MET	-	expression tag	UNP A8JE91
C	138	VAL	-	see sequence details	UNP A8JE91
D	1	MET	-	expression tag	UNP A8JE91
D	138	VAL	-	see sequence details	UNP A8JE91
E	1	MET	-	expression tag	UNP A8JE91
E	138	VAL	-	see sequence details	UNP A8JE91
F	1	MET	-	expression tag	UNP A8JE91
F	138	VAL	-	see sequence details	UNP A8JE91
G	1	MET	-	expression tag	UNP A8JE91
G	138	VAL	-	see sequence details	UNP A8JE91
H	1	MET	-	expression tag	UNP A8JE91
H	138	VAL	-	see sequence details	UNP A8JE91
I	1	MET	-	expression tag	UNP A8JE91
I	138	VAL	-	see sequence details	UNP A8JE91
J	1	MET	-	expression tag	UNP A8JE91
J	138	VAL	-	see sequence details	UNP A8JE91
K	1	MET	-	expression tag	UNP A8JE91
K	138	VAL	-	see sequence details	UNP A8JE91
L	1	MET	-	expression tag	UNP A8JE91
L	138	VAL	-	see sequence details	UNP A8JE91
M	1	MET	-	expression tag	UNP A8JE91
M	138	VAL	-	see sequence details	UNP A8JE91

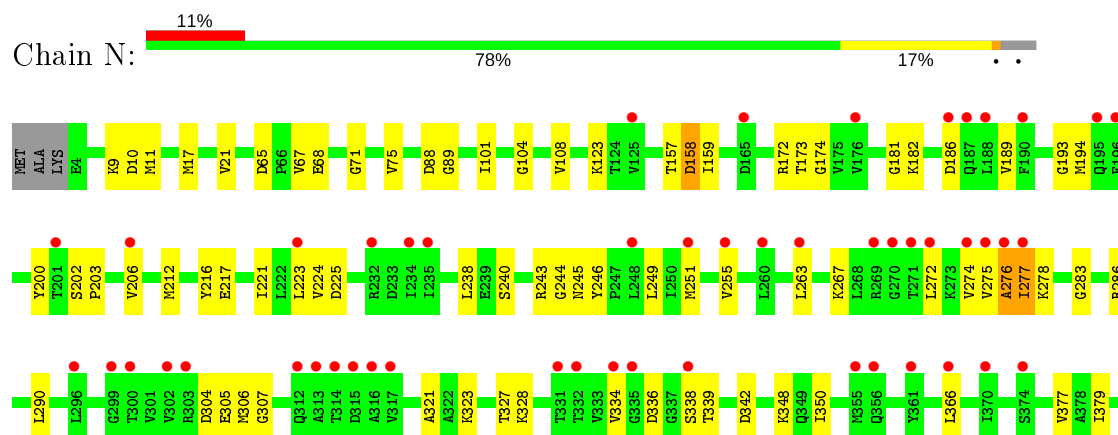
### 3 Residue-property plots [i](#)

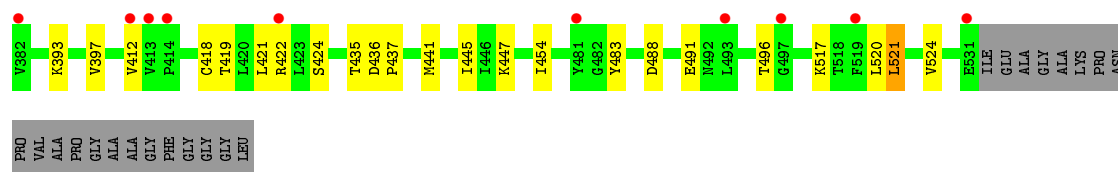
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Chaperonin 60B1

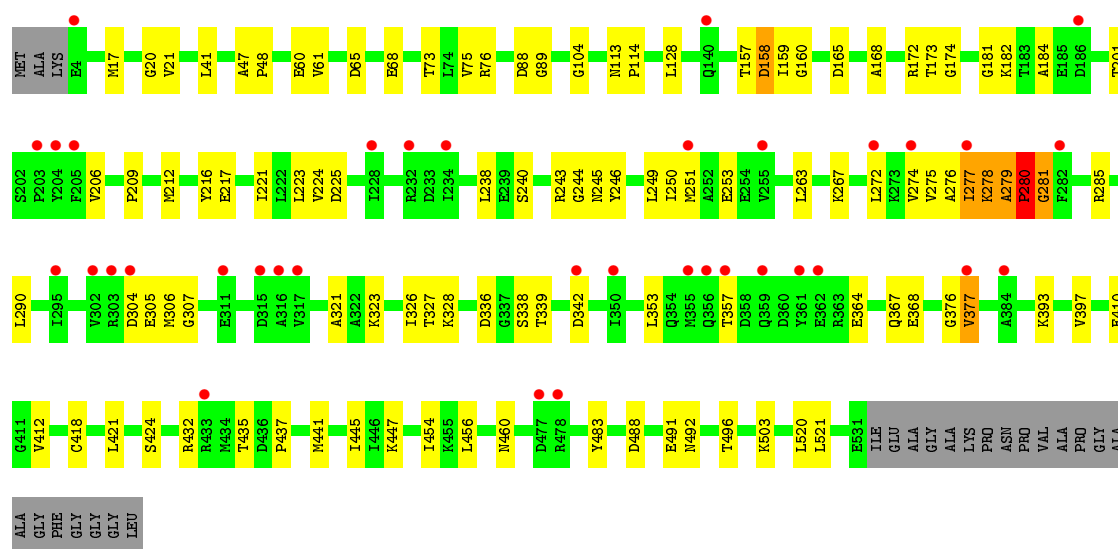
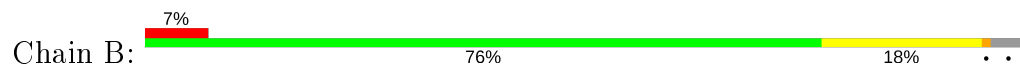


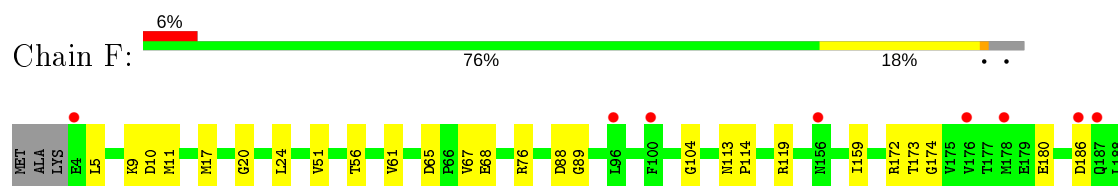
#### • Molecule 1: Chaperonin 60B1



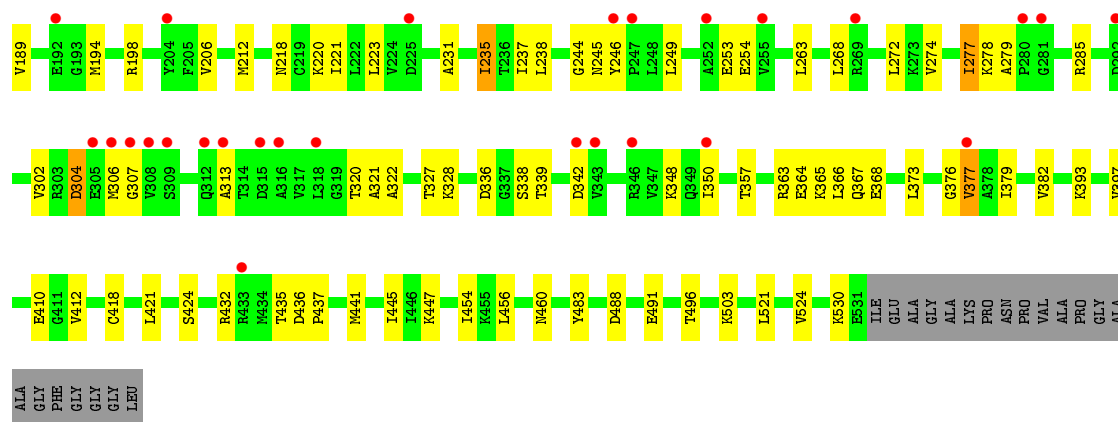


• Molecule 1: Chaperonin 60B1

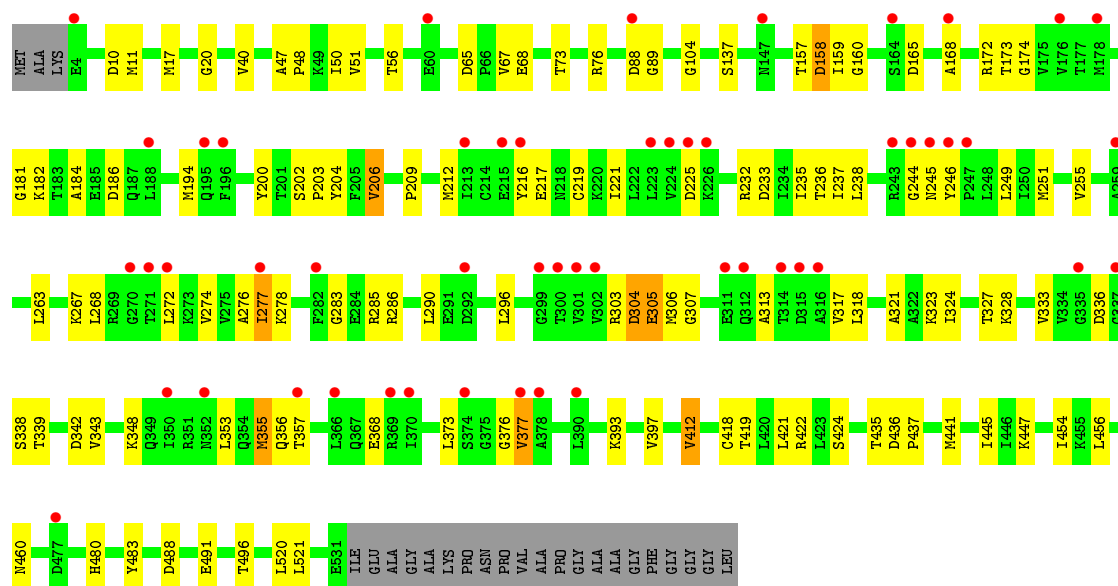
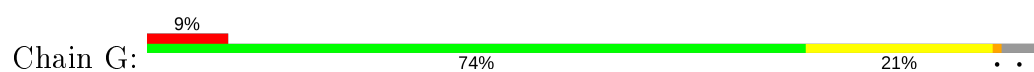




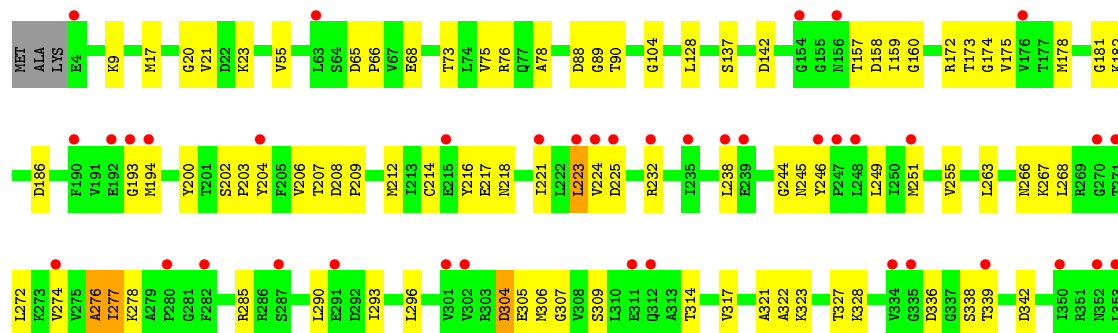
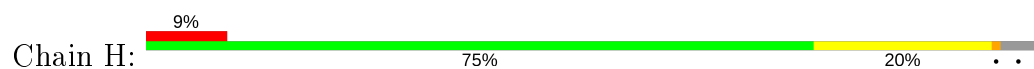


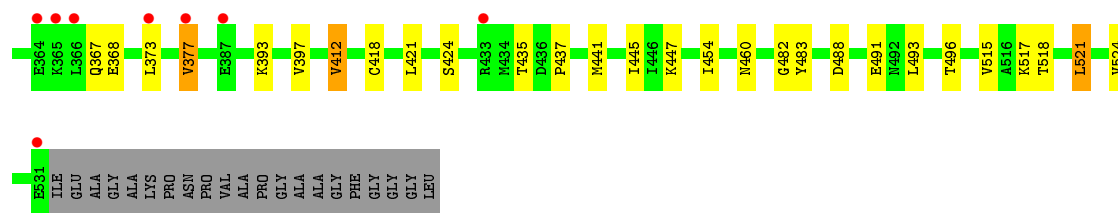


• Molecule 1: Chaperonin 60B1

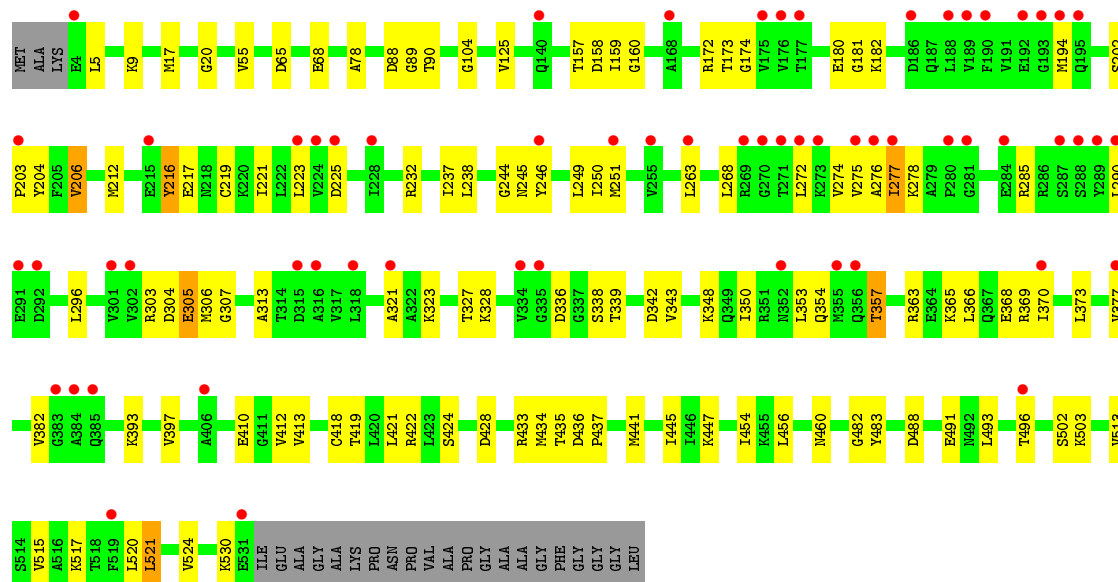
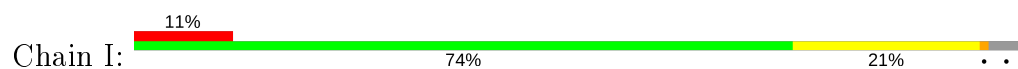


• Molecule 1: Chaperonin 60B1

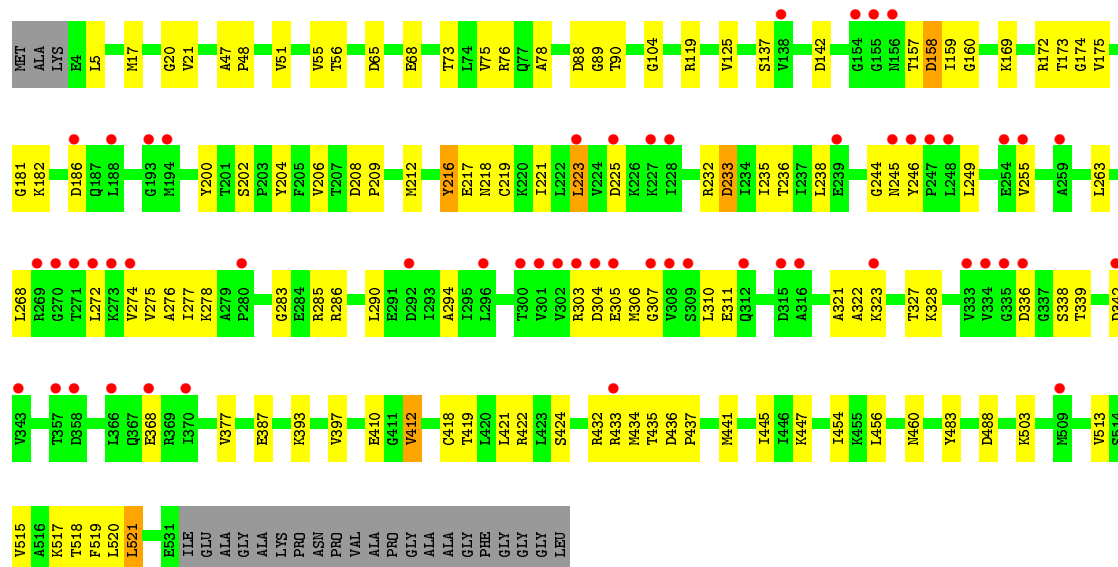
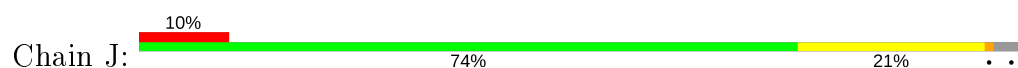




