Full wwPDB X-ray Structure Validation Report (i)

May 1, 2016 – 11:11 PM EDT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

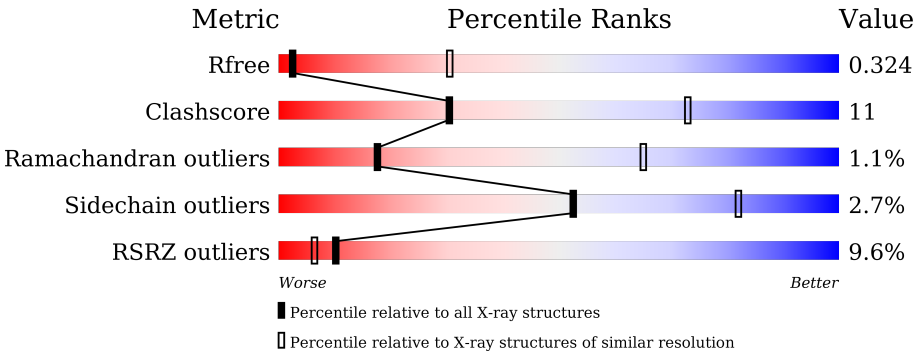
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	9% 69% 25%
1	B	552	7% 76% 18%
1	C	552	7% 74% 21%
1	D	552	6% 73% 22%
1	E	552	5% 65% 26%
1	F	552	6% 76% 18%

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Mol	Chain	Length	Quality of chain
1	G	552	9% 74% 21%
1	H	552	8% 75% 20%
1	I	552	11% 74% 21%
1	J	552	11% 74% 21%
1	K	552	13% 76% 19%
1	L	552	13% 75% 20%
1	M	552	14% 75% 20%
1	N	552	11% 78% 17%

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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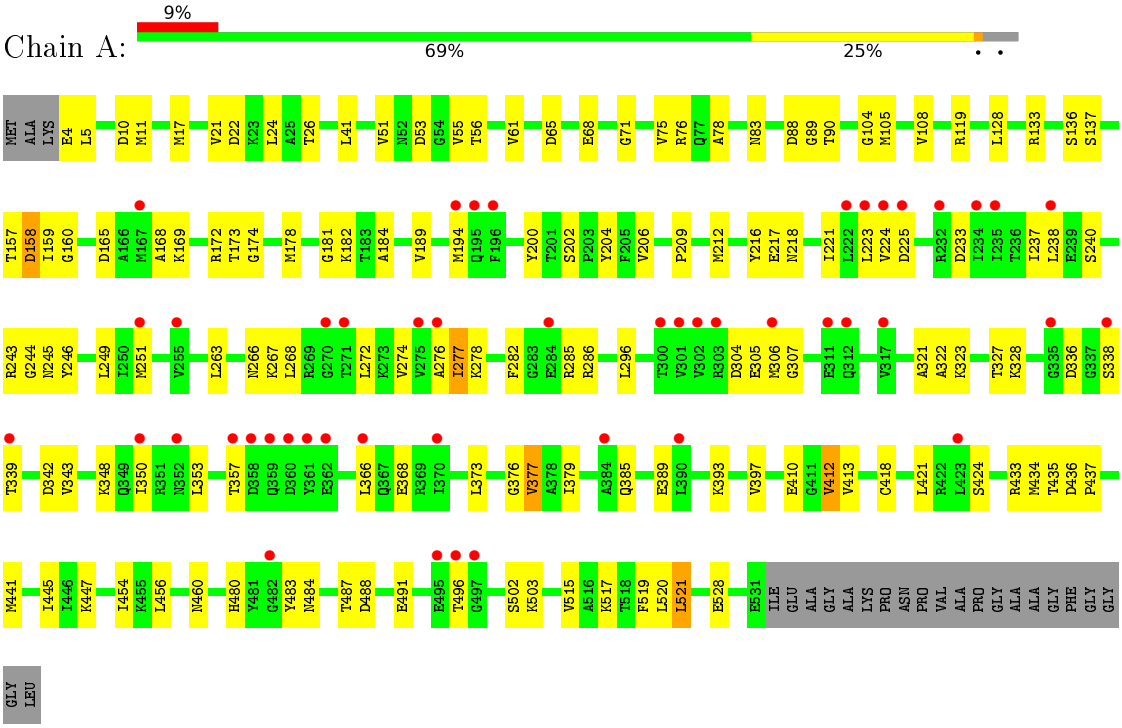
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	VAL	-	see sequence details	UNP A8JE91
N	1	MET	-	expression tag	UNP A8JE91
N	138	VAL	-	see sequence details	UNP A8JE91
B	1	MET	-	expression tag	UNP A8JE91
B	138	VAL	-	see sequence details	UNP A8JE91
C	1	MET	-	expression tag	UNP A8JE91
C	138	VAL	-	see 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