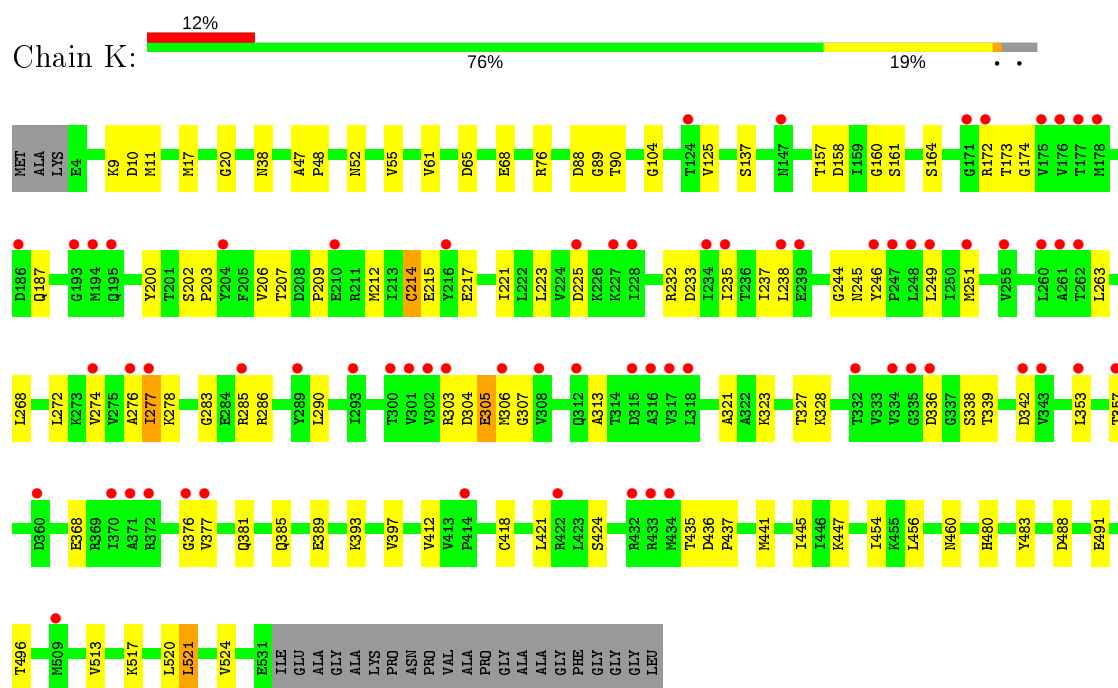
• Molecule 1: Chaperonin 60B1



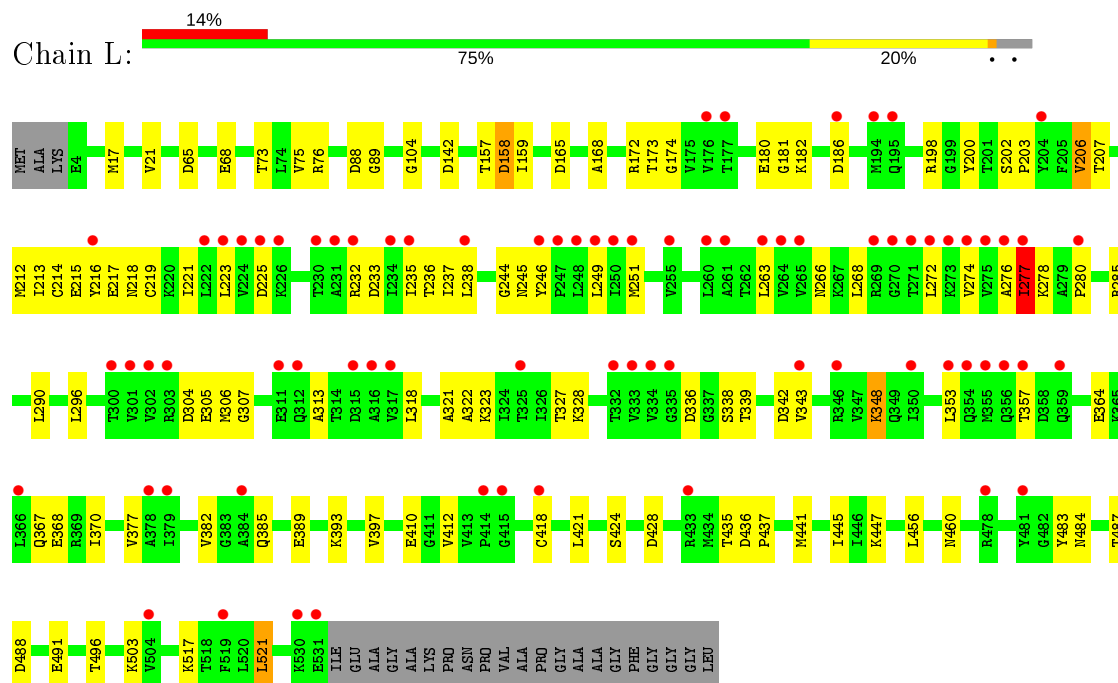
• Molecule 1: Chaperonin 60B1



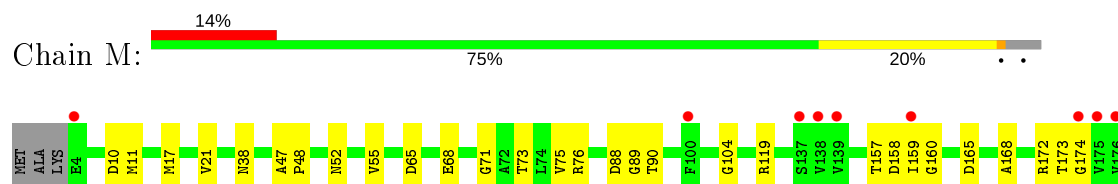
• Molecule 1: Chaperonin 60B1

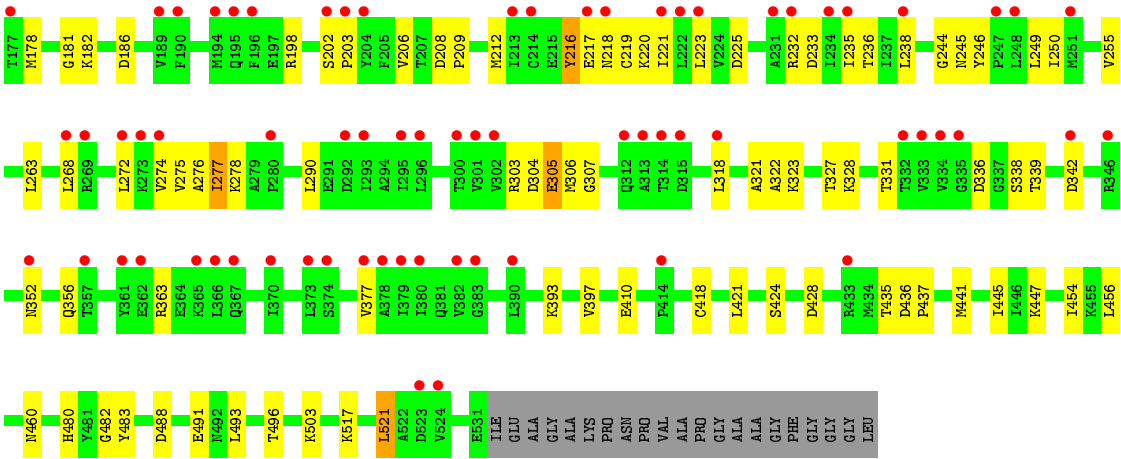


• Molecule 1: Chaperonin 60B1



• Molecule 1: Chaperonin 60B1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.34Å 174.39Å 213.68Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	48.66 – 3.81 48.66 – 3.81	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.66-3.81) 85.1 (48.66-3.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.275 , 0.325 0.296 , 0.340	Depositor DCC
$R_{free}$ test set	2003 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	129.8	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 114.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	55706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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	0.21	0/4011	0.40	0/5417
1	B	0.25	1/4011 (0.0%)	0.43	1/5417 (0.0%)
1	C	0.25	0/4011	0.44	3/5417 (0.1%)
1	D	0.23	0/4011	0.41	0/5417
1	E	0.32	3/4011 (0.1%)	0.49	4/5417 (0.1%)
1	F	0.23	0/4011	0.41	0/5417
1	G	0.25	1/4011 (0.0%)	0.40	0/5417
1	H	0.23	0/4011	0.43	2/5417 (0.0%)
1	I	0.22	0/4011	0.41	0/5417
1	J	0.24	0/4011	0.40	0/5417
1	K	0.21	0/4011	0.43	1/5417 (0.0%)
1	L	0.22	0/4011	0.41	0/5417
1	M	0.24	0/4011	0.40	0/5417
1	N	0.24	1/4011 (0.0%)	0.41	0/5417
All	All	0.24	6/56154 (0.0%)	0.42	11/75838 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	E	0	1
1	L	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	377	VAL	C-N	10.25	1.57	1.34
1	N	276	ALA	C-N	-5.80	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	206	VAL	C-N	-5.68	1.21	1.34
1	E	209	PRO	N-CD	5.45	1.55	1.47
1	B	280	PRO	N-CD	5.40	1.55	1.47
1	E	203	PRO	N-CD	5.32	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ALA	O-C-N	-7.55	110.61	122.70
1	H	276	ALA	O-C-N	-6.88	111.69	122.70
1	B	277	ILE	N-CA-C	6.17	127.65	111.00
1	C	277	ILE	O-C-N	-5.72	113.55	122.70
1	K	376	GLY	O-C-N	-5.68	113.61	122.70
1	E	202	SER	C-N-CD	5.51	139.97	128.40
1	E	208	ASP	C-N-CD	5.51	139.97	128.40
1	C	276	ALA	C-N-CA	5.45	135.32	121.70
1	E	376	GLY	O-C-N	-5.32	114.18	122.70
1	E	377	VAL	O-C-N	-5.22	114.35	122.70
1	H	276	ALA	C-N-CA	5.13	134.53	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	279	ALA	Peptide
1	C	277	ILE	Mainchain
1	E	202	SER	Peptide
1	L	277	ILE	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3979	0	4104	88	0
1	B	3979	0	4104	88	0
1	C	3979	0	4103	82	0
1	D	3979	0	4104	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3979	0	4104	212	0
1	F	3979	0	4104	87	0
1	G	3979	0	4103	82	0
1	H	3979	0	4103	75	0
1	I	3979	0	4104	71	0
1	J	3979	0	4104	81	0
1	K	3979	0	4104	71	0
1	L	3979	0	4104	71	0
1	M	3979	0	4103	69	0
1	N	3979	0	4103	75	0
All	All	55706	0	57451	1242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1242) 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:E:205:PHE:CE2	1:E:267:LYS:CB	1.85	1.55
1:E:205:PHE:CE2	1:E:267:LYS:HB3	0.97	1.47
1:E:59:ARG:HH22	1:E:212:MET:CE	1.27	1.46
1:E:251:MET:HA	1:E:277:ILE:CG2	1.46	1.46
1:E:277:ILE:HD12	1:E:278:LYS:N	1.27	1.43
1:F:277:ILE:HD12	1:F:278:LYS:N	1.33	1.41
1:E:205:PHE:HZ	1:E:267:LYS:C	1.25	1.36
1:E:205:PHE:CZ	1:E:267:LYS:C	2.03	1.30
1:L:276:ALA:O	1:L:277:ILE:HG23	1.31	1.24
1:N:193:GLY:HA3	1:N:377:VAL:CG2	1.67	1.24
1:I:250:ILE:O	1:I:277:ILE:HD12	1.07	1.23
1:I:250:ILE:O	1:I:277:ILE:CD1	1.86	1.20
1:N:193:GLY:CA	1:N:377:VAL:HG23	1.71	1.20
1:E:201:THR:O	1:E:203:PRO:N	1.71	1.19
1:E:59:ARG:NH2	1:E:212:MET:HE1	1.56	1.19
1:N:193:GLY:C	1:N:377:VAL:CG2	2.11	1.18
1:E:205:PHE:CG	1:E:267:LYS:HE3	1.77	1.18
1:E:267:LYS:NZ	1:E:273:LYS:HG3	1.59	1.18
1:N:193:GLY:CA	1:N:377:VAL:CG2	2.22	1.17
1:E:205:PHE:CD2	1:E:267:LYS:HB3	1.80	1.16
1:N:276:ALA:O	1:N:277:ILE:HG23	1.40	1.16
1:B:251:MET:HB3	1:B:277:ILE:HG13	1.17	1.16
1:E:200:TYR:CE1	1:E:328:LYS:HE3	1.81	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:ARG:NH2	1:E:212:MET:CE	2.08	1.15
1:K:276:ALA:O	1:K:277:ILE:HG23	1.42	1.15
1:G:251:MET:CB	1:G:277:ILE:HD11	1.74	1.14
1:N:193:GLY:C	1:N:377:VAL:HG23	1.66	1.14
1:E:205:PHE:CZ	1:E:267:LYS:CB	2.31	1.14
1:E:251:MET:HG3	1:E:277:ILE:HG21	1.21	1.13
1:G:276:ALA:O	1:G:277:ILE:HG23	1.47	1.13
1:C:276:ALA:O	1:C:277:ILE:HG23	1.45	1.12
1:E:251:MET:CA	1:E:277:ILE:CG2	2.28	1.12
1:L:276:ALA:O	1:L:277:ILE:CG2	1.98	1.11
1:H:276:ALA:O	1:H:277:ILE:HG23	1.47	1.11
1:E:277:ILE:CD1	1:E:278:LYS:H	1.63	1.10
1:D:200:TYR:HA	1:D:277:ILE:HG12	1.11	1.09
1:F:277:ILE:HD11	1:F:278:LYS:O	1.52	1.09
1:D:334:VAL:HG23	1:D:377:VAL:HG11	1.10	1.09
1:E:205:PHE:CZ	1:E:267:LYS:HG2	1.88	1.08
1:F:277:ILE:CD1	1:F:278:LYS:O	2.03	1.06
1:E:205:PHE:CE1	1:E:267:LYS:HG2	1.90	1.05
1:E:205:PHE:CD1	1:E:267:LYS:HE3	1.92	1.05
1:K:200:TYR:HA	1:K:277:ILE:HG22	1.38	1.04
1:A:276:ALA:O	1:A:277:ILE:HG23	1.57	1.04
1:A:251:MET:CB	1:A:277:ILE:HD11	1.87	1.03
1:E:205:PHE:CZ	1:E:268:LEU:N	2.25	1.03
1:E:251:MET:CG	1:E:277:ILE:HG21	1.88	1.03
1:N:276:ALA:O	1:N:277:ILE:CG2	2.06	1.03
1:L:251:MET:HB3	1:L:277:ILE:HD11	1.41	1.02
1:E:205:PHE:CZ	1:E:267:LYS:HB3	1.90	1.02
1:G:251:MET:HB3	1:G:277:ILE:CD1	1.89	1.02
1:C:251:MET:CB	1:C:277:ILE:HD11	1.88	1.02
1:L:251:MET:CB	1:L:277:ILE:HD11	1.90	1.02
1:E:251:MET:CA	1:E:277:ILE:HG23	1.88	1.01
1:F:253:GLU:C	1:F:278:LYS:NZ	2.13	1.01
1:N:193:GLY:HA3	1:N:377:VAL:HG21	1.39	1.01
1:E:251:MET:HG3	1:E:277:ILE:CG2	1.91	1.01
1:E:251:MET:HA	1:E:277:ILE:HG23	1.04	1.00
1:E:301:VAL:HB	1:E:302:VAL:HA	1.42	1.00
1:K:251:MET:CB	1:K:277:ILE:HD11	1.91	1.00
1:E:277:ILE:CD1	1:E:278:LYS:N	2.20	1.00
1:E:267:LYS:HD2	1:E:274:VAL:H	1.26	1.00
1:G:251:MET:HB3	1:G:277:ILE:HD11	1.39	1.00
1:A:200:TYR:HA	1:A:277:ILE:HG22	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:PHE:CZ	1:E:267:LYS:CG	2.46	0.99
1:D:334:VAL:HG23	1:D:377:VAL:CG1	1.92	0.99
1:A:251:MET:HB3	1:A:277:ILE:HD11	1.42	0.99
1:G:251:MET:CB	1:G:277:ILE:CD1	2.40	0.99
1:K:276:ALA:O	1:K:277:ILE:CG2	2.11	0.98
1:H:200:TYR:HA	1:H:277:ILE:HG22	1.46	0.98
1:D:277:ILE:HD12	1:D:278:LYS:H	1.28	0.97
1:F:277:ILE:CD1	1:F:278:LYS:N	2.28	0.96
1:D:200:TYR:CA	1:D:277:ILE:HG12	1.95	0.96
1:G:276:ALA:O	1:G:277:ILE:CG2	2.12	0.96
1:D:334:VAL:HG21	1:D:377:VAL:HG21	1.42	0.96
1:D:334:VAL:CG2	1:D:377:VAL:HG21	1.95	0.96
1:E:201:THR:O	1:E:203:PRO:CD	2.13	0.96
1:E:267:LYS:HD2	1:E:274:VAL:N	1.81	0.95
1:N:251:MET:CB	1:N:277:ILE:HD11	1.96	0.95
1:K:251:MET:HB3	1:K:277:ILE:HD11	1.46	0.95
1:H:251:MET:HB3	1:H:277:ILE:HD11	1.46	0.95
1:B:253:GLU:O	1:B:278:LYS:NZ	1.99	0.94
1:C:276:ALA:O	1:C:277:ILE:CG2	2.15	0.94
1:E:251:MET:HA	1:E:277:ILE:HG22	1.49	0.94
1:N:200:TYR:HA	1:N:277:ILE:HG22	1.50	0.94
1:E:205:PHE:CD1	1:E:267:LYS:CE	2.51	0.93
1:C:251:MET:HB3	1:C:277:ILE:HD11	1.48	0.93
1:H:276:ALA:O	1:H:277:ILE:CG2	2.16	0.93
1:D:200:TYR:HA	1:D:277:ILE:CG1	1.99	0.93
1:G:200:TYR:HA	1:G:277:ILE:HG22	1.49	0.92
1:E:209:PRO:HA	1:E:212:MET:H	1.34	0.92
1:L:200:TYR:HA	1:L:277:ILE:HG22	1.52	0.92
1:F:253:GLU:O	1:F:278:LYS:CE	2.18	0.92
1:I:206:VAL:HG21	1:I:212:MET:HA	1.51	0.92
1:C:200:TYR:HA	1:C:277:ILE:HG22	1.50	0.91
1:E:200:TYR:CE2	1:E:202:SER:O	2.24	0.91
1:H:251:MET:CB	1:H:277:ILE:HD11	1.99	0.91
1:N:251:MET:HB3	1:N:277:ILE:HD11	1.52	0.90
1:F:277:ILE:HD12	1:F:278:LYS:H	1.09	0.89
1:E:267:LYS:HZ1	1:E:273:LYS:HG3	1.34	0.89
1:E:211:ARG:HH11	1:E:211:ARG:HG2	1.35	0.89
1:E:267:LYS:HZ3	1:E:273:LYS:HG3	1.32	0.89
1:E:59:ARG:HH22	1:E:212:MET:HE1	0.73	0.88
1:J:276:ALA:C	1:J:277:ILE:HD12	1.94	0.88
1:H:207:THR:OG1	1:H:214:CYS:HA	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:TYR:CE1	1:E:328:LYS:CE	2.57	0.87
1:D:334:VAL:CG2	1:D:377:VAL:HG11	1.99	0.87
1:F:253:GLU:C	1:F:278:LYS:HZ2	1.77	0.86
1:N:193:GLY:CA	1:N:377:VAL:HG21	1.97	0.86
1:E:205:PHE:HZ	1:E:267:LYS:O	1.59	0.86
1:E:205:PHE:CG	1:E:267:LYS:CE	2.58	0.85
1:E:205:PHE:CE2	1:E:267:LYS:CG	2.57	0.85
1:A:276:ALA:O	1:A:277:ILE:CG2	2.24	0.85
1:G:251:MET:HB3	1:G:277:ILE:CG1	2.06	0.84
1:E:205:PHE:CB	1:E:267:LYS:HE3	2.05	0.84
1:B:278:LYS:HA	1:B:278:LYS:CE	2.06	0.84
1:B:251:MET:HB3	1:B:277:ILE:CG1	2.03	0.84
1:E:205:PHE:HZ	1:E:268:LEU:N	1.67	0.83
1:C:251:MET:HB2	1:C:277:ILE:HD11	1.59	0.83
1:L:207:THR:OG1	1:L:214:CYS:HA	1.78	0.83
1:B:250:ILE:O	1:B:277:ILE:HG12	1.78	0.83
1:A:251:MET:HB3	1:A:277:ILE:CD1	2.08	0.82
1:M:275:VAL:HG12	1:M:277:ILE:HD11	1.59	0.82
1:G:251:MET:HB2	1:G:277:ILE:CD1	2.09	0.81
1:E:251:MET:CB	1:E:277:ILE:HG21	2.09	0.81
1:E:251:MET:CG	1:E:277:ILE:CG2	2.55	0.81
1:E:205:PHE:HE2	1:E:267:LYS:HB3	1.00	0.81
1:K:200:TYR:CA	1:K:277:ILE:HG22	2.11	0.81
1:B:274:VAL:O	1:B:275:VAL:CG2	2.28	0.81
1:B:280:PRO:O	1:B:281:GLY:O	1.97	0.81
1:F:253:GLU:O	1:F:278:LYS:NZ	2.14	0.81
1:E:205:PHE:CE2	1:E:267:LYS:CA	2.64	0.80
1:G:251:MET:SD	1:G:277:ILE:HD11	2.21	0.80
1:K:251:MET:HB3	1:K:277:ILE:CD1	2.11	0.79
1:J:200:TYR:HA	1:J:277:ILE:HG13	1.63	0.79
1:L:251:MET:HB3	1:L:277:ILE:CD1	2.13	0.79
1:E:205:PHE:HB3	1:E:267:LYS:HE3	1.64	0.78
1:E:205:PHE:CZ	1:E:267:LYS:CA	2.65	0.78
1:E:200:TYR:HE1	1:E:328:LYS:HE3	1.49	0.78
1:D:334:VAL:HG21	1:D:377:VAL:CG2	2.14	0.78
1:G:251:MET:HB2	1:G:277:ILE:HD11	1.60	0.78
1:A:251:MET:CB	1:A:277:ILE:CD1	2.60	0.77
1:A:251:MET:HB2	1:A:277:ILE:HD11	1.66	0.77
1:E:201:THR:O	1:E:203:PRO:HD3	1.83	0.77
1:E:205:PHE:CE2	1:E:268:LEU:N	2.53	0.76
1:E:249:LEU:HD22	1:E:324:ILE:HD13	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:251:MET:HB3	1:H:277:ILE:CD1	2.15	0.76
1:F:278:LYS:HA	1:F:278:LYS:HE3	1.67	0.76
1:B:253:GLU:H	1:B:279:ALA:HB2	1.49	0.76
1:K:251:MET:CB	1:K:277:ILE:CD1	2.63	0.75
1:E:251:MET:CB	1:E:277:ILE:CG2	2.63	0.75
1:C:251:MET:CB	1:C:277:ILE:CD1	2.65	0.75
1:E:219:CYS:SG	1:E:220:LYS:N	2.60	0.75
1:E:295:ILE:HD12	1:E:346:ARG:HH11	1.51	0.75
1:E:205:PHE:CD1	1:E:267:LYS:NZ	2.55	0.75
1:E:202:SER:OG	1:E:204:TYR:HB2	1.86	0.74
1:N:251:MET:HB3	1:N:277:ILE:CD1	2.17	0.74
1:L:251:MET:HB2	1:L:277:ILE:HD11	1.69	0.74
1:L:276:ALA:C	1:L:277:ILE:HG23	2.08	0.74
1:C:251:MET:HB3	1:C:277:ILE:CD1	2.18	0.74
1:B:251:MET:CB	1:B:277:ILE:HG13	2.09	0.74
1:D:390:LEU:HA	1:D:393:LYS:HB2	1.69	0.74
1:E:209:PRO:HB2	1:E:210:GLU:HA	1.69	0.73
1:E:205:PHE:CE2	1:E:267:LYS:C	2.62	0.73
1:L:251:MET:CB	1:L:277:ILE:CD1	2.66	0.73
1:E:201:THR:O	1:E:202:SER:C	2.26	0.73
1:I:206:VAL:CG2	1:I:212:MET:HA	2.18	0.73
1:D:193:GLY:HA3	1:D:377:VAL:CG1	2.18	0.73
1:J:275:VAL:HG12	1:J:277:ILE:CD1	2.18	0.72
1:D:277:ILE:CD1	1:D:278:LYS:H	2.01	0.72
1:E:211:ARG:HG2	1:E:211:ARG:NH1	2.03	0.72
1:J:274:VAL:O	1:J:275:VAL:CG2	2.38	0.72
1:J:274:VAL:O	1:J:275:VAL:HG23	1.90	0.72
1:E:244:GLY:O	1:E:245:ASN:ND2	2.22	0.71
1:K:251:MET:HB2	1:K:277:ILE:HD11	1.70	0.71
1:N:251:MET:HB2	1:N:277:ILE:HD11	1.72	0.71
1:M:277:ILE:HD12	1:M:277:ILE:N	2.05	0.71
1:N:251:MET:CB	1:N:277:ILE:CD1	2.68	0.71
1:E:200:TYR:HE2	1:E:202:SER:O	1.72	0.71
1:E:199:GLY:O	1:E:277:ILE:HD13	1.91	0.71
1:I:276:ALA:C	1:I:277:ILE:HG13	2.10	0.71
1:M:250:ILE:O	1:M:277:ILE:CD1	2.38	0.71
1:E:209:PRO:HB3	1:E:212:MET:HB3	1.73	0.71
1:K:206:VAL:HG11	1:K:212:MET:HB2	1.73	0.71
1:E:249:LEU:HG	1:E:275:VAL:HB	1.70	0.70
1:E:250:ILE:O	1:E:277:ILE:HG22	1.91	0.70
1:F:277:ILE:CD1	1:F:278:LYS:H	1.97	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:GLU:O	1:F:278:LYS:HE3	1.92	0.70
1:G:251:MET:HB3	1:G:277:ILE:HG13	1.71	0.70
1:C:17:MET:HA	1:C:68:GLU:HA	1.73	0.70
1:F:254:GLU:HA	1:F:278:LYS:HZ2	1.56	0.69
1:E:209:PRO:HA	1:E:212:MET:N	2.06	0.69
1:E:59:ARG:NH2	1:E:212:MET:HE3	2.03	0.69
1:L:277:ILE:HD12	1:L:278:LYS:N	2.07	0.69
1:J:276:ALA:O	1:J:277:ILE:HD12	1.93	0.69
1:E:296:LEU:HD12	1:E:297:THR:HG23	1.73	0.69
1:E:203:PRO:HG2	1:E:205:PHE:O	1.92	0.69
1:E:282:PHE:O	1:E:286:ARG:N	2.19	0.68
1:E:209:PRO:HB2	1:E:210:GLU:CA	2.23	0.68
1:B:253:GLU:HA	1:B:279:ALA:HB3	1.76	0.68
1:F:253:GLU:C	1:F:278:LYS:HZ1	1.97	0.68
1:B:278:LYS:HA	1:B:278:LYS:HE2	1.75	0.67
1:M:250:ILE:O	1:M:277:ILE:HD13	1.94	0.67
1:F:254:GLU:CA	1:F:278:LYS:HZ2	2.06	0.67
1:F:277:ILE:HD12	1:F:278:LYS:CA	2.21	0.67
1:B:274:VAL:O	1:B:275:VAL:HG23	1.95	0.67
1:D:334:VAL:CG2	1:D:377:VAL:CG2	2.71	0.67
1:E:200:TYR:HE1	1:E:328:LYS:CE	2.04	0.67
1:N:334:VAL:HG23	1:N:377:VAL:HB	1.77	0.66
1:B:274:VAL:O	1:B:275:VAL:HG22	1.95	0.66
1:F:456:LEU:O	1:F:460:ASN:ND2	2.23	0.66
1:N:194:MET:N	1:N:377:VAL:CG2	2.59	0.66
1:G:276:ALA:C	1:G:277:ILE:HG23	2.15	0.66
1:D:277:ILE:CD1	1:D:278:LYS:HG2	2.26	0.65
1:I:353:LEU:O	1:I:357:THR:OG1	2.14	0.65
1:N:193:GLY:C	1:N:377:VAL:HG21	2.10	0.65
1:N:17:MET:HA	1:N:68:GLU:HA	1.76	0.65
1:A:17:MET:HA	1:A:68:GLU:HA	1.77	0.65
1:E:207:THR:CB	1:E:214:CYS:HA	2.27	0.65
1:D:17:MET:HA	1:D:68:GLU:HA	1.78	0.65
1:M:17:MET:HA	1:M:68:GLU:HA	1.77	0.65
1:N:193:GLY:O	1:N:377:VAL:HG23	1.95	0.65
1:E:277:ILE:HD12	1:E:278:LYS:H	0.73	0.64
1:E:321:ALA:HA	1:E:336:ASP:HB3	1.78	0.64
1:B:278:LYS:HA	1:B:278:LYS:NZ	2.12	0.64
1:F:253:GLU:C	1:F:278:LYS:CE	2.64	0.64
1:E:220:LYS:HG3	1:E:318:LEU:HD23	1.80	0.64
1:E:456:LEU:O	1:E:460:ASN:ND2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:MET:HB3	1:I:277:ILE:HD13	1.80	0.63
1:I:277:ILE:HG22	1:I:278:LYS:H	1.64	0.63
1:A:276:ALA:C	1:A:277:ILE:HG23	2.19	0.63
1:H:137:SER:HB3	1:H:412:VAL:HG12	1.78	0.63
1:A:251:MET:HB2	1:A:277:ILE:CD1	2.26	0.63
1:C:251:MET:HB2	1:C:277:ILE:CD1	2.25	0.63
1:I:418:CYS:HA	1:I:421:LEU:HD13	1.81	0.63
1:D:456:LEU:O	1:D:460:ASN:ND2	2.25	0.63
1:B:327:THR:OG1	1:B:328:LYS:N	2.32	0.63
1:G:137:SER:HB3	1:G:412:VAL:HG12	1.81	0.63
1:K:200:TYR:HA	1:K:277:ILE:CG2	2.24	0.62
1:E:267:LYS:HG3	1:E:273:LYS:HA	1.81	0.62
1:H:327:THR:OG1	1:H:328:LYS:N	2.31	0.62
1:D:277:ILE:HD12	1:D:278:LYS:N	2.10	0.62
1:F:483:TYR:OH	1:F:488:ASP:OD1	2.17	0.62
1:F:277:ILE:C	1:F:277:ILE:HD12	2.15	0.62
1:B:17:MET:HA	1:B:68:GLU:HA	1.82	0.62
1:F:17:MET:HA	1:F:68:GLU:HA	1.82	0.62
1:G:17:MET:HA	1:G:68:GLU:HA	1.82	0.62
1:D:245:ASN:ND2	1:E:233:ASP:OD2	2.32	0.61
1:G:327:THR:OG1	1:G:328:LYS:N	2.33	0.61
1:M:276:ALA:O	1:M:277:ILE:HG13	2.00	0.61
1:I:206:VAL:HG21	1:I:212:MET:CA	2.26	0.61
1:M:276:ALA:C	1:M:277:ILE:HD12	2.21	0.61
1:E:231:ALA:HB2	1:E:259:ALA:HA	1.83	0.61
1:C:277:ILE:HD12	1:C:278:LYS:N	2.15	0.61
1:E:201:THR:O	1:E:203:PRO:CA	2.49	0.61
1:J:17:MET:HA	1:J:68:GLU:HA	1.82	0.61
1:B:253:GLU:O	1:B:278:LYS:CE	2.48	0.61
1:D:157:THR:O	1:D:159:ILE:N	2.34	0.61
1:D:206:VAL:HG11	1:D:212:MET:HB2	1.83	0.61
1:E:216:TYR:HD2	1:E:247:PRO:HG2	1.65	0.61
1:L:483:TYR:OH	1:L:488:ASP:OD1	2.17	0.61
1:F:254:GLU:N	1:F:278:LYS:HZ2	1.98	0.60
1:F:254:GLU:N	1:F:278:LYS:NZ	2.49	0.60
1:B:418:CYS:HA	1:B:421:LEU:HD13	1.82	0.60
1:D:193:GLY:HA3	1:D:377:VAL:HG11	1.83	0.60
1:H:17:MET:HA	1:H:68:GLU:HA	1.82	0.60
1:B:253:GLU:H	1:B:279:ALA:CB	2.12	0.60
1:D:418:CYS:HA	1:D:421:LEU:HD13	1.83	0.60
1:K:277:ILE:HD12	1:K:278:LYS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:221:ILE:HA	1:L:249:LEU:HB2	1.84	0.60
1:L:353:LEU:O	1:L:357:THR:OG1	2.11	0.60
1:A:327:THR:OG1	1:A:328:LYS:N	2.33	0.60
1:C:327:THR:OG1	1:C:328:LYS:N	2.33	0.60
1:D:327:THR:OG1	1:D:328:LYS:N	2.32	0.60
1:K:277:ILE:HD12	1:K:278:LYS:N	2.17	0.60
1:B:483:TYR:OH	1:B:488:ASP:OD1	2.19	0.59
1:H:251:MET:CB	1:H:277:ILE:CD1	2.74	0.59
1:N:251:MET:HB2	1:N:277:ILE:CD1	2.32	0.59
1:D:339:THR:HG22	1:D:342:ASP:H	1.67	0.59
1:E:267:LYS:CD	1:E:274:VAL:H	2.10	0.59
1:A:200:TYR:CA	1:A:277:ILE:HG22	2.28	0.59
1:F:253:GLU:HG2	1:F:278:LYS:HZ1	1.67	0.59
1:J:321:ALA:HA	1:J:336:ASP:HB3	1.84	0.59
1:A:456:LEU:O	1:A:460:ASN:ND2	2.27	0.59
1:K:251:MET:HB2	1:K:277:ILE:CD1	2.29	0.59
1:E:267:LYS:NZ	1:E:273:LYS:CG	2.51	0.58
1:K:483:TYR:OH	1:K:488:ASP:OD1	2.20	0.58
1:L:157:THR:O	1:L:159:ILE:N	2.35	0.58
1:N:157:THR:O	1:N:159:ILE:N	2.35	0.58
1:A:206:VAL:HG11	1:A:212:MET:HB2	1.86	0.58
1:G:483:TYR:OH	1:G:488:ASP:OD1	2.21	0.58
1:F:206:VAL:HG11	1:F:212:MET:HB2	1.86	0.58
1:K:65:ASP:HB3	1:K:68:GLU:HG2	1.85	0.58
1:M:321:ALA:HA	1:M:336:ASP:HB3	1.84	0.58
1:M:327:THR:OG1	1:M:328:LYS:N	2.36	0.58
1:J:327:THR:OG1	1:J:328:LYS:N	2.36	0.58
1:A:277:ILE:HD12	1:A:278:LYS:O	2.04	0.58
1:K:321:ALA:HA	1:K:336:ASP:HB3	1.86	0.58
1:F:321:ALA:HA	1:F:336:ASP:HB3	1.84	0.58
1:K:327:THR:OG1	1:K:328:LYS:N	2.35	0.58
1:K:17:MET:HA	1:K:68:GLU:HA	1.85	0.58
1:E:205:PHE:CE2	1:E:264:VAL:O	2.57	0.58
1:N:321:ALA:HA	1:N:336:ASP:HB3	1.86	0.58
1:A:483:TYR:OH	1:A:488:ASP:OD1	2.20	0.58
1:K:418:CYS:HA	1:K:421:LEU:HD13	1.86	0.58
1:L:327:THR:OG1	1:L:328:LYS:N	2.31	0.58
1:D:385:GLN:HB2	1:D:389:GLU:HG2	1.86	0.58
1:E:218:ASN:N	1:E:322:ALA:O	2.37	0.58
1:L:321:ALA:HA	1:L:336:ASP:HB3	1.86	0.58
1:I:17:MET:HA	1:I:68:GLU:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:251:MET:HB2	1:L:277:ILE:CD1	2.33	0.57
1:F:253:GLU:HA	1:F:278:LYS:HE3	1.86	0.57
1:G:221:ILE:HA	1:G:249:LEU:HB2	1.86	0.57
1:C:456:LEU:O	1:C:460:ASN:ND2	2.26	0.57
1:G:237:ILE:HG12	1:G:313:ALA:HB3	1.86	0.57
1:I:20:GLY:HA3	1:I:68:GLU:HB2	1.85	0.57
1:K:20:GLY:HA3	1:K:68:GLU:HB2	1.87	0.57
1:L:277:ILE:HD12	1:L:278:LYS:O	2.05	0.57
1:B:274:VAL:C	1:B:275:VAL:HG23	2.23	0.57
1:E:231:ALA:O	1:E:233:ASP:N	2.38	0.57
1:C:9:LYS:HG2	1:C:524:VAL:HG22	1.86	0.57
1:H:277:ILE:HD12	1:H:278:LYS:N	2.20	0.57
1:N:483:TYR:OH	1:N:488:ASP:OD1	2.19	0.57
1:E:207:THR:HB	1:E:214:CYS:HA	1.87	0.57
1:I:327:THR:OG1	1:I:328:LYS:N	2.37	0.57
1:J:275:VAL:HG12	1:J:276:ALA:N	2.18	0.57
1:E:205:PHE:CE1	1:E:267:LYS:CG	2.77	0.57
1:M:38:ASN:OD1	1:M:52:ASN:ND2	2.38	0.57
1:N:418:CYS:HA	1:N:421:LEU:HD13	1.86	0.57
1:D:238:LEU:HD12	1:D:272:LEU:HD22	1.86	0.57
1:G:313:ALA:HB1	1:G:317:VAL:HG21	1.86	0.57
1:I:354:GLN:O	1:I:363:ARG:NH1	2.38	0.57
1:B:157:THR:O	1:B:159:ILE:N	2.37	0.57
1:F:327:THR:OG1	1:F:328:LYS:N	2.37	0.57
1:M:250:ILE:O	1:M:277:ILE:HD12	2.05	0.57
1:D:421:LEU:HD11	1:D:454:ILE:HG21	1.87	0.56
1:E:17:MET:HA	1:E:68:GLU:HA	1.86	0.56
1:A:137:SER:HB3	1:A:412:VAL:HG12	1.86	0.56
1:M:206:VAL:HG11	1:M:212:MET:HB2	1.86	0.56
1:A:282:PHE:HA	1:A:286:ARG:HE	1.70	0.56
1:F:253:GLU:O	1:F:278:LYS:CD	2.54	0.56
1:F:278:LYS:HA	1:F:278:LYS:CE	2.31	0.56
1:G:251:MET:CG	1:G:277:ILE:HD11	2.34	0.56
1:B:253:GLU:C	1:B:278:LYS:HZ1	2.05	0.56
1:B:277:ILE:HG22	1:B:326:ILE:HD13	1.87	0.56
1:C:206:VAL:HG11	1:C:212:MET:HB2	1.87	0.56
1:M:418:CYS:HA	1:M:421:LEU:HD13	1.87	0.56
1:L:277:ILE:HD12	1:L:278:LYS:H	1.69	0.56
1:A:251:MET:HB3	1:A:277:ILE:CG1	2.36	0.56
1:E:247:PRO:HG3	1:E:273:LYS:HB3	1.87	0.56
1:D:387:GLU:HA	1:E:282:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ARG:O	1:E:290:LEU:HB2	2.06	0.56
1:G:339:THR:HG22	1:G:342:ASP:H	1.70	0.56
1:N:221:ILE:HA	1:N:249:LEU:HB2	1.88	0.56
1:I:221:ILE:HA	1:I:249:LEU:HB2	1.87	0.55
1:I:65:ASP:HB3	1:I:68:GLU:HG2	1.88	0.55
1:A:321:ALA:HA	1:A:336:ASP:HB3	1.87	0.55
1:B:321:ALA:HA	1:B:336:ASP:HB3	1.87	0.55
1:D:321:ALA:HA	1:D:336:ASP:HB3	1.88	0.55
1:G:491:GLU:HB3	1:G:496:THR:HG21	1.88	0.55
1:I:491:GLU:HB3	1:I:496:THR:HG21	1.87	0.55
1:C:277:ILE:HD12	1:C:278:LYS:O	2.06	0.55
1:D:221:ILE:HA	1:D:249:LEU:HB2	1.88	0.55
1:H:491:GLU:HB3	1:H:496:THR:HG21	1.88	0.55
1:M:221:ILE:HA	1:M:249:LEU:HB2	1.87	0.55
1:A:216:TYR:OH	1:A:267:LYS:NZ	2.37	0.55
1:C:418:CYS:HA	1:C:421:LEU:HD13	1.88	0.55
1:B:216:TYR:OH	1:B:267:LYS:NZ	2.35	0.55
1:D:277:ILE:CD1	1:D:278:LYS:N	2.68	0.55
1:K:276:ALA:C	1:K:277:ILE:HG23	2.22	0.55
1:N:277:ILE:HD12	1:N:278:LYS:N	2.21	0.55
1:A:424:SER:HB2	1:A:447:LYS:HD2	1.88	0.55
1:D:216:TYR:OH	1:D:267:LYS:NZ	2.37	0.55
1:G:88:ASP:OD1	1:G:89:GLY:N	2.39	0.55
1:L:157:THR:OG1	1:L:158:ASP:N	2.39	0.55
1:L:17:MET:HA	1:L:68:GLU:HA	1.88	0.55
1:L:65:ASP:HB3	1:L:68:GLU:HG2	1.89	0.55
1:B:244:GLY:O	1:B:246:TYR:N	2.40	0.55
1:E:418:CYS:HA	1:E:421:LEU:HD13	1.89	0.55
1:G:216:TYR:OH	1:G:267:LYS:NZ	2.40	0.55
1:G:353:LEU:O	1:G:357:THR:OG1	2.19	0.55
1:H:277:ILE:HD12	1:H:278:LYS:O	2.07	0.55
1:A:244:GLY:O	1:A:246:TYR:N	2.40	0.55
1:H:263:LEU:HG	1:H:274:VAL:HG21	1.89	0.55
1:N:157:THR:OG1	1:N:158:ASP:N	2.39	0.55
1:N:339:THR:HG22	1:N:342:ASP:H	1.71	0.55
1:I:157:THR:O	1:I:160:GLY:N	2.39	0.54
1:K:55:VAL:HG22	1:K:90:THR:HG21	1.89	0.54
1:N:244:GLY:O	1:N:246:TYR:N	2.40	0.54
1:B:277:ILE:O	1:B:277:ILE:HG13	2.06	0.54
1:H:321:ALA:HA	1:H:336:ASP:HB3	1.89	0.54
1:J:275:VAL:HG12	1:J:277:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:O	1:B:281:GLY:C	2.45	0.54
1:D:244:GLY:O	1:D:246:TYR:N	2.41	0.54
1:F:221:ILE:HA	1:F:249:LEU:HB2	1.90	0.54
1:H:251:MET:HB2	1:H:277:ILE:HD11	1.83	0.54
1:I:483:TYR:OH	1:I:488:ASP:OD1	2.20	0.54
1:N:276:ALA:C	1:N:277:ILE:HG23	2.18	0.54
1:E:88:ASP:OD1	1:E:89:GLY:N	2.41	0.54
1:G:251:MET:HB2	1:G:277:ILE:HD12	1.88	0.54
1:I:339:THR:HG22	1:I:342:ASP:H	1.72	0.54
1:K:221:ILE:HA	1:K:249:LEU:HB2	1.89	0.54
1:B:424:SER:HB2	1:B:447:LYS:HD2	1.90	0.54
1:E:267:LYS:CD	1:E:274:VAL:O	2.56	0.54
1:J:65:ASP:HB3	1:J:68:GLU:HG2	1.90	0.54
1:A:353:LEU:O	1:A:357:THR:OG1	2.21	0.54
1:B:250:ILE:O	1:B:277:ILE:CG1	2.53	0.54
1:D:263:LEU:HG	1:D:274:VAL:HG21	1.90	0.54
1:D:193:GLY:N	1:D:377:VAL:HG12	2.23	0.54
1:B:278:LYS:CB	1:B:278:LYS:HZ2	2.21	0.54
1:B:277:ILE:HG22	1:B:326:ILE:CD1	2.38	0.54
1:D:483:TYR:OH	1:D:488:ASP:OD1	2.25	0.54
1:E:202:SER:HB3	1:E:203:PRO:HA	1.89	0.54
1:E:200:TYR:HB3	1:E:328:LYS:HA	1.90	0.54
1:K:251:MET:HB3	1:K:277:ILE:CG1	2.38	0.54
1:G:157:THR:O	1:G:159:ILE:N	2.40	0.53
1:H:159:ILE:HG12	1:H:397:VAL:HG12	1.89	0.53
1:L:263:LEU:HG	1:L:274:VAL:HG21	1.90	0.53
1:C:216:TYR:OH	1:C:267:LYS:NZ	2.36	0.53
1:E:483:TYR:OH	1:E:488:ASP:OD1	2.24	0.53
1:H:418:CYS:HA	1:H:421:LEU:HD13	1.89	0.53
1:B:201:THR:HB	1:B:276:ALA:HB1	1.90	0.53
1:D:157:THR:OG1	1:D:158:ASP:N	2.40	0.53
1:A:263:LEU:HG	1:A:274:VAL:HG21	1.91	0.53
1:C:157:THR:O	1:C:160:GLY:N	2.38	0.53
1:E:281:GLY:HA3	1:E:285:ARG:HB2	1.90	0.53
1:D:73:THR:HA	1:D:76:ARG:HD3	1.90	0.53
1:J:339:THR:HG22	1:J:342:ASP:H	1.74	0.53
1:G:244:GLY:O	1:G:246:TYR:N	2.42	0.53
1:K:157:THR:O	1:K:160:GLY:N	2.42	0.53
1:K:424:SER:HB2	1:K:447:LYS:HD2	1.91	0.53
1:K:421:LEU:HD11	1:K:454:ILE:HG21	1.91	0.53
1:M:491:GLU:HB3	1:M:496:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:SER:HB3	1:G:204:TYR:HD1	1.73	0.53
1:H:238:LEU:HD12	1:H:272:LEU:HD22	1.91	0.53
1:K:456:LEU:O	1:K:460:ASN:ND2	2.26	0.53
1:K:491:GLU:HB3	1:K:496:THR:HG21	1.91	0.53
1:G:233:ASP:O	1:G:236:THR:OG1	2.27	0.53
1:D:137:SER:HB3	1:D:412:VAL:HG12	1.91	0.53
1:D:334:VAL:CG2	1:D:377:VAL:CG1	2.75	0.53
1:F:198:ARG:NH1	1:F:279:ALA:O	2.42	0.53
1:G:338:SER:OG	1:G:339:THR:N	2.42	0.53
1:A:88:ASP:OD1	1:A:89:GLY:N	2.41	0.53
1:B:238:LEU:HD12	1:B:272:LEU:HD22	1.92	0.53
1:E:202:SER:N	1:E:203:PRO:HA	2.24	0.53
1:J:88:ASP:OD1	1:J:89:GLY:N	2.41	0.53
1:C:244:GLY:O	1:C:246:TYR:N	2.42	0.52
1:C:277:ILE:HD12	1:C:278:LYS:H	1.72	0.52
1:E:491:GLU:HB3	1:E:496:THR:HG21	1.90	0.52
1:I:321:ALA:HA	1:I:336:ASP:HB3	1.90	0.52
1:J:421:LEU:HD11	1:J:454:ILE:HG21	1.91	0.52
1:A:238:LEU:HD12	1:A:272:LEU:HD22	1.90	0.52
1:D:277:ILE:HD13	1:D:278:LYS:HG2	1.90	0.52
1:I:159:ILE:HG12	1:I:397:VAL:HG12	1.91	0.52
1:E:233:ASP:OD1	1:E:234:ILE:N	2.40	0.52
1:F:491:GLU:HB3	1:F:496:THR:HG21	1.91	0.52
1:I:456:LEU:O	1:I:460:ASN:ND2	2.28	0.52
1:L:456:LEU:O	1:L:460:ASN:ND2	2.25	0.52
1:M:244:GLY:O	1:M:246:TYR:N	2.43	0.52
1:B:206:VAL:HG11	1:B:212:MET:HB2	1.91	0.52
1:H:424:SER:HB2	1:H:447:LYS:HD2	1.91	0.52
1:B:339:THR:HG22	1:B:342:ASP:H	1.73	0.52
1:E:211:ARG:CG	1:E:211:ARG:NH1	2.73	0.52
1:J:157:THR:O	1:J:159:ILE:N	2.43	0.52
1:L:276:ALA:O	1:L:277:ILE:HG22	2.04	0.52
1:E:291:GLU:O	1:E:295:ILE:HB	2.10	0.52
1:M:456:LEU:O	1:M:460:ASN:ND2	2.29	0.52
1:C:238:LEU:HD12	1:C:272:LEU:HD22	1.91	0.52
1:J:157:THR:O	1:J:160:GLY:N	2.40	0.52
1:J:285:ARG:NH2	1:J:368:GLU:OE2	2.43	0.52
1:K:263:LEU:HG	1:K:274:VAL:HG21	1.91	0.52
1:G:238:LEU:HD12	1:G:272:LEU:HD22	1.92	0.52
1:N:238:LEU:HD12	1:N:272:LEU:HD22	1.91	0.52
1:B:221:ILE:HA	1:B:249:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LEU:O	1:B:460:ASN:ND2	2.28	0.52
1:C:88:ASP:OD1	1:C:89:GLY:N	2.41	0.52
1:D:306:MET:HB2	1:D:307:GLY:HA2	1.92	0.52
1:E:205:PHE:CD2	1:E:267:LYS:CB	2.63	0.52
1:A:51:VAL:HG12	1:A:53:ASP:H	1.74	0.52
1:G:456:LEU:O	1:G:460:ASN:ND2	2.27	0.52
1:H:88:ASP:OD1	1:H:89:GLY:N	2.42	0.52
1:J:483:TYR:OH	1:J:488:ASP:OD1	2.26	0.52
1:I:244:GLY:O	1:I:246:TYR:N	2.43	0.51
1:J:221:ILE:HA	1:J:249:LEU:HB2	1.91	0.51
1:K:88:ASP:OD1	1:K:89:GLY:N	2.38	0.51
1:L:339:THR:HG22	1:L:342:ASP:H	1.74	0.51
1:M:421:LEU:HD11	1:M:454:ILE:HG21	1.91	0.51
1:B:157:THR:OG1	1:B:158:ASP:N	2.42	0.51
1:B:278:LYS:CB	1:B:278:LYS:NZ	2.73	0.51
1:E:421:LEU:HD11	1:E:454:ILE:HG21	1.92	0.51
1:M:424:SER:HB2	1:M:447:LYS:HD2	1.92	0.51
1:N:240:SER:OG	1:N:243:ARG:NH1	2.43	0.51
1:B:201:THR:CB	1:B:276:ALA:HB1	2.41	0.51
1:C:73:THR:HA	1:C:76:ARG:HD3	1.92	0.51
1:G:206:VAL:HG11	1:G:212:MET:HB2	1.90	0.51
1:I:338:SER:OG	1:I:339:THR:N	2.43	0.51
1:J:137:SER:HB3	1:J:412:VAL:HG12	1.92	0.51
1:N:277:ILE:HD12	1:N:278:LYS:O	2.10	0.51
1:A:105:MET:HA	1:A:108:VAL:HB	1.91	0.51
1:B:285:ARG:NH2	1:B:368:GLU:OE2	2.43	0.51
1:E:306:MET:N	1:E:307:GLY:HA2	2.26	0.51
1:H:206:VAL:HG11	1:H:212:MET:HB2	1.92	0.51
1:A:240:SER:OG	1:A:243:ARG:NH1	2.43	0.51
1:E:241:ALA:O	1:E:245:ASN:N	2.39	0.51
1:F:244:GLY:O	1:F:246:TYR:N	2.44	0.51
1:F:253:GLU:C	1:F:278:LYS:HE3	2.30	0.51
1:J:104:GLY:HA2	1:J:445:ILE:HD13	1.93	0.51
1:L:244:GLY:O	1:L:246:TYR:N	2.44	0.51
1:L:238:LEU:HD12	1:L:272:LEU:HD22	1.92	0.51
1:M:55:VAL:HG22	1:M:90:THR:HG21	1.93	0.51
1:A:418:CYS:HA	1:A:421:LEU:HD13	1.91	0.51
1:B:278:LYS:NZ	1:B:278:LYS:CA	2.73	0.51
1:E:194:MET:HG3	1:E:296:LEU:HD22	1.93	0.51
1:G:20:GLY:HA3	1:G:68:GLU:HB2	1.92	0.51
1:A:157:THR:O	1:A:159:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:285:ARG:NH2	1:L:368:GLU:OE2	2.44	0.51
1:D:251:MET:HB3	1:D:277:ILE:HG22	1.92	0.51
1:G:40:VAL:HG22	1:G:50:ILE:HG22	1.92	0.51
1:G:424:SER:HB2	1:G:447:LYS:HD2	1.92	0.51
1:H:20:GLY:HA3	1:H:68:GLU:HB2	1.92	0.51
1:H:483:TYR:OH	1:H:488:ASP:OD1	2.24	0.51
1:M:277:ILE:HG22	1:M:278:LYS:H	1.75	0.51
1:N:194:MET:N	1:N:377:VAL:HG21	2.26	0.51
1:B:278:LYS:HA	1:B:278:LYS:HZ3	1.75	0.51
1:C:240:SER:OG	1:C:243:ARG:NH1	2.44	0.51
1:D:217:GLU:HG2	1:D:323:LYS:HG2	1.93	0.51
1:F:253:GLU:O	1:F:278:LYS:HD2	2.10	0.51
1:F:263:LEU:HG	1:F:274:VAL:HG21	1.92	0.51
1:J:263:LEU:HG	1:J:274:VAL:HG21	1.92	0.51
1:J:387:GLU:OE2	1:M:198:ARG:NH2	2.44	0.51
1:D:424:SER:HB2	1:D:447:LYS:HD2	1.93	0.51
1:G:157:THR:O	1:G:160:GLY:N	2.41	0.51
1:G:232:ARG:H	1:G:232:ARG:HD2	1.76	0.51
1:G:277:ILE:HD12	1:G:278:LYS:O	2.10	0.51
1:K:244:GLY:O	1:K:246:TYR:N	2.44	0.51
1:N:88:ASP:OD1	1:N:89:GLY:N	2.43	0.51
1:C:65:ASP:HB3	1:C:68:GLU:HG2	1.92	0.50
1:F:278:LYS:HE3	1:F:278:LYS:CA	2.38	0.50
1:K:38:ASN:OD1	1:K:52:ASN:ND2	2.43	0.50
1:C:338:SER:OG	1:C:339:THR:N	2.42	0.50
1:E:195:GLN:HB2	1:E:332:THR:HG22	1.93	0.50
1:F:376:GLY:O	1:F:377:VAL:HG23	2.11	0.50
1:N:216:TYR:OH	1:N:267:LYS:NZ	2.36	0.50
1:N:491:GLU:HB3	1:N:496:THR:HG21	1.92	0.50
1:C:83:ASN:HB2	1:C:90:THR:HG22	1.94	0.50
1:E:209:PRO:CA	1:E:212:MET:H	2.16	0.50
1:E:73:THR:HA	1:E:76:ARG:HD3	1.94	0.50
1:M:338:SER:OG	1:M:339:THR:N	2.43	0.50
1:M:88:ASP:OD1	1:M:89:GLY:N	2.39	0.50
1:N:424:SER:HB2	1:N:447:LYS:HD2	1.93	0.50
1:B:217:GLU:HG2	1:B:323:LYS:HG2	1.93	0.50
1:C:421:LEU:HD11	1:C:454:ILE:HG21	1.92	0.50
1:E:205:PHE:CD2	1:E:267:LYS:HD3	2.46	0.50
1:F:218:ASN:N	1:F:322:ALA:O	2.33	0.50
1:M:104:GLY:HA2	1:M:445:ILE:HD13	1.92	0.50
1:M:238:LEU:HD12	1:M:272:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:SER:HB3	1:E:203:PRO:CA	2.42	0.50
1:J:73:THR:HA	1:J:76:ARG:HD3	1.94	0.50
1:E:137:SER:HB3	1:E:412:VAL:HG12	1.94	0.50
1:E:202:SER:OG	1:E:204:TYR:CB	2.58	0.50
1:F:61:VAL:O	1:F:76:ARG:NH1	2.44	0.50
1:I:263:LEU:HG	1:I:274:VAL:HG21	1.94	0.50
1:K:339:THR:HG22	1:K:342:ASP:H	1.77	0.50
1:L:207:THR:OG1	1:L:213:ILE:O	2.29	0.50
1:J:275:VAL:CG1	1:J:276:ALA:N	2.74	0.50
1:J:456:LEU:O	1:J:460:ASN:ND2	2.29	0.50
1:M:277:ILE:HG21	1:M:331:THR:HG21	1.94	0.50
1:N:338:SER:OG	1:N:339:THR:N	2.44	0.50
1:N:104:GLY:HA2	1:N:445:ILE:HD13	1.93	0.50
1:A:157:THR:O	1:A:160:GLY:N	2.41	0.50
1:C:483:TYR:OH	1:C:488:ASP:OD1	2.25	0.50
1:E:205:PHE:CG	1:E:267:LYS:CD	2.94	0.50
1:E:424:SER:HB2	1:E:447:LYS:HD2	1.94	0.50
1:J:277:ILE:CG2	1:J:278:LYS:N	2.75	0.50
1:K:207:THR:OG1	1:K:214:CYS:HA	2.12	0.50
1:N:217:GLU:HG2	1:N:323:LYS:HG2	1.93	0.50
1:B:491:GLU:HB3	1:B:496:THR:HG21	1.94	0.49
1:K:9:LYS:HG2	1:K:524:VAL:HG22	1.94	0.49
1:B:278:LYS:CE	1:B:278:LYS:CA	2.85	0.49
1:E:118:VAL:HG21	1:E:517:LYS:HG3	1.92	0.49
1:G:418:CYS:HA	1:G:421:LEU:HD13	1.94	0.49
1:H:276:ALA:C	1:H:277:ILE:HG23	2.26	0.49
1:E:350:ILE:HG21	1:E:370:ILE:HB	1.94	0.49
1:H:339:THR:HG22	1:H:342:ASP:H	1.76	0.49
1:J:104:GLY:HA3	1:J:520:LEU:HD21	1.94	0.49
1:L:233:ASP:O	1:L:236:THR:OG1	2.30	0.49
1:C:20:GLY:HA3	1:C:68:GLU:HB2	1.94	0.49