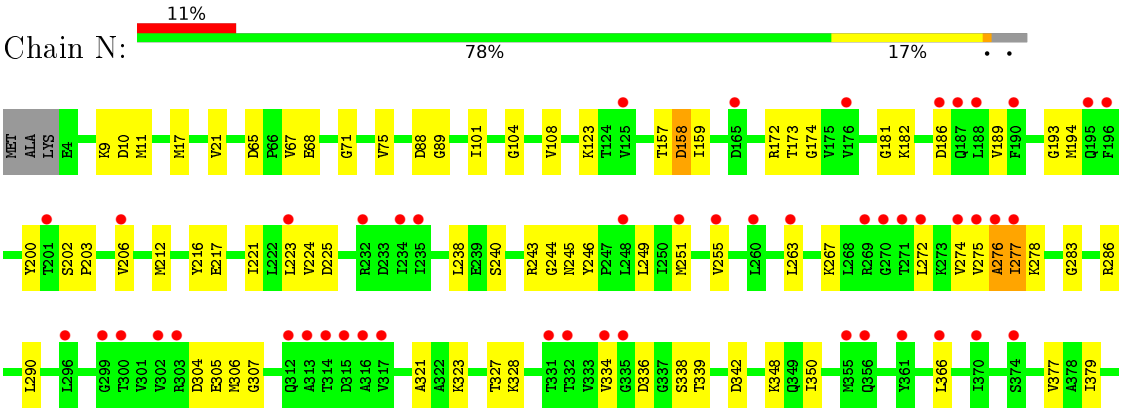
- Molecule 1: Chaperonin 60B1

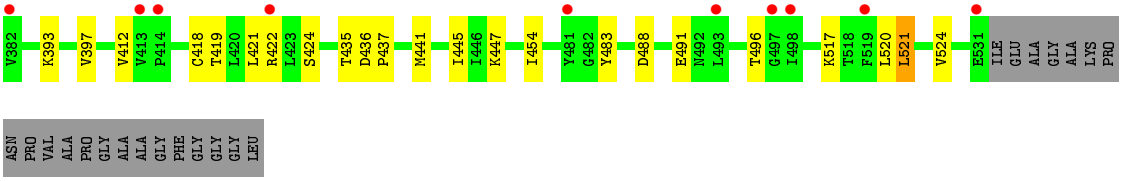
Chain A:



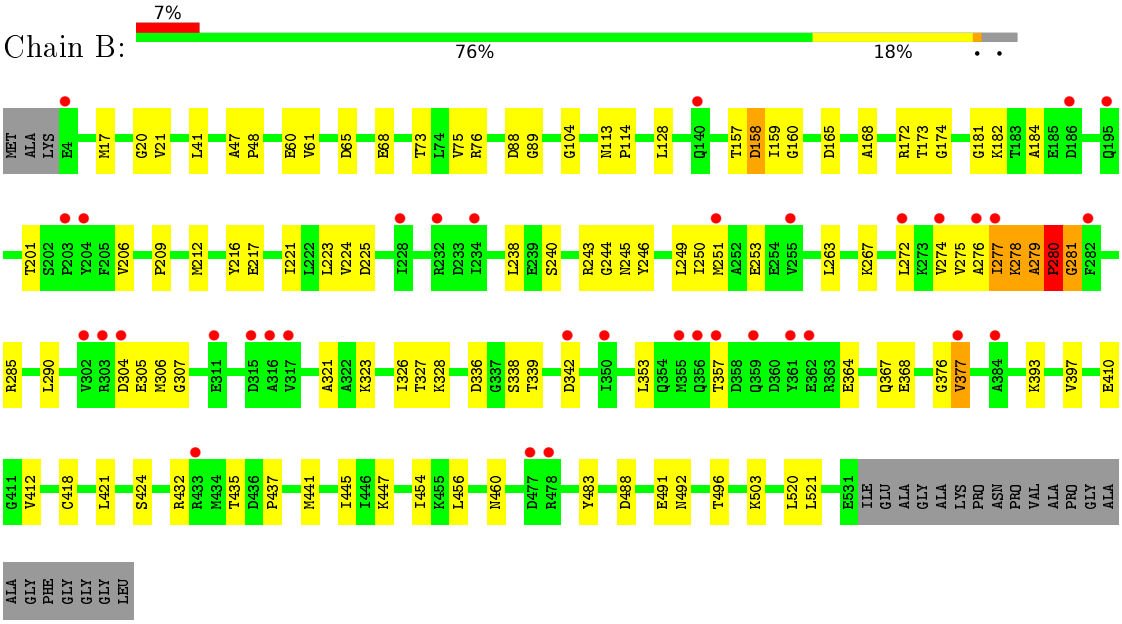
- Molecule 1: Chaperonin 60B1

Chain N:

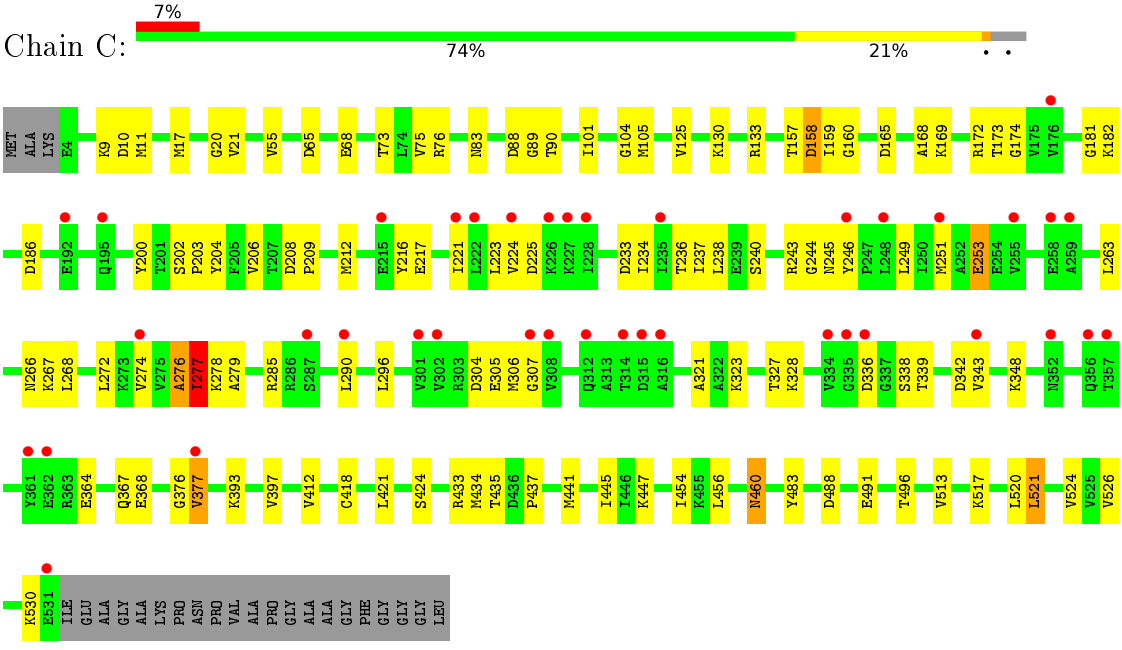




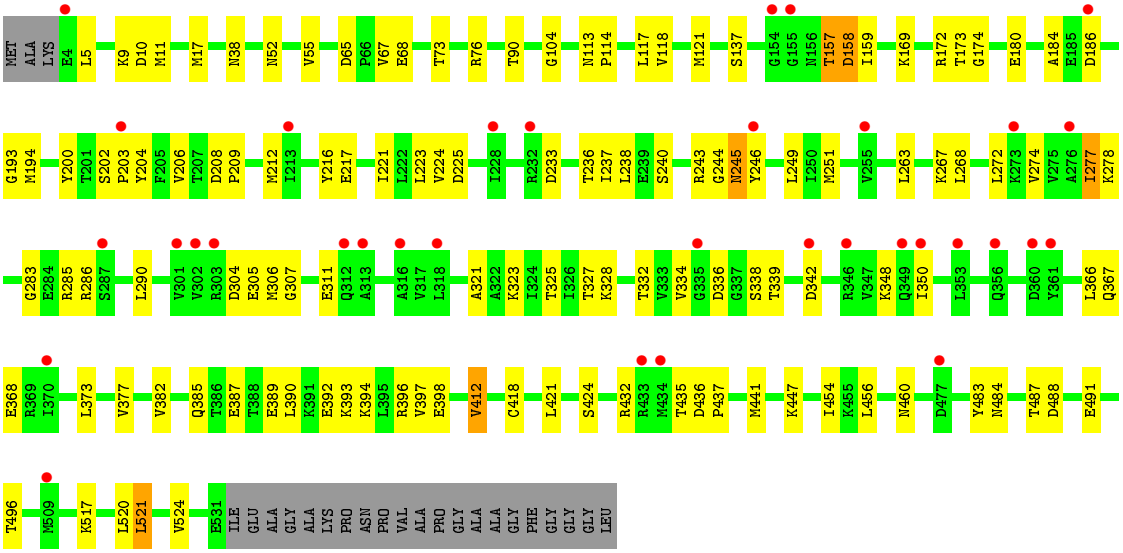
• Molecule 1: Chaperonin 60B1



• Molecule 1: Chaperonin 60B1

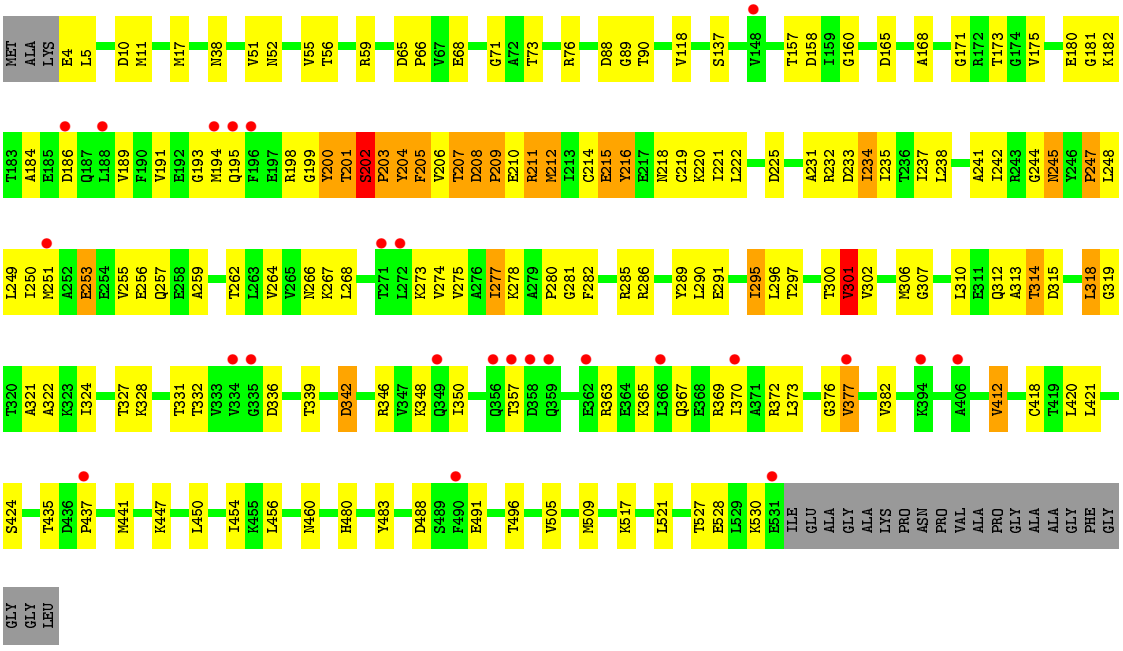


• Molecule 1: Chaperonin 60B1