1:C:200:TYR:CA	1:C:277:ILE:HG22	2.34	0.49
1:C:217:GLU:HG2	1:C:323:LYS:HG2	1.94	0.49
1:E:216:TYR:CD2	1:E:247:PRO:HG2	2.44	0.49
1:F:194:MET:HE1	1:F:373:LEU:HA	1.93	0.49
1:H:327:THR:HG1	1:H:328:LYS:H	1.59	0.49
1:K:217:GLU:HG2	1:K:323:LYS:HG2	1.93	0.49
1:M:483:TYR:OH	1:M:488:ASP:OD1	2.27	0.49
1:C:221:ILE:HA	1:C:249:LEU:HB2	1.94	0.49
1:G:263:LEU:HG	1:G:274:VAL:HG21	1.95	0.49
1:H:393:LYS:O	1:H:397:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:285:ARG:NH2	1:K:368:GLU:OE2	2.46	0.49
1:B:263:LEU:HG	1:B:274:VAL:HG21	1.94	0.49
1:E:205:PHE:HE2	1:E:264:VAL:O	1.95	0.49
1:I:424:SER:HB2	1:I:447:LYS:HD2	1.93	0.49
1:K:137:SER:HB3	1:K:412:VAL:HG12	1.93	0.49
1:L:338:SER:OG	1:L:339:THR:N	2.44	0.49
1:A:217:GLU:HG2	1:A:323:LYS:HG2	1.93	0.49
1:B:253:GLU:O	1:B:278:LYS:HE3	2.13	0.49
1:B:274:VAL:C	1:B:275:VAL:CG2	2.80	0.49
1:E:205:PHE:CD2	1:E:267:LYS:CD	2.95	0.49
1:F:104:GLY:HA2	1:F:445:ILE:HD13	1.94	0.49
1:K:238:LEU:HD12	1:K:272:LEU:HD22	1.94	0.49
1:A:137:SER:N	1:A:412:VAL:O	2.38	0.49
1:B:104:GLY:HA2	1:B:445:ILE:HD13	1.94	0.49
1:C:424:SER:HB2	1:C:447:LYS:HD2	1.94	0.49
1:E:180:GLU:HA	1:E:382:VAL:HG12	1.93	0.49
1:F:285:ARG:NH2	1:F:368:GLU:OE2	2.46	0.49
1:G:65:ASP:HB3	1:G:68:GLU:HG2	1.95	0.49
1:H:306:MET:HB2	1:H:307:GLY:HA2	1.95	0.49
1:K:232:ARG:H	1:K:232:ARG:HD2	1.78	0.49
1:M:157:THR:O	1:M:160:GLY:N	2.45	0.49
1:B:157:THR:O	1:B:160:GLY:N	2.43	0.48
1:C:181:GLY:HA2	1:C:182:LYS:HA	1.64	0.48
1:E:175:VAL:CG1	1:E:377:VAL:HG22	2.42	0.48
1:G:321:ALA:HA	1:G:336:ASP:HB3	1.94	0.48
1:J:424:SER:HB2	1:J:447:LYS:HD2	1.95	0.48
1:K:206:VAL:HB	1:K:212:MET:HA	1.94	0.48
1:L:266:ASN:HB3	1:L:272:LEU:HB3	1.95	0.48
1:N:421:LEU:HD11	1:N:454:ILE:HG21	1.94	0.48
1:C:104:GLY:HA2	1:C:445:ILE:HD13	1.94	0.48
1:E:157:THR:O	1:E:160:GLY:N	2.46	0.48
1:E:209:PRO:HA	1:E:211:ARG:N	2.28	0.48
1:J:217:GLU:HG2	1:J:323:LYS:HG2	1.96	0.48
1:C:306:MET:HB2	1:C:307:GLY:HA2	1.94	0.48
1:E:200:TYR:CD1	1:E:328:LYS:HD3	2.48	0.48
1:E:38:ASN:OD1	1:E:52:ASN:ND2	2.44	0.48
1:J:418:CYS:HA	1:J:421:LEU:HD13	1.95	0.48
1:L:73:THR:HA	1:L:76:ARG:HD3	1.94	0.48
1:C:21:VAL:HG11	1:C:101:ILE:HD12	1.94	0.48
1:D:377:VAL:O	1:D:377:VAL:HG13	2.12	0.48
1:G:355:MET:SD	1:G:356:GLN:HG2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:306:MET:H	1:J:307:GLY:HA3	1.78	0.48
1:J:338:SER:OG	1:J:339:THR:N	2.45	0.48
1:N:65:ASP:HB3	1:N:68:GLU:HG2	1.95	0.48
1:E:212:MET:HG2	1:E:212:MET:O	2.13	0.48
1:F:338:SER:OG	1:F:339:THR:N	2.44	0.48
1:I:421:LEU:HD11	1:I:454:ILE:HG21	1.95	0.48
1:I:88:ASP:OD1	1:I:89:GLY:N	2.42	0.48
1:L:424:SER:HB2	1:L:447:LYS:HD2	1.95	0.48
1:B:437:PRO:O	1:B:441:MET:HG2	2.14	0.48
1:D:285:ARG:NH2	1:D:368:GLU:OE2	2.47	0.48
1:M:263:LEU:HG	1:M:274:VAL:HG21	1.93	0.48
1:N:263:LEU:HG	1:N:274:VAL:HG21	1.95	0.48
1:C:157:THR:O	1:C:159:ILE:N	2.47	0.48
1:C:276:ALA:C	1:C:277:ILE:HG23	2.26	0.48
1:H:338:SER:OG	1:H:339:THR:N	2.45	0.48
1:J:275:VAL:CG1	1:J:277:ILE:HD11	2.44	0.48
1:K:517:LYS:O	1:K:521:LEU:HB2	2.14	0.48
1:N:251:MET:HB3	1:N:277:ILE:CG1	2.43	0.48
1:C:321:ALA:HA	1:C:336:ASP:HB3	1.96	0.48
1:I:393:LYS:O	1:I:397:VAL:HG13	2.14	0.48
1:L:418:CYS:HA	1:L:421:LEU:HD13	1.94	0.48
1:N:21:VAL:HG13	1:N:75:VAL:HG21	1.95	0.48
1:N:306:MET:HB2	1:N:307:GLY:HA2	1.96	0.48
1:B:353:LEU:O	1:B:357:THR:OG1	2.24	0.48
1:G:277:ILE:HD12	1:G:278:LYS:N	2.29	0.48
1:J:200:TYR:CA	1:J:277:ILE:HG13	2.40	0.48
1:G:306:MET:HB2	1:G:307:GLY:HA2	1.96	0.47
1:H:437:PRO:O	1:H:441:MET:HG2	2.14	0.47
1:A:218:ASN:N	1:A:322:ALA:O	2.34	0.47
1:B:253:GLU:CA	1:B:279:ALA:HB3	2.43	0.47
1:E:208:ASP:OD1	1:E:209:PRO:HD2	2.13	0.47
1:F:339:THR:HG22	1:F:342:ASP:H	1.79	0.47
1:I:232:ARG:H	1:I:232:ARG:HD2	1.79	0.47
1:N:181:GLY:HA2	1:N:182:LYS:HA	1.68	0.47
1:N:327:THR:OG1	1:N:328:LYS:N	2.32	0.47
1:A:491:GLU:HB3	1:A:496:THR:HG21	1.95	0.47
1:E:189:VAL:HG12	1:E:191:VAL:HG13	1.95	0.47
1:G:47:ALA:HA	1:G:48:PRO:HD3	1.79	0.47
1:H:104:GLY:HA2	1:H:445:ILE:HD13	1.96	0.47
1:L:306:MET:HB2	1:L:307:GLY:HA2	1.95	0.47
1:C:251:MET:HB3	1:C:277:ILE:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:SER:HB2	1:F:447:LYS:HD2	1.95	0.47
1:G:437:PRO:O	1:G:441:MET:HG2	2.15	0.47
1:I:251:MET:HB3	1:I:277:ILE:HB	1.95	0.47
1:M:339:THR:HG22	1:M:342:ASP:H	1.79	0.47
1:B:306:MET:HB2	1:B:307:GLY:HA2	1.95	0.47
1:B:41:LEU:HD21	1:B:60:GLU:HG3	1.96	0.47
1:C:263:LEU:HG	1:C:274:VAL:HG21	1.96	0.47
1:E:200:TYR:CZ	1:E:328:LYS:HE3	2.44	0.47
1:F:437:PRO:O	1:F:441:MET:HG2	2.14	0.47
1:H:202:SER:HB3	1:H:204:TYR:HD1	1.79	0.47
1:M:306:MET:HB2	1:M:307:GLY:HA2	1.95	0.47
1:D:193:GLY:CA	1:D:377:VAL:HG12	2.44	0.47
1:F:277:ILE:HD12	1:F:278:LYS:O	2.00	0.47
1:F:418:CYS:HA	1:F:421:LEU:HD13	1.96	0.47
1:G:104:GLY:HA2	1:G:445:ILE:HD13	1.96	0.47
1:A:221:ILE:HA	1:A:249:LEU:HB2	1.97	0.47
1:A:65:ASP:HB3	1:A:68:GLU:HG2	1.95	0.47
1:E:200:TYR:CD1	1:E:201:THR:N	2.83	0.47
1:E:66:PRO:HB2	1:E:527:THR:HG21	1.97	0.47
1:H:172:ARG:O	1:H:174:GLY:N	2.48	0.47
1:J:517:LYS:O	1:J:521:LEU:HB2	2.14	0.47
1:A:104:GLY:HA2	1:A:445:ILE:HD13	1.96	0.47
1:A:410:GLU:HB2	1:A:503:LYS:HB2	1.97	0.47
1:B:88:ASP:OD1	1:B:89:GLY:N	2.44	0.47
1:E:255:VAL:HG23	1:E:259:ALA:HB3	1.97	0.47
1:E:310:LEU:HD22	1:E:310:LEU:H	1.79	0.47
1:F:421:LEU:HD11	1:F:454:ILE:HG21	1.97	0.47
1:J:20:GLY:HA3	1:J:68:GLU:HB2	1.95	0.47
1:N:9:LYS:HG2	1:N:524:VAL:HG22	1.97	0.47
1:E:205:PHE:O	1:E:206:VAL:HG22	2.15	0.47
1:E:350:ILE:HG12	1:E:369:ARG:HH21	1.80	0.47
1:I:276:ALA:O	1:I:277:ILE:HG13	2.14	0.47
1:L:217:GLU:HG2	1:L:323:LYS:HG2	1.96	0.47
1:A:133:ARG:O	1:A:136:SER:OG	2.30	0.47
1:D:65:ASP:HB3	1:D:68:GLU:HG2	1.96	0.47
1:F:238:LEU:HD12	1:F:272:LEU:HD22	1.97	0.47
1:L:232:ARG:H	1:L:232:ARG:HD2	1.80	0.47
1:A:22:ASP:O	1:A:26:THR:OG1	2.24	0.47
1:D:437:PRO:O	1:D:441:MET:HG2	2.15	0.47
1:H:421:LEU:HD11	1:H:454:ILE:HG21	1.97	0.47
1:L:21:VAL:HG13	1:L:75:VAL:HG21	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LYS:O	1:A:397:VAL:HG13	2.15	0.46
1:A:437:PRO:O	1:A:441:MET:HG2	2.16	0.46
1:E:198:ARG:HB3	1:E:277:ILE:HD11	1.97	0.46
1:I:306:MET:HB2	1:I:307:GLY:HA2	1.95	0.46
1:J:274:VAL:C	1:J:275:VAL:HG23	2.35	0.46
1:K:137:SER:N	1:K:412:VAL:O	2.41	0.46
1:L:491:GLU:HB3	1:L:496:THR:HG21	1.97	0.46
1:A:24:LEU:HD11	1:A:76:ARG:HG3	1.97	0.46
1:A:338:SER:OG	1:A:339:THR:N	2.46	0.46
1:B:201:THR:HB	1:B:276:ALA:CB	2.45	0.46
1:B:201:THR:OG1	1:B:276:ALA:HB1	2.15	0.46
1:G:172:ARG:O	1:G:174:GLY:N	2.48	0.46
1:H:244:GLY:O	1:H:246:TYR:N	2.48	0.46
1:M:232:ARG:H	1:M:232:ARG:HD2	1.81	0.46
1:C:339:THR:HG22	1:C:342:ASP:H	1.81	0.46
1:E:437:PRO:O	1:E:441:MET:HG2	2.15	0.46
1:F:410:GLU:HB2	1:F:503:LYS:HB2	1.96	0.46
1:G:296:LEU:HG	1:G:343:VAL:HG22	1.97	0.46
1:G:303:ARG:HE	1:G:305:GLU:HB2	1.79	0.46
1:H:142:ASP:N	1:H:142:ASP:OD1	2.48	0.46
1:I:216:TYR:HB3	1:I:219:CYS:SG	2.55	0.46
1:K:306:MET:HB2	1:K:307:GLY:HA2	1.95	0.46
1:A:285:ARG:NH2	1:A:368:GLU:OE2	2.49	0.46
1:A:436:ASP:N	1:A:436:ASP:OD1	2.48	0.46
1:C:376:GLY:O	1:C:377:VAL:HG23	2.15	0.46
1:E:194:MET:HE1	1:E:372:ARG:HG3	1.98	0.46
1:H:251:MET:HB2	1:H:277:ILE:CD1	2.45	0.46
1:I:275:VAL:HG12	1:I:277:ILE:HD11	1.97	0.46
1:B:172:ARG:O	1:B:174:GLY:N	2.48	0.46
1:D:338:SER:OG	1:D:339:THR:N	2.44	0.46
1:D:393:LYS:O	1:D:397:VAL:HG13	2.15	0.46
1:G:421:LEU:HD11	1:G:454:ILE:HG21	1.97	0.46
1:L:172:ARG:O	1:L:174:GLY:N	2.49	0.46
1:M:65:ASP:HB3	1:M:68:GLU:HG2	1.96	0.46
1:B:251:MET:CB	1:B:277:ILE:O	2.64	0.46
1:E:202:SER:CB	1:E:203:PRO:CA	2.93	0.46
1:K:209:PRO:HA	1:K:212:MET:H	1.80	0.46
1:M:181:GLY:HA2	1:M:182:LYS:HA	1.68	0.46
1:M:159:ILE:HG12	1:M:397:VAL:HG12	1.98	0.46
1:N:437:PRO:O	1:N:441:MET:HG2	2.16	0.46
1:A:339:THR:HG22	1:A:342:ASP:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:PHE:CD2	1:E:267:LYS:CG	2.97	0.46
1:F:172:ARG:O	1:F:174:GLY:N	2.49	0.46
1:F:253:GLU:CA	1:F:278:LYS:HE3	2.45	0.46
1:H:78:ALA:HB2	1:H:515:VAL:HG11	1.98	0.46
1:H:65:ASP:HB3	1:H:68:GLU:HG2	1.97	0.46
1:J:410:GLU:HB2	1:J:503:LYS:HB2	1.97	0.46
1:K:104:GLY:HA2	1:K:445:ILE:HD13	1.96	0.46
1:L:207:THR:HG23	1:L:214:CYS:SG	2.56	0.46
1:D:334:VAL:HG23	1:D:377:VAL:HG21	1.91	0.46
1:D:104:GLY:HA3	1:D:520:LEU:HD21	1.96	0.46
1:H:206:VAL:HB	1:H:212:MET:HA	1.96	0.46
1:J:172:ARG:O	1:J:174:GLY:N	2.48	0.46
1:J:238:LEU:HD12	1:J:272:LEU:HD22	1.97	0.46
1:L:251:MET:HB3	1:L:277:ILE:CG1	2.45	0.46
1:N:172:ARG:O	1:N:174:GLY:N	2.48	0.46
1:C:437:PRO:O	1:C:441:MET:HG2	2.16	0.46
1:D:325:THR:O	1:D:332:THR:OG1	2.28	0.46
1:E:202:SER:HB3	1:E:203:PRO:C	2.36	0.46
1:E:277:ILE:HG12	1:E:331:THR:HG21	1.97	0.46
1:F:393:LYS:O	1:F:397:VAL:HG13	2.16	0.46
1:I:172:ARG:O	1:I:174:GLY:N	2.49	0.46
1:J:119:ARG:O	1:J:119:ARG:NH1	2.48	0.46
1:K:215:GLU:O	1:K:215:GLU:HG3	2.15	0.46
1:K:353:LEU:O	1:K:357:THR:OG1	2.25	0.46
1:C:172:ARG:O	1:C:174:GLY:N	2.49	0.46
1:E:205:PHE:CZ	1:E:267:LYS:O	2.45	0.46
1:F:65:ASP:HB3	1:F:68:GLU:HG2	1.97	0.46
1:K:437:PRO:O	1:K:441:MET:HG2	2.16	0.46
1:A:306:MET:HB2	1:A:307:GLY:HA2	1.98	0.45
1:A:17:MET:HB2	1:A:71:GLY:HA3	1.98	0.45
1:C:130:LYS:HG2	1:C:133:ARG:HH21	1.81	0.45
1:C:224:VAL:HG12	1:C:225:ASP:H	1.79	0.45
1:E:209:PRO:HB2	1:E:210:GLU:C	2.35	0.45
1:G:157:THR:OG1	1:G:158:ASP:N	2.47	0.45
1:G:104:GLY:HA3	1:G:520:LEU:HD21	1.97	0.45
1:I:9:LYS:HG2	1:I:524:VAL:HG22	1.97	0.45
1:I:55:VAL:HG22	1:I:90:THR:HG21	1.98	0.45
1:J:225:ASP:HB3	1:J:290:LEU:HD21	1.98	0.45
1:M:517:LYS:O	1:M:521:LEU:HB2	2.16	0.45
1:H:232:ARG:H	1:H:232:ARG:HD2	1.81	0.45
1:I:238:LEU:HD12	1:I:272:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:216:TYR:HB3	1:L:219:CYS:SG	2.56	0.45
1:M:73:THR:HA	1:M:76:ARG:HD3	1.99	0.45
1:A:348:LYS:HB3	1:A:348:LYS:HE2	1.87	0.45
1:A:517:LYS:O	1:A:521:LEU:HB2	2.17	0.45
1:H:304:ASP:OD1	1:H:309:SER:OG	2.30	0.45
1:I:157:THR:O	1:I:159:ILE:N	2.50	0.45
1:I:202:SER:HA	1:I:203:PRO:HD3	1.84	0.45
1:B:21:VAL:HG13	1:B:75:VAL:HG21	1.98	0.45
1:D:225:ASP:HB3	1:D:290:LEU:HD21	1.99	0.45
1:G:393:LYS:O	1:G:397:VAL:HG13	2.16	0.45
1:J:437:PRO:O	1:J:441:MET:HG2	2.16	0.45
1:K:303:ARG:HE	1:K:305:GLU:HB2	1.81	0.45
1:L:437:PRO:O	1:L:441:MET:HG2	2.17	0.45
1:A:10:ASP:CG	1:A:11:MET:H	2.20	0.45
1:C:233:ASP:O	1:C:236:THR:OG1	2.30	0.45
1:C:285:ARG:NH2	1:C:368:GLU:OE2	2.50	0.45
1:G:217:GLU:HG2	1:G:323:LYS:HG2	1.97	0.45
1:H:285:ARG:NH2	1:H:368:GLU:OE2	2.49	0.45
1:L:436:ASP:N	1:L:436:ASP:OD1	2.49	0.45
1:M:216:TYR:HB3	1:M:219:CYS:SG	2.56	0.45
1:N:206:VAL:HG11	1:N:212:MET:HB2	1.97	0.45
1:E:198:ARG:HA	1:E:198:ARG:HD3	1.68	0.45
1:F:376:GLY:O	1:F:377:VAL:CG2	2.65	0.45
1:K:385:GLN:HB2	1:K:389:GLU:HG2	1.99	0.45
1:L:202:SER:HA	1:L:203:PRO:HD3	1.85	0.45
1:M:233:ASP:O	1:M:236:THR:OG1	2.34	0.45
1:M:303:ARG:HE	1:M:305:GLU:HB2	1.81	0.45
1:B:338:SER:OG	1:B:339:THR:N	2.46	0.45
1:D:172:ARG:O	1:D:174:GLY:N	2.49	0.45
1:D:240:SER:OG	1:D:243:ARG:NH1	2.49	0.45
1:E:202:SER:CB	1:E:203:PRO:C	2.85	0.45
1:E:65:ASP:HB3	1:E:68:GLU:HG2	1.98	0.45
1:H:202:SER:HA	1:H:203:PRO:HD3	1.86	0.45
1:H:55:VAL:HG22	1:H:90:THR:HG21	1.97	0.45
1:L:198:ARG:HE	1:L:280:PRO:HA	1.81	0.45
1:M:276:ALA:C	1:M:277:ILE:CD1	2.85	0.45
1:M:437:PRO:O	1:M:441:MET:HG2	2.16	0.45
1:N:200:TYR:CA	1:N:277:ILE:HG22	2.33	0.45
1:A:172:ARG:O	1:A:174:GLY:N	2.50	0.45
1:D:200:TYR:CA	1:D:277:ILE:CG1	2.77	0.45
1:D:202:SER:HB3	1:D:204:TYR:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:PRO:CA	1:E:210:GLU:C	2.85	0.45
1:F:348:LYS:HE2	1:F:348:LYS:HB3	1.85	0.45
1:H:200:TYR:CA	1:H:277:ILE:HG22	2.33	0.45
1:H:517:LYS:O	1:H:521:LEU:HB2	2.17	0.45
1:J:142:ASP:OD1	1:J:142:ASP:N	2.49	0.45
1:M:172:ARG:O	1:M:174:GLY:N	2.50	0.45
1:D:55:VAL:HG22	1:D:90:THR:HG21	1.99	0.45
1:E:209:PRO:CB	1:E:210:GLU:C	2.85	0.45
1:J:275:VAL:CG1	1:J:277:ILE:CD1	2.92	0.45
1:L:165:ASP:HA	1:L:168:ALA:HB3	1.98	0.45
1:M:202:SER:HA	1:M:203:PRO:HD3	1.83	0.45
1:M:393:LYS:O	1:M:397:VAL:HG13	2.17	0.45
1:E:267:LYS:HZ1	1:E:273:LYS:CG	2.19	0.45
1:J:277:ILE:HG22	1:J:278:LYS:N	2.31	0.45
1:J:47:ALA:HA	1:J:48:PRO:HD3	1.86	0.45
1:M:276:ALA:C	1:M:277:ILE:CG1	2.85	0.45
1:E:59:ARG:NH2	1:E:212:MET:SD	2.89	0.44
1:J:274:VAL:O	1:J:275:VAL:HG22	2.16	0.44
1:L:517:LYS:O	1:L:521:LEU:HB2	2.17	0.44
1:M:277:ILE:N	1:M:277:ILE:CD1	2.74	0.44
1:D:233:ASP:O	1:D:236:THR:OG1	2.29	0.44
1:D:392:GLU:OE2	1:D:396:ARG:NH2	2.50	0.44
1:E:280:PRO:HG2	1:E:289:TYR:HD2	1.81	0.44
1:H:194:MET:HE1	1:H:373:LEU:HA	1.98	0.44
1:I:437:PRO:O	1:I:441:MET:HG2	2.16	0.44
1:K:61:VAL:O	1:K:76:ARG:NH1	2.50	0.44
1:M:10:ASP:OD1	1:M:11:MET:N	2.49	0.44
1:M:352:ASN:O	1:M:356:GLN:HG2	2.17	0.44
1:A:157:THR:OG1	1:A:158:ASP:N	2.50	0.44
1:A:202:SER:HB3	1:A:204:TYR:HD1	1.82	0.44
1:A:421:LEU:HD11	1:A:454:ILE:HG21	1.97	0.44
1:D:10:ASP:OD1	1:D:11:MET:N	2.50	0.44
1:E:17:MET:HB2	1:E:71:GLY:HA3	1.99	0.44
1:G:233:ASP:O	1:G:237:ILE:HG13	2.18	0.44
1:H:216:TYR:OH	1:H:267:LYS:NZ	2.43	0.44
1:L:484:ASN:HB3	1:L:487:THR:HG22	1.99	0.44
1:H:515:VAL:HA	1:H:518:THR:HG22	1.98	0.44
1:I:104:GLY:HA2	1:I:445:ILE:HD13	1.99	0.44
1:J:393:LYS:O	1:J:397:VAL:HG13	2.17	0.44
1:J:78:ALA:HB2	1:J:515:VAL:HG11	2.00	0.44
1:B:364:GLU:HA	1:B:367:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ASP:OD1	1:E:186:ASP:N	2.51	0.44
1:E:251:MET:CG	1:E:277:ILE:HG23	2.44	0.44
1:G:216:TYR:HB3	1:G:219:CYS:SG	2.57	0.44
1:H:266:ASN:HB3	1:H:272:LEU:HB3	1.99	0.44
1:K:187:GLN:HB3	1:K:381:GLN:HB2	1.99	0.44
1:A:181:GLY:HA2	1:A:182:LYS:HA	1.69	0.44
1:D:180:GLU:HA	1:D:382:VAL:HG12	1.99	0.44
1:F:254:GLU:CA	1:F:278:LYS:NZ	2.79	0.44
1:G:51:VAL:HG11	1:G:56:THR:HB	1.99	0.44
1:H:181:GLY:HA2	1:H:182:LYS:HA	1.64	0.44
1:H:314:THR:O	1:H:317:VAL:HG22	2.18	0.44
1:I:517:LYS:O	1:I:521:LEU:HB2	2.18	0.44
1:J:436:ASP:OD1	1:J:436:ASP:N	2.51	0.44
1:J:51:VAL:HG11	1:J:56:THR:HB	1.98	0.44
1:B:432:ARG:HA	1:B:432:ARG:HD3	1.87	0.44
1:G:209:PRO:HA	1:G:212:MET:H	1.83	0.44
1:H:221:ILE:HA	1:H:249:LEU:HB2	1.98	0.44
1:H:217:GLU:HG2	1:H:323:LYS:HG2	2.00	0.44
1:N:348:LYS:HE2	1:N:348:LYS:HB3	1.85	0.44
1:C:517:LYS:O	1:C:521:LEU:HB2	2.18	0.44
1:E:215:GLU:O	1:E:216:TYR:HD1	2.01	0.44
1:E:346:ARG:HD2	1:E:346:ARG:HA	1.77	0.44
1:E:420:LEU:HD22	1:E:450:LEU:HD22	1.99	0.44
1:G:159:ILE:HG12	1:G:397:VAL:HG12	1.99	0.44
1:G:276:ALA:O	1:G:277:ILE:HG22	2.13	0.44
1:G:376:GLY:O	1:G:377:VAL:HG23	2.18	0.44
1:K:172:ARG:O	1:K:174:GLY:N	2.51	0.44
1:M:21:VAL:HG13	1:M:75:VAL:HG21	2.00	0.44
1:A:159:ILE:HG12	1:A:397:VAL:HG12	1.99	0.44
1:B:376:GLY:O	1:B:377:VAL:HG23	2.18	0.44
1:B:65:ASP:HB3	1:B:68:GLU:HG2	2.00	0.44
1:C:104:GLY:HA3	1:C:520:LEU:HD21	2.00	0.44
1:E:225:ASP:HB2	1:E:290:LEU:HD22	2.00	0.44
1:F:20:GLY:HA3	1:F:68:GLU:HB2	2.00	0.44
1:J:216:TYR:HB3	1:J:219:CYS:SG	2.58	0.44
1:N:393:LYS:O	1:N:397:VAL:HG13	2.18	0.44
1:C:202:SER:HA	1:C:203:PRO:HD3	1.86	0.43
1:C:376:GLY:O	1:C:377:VAL:CG2	2.66	0.43
1:D:113:ASN:HA	1:D:114:PRO:HD3	1.85	0.43
1:E:193:GLY:HA3	1:E:377:VAL:HB	1.99	0.43
1:E:205:PHE:C	1:E:206:VAL:CG2	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:PHE:CD1	1:E:267:LYS:HG2	2.49	0.43
1:E:327:THR:OG1	1:E:328:LYS:N	2.46	0.43
1:G:324:ILE:HD12	1:G:333:VAL:HG12	1.99	0.43
1:J:186:ASP:OD1	1:J:186:ASP:N	2.51	0.43
1:J:283:GLY:H	1:J:286:ARG:NH1	2.16	0.43
1:L:410:GLU:HB2	1:L:503:LYS:HB2	1.99	0.43
1:C:21:VAL:HG13	1:C:75:VAL:HG21	2.01	0.43
1:J:206:VAL:HG11	1:J:212:MET:HB2	1.98	0.43
1:M:220:LYS:HD2	1:M:318:LEU:HD13	1.99	0.43
1:E:10:ASP:CG	1:E:11:MET:H	2.21	0.43
1:E:198:ARG:HG2	1:E:280:PRO:HB3	2.00	0.43
1:H:208:ASP:HA	1:H:209:PRO:HD2	1.90	0.43
1:J:433:ARG:HA	1:J:434:MET:HA	1.79	0.43
1:N:189:VAL:HB	1:N:379:ILE:HG23	2.00	0.43
1:E:222:LEU:HD13	1:E:237:ILE:HD13	2.00	0.43
1:F:364:GLU:HA	1:F:367:GLN:HB2	2.00	0.43
1:H:277:ILE:HD12	1:H:278:LYS:H	1.83	0.43
1:I:413:VAL:HG13	1:I:502:SER:HB2	2.01	0.43
1:J:157:THR:OG1	1:J:158:ASP:N	2.50	0.43
1:K:104:GLY:HA3	1:K:520:LEU:HD21	2.01	0.43
1:B:393:LYS:O	1:B:397:VAL:HG13	2.17	0.43
1:C:186:ASP:N	1:C:186:ASP:OD1	2.52	0.43
1:C:393:LYS:O	1:C:397:VAL:HG13	2.18	0.43
1:E:233:ASP:C	1:E:235:ILE:H	2.22	0.43
1:E:51:VAL:HG11	1:E:56:THR:HB	2.01	0.43
1:F:365:LYS:HA	1:F:368:GLU:HG2	2.00	0.43
1:G:186:ASP:N	1:G:186:ASP:OD1	2.51	0.43
1:M:218:ASN:N	1:M:322:ALA:O	2.32	0.43
1:N:186:ASP:N	1:N:186:ASP:OD1	2.51	0.43
1:A:119:ARG:NH1	1:A:119:ARG:O	2.52	0.43
1:B:225:ASP:HB3	1:B:290:LEU:HD21	2.00	0.43
1:C:55:VAL:HG22	1:C:90:THR:HG21	2.00	0.43
1:D:348:LYS:HE2	1:D:348:LYS:HB3	1.87	0.43
1:E:205:PHE:CZ	1:E:268:LEU:CA	3.01	0.43
1:E:215:GLU:O	1:E:216:TYR:CD1	2.72	0.43
1:G:165:ASP:HA	1:G:168:ALA:HB3	2.00	0.43
1:G:181:GLY:HA2	1:G:182:LYS:HA	1.67	0.43
1:L:393:LYS:O	1:L:397:VAL:HG13	2.18	0.43
1:A:51:VAL:HG11	1:A:56:THR:HB	2.00	0.43
1:D:194:MET:HE1	1:D:373:LEU:HA	2.00	0.43
1:F:159:ILE:HG12	1:F:397:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:ASP:OD1	1:G:304:ASP:N	2.52	0.43
1:I:181:GLY:HA2	1:I:182:LYS:HA	1.66	0.43
1:K:283:GLY:H	1:K:286:ARG:NH1	2.16	0.43
1:M:217:GLU:HG2	1:M:323:LYS:HG2	2.00	0.43
1:B:181:GLY:HA2	1:B:182:LYS:HA	1.70	0.43
1:C:491:GLU:HB3	1:C:496:THR:HG21	2.00	0.43
1:D:117:LEU:O	1:D:121:MET:HG3	2.19	0.43
1:E:181:GLY:HA2	1:E:182:LYS:HA	1.65	0.43
1:E:205:PHE:CE1	1:E:267:LYS:NZ	2.82	0.43
1:E:220:LYS:HG2	1:E:248:LEU:HD13	2.00	0.43
1:E:313:ALA:O	1:E:314:THR:OG1	2.31	0.43
1:G:10:ASP:OD1	1:G:11:MET:N	2.51	0.43
1:I:436:ASP:N	1:I:436:ASP:OD1	2.52	0.43
1:J:233:ASP:O	1:J:236:THR:OG1	2.35	0.43
1:L:186:ASP:N	1:L:186:ASP:OD1	2.52	0.43
1:L:88:ASP:OD1	1:L:89:GLY:N	2.41	0.43
1:M:186:ASP:OD1	1:M:186:ASP:N	2.52	0.43
1:N:17:MET:HB2	1:N:71:GLY:HA3	2.00	0.43
1:A:266:ASN:HB3	1:A:272:LEU:HB3	2.01	0.43
1:A:41:LEU:HA	1:C:526:VAL:HG22	2.00	0.43
1:E:339:THR:HG22	1:E:342:ASP:H	1.83	0.43
1:E:285:ARG:HE	1:E:365:LYS:HE2	1.84	0.43
1:F:306:MET:N	1:F:307:GLY:HA2	2.32	0.43
1:F:432:ARG:HD3	1:F:432:ARG:HA	1.87	0.43
1:J:232:ARG:H	1:J:232:ARG:HD2	1.84	0.43
1:J:21:VAL:HG13	1:J:75:VAL:HG21	1.99	0.43
1:K:277:ILE:HD12	1:K:278:LYS:H	1.81	0.43
1:L:218:ASN:N	1:L:322:ALA:O	2.29	0.43
1:B:104:GLY:HA3	1:B:520:LEU:HD21	2.00	0.43
1:D:9:LYS:HG2	1:D:524:VAL:HG22	2.01	0.43
1:I:202:SER:HB3	1:I:204:TYR:HD1	1.84	0.43
1:I:285:ARG:NH2	1:I:368:GLU:OE2	2.52	0.43
1:J:208:ASP:HA	1:J:209:PRO:HD2	1.88	0.43
1:M:428:ASP:N	1:M:428:ASP:OD1	2.52	0.43
1:N:517:LYS:O	1:N:521:LEU:HB2	2.19	0.43
1:A:61:VAL:O	1:A:76:ARG:NH1	2.52	0.42
1:D:517:LYS:O	1:D:521:LEU:HB2	2.19	0.42
1:G:436:ASP:OD1	1:G:436:ASP:N	2.52	0.42
1:H:174:GLY:HA3	1:H:175:VAL:HA	1.85	0.42
1:I:348:LYS:HB3	1:I:348:LYS:HE2	1.88	0.42
1:K:202:SER:HA	1:K:203:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ALA:HA	1:K:48:PRO:HD3	1.85	0.42
1:L:237:ILE:HG12	1:L:313:ALA:HB3	2.00	0.42
1:C:225:ASP:HB3	1:C:290:LEU:HD21	2.02	0.42
1:E:204:TYR:HD1	1:E:204:TYR:HA	1.71	0.42
1:F:10:ASP:CG	1:F:11:MET:H	2.21	0.42
1:I:350:ILE:HG12	1:I:369:ARG:HH21	1.84	0.42
1:J:244:GLY:O	1:J:246:TYR:N	2.52	0.42
1:L:225:ASP:HB3	1:L:290:LEU:HD21	2.01	0.42
1:L:296:LEU:HG	1:L:343:VAL:HG22	2.01	0.42
1:N:225:ASP:HB3	1:N:290:LEU:HD21	2.01	0.42
1:C:376:GLY:C	1:C:377:VAL:HG23	2.40	0.42
1:E:203:PRO:CG	1:E:205:PHE:O	2.66	0.42
1:E:300:THR:O	1:E:302:VAL:HG23	2.19	0.42
1:I:180:GLU:HA	1:I:382:VAL:HG12	2.01	0.42
1:M:208:ASP:HA	1:M:209:PRO:HD2	1.89	0.42
1:N:104:GLY:HA3	1:N:520:LEU:HD21	2.01	0.42
1:B:159:ILE:HG12	1:B:397:VAL:HG12	2.01	0.42
1:C:169:LYS:HD2	1:C:169:LYS:HA	1.94	0.42
1:D:38:ASN:OD1	1:D:52:ASN:ND2	2.53	0.42
1:F:88:ASP:OD1	1:F:89:GLY:N	2.44	0.42
1:H:193:GLY:HA3	1:H:377:VAL:HB	2.02	0.42
1:H:23:LYS:HD3	1:H:23:LYS:HA	1.89	0.42
1:I:419:THR:HA	1:I:422:ARG:HD3	2.01	0.42
1:C:10:ASP:CG	1:C:11:MET:H	2.23	0.42
1:E:55:VAL:HG22	1:E:90:THR:HG21	2.01	0.42
1:F:186:ASP:OD1	1:F:186:ASP:N	2.52	0.42
1:H:21:VAL:HG13	1:H:75:VAL:HG21	2.01	0.42
1:N:21:VAL:HG11	1:N:101:ILE:HD12	2.02	0.42
1:A:515:VAL:O	1:A:519:PHE:HB2	2.18	0.42
1:B:224:VAL:HG12	1:B:225:ASP:H	1.83	0.42
1:B:421:LEU:HD11	1:B:454:ILE:HG21	2.01	0.42
1:B:61:VAL:O	1:B:76:ARG:NH1	2.52	0.42
1:C:157:THR:OG1	1:C:158:ASP:N	2.52	0.42
1:C:202:SER:HB3	1:C:204:TYR:HD1	1.85	0.42
1:D:169:LYS:HD2	1:D:169:LYS:HA	1.94	0.42
1:E:267:LYS:CE	1:E:273:LYS:HG3	2.45	0.42
1:E:295:ILE:HG23	1:E:342:ASP:OD1	2.20	0.42
1:E:221:ILE:HG13	1:E:319:GLY:O	2.19	0.42
1:F:350:ILE:HG23	1:F:366:LEU:HD22	2.02	0.42
1:G:194:MET:HE1	1:G:373:LEU:HA	2.01	0.42
1:A:4:GLU:O	1:A:528:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:CG2	1:B:326:ILE:HD13	2.48	0.42
1:E:251:MET:HG3	1:E:277:ILE:HG13	2.01	0.42
1:E:348:LYS:HE2	1:E:348:LYS:HB3	1.88	0.42
1:F:277:ILE:HD12	1:F:278:LYS:C	2.39	0.42
1:G:419:THR:HA	1:G:422:ARG:HD3	2.02	0.42
1:I:433:ARG:HA	1:I:434:MET:HA	1.80	0.42
1:K:200:TYR:HA	1:K:277:ILE:HA	2.02	0.42
1:M:436:ASP:OD1	1:M:436:ASP:N	2.53	0.42
1:D:208:ASP:HA	1:D:209:PRO:HD2	1.88	0.42
1:E:267:LYS:HD3	1:E:274:VAL:O	2.20	0.42
1:G:73:THR:HA	1:G:76:ARG:HD3	2.00	0.42
1:J:432:ARG:HA	1:J:432:ARG:HD3	1.90	0.42
1:J:55:VAL:HG22	1:J:90:THR:HG21	2.01	0.42
1:D:350:ILE:HG23	1:D:366:LEU:HD22	2.02	0.42
1:H:223:LEU:HD23	1:H:290:LEU:HB2	2.02	0.42
1:J:181:GLY:HA2	1:J:182:LYS:HA	1.67	0.42
1:L:181:GLY:HA2	1:L:182:LYS:HA	1.73	0.42
1:A:169:LYS:HA	1:A:169:LYS:HD2	1.95	0.42
1:A:433:ARG:HA	1:A:434:MET:HA	1.75	0.42
1:E:301:VAL:CB	1:E:302:VAL:HA	2.31	0.42
1:I:350:ILE:HG23	1:I:366:LEU:HD22	2.01	0.42
1:J:515:VAL:HA	1:J:518:THR:HG22	2.02	0.42
1:L:233:ASP:O	1:L:237:ILE:HG13	2.19	0.42
1:L:385:GLN:HB2	1:L:389:GLU:HG2	2.02	0.42
1:M:225:ASP:HB3	1:M:290:LEU:HD21	2.00	0.42
1:M:276:ALA:C	1:M:277:ILE:HG13	2.40	0.42
1:A:104:GLY:HA3	1:A:520:LEU:HD21	2.02	0.41
1:A:55:VAL:HG22	1:A:90:THR:HG21	2.02	0.41
1:D:277:ILE:HD13	1:D:277:ILE:HA	1.84	0.41
1:D:484:ASN:HB3	1:D:487:THR:HG22	2.01	0.41
1:E:277:ILE:HD12	1:E:278:LYS:CA	2.30	0.41
1:F:221:ILE:HG13	1:F:249:LEU:HB3	2.02	0.41
1:F:357:THR:HB	1:F:363:ARG:HD3	2.02	0.41
1:F:180:GLU:HA	1:F:382:VAL:HG12	2.02	0.41
1:G:283:GLY:H	1:G:286:ARG:NH1	2.18	0.41
1:H:482:GLY:HA3	1:H:493:LEU:HG	2.02	0.41
1:J:174:GLY:HA3	1:J:175:VAL:HA	1.85	0.41
1:J:223:LEU:HD21	1:J:294:ALA:HB2	2.01	0.41
1:J:419:THR:HA	1:J:422:ARG:HD3	2.02	0.41
1:N:202:SER:HA	1:N:203:PRO:HD3	1.86	0.41
1:D:202:SER:HA	1:D:203:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ASP:O	1:D:237:ILE:HG13	2.20	0.41
1:I:217:GLU:HG2	1:I:323:LYS:HG2	2.01	0.41
1:K:338:SER:OG	1:K:339:THR:N	2.45	0.41
1:M:165:ASP:HA	1:M:168:ALA:HB3	2.02	0.41
1:B:278:LYS:HZ3	1:B:279:ALA:N	2.19	0.41
1:C:348:LYS:HE2	1:C:348:LYS:HB3	1.84	0.41
1:D:283:GLY:H	1:D:286:ARG:NH1	2.18	0.41
1:D:334:VAL:HG23	1:D:377:VAL:CB	2.47	0.41
1:F:113:ASN:HA	1:F:114:PRO:HD3	1.86	0.41
1:H:209:PRO:HA	1:H:212:MET:H	1.85	0.41
1:I:277:ILE:HG22	1:I:278:LYS:N	2.33	0.41
1:I:296:LEU:HG	1:I:343:VAL:HG22	2.02	0.41
1:L:206:VAL:HB	1:L:212:MET:HA	2.03	0.41
1:L:364:GLU:HA	1:L:367:GLN:HB2	2.02	0.41
1:C:165:ASP:HA	1:C:168:ALA:HB3	2.01	0.41
1:C:209:PRO:HA	1:C:212:MET:H	1.85	0.41
1:C:234:ILE:O	1:C:238:LEU:N	2.49	0.41
1:C:253:GLU:H	1:C:279:ALA:HB2	1.85	0.41
1:F:220:LYS:HA	1:F:320:THR:HA	2.02	0.41
1:F:24:LEU:HD11	1:F:76:ARG:HG3	2.01	0.41
1:F:436:ASP:OD1	1:F:436:ASP:N	2.50	0.41
1:G:285:ARG:NH2	1:G:368:GLU:OE2	2.53	0.41
1:H:251:MET:HB3	1:H:277:ILE:CG1	2.49	0.41
1:H:73:THR:HA	1:H:76:ARG:HD3	2.02	0.41
1:J:303:ARG:HG2	1:J:305:GLU:HB2	2.01	0.41
1:M:119:ARG:O	1:M:119:ARG:NH1	2.53	0.41
1:M:47:ALA:HA	1:M:48:PRO:HD3	1.89	0.41
1:N:104:GLY:O	1:N:108:VAL:HG23	2.21	0.41
1:A:194:MET:HE1	1:A:373:LEU:HA	2.03	0.41
1:A:224:VAL:HG12	1:A:225:ASP:H	1.86	0.41
1:A:296:LEU:HG	1:A:343:VAL:HG22	2.02	0.41
1:C:125:VAL:HG11	1:C:513:VAL:HG21	2.01	0.41
1:G:202:SER:HA	1:G:203:PRO:HD3	1.87	0.41
1:I:365:LYS:HA	1:I:368:GLU:HG2	2.02	0.41
1:I:428:ASP:OD1	1:I:428:ASP:N	2.48	0.41
1:J:306:MET:HB2	1:J:307:GLY:HA2	2.03	0.41
1:J:515:VAL:O	1:J:519:PHE:HB2	2.19	0.41
1:N:276:ALA:O	1:N:277:ILE:HG22	2.12	0.41
1:A:209:PRO:HA	1:A:212:MET:H	1.84	0.41
1:A:350:ILE:HG23	1:A:366:LEU:HD22	2.02	0.41
1:A:376:GLY:O	1:A:377:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ASP:HA	1:E:168:ALA:HB3	2.02	0.41
1:F:51:VAL:HG11	1:F:56:THR:HB	2.02	0.41
1:F:9:LYS:HG2	1:F:524:VAL:HG13	2.03	0.41
1:J:169:LYS:HA	1:J:169:LYS:HD2	1.95	0.41
1:A:83:ASN:HB2	1:A:90:THR:HG22	2.02	0.41
1:B:240:SER:OG	1:B:243:ARG:NH1	2.54	0.41
1:B:47:ALA:HA	1:B:48:PRO:HD3	1.84	0.41
1:C:433:ARG:HA	1:C:434:MET:HA	1.77	0.41
1:E:175:VAL:HG13	1:E:377:VAL:HG13	2.01	0.41
1:H:218:ASN:N	1:H:322:ALA:O	2.28	0.41
1:J:218:ASN:N	1:J:322:ALA:O	2.37	0.41
1:L:142:ASP:OD1	1:L:142:ASP:N	2.52	0.41
1:N:419:THR:HA	1:N:422:ARG:HD3	2.03	0.41
1:N:436:ASP:N	1:N:436:ASP:OD1	2.54	0.41
1:A:385:GLN:HB2	1:A:389:GLU:HG2	2.03	0.41
1:A:484:ASN:HB3	1:A:487:THR:HG22	2.03	0.41
1:D:436:ASP:N	1:D:436:ASP:OD1	2.51	0.41
1:E:238:LEU:O	1:E:242:ILE:HG13	2.21	0.41
1:H:293:ILE:HD12	1:H:296:LEU:HD13	2.03	0.41
1:I:237:ILE:HG12	1:I:313:ALA:HB3	2.03	0.41
1:I:482:GLY:HA3	1:I:493:LEU:HG	2.02	0.41
1:K:225:ASP:HB3	1:K:290:LEU:HD21	2.03	0.41
1:M:410:GLU:HB2	1:M:503:LYS:HB2	2.03	0.41
1:B:376:GLY:O	1:B:377:VAL:CG2	2.69	0.41
1:D:491:GLU:HB3	1:D:496:THR:HG21	2.02	0.41
1:E:251:MET:HG3	1:E:277:ILE:CG1	2.51	0.41
1:F:119:ARG:NH1	1:F:119:ARG:O	2.53	0.41
1:G:206:VAL:HG23	1:G:206:VAL:O	2.21	0.41
1:G:348:LYS:HE2	1:G:348:LYS:HB3	1.87	0.41
1:I:303:ARG:HE	1:I:305:GLU:HB2	1.85	0.41
1:K:393:LYS:O	1:K:397:VAL:HG13	2.21	0.41
1:L:428:ASP:OD1	1:L:428:ASP:N	2.54	0.41
1:A:165:ASP:HA	1:A:168:ALA:HB3	2.02	0.41
1:A:21:VAL:HG13	1:A:75:VAL:HG21	2.03	0.41
1:A:233:ASP:O	1:A:237:ILE:HG13	2.20	0.41
1:B:113:ASN:HA	1:B:114:PRO:HD3	1.91	0.41
1:B:410:GLU:HB2	1:B:503:LYS:HB2	2.03	0.41
1:B:20:GLY:HA3	1:B:68:GLU:HB2	2.03	0.41
1:B:73:THR:HA	1:B:76:ARG:HD3	2.03	0.41
1:C:233:ASP:O	1:C:237:ILE:HG13	2.20	0.41
1:D:186:ASP:N	1:D:186:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:SER:N	1:E:203:PRO:CA	2.84	0.41
1:F:306:MET:H	1:F:307:GLY:HA2	1.86	0.41
1:I:78:ALA:HB2	1:I:515:VAL:HG11	2.03	0.41
1:J:310:LEU:HB3	1:J:311:GLU:H	1.66	0.41
1:K:10:ASP:OD1	1:K:11:MET:N	2.47	0.41
1:M:277:ILE:HG22	1:M:278:LYS:N	2.35	0.41
1:N:249:LEU:HD13	1:N:275:VAL:HB	2.03	0.41
1:A:189:VAL:HB	1:A:379:ILE:HG23	2.03	0.41
1:B:209:PRO:HA	1:B:212:MET:H	1.86	0.41
1:C:296:LEU:HG	1:C:343:VAL:HG22	2.03	0.41
1:C:364:GLU:HA	1:C:367:GLN:HB2	2.03	0.41
1:E:211:ARG:O	1:E:212:MET:SD	2.79	0.41
1:F:231:ALA:O	1:F:235:ILE:HG23	2.21	0.41
1:K:125:VAL:HG11	1:K:513:VAL:HG21	2.01	0.41
1:K:233:ASP:O	1:K:237:ILE:HG13	2.21	0.41
1:L:348:LYS:HB3	1:L:348:LYS:HE2	1.82	0.41
1:M:363:ARG:HD2	1:M:363:ARG:HA	1.95	0.41
1:N:283:GLY:H	1:N:286:ARG:NH1	2.19	0.41
1:N:350:ILE:HG23	1:N:366:LEU:HD22	2.02	0.41
1:C:208:ASP:HA	1:C:209:PRO:HD2	1.91	0.40
1:E:517:LYS:O	1:E:521:LEU:HB2	2.20	0.40
1:E:4:GLU:O	1:E:528:GLU:HG3	2.21	0.40
1:F:206:VAL:O	1:F:206:VAL:HG23	2.21	0.40
1:H:9:LYS:HG2	1:H:524:VAL:HG22	2.03	0.40
1:H:65:ASP:HA	1:H:66:PRO:HD3	1.92	0.40
1:M:206:VAL:O	1:M:206:VAL:HG23	2.21	0.40
1:B:165:ASP:HA	1:B:168:ALA:HB3	2.03	0.40
1:C:206:VAL:O	1:C:206:VAL:HG23	2.21	0.40
1:C:266:ASN:HB3	1:C:272:LEU:HB3	2.03	0.40
1:D:224:VAL:HG12	1:D:225:ASP:H	1.87	0.40
1:D:394:LYS:O	1:D:398:GLU:HB2	2.21	0.40
1:E:262:THR:O	1:E:266:ASN:ND2	2.30	0.40
1:E:312:GLN:O	1:E:314:THR:HG23	2.22	0.40
1:F:304:ASP:N	1:F:304:ASP:OD1	2.54	0.40
1:G:225:ASP:HB3	1:G:290:LEU:HD21	2.02	0.40
1:I:225:ASP:HB3	1:I:290:LEU:HD21	2.03	0.40
1:I:194:MET:HE1	1:I:373:LEU:HA	2.03	0.40
1:I:104:GLY:HA3	1:I:520:LEU:HD21	2.02	0.40
1:J:283:GLY:H	1:J:286:ARG:CZ	2.35	0.40
1:N:10:ASP:CG	1:N:11:MET:H	2.25	0.40
1:D:118:VAL:HG21	1:D:517:LYS:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ARG:HD3	1:D:432:ARG:HA	1.85	0.40
1:E:505:VAL:O	1:E:509:MET:HB2	2.21	0.40
1:F:189:VAL:HB	1:F:379:ILE:HG23	2.03	0.40
1:H:157:THR:O	1:H:160:GLY:N	2.53	0.40
1:I:410:GLU:HB2	1:I:503:LYS:HB2	2.02	0.40
1:J:202:SER:HB3	1:J:204:TYR:HD1	1.86	0.40
1:K:161:SER:O	1:K:164:SER:OG	2.34	0.40
1:M:482:GLY:HA3	1:M:493:LEU:HG	2.04	0.40
1:A:413:VAL:HG13	1:A:502:SER:HB2	2.03	0.40
1:A:78:ALA:HB2	1:A:515:VAL:HG11	2.04	0.40
1:D:159:ILE:HG12	1:D:397:VAL:HG12	2.02	0.40
1:D:193:GLY:CA	1:D:377:VAL:CG1	2.93	0.40
1:E:357:THR:HB	1:E:363:ARG:HD3	2.04	0.40
1:F:237:ILE:HG12	1:F:313:ALA:HB3	2.03	0.40
1:H:224:VAL:HG12	1:H:225:ASP:H	1.87	0.40
1:I:250:ILE:C	1:I:277:ILE:CD1	2.79	0.40
1:K:237:ILE:HG12	1:K:313:ALA:HB3	2.02	0.40
1:L:180:GLU:HA	1:L:382:VAL:HG12	2.03	0.40
1:M:17:MET:HB2	1:M:71:GLY:HA3	2.04	0.40
1:N:123:LYS:HA	1:N:123:LYS:HD2	1.86	0.40
1:N:224:VAL:HG12	1:N:225:ASP:H	1.86	0.40
1:C:221:ILE:HG13	1:C:249:LEU:HB3	2.03	0.40
1:D:193:GLY:HA3	1:D:377:VAL:HG12	1.98	0.40
1:D:206:VAL:O	1:D:206:VAL:HG23	2.21	0.40
1:D:236:THR:OG1	1:D:311:GLU:O	2.40	0.40
1:H:186:ASP:OD1	1:H:186:ASP:N	2.52	0.40
1:I:125:VAL:HG11	1:I:513:VAL:HG21	2.04	0.40
1:J:125:VAL:HG11	1:J:513:VAL:HG21	2.03	0.40
1:K:436:ASP:OD1	1:K:436:ASP:N	2.54	0.40
1:L:104:GLY:HA2	1:L:445:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

## 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	526/552 (95%)	480 (91%)	40 (8%)	6 (1%)	14	51
1	B	526/552 (95%)	473 (90%)	46 (9%)	7 (1%)	12	48
1	C	526/552 (95%)	479 (91%)	40 (8%)	7 (1%)	12	48
1	D	526/552 (95%)	479 (91%)	42 (8%)	5 (1%)	15	52
1	E	526/552 (95%)	472 (90%)	40 (8%)	14 (3%)	5	35
1	F	526/552 (95%)	480 (91%)	42 (8%)	4 (1%)	19	57
1	G	526/552 (95%)	483 (92%)	37 (7%)	6 (1%)	14	51
1	H	526/552 (95%)	478 (91%)	43 (8%)	5 (1%)	15	52
1	I	526/552 (95%)	482 (92%)	39 (7%)	5 (1%)	15	52
1	J	526/552 (95%)	480 (91%)	42 (8%)	4 (1%)	19	57
1	K	526/552 (95%)	478 (91%)	43 (8%)	5 (1%)	15	52
1	L	526/552 (95%)	478 (91%)	43 (8%)	5 (1%)	15	52
1	M	526/552 (95%)	475 (90%)	47 (9%)	4 (1%)	19	57
1	N	526/552 (95%)	480 (91%)	42 (8%)	4 (1%)	19	57
All	All	7364/7728 (95%)	6697 (91%)	586 (8%)	81 (1%)	14	51

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	173	THR
1	A	245	ASN
1	N	158	ASP
1	N	173	THR
1	N	245	ASN
1	N	277	ILE
1	B	158	ASP
1	B	173	THR
1	B	245	ASN
1	B	281	GLY
1	C	158	ASP
1	C	173	THR
1	C	245	ASN
1	C	277	ILE
1	D	158	ASP

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Mol	Chain	Res	Type
1	D	173	THR
1	D	245	ASN
1	E	173	THR
1	E	247	PRO
1	F	173	THR
1	F	245	ASN
1	G	158	ASP
1	G	173	THR
1	G	245	ASN
1	G	277	ILE
1	H	173	THR
1	H	277	ILE
1	I	158	ASP
1	I	173	THR
1	I	245	ASN
1	J	158	ASP
1	J	173	THR
1	K	158	ASP
1	K	173	THR
1	K	245	ASN
1	K	277	ILE
1	L	158	ASP
1	L	173	THR
1	L	245	ASN
1	L	277	ILE
1	M	173	THR
1	M	245	ASN
1	A	277	ILE
1	B	377	VAL
1	E	232	ARG
1	E	256	GLU
1	E	301	VAL
1	F	377	VAL
1	H	245	ASN
1	J	245	ASN
1	B	280	PRO
1	C	253	GLU
1	C	377	VAL
1	E	202	SER
1	E	314	THR
1	G	377	VAL
1	M	158	ASP

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Mol	Chain	Res	Type
1	D	184	ALA
1	E	158	ASP
1	E	257	GLN
1	G	184	ALA
1	A	184	ALA
1	A	377	VAL
1	B	184	ALA
1	D	157	THR
1	E	253	GLU
1	E	530	LYS
1	F	530	LYS
1	I	530	LYS
1	K	377	VAL
1	C	530	LYS
1	E	184	ALA
1	H	158	ASP
1	L	377	VAL
1	E	171	GLY
1	E	234	ILE
1	J	377	VAL
1	H	377	VAL
1	M	377	VAL
1	I	377	VAL

### 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	433/445 (97%)	422 (98%)	11 (2%)	47	70
1	B	433/445 (97%)	424 (98%)	9 (2%)	53	74
1	C	433/445 (97%)	424 (98%)	9 (2%)	53	74
1	D	433/445 (97%)	422 (98%)	11 (2%)	47	70
1	E	433/445 (97%)	410 (95%)	23 (5%)	22	54
1	F	433/445 (97%)	422 (98%)	11 (2%)	47	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	433/445 (97%)	421 (97%)	12 (3%)	43	68
1	H	433/445 (97%)	421 (97%)	12 (3%)	43	68
1	I	433/445 (97%)	420 (97%)	13 (3%)	41	66
1	J	433/445 (97%)	422 (98%)	11 (2%)	47	70
1	K	433/445 (97%)	424 (98%)	9 (2%)	53	74
1	L	433/445 (97%)	420 (97%)	13 (3%)	41	66
1	M	433/445 (97%)	421 (97%)	12 (3%)	43	68
1	N	433/445 (97%)	425 (98%)	8 (2%)	59	77
All	All	6062/6230 (97%)	5898 (97%)	164 (3%)	44	69

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	128	LEU
1	A	178	MET
1	A	223	LEU
1	A	268	LEU
1	A	304	ASP
1	A	305	GLU
1	A	412	VAL
1	A	435	THR
1	A	480	HIS
1	A	521	LEU
1	N	67	VAL
1	N	223	LEU
1	N	255	VAL
1	N	304	ASP
1	N	305	GLU
1	N	412	VAL
1	N	435	THR
1	N	521	LEU
1	B	128	LEU
1	B	223	LEU
1	B	278	LYS
1	B	304	ASP
1	B	305	GLU
1	B	412	VAL
1	B	435	THR

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Mol	Chain	Res	Type
1	B	492	ASN
1	B	521	LEU
1	C	105	MET
1	C	223	LEU
1	C	268	LEU
1	C	304	ASP
1	C	305	GLU
1	C	412	VAL
1	C	435	THR
1	C	460	ASN
1	C	521	LEU
1	D	5	LEU
1	D	67	VAL
1	D	223	LEU
1	D	268	LEU
1	D	277	ILE
1	D	304	ASP
1	D	305	GLU
1	D	367	GLN
1	D	412	VAL
1	D	435	THR
1	D	521	LEU
1	E	5	LEU
1	E	200	TYR
1	E	201	THR
1	E	204	TYR
1	E	205	PHE
1	E	207	THR
1	E	211	ARG
1	E	212	MET
1	E	215	GLU
1	E	216	TYR
1	E	245	ASN
1	E	253	GLU
1	E	277	ILE
1	E	295	ILE
1	E	301	VAL
1	E	315	ASP
1	E	318	LEU
1	E	342	ASP
1	E	367	GLN
1	E	373	LEU

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Mol	Chain	Res	Type
1	E	412	VAL
1	E	435	THR
1	E	480	HIS
1	F	5	LEU
1	F	67	VAL
1	F	223	LEU
1	F	235	ILE
1	F	268	LEU
1	F	277	ILE
1	F	302	VAL
1	F	304	ASP
1	F	412	VAL
1	F	435	THR
1	F	521	LEU
1	G	67	VAL
1	G	235	ILE
1	G	255	VAL
1	G	268	LEU
1	G	304	ASP
1	G	305	GLU
1	G	318	LEU
1	G	355	MET
1	G	412	VAL
1	G	435	THR
1	G	480	HIS
1	G	521	LEU
1	H	128	LEU
1	H	178	MET
1	H	223	LEU
1	H	255	VAL
1	H	268	LEU
1	H	304	ASP
1	H	305	GLU
1	H	367	GLN
1	H	412	VAL
1	H	435	THR
1	H	460	ASN
1	H	521	LEU
1	I	5	LEU
1	I	206	VAL
1	I	216	TYR
1	I	223	LEU

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Mol	Chain	Res	Type
1	I	268	LEU
1	I	277	ILE
1	I	304	ASP
1	I	305	GLU
1	I	357	THR
1	I	370	ILE
1	I	412	VAL
1	I	435	THR
1	I	521	LEU
1	J	5	LEU
1	J	216	TYR
1	J	223	LEU
1	J	233	ASP
1	J	235	ILE
1	J	255	VAL
1	J	268	LEU
1	J	304	ASP
1	J	412	VAL
1	J	435	THR
1	J	521	LEU
1	K	214	CYS
1	K	223	LEU
1	K	235	ILE
1	K	268	LEU
1	K	304	ASP
1	K	305	GLU
1	K	435	THR
1	K	480	HIS
1	K	521	LEU
1	L	206	VAL
1	L	215	GLU
1	L	223	LEU
1	L	235	ILE
1	L	268	LEU
1	L	304	ASP
1	L	305	GLU
1	L	318	LEU
1	L	348	LYS
1	L	370	ILE
1	L	412	VAL
1	L	435	THR
1	L	521	LEU

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Mol	Chain	Res	Type
1	M	178	MET
1	M	216	TYR
1	M	223	LEU
1	M	235	ILE
1	M	255	VAL
1	M	268	LEU
1	M	277	ILE
1	M	304	ASP
1	M	305	GLU
1	M	435	THR
1	M	480	HIS
1	M	521	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

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	528/552 (95%)	0.41	45 (8%)	10	9	64, 175, 274, 319	0
1	B	528/552 (95%)	0.41	36 (6%)	17	13	49, 165, 283, 325	0
1	C	528/552 (95%)	0.40	41 (7%)	13	10	50, 166, 284, 318	0
1	D	528/552 (95%)	0.31	34 (6%)	19	15	55, 153, 262, 292	0
1	E	528/552 (95%)	0.30	26 (4%)	29	25	26, 159, 234, 301	0
1	F	528/552 (95%)	0.41	35 (6%)	18	14	69, 184, 271, 303	0
1	G	528/552 (95%)	0.56	52 (9%)	7	7	55, 193, 280, 315	0
1	H	528/552 (95%)	0.43	48 (9%)	9	7	57, 182, 288, 319	0
1	I	528/552 (95%)	0.54	61 (11%)	4	5	57, 192, 299, 325	0
1	J	528/552 (95%)	0.51	55 (10%)	6	5	84, 203, 315, 369	0
1	K	528/552 (95%)	0.65	68 (12%)	3	4	71, 189, 307, 340	0
1	L	528/552 (95%)	0.70	77 (14%)	2	2	70, 185, 310, 357	0
1	M	528/552 (95%)	0.71	78 (14%)	2	2	81, 207, 326, 366	0
1	N	528/552 (95%)	0.64	60 (11%)	5	5	77, 194, 294, 335	0
All	All	7392/7728 (95%)	0.50	716 (9%)	7	7	26, 178, 296, 369	0

All (716) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	302	VAL	18.9
1	C	302	VAL	11.9
1	G	316	ALA	10.4
1	M	362	GLU	9.8
1	L	225	ASP	9.1
1	B	302	VAL	8.8
1	G	312	GLN	8.6
1	I	384	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
1	H	302	VAL	8.0
1	K	194	MET	7.9
1	E	272	LEU	7.8
1	M	195	GLN	7.8
1	N	313	ALA	7.6
1	F	307	GLY	7.5
1	K	300	THR	7.4
1	F	308	VAL	7.3
1	N	312	GLN	7.2
1	G	300	THR	7.2
1	L	301	VAL	7.2
1	B	315	ASP	7.1
1	D	302	VAL	7.1
1	G	311	GLU	7.1
1	M	194	MET	7.0
1	K	316	ALA	7.0
1	N	186	ASP	7.0
1	J	302	VAL	6.9
1	H	312	GLN	6.7
1	G	315	ASP	6.7
1	L	312	GLN	6.6
1	K	195	GLN	6.5
1	L	231	ALA	6.5
1	L	223	LEU	6.4
1	N	302	VAL	6.4
1	I	271	THR	6.3
1	A	300	THR	6.3
1	F	306	MET	6.3
1	M	177	THR	6.3
1	K	315	ASP	6.3
1	C	356	GLN	6.3
1	A	312	GLN	6.2
1	A	302	VAL	6.2
1	B	303	ARG	6.1
1	L	275	VAL	6.1
1	L	248	LEU	6.1
1	J	292	ASP	6.0
1	L	316	ALA	6.0
1	L	274	VAL	5.8
1	E	271	THR	5.8
1	N	314	THR	5.8
1	N	190	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
1	G	225	ASP	5.7
1	J	316	ALA	5.7
1	B	356	GLN	5.7
1	J	303	ARG	5.7
1	N	195	GLN	5.7
1	A	270	GLY	5.7
1	N	276	ALA	5.7
1	L	195	GLN	5.7
1	J	315	ASP	5.6
1	L	276	ALA	5.6
1	J	246	TYR	5.6
1	N	275	VAL	5.6
1	A	359	GLN	5.6
1	K	235	ILE	5.5
1	L	311	GLU	5.5
1	L	255	VAL	5.5
1	C	335	GLY	5.4
1	M	335	GLY	5.4
1	M	235	ILE	5.4
1	L	247	PRO	5.4
1	J	194	MET	5.4
1	F	343	VAL	5.4
1	M	361	TYR	5.3
1	C	531	GLU	5.3
1	C	336	ASP	5.3
1	G	246	TYR	5.2
1	J	358	ASP	5.2
1	A	301	VAL	5.2
1	J	273	LYS	5.2
1	M	366	LEU	5.2
1	B	277	ILE	5.1
1	G	195	GLN	5.1
1	J	225	ASP	5.1
1	L	224	VAL	5.1
1	K	301	VAL	5.1
1	L	194	MET	5.1
1	N	315	ASP	5.0
1	M	231	ALA	5.0
1	F	433	ARG	5.0
1	M	334	VAL	5.0
1	D	154	GLY	5.0
1	K	302	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	I	251	MET	4.9
1	I	176	VAL	4.9
1	F	186	ASP	4.8
1	B	359	GLN	4.8
1	N	188	LEU	4.8
1	M	333	VAL	4.8
1	F	4	GLU	4.8
1	A	195	GLN	4.8
1	M	272	LEU	4.8
1	M	313	ALA	4.7
1	I	383	GLY	4.7
1	J	255	VAL	4.7
1	J	335	GLY	4.7
1	B	316	ALA	4.7
1	F	316	ALA	4.7
1	J	300	THR	4.7
1	I	291	GLU	4.6
1	E	186	ASP	4.6
1	G	270	GLY	4.6
1	L	315	ASP	4.6
1	M	280	PRO	4.6
1	B	361	TYR	4.6
1	A	194	MET	4.6
1	J	272	LEU	4.6
1	J	304	ASP	4.5
1	N	370	ILE	4.5
1	K	317	VAL	4.5
1	I	246	TYR	4.5
1	G	226	LYS	4.5
1	N	271	THR	4.4
1	L	303	ARG	4.4
1	K	335	GLY	4.4
1	N	531	GLU	4.4
1	J	301	VAL	4.4
1	B	255	VAL	4.4
1	M	175	VAL	4.4
1	K	171	GLY	4.4
1	M	176	VAL	4.4
1	H	352	ASN	4.3
1	E	359	GLN	4.3
1	C	308	VAL	4.3
1	G	366	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	434	MET	4.3
1	N	422	ARG	4.3
1	G	147	ASN	4.3
1	F	312	GLN	4.3
1	I	496	THR	4.3
1	H	232	ARG	4.3
1	H	239	GLU	4.3
1	L	235	ILE	4.2
1	M	217	GLU	4.2
1	M	379	ILE	4.2
1	F	309	SER	4.2
1	J	343	VAL	4.2
1	K	312	GLN	4.2
1	C	259	ALA	4.2
1	H	248	LEU	4.2
1	N	270	GLY	4.2
1	G	370	ILE	4.1
1	A	338	SER	4.1
1	N	235	ILE	4.1
1	E	196	PHE	4.1
1	A	482	GLY	4.1
1	M	312	GLN	4.1
1	B	232	ARG	4.1
1	J	368	GLU	4.1
1	I	223	LEU	4.1
1	I	316	ALA	4.1
1	G	357	THR	4.1
1	C	227	LYS	4.0
1	G	245	ASN	4.0
1	A	390	LEU	4.0
1	M	223	LEU	4.0
1	B	274	VAL	4.0
1	M	4	GLU	4.0
1	K	216	TYR	4.0
1	A	311	GLU	4.0
1	G	377	VAL	3.9
1	K	147	ASN	3.9
1	D	433	ARG	3.9
1	L	270	GLY	3.9
1	L	356	GLN	3.9
1	B	203	PRO	3.9
1	F	315	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	M	269	ARG	3.8
1	F	305	GLU	3.8
1	N	274	VAL	3.8
1	J	270	GLY	3.8
1	M	370	ILE	3.8
1	N	316	ALA	3.8
1	M	314	THR	3.8
1	D	350	ILE	3.8
1	F	178	MET	3.8
1	L	271	THR	3.8
1	J	357	THR	3.8
1	N	356	GLN	3.8
1	M	302	VAL	3.8
1	H	377	VAL	3.8
1	E	195	GLN	3.8
1	D	349	GLN	3.8
1	H	274	VAL	3.7
1	K	248	LEU	3.7
1	J	271	THR	3.7
1	M	390	LEU	3.7
1	L	226	LYS	3.7
1	L	263	LEU	3.7
1	D	477	ASP	3.7
1	J	342	ASP	3.7
1	K	247	PRO	3.7
1	H	204	TYR	3.7
1	H	335	GLY	3.7
1	L	250	ILE	3.7
1	L	269	ARG	3.7
1	N	317	VAL	3.7
1	L	273	LYS	3.7
1	I	224	VAL	3.7
1	H	223	LEU	3.7
1	L	264	VAL	3.7
1	K	318	LEU	3.7
1	H	235	ILE	3.6
1	I	292	ASP	3.6
1	M	238	LEU	3.6
1	J	274	VAL	3.6
1	E	531	GLU	3.6
1	M	234	ILE	3.6
1	H	271	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	156	ASN	3.6
1	N	277	ILE	3.6
1	G	196	PHE	3.6
1	H	531	GLU	3.6
1	A	362	GLU	3.6
1	L	353	LEU	3.6
1	C	228	ILE	3.6
1	A	361	TYR	3.6
1	J	155	GLY	3.6
1	M	189	VAL	3.6
1	C	301	VAL	3.6
1	B	251	MET	3.6
1	E	357	THR	3.5
1	I	335	GLY	3.5
1	N	366	LEU	3.5
1	N	497	GLY	3.5
1	D	361	TYR	3.5
1	L	334	VAL	3.5
1	M	274	VAL	3.5
1	G	378	ALA	3.5
1	M	296	LEU	3.5
1	L	378	ALA	3.5
1	J	333	VAL	3.5
1	H	224	VAL	3.5
1	I	272	LEU	3.4
1	G	271	THR	3.4
1	L	272	LEU	3.4
1	N	355	MET	3.4
1	K	178	MET	3.4
1	E	335	GLY	3.4
1	L	379	ILE	3.4
1	A	352	ASN	3.4
1	K	234	ILE	3.4
1	I	302	VAL	3.4
1	C	307	GLY	3.4
1	M	273	LYS	3.4
1	N	269	ARG	3.4
1	L	333	VAL	3.4
1	G	335	GLY	3.4
1	I	194	MET	3.4
1	H	350	ILE	3.4
1	M	292	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	255	VAL	3.4
1	B	362	GLU	3.3
1	H	194	MET	3.3
1	L	260	LEU	3.3
1	N	206	VAL	3.3
1	K	176	VAL	3.3
1	H	238	LEU	3.3
1	C	287	SER	3.3
1	D	4	GLU	3.3
1	F	255	VAL	3.3
1	G	272	LEU	3.3
1	L	222	LEU	3.3
1	M	202	SER	3.3
1	L	343	VAL	3.3
1	L	335	GLY	3.3
1	B	140	GLN	3.3
1	N	481	TYR	3.3
1	K	336	ASP	3.3
1	K	343	VAL	3.3
1	J	245	ASN	3.2
1	A	350	ILE	3.2
1	B	384	ALA	3.2
1	L	204	TYR	3.2
1	K	377	VAL	3.2
1	K	277	ILE	3.2
1	A	235	ILE	3.2
1	I	315	ASP	3.2
1	N	332	THR	3.2
1	I	280	PRO	3.2
1	G	215	GLU	3.2
1	K	261	ALA	3.2
1	M	232	ARG	3.2
1	M	218	ASN	3.2
1	G	277	ILE	3.2
1	I	175	VAL	3.2
1	M	213	ILE	3.2
1	K	239	GLU	3.2
1	K	186	ASP	3.1
1	M	523	ASP	3.1
1	N	234	ILE	3.1
1	G	390	LEU	3.1
1	H	280	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	477	ASP	3.1
1	J	308	VAL	3.1
1	A	339	THR	3.1
1	K	353	LEU	3.1
1	B	317	VAL	3.1
1	A	303	ARG	3.1
1	G	213	ILE	3.1
1	K	260	LEU	3.1
1	J	305	GLU	3.1
1	K	262	THR	3.1
1	G	352	ASN	3.1
1	E	370	ILE	3.1
1	I	370	ILE	3.1
1	J	269	ARG	3.1
1	L	186	ASP	3.1
1	I	289	TYR	3.1
1	N	382	VAL	3.1
1	D	155	GLY	3.1
1	J	247	PRO	3.1
1	N	263	LEU	3.1
1	M	221	ILE	3.1
1	K	274	VAL	3.0
1	D	312	GLN	3.0
1	D	301	VAL	3.0
1	K	193	GLY	3.0
1	N	196	PHE	3.0
1	C	258	GLU	3.0
1	I	225	ASP	3.0
1	C	290	LEU	3.0
1	H	387	GLU	3.0
1	M	251	MET	3.0
1	E	356	GLN	3.0
1	M	378	ALA	3.0
1	J	186	ASP	3.0
1	I	287	SER	3.0
1	M	300	THR	3.0
1	L	234	ILE	3.0
1	A	225	ASP	3.0
1	C	343	VAL	2.9
1	I	356	GLN	2.9
1	N	296	LEU	2.9
1	G	302	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	271	THR	2.9
1	I	140	GLN	2.9
1	I	277	ILE	2.9
1	H	291	GLU	2.9
1	C	226	LYS	2.9
1	K	376	GLY	2.9
1	B	433	ARG	2.9
1	F	269	ARG	2.9
1	K	172	ARG	2.9
1	M	204	TYR	2.9
1	I	193	GLY	2.9
1	J	223	LEU	2.9
1	L	519	PHE	2.9
1	A	224	VAL	2.9
1	A	335	GLY	2.9
1	N	251	MET	2.9
1	H	225	ASP	2.9
1	F	377	VAL	2.9
1	J	433	ARG	2.9
1	M	373	LEU	2.9
1	J	193	GLY	2.8
1	H	251	MET	2.8
1	H	364	GLU	2.8
1	B	357	THR	2.8
1	A	384	ALA	2.8
1	L	317	VAL	2.8
1	I	284	GLU	2.8
1	B	228	ILE	2.8
1	F	247	PRO	2.8
1	N	125	VAL	2.8
1	N	176	VAL	2.8
1	E	194	MET	2.8
1	H	366	LEU	2.8
1	I	406	ALA	2.8
1	K	238	LEU	2.8
1	B	304	ASP	2.8
1	A	497	GLY	2.8
1	K	306	MET	2.8
1	G	259	ALA	2.8
1	E	366	LEU	2.8
1	F	346	ARG	2.8
1	E	437	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	276	ALA	2.8
1	M	365	LYS	2.8
1	A	196	PHE	2.8
1	B	282	PHE	2.8
1	G	168	ALA	2.8
1	J	509	MET	2.8
1	B	4	GLU	2.7
1	M	196	PHE	2.7
1	M	248	LEU	2.7
1	L	357	THR	2.7
1	M	214	CYS	2.7
1	I	192	GLU	2.7
1	G	223	LEU	2.7
1	I	203	PRO	2.7
1	C	334	VAL	2.7
1	L	478	ARG	2.7
1	G	4	GLU	2.7
1	J	296	LEU	2.7
1	N	303	ARG	2.7
1	E	377	VAL	2.7
1	M	174	GLY	2.7
1	F	204	TYR	2.7
1	I	269	ARG	2.7
1	J	309	SER	2.7
1	F	313	ALA	2.7
1	L	332	THR	2.7
1	F	350	ILE	2.7
1	A	306	MET	2.7
1	E	490	PHE	2.7
1	G	477	ASP	2.7
1	B	234	ILE	2.7
1	H	193	GLY	2.7
1	D	186	ASP	2.7
1	D	273	LYS	2.7
1	M	100	PHE	2.7
1	A	234	ILE	2.7
1	F	225	ASP	2.7
1	I	215	GLU	2.7
1	B	350	ILE	2.7
1	I	321	ALA	2.7
1	F	292	ASP	2.6
1	E	188	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	334	VAL	2.6
1	I	263	LEU	2.6
1	L	232	ARG	2.6
1	M	203	PRO	2.6
1	D	353	LEU	2.6
1	B	186	ASP	2.6
1	M	315	ASP	2.6
1	L	325	THR	2.6
1	G	247	PRO	2.6
1	N	223	LEU	2.6
1	L	277	ILE	2.6
1	D	203	PRO	2.6
1	H	270	GLY	2.6
1	E	362	GLU	2.6
1	K	249	LEU	2.6
1	A	275	VAL	2.6
1	E	148	VAL	2.6
1	M	382	VAL	2.6
1	A	360	ASP	2.6
1	D	276	ALA	2.6
1	G	337	GLY	2.6
1	L	354	GLN	2.6
1	C	377	VAL	2.6
1	G	299	GLY	2.6
1	M	139	VAL	2.6
1	F	281	GLY	2.6
1	K	432	ARG	2.6
1	M	159	ILE	2.6
1	N	413	VAL	2.6
1	H	287	SER	2.6
1	A	495	GLU	2.5
1	F	192	GLU	2.5
1	H	192	GLU	2.5
1	F	187	GLN	2.5
1	K	433	ARG	2.5
1	N	272	LEU	2.5
1	M	268	LEU	2.5
1	I	377	VAL	2.5
1	C	315	ASP	2.5
1	A	284	GLU	2.5
1	I	290	LEU	2.5
1	B	478	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	285	ARG	2.5
1	B	342	ASP	2.5
1	N	493	LEU	2.5
1	H	63	LEU	2.5
1	A	358	ASP	2.5
1	G	224	VAL	2.5
1	K	293	ILE	2.5
1	K	334	VAL	2.5
1	A	276	ALA	2.5
1	C	352	ASN	2.5
1	I	190	PHE	2.5
1	A	366	LEU	2.5
1	D	287	SER	2.5
1	N	232	ARG	2.5
1	G	369	ARG	2.5
1	I	168	ALA	2.5
1	J	154	GLY	2.5
1	C	357	THR	2.5
1	D	213	ILE	2.5
1	L	530	LYS	2.5
1	A	251	MET	2.5
1	J	227	LYS	2.5
1	D	356	GLN	2.5
1	I	255	VAL	2.5
1	M	433	ARG	2.5
1	L	300	THR	2.5
1	E	349	GLN	2.5
1	J	188	LEU	2.5
1	A	255	VAL	2.5
1	N	255	VAL	2.5
1	G	176	VAL	2.5
1	K	303	ARG	2.5
1	F	100	PHE	2.5
1	L	414	PRO	2.5
1	E	334	VAL	2.5
1	G	292	ASP	2.4
1	A	223	LEU	2.4
1	B	272	LEU	2.4
1	I	195	GLN	2.4
1	N	519	PHE	2.4
1	A	423	LEU	2.4
1	C	246	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	336	ASP	2.4
1	L	251	MET	2.4
1	L	176	VAL	2.4
1	G	350	ILE	2.4
1	J	239	GLU	2.4
1	M	301	VAL	2.4
1	D	316	ALA	2.4
1	K	225	ASP	2.4
1	M	383	GLY	2.4
1	L	418	CYS	2.4
1	M	357	THR	2.4
1	L	249	LEU	2.4
1	L	346	ARG	2.4
1	D	370	ILE	2.4
1	D	360	ASP	2.4
1	J	254	GLU	2.4
1	K	204	TYR	2.4
1	D	303	ARG	2.4
1	E	394	LYS	2.4
1	L	355	MET	2.4
1	H	176	VAL	2.4
1	I	275	VAL	2.4
1	K	289	TYR	2.4
1	M	374	SER	2.4
1	C	361	TYR	2.4
1	N	299	GLY	2.4
1	G	88	ASP	2.4
1	I	177	THR	2.4
1	K	251	MET	2.4
1	G	282	PHE	2.4
1	A	167	MET	2.4
1	G	243	ARG	2.4
1	H	373	LEU	2.4
1	N	300	THR	2.4
1	N	334	VAL	2.4
1	H	353	LEU	2.4
1	A	370	ILE	2.4
1	N	414	PRO	2.4
1	B	204	TYR	2.4
1	C	195	GLN	2.4
1	H	433	ARG	2.4
1	L	177	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	189	VAL	2.3
1	D	246	TYR	2.3
1	D	342	ASP	2.3
1	M	318	LEU	2.3
1	G	374	SER	2.3
1	C	222	LEU	2.3
1	N	187	GLN	2.3
1	J	312	GLN	2.3
1	N	335	GLY	2.3
1	F	176	VAL	2.3
1	M	138	VAL	2.3
1	K	370	ILE	2.3
1	B	311	GLU	2.3
1	B	377	VAL	2.3
1	H	311	GLU	2.3
1	I	4	GLU	2.3
1	D	255	VAL	2.3
1	G	188	LEU	2.3
1	I	301	VAL	2.3
1	K	357	THR	2.3
1	I	355	MET	2.3
1	C	362	GLU	2.3
1	M	377	VAL	2.3
1	L	230	THR	2.3
1	L	433	ARG	2.3
1	J	370	ILE	2.3
1	F	280	PRO	2.3
1	K	246	TYR	2.3
1	G	244	GLY	2.3
1	N	248	LEU	2.3
1	I	288	SER	2.3
1	K	227	LYS	2.3
1	M	367	GLN	2.3
1	M	414	PRO	2.3
1	I	281	GLY	2.3
1	M	137	SER	2.2
1	L	261	ALA	2.2
1	C	192	GLU	2.2
1	A	496	THR	2.2
1	C	215	GLU	2.2
1	L	359	GLN	2.2
1	C	274	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	259	ALA	2.2
1	B	355	MET	2.2
1	K	372	ARG	2.2
1	A	238	LEU	2.2
1	E	358	ASP	2.2
1	I	273	LYS	2.2
1	D	318	LEU	2.2
1	J	248	LEU	2.2
1	H	247	PRO	2.2
1	N	374	SER	2.2
1	L	366	LEU	2.2
1	F	246	TYR	2.2
1	C	316	ALA	2.2
1	D	313	ALA	2.2
1	K	360	ASP	2.2
1	J	228	ILE	2.2
1	M	524	VAL	2.2
1	I	228	ILE	2.2
1	K	177	THR	2.2
1	E	251	MET	2.2
1	K	332	THR	2.2
1	M	342	ASP	2.2
1	N	361	TYR	2.2
1	C	176	VAL	2.2
1	G	301	VAL	2.2
1	H	334	VAL	2.2
1	I	334	VAL	2.2
1	J	307	GLY	2.2
1	D	434	MET	2.2
1	D	232	ARG	2.2
1	H	301	VAL	2.2
1	L	246	TYR	2.2
1	L	504	VAL	2.2
1	L	280	PRO	2.2
1	L	531	GLU	2.2
1	M	295	ILE	2.2
1	H	339	THR	2.2
1	C	224	VAL	2.2
1	K	371	ALA	2.1
1	N	338	SER	2.1
1	M	346	ARG	2.1
1	N	201	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	352	ASN	2.1
1	L	350	ILE	2.1
1	K	509	MET	2.1
1	H	190	PHE	2.1
1	A	357	THR	2.1
1	H	156	ASN	2.1
1	C	251	MET	2.1
1	E	406	ALA	2.1
1	J	323	LYS	2.1
1	I	519	PHE	2.1
1	A	317	VAL	2.1
1	C	312	GLN	2.1
1	M	332	THR	2.1
1	J	138	VAL	2.1
1	L	265	VAL	2.1
1	M	222	LEU	2.1
1	K	124	THR	2.1
1	H	154	GLY	2.1
1	F	252	ALA	2.1
1	H	221	ILE	2.1
1	M	247	PRO	2.1
1	C	248	LEU	2.1
1	G	178	MET	2.1
1	L	481	TYR	2.1
1	D	272	LEU	2.1
1	I	270	GLY	2.1
1	K	308	VAL	2.1
1	G	164	SER	2.1
1	C	255	VAL	2.1
1	C	314	THR	2.1
1	F	342	ASP	2.1
1	J	366	LEU	2.1
1	H	282	PHE	2.1
1	B	295	ILE	2.1
1	N	331	THR	2.1
1	H	215	GLU	2.1
1	K	210	GLU	2.1
1	D	346	ARG	2.1
1	K	276	ALA	2.1
1	H	365	LYS	2.0
1	C	231	ALA	2.0
1	D	509	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	314	THR	2.0
1	G	60	GLU	2.0
1	I	318	LEU	2.0
1	I	531	GLU	2.0
1	C	235	ILE	2.0
1	K	228	ILE	2.0
1	M	293	ILE	2.0
1	N	165	ASP	2.0
1	E	142	ASP	2.0
1	H	246	TYR	2.0
1	N	412	VAL	2.0
1	I	188	LEU	2.0
1	L	238	LEU	2.0
1	K	414	PRO	2.0
1	K	422	ARG	2.0
1	M	380	ILE	2.0
1	F	96	LEU	2.0
1	M	190	PHE	2.0
1	C	350	ILE	2.0
1	L	384	ALA	2.0
1	L	216	TYR	2.0
1	I	186	ASP	2.0
1	K	342	ASP	2.0
1	B	205	PHE	2.0
1	F	318	LEU	2.0
1	K	175	VAL	2.0
1	H	4	GLU	2.0
1	L	415	GLY	2.0
1	C	243	ARG	2.0
1	J	280	PRO	2.0
1	I	385	GLN	2.0
1	N	260	LEU	2.0
1	G	216	TYR	2.0
1	F	156	ASN	2.0
1	M	352	ASN	2.0
1	D	270	GLY	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.