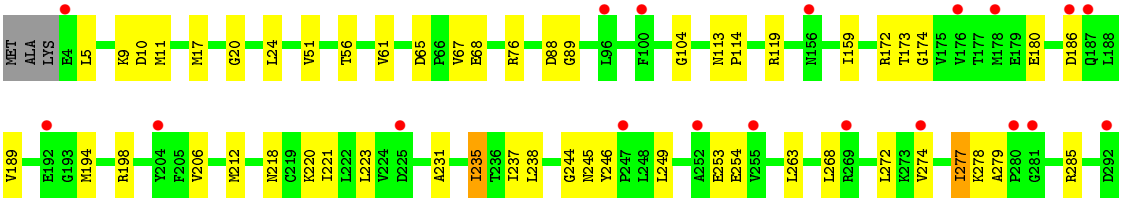
• Molecule 1: Chaperonin 60B1

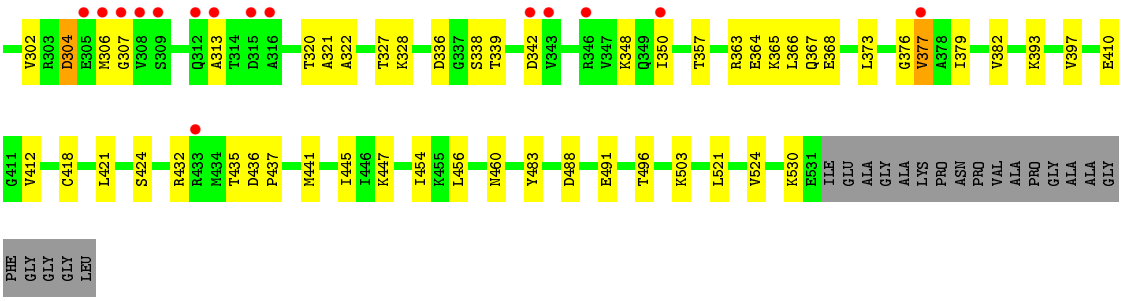
Chain E:



• Molecule 1: Chaperonin 60B1

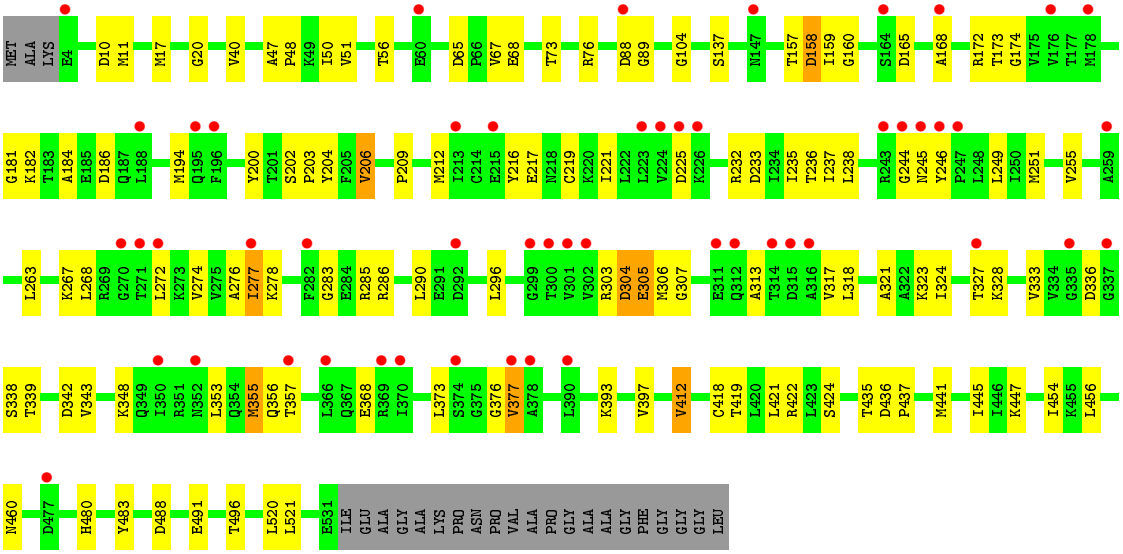
Chain F:





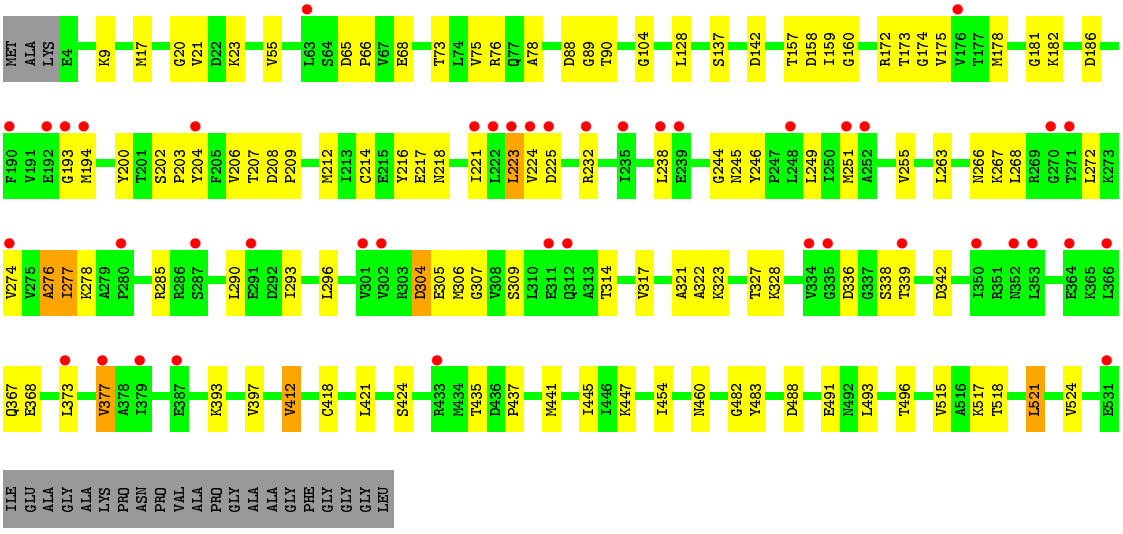
• Molecule 1: Chaperonin 60B1

Chain G:



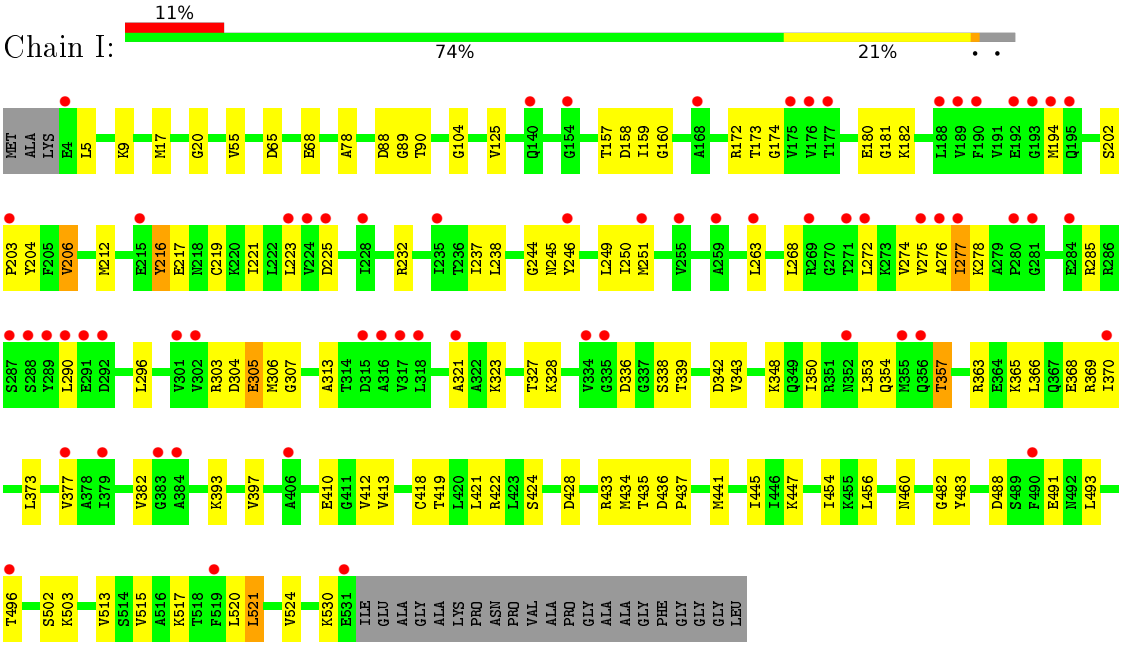
• Molecule 1: Chaperonin 60B1

Chain H:



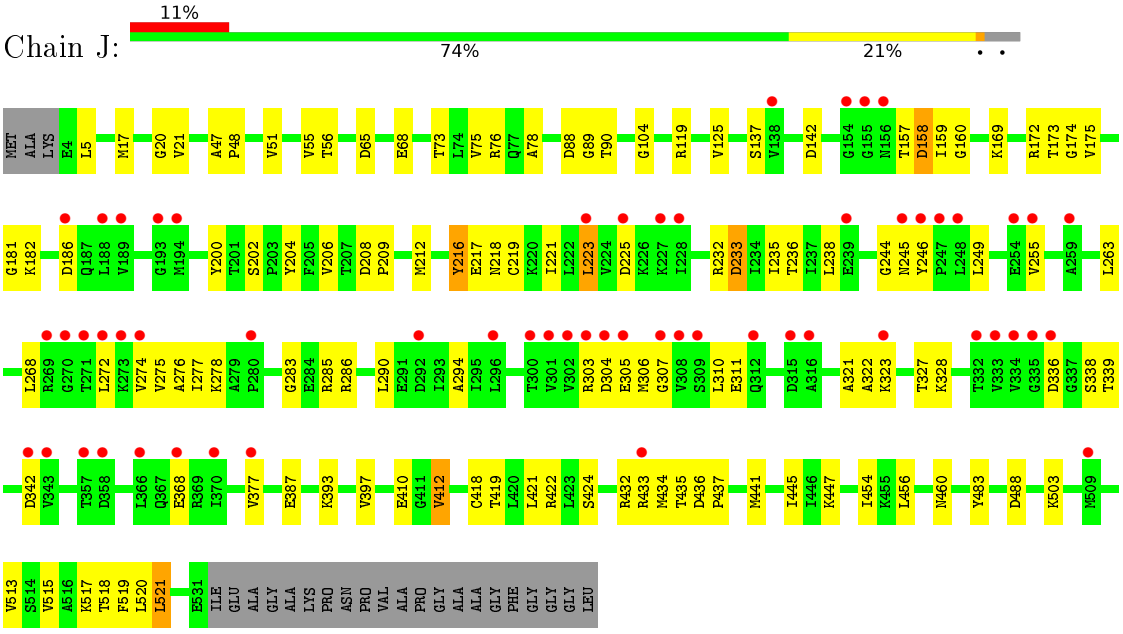
• Molecule 1: Chaperonin 60B1

Chain I:



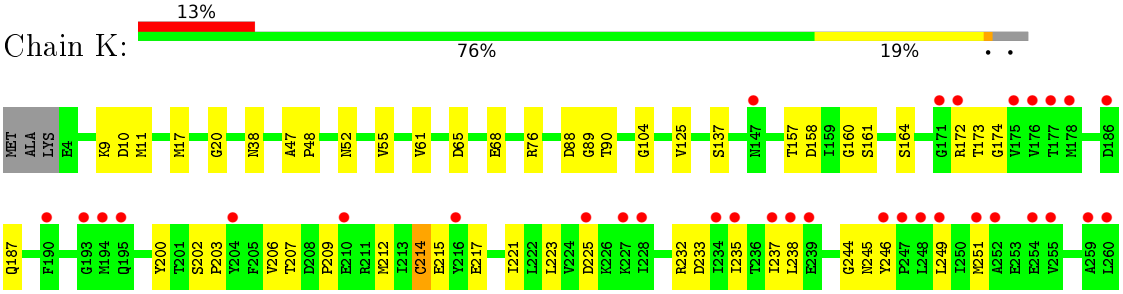
• Molecule 1: Chaperonin 60B1

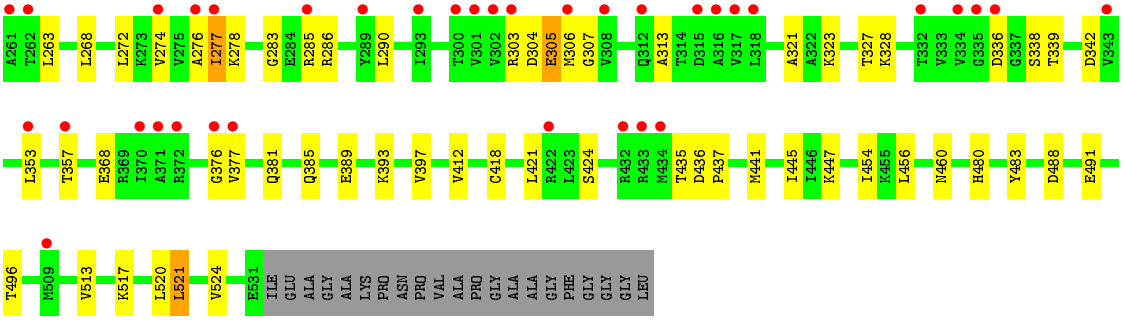
Chain J:



• Molecule 1: Chaperonin 60B1

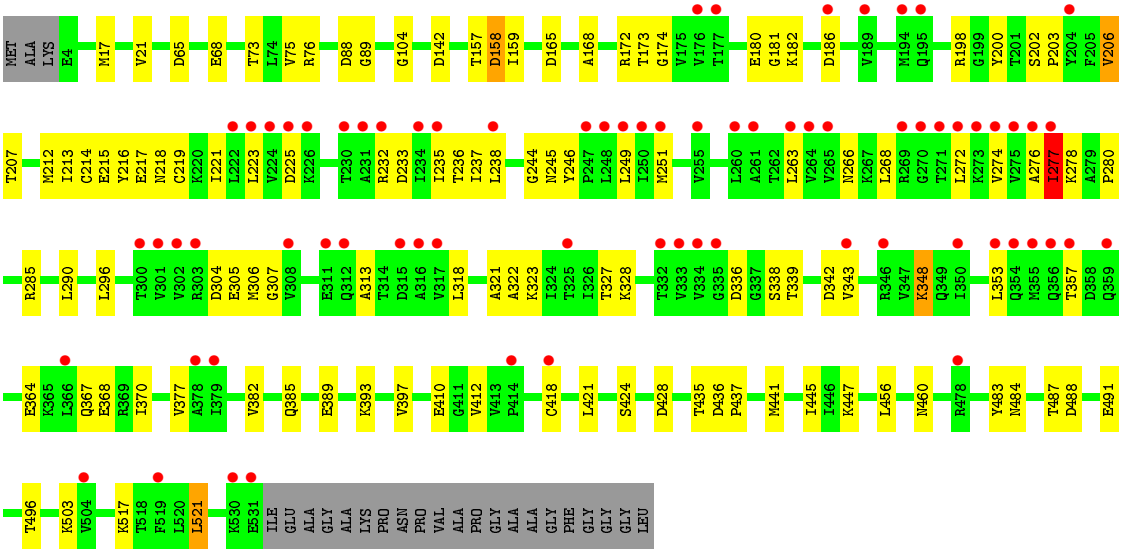
Chain K:





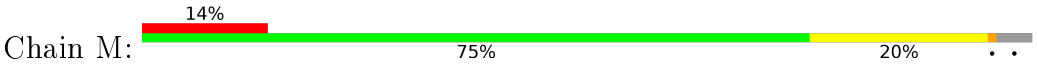
• Molecule 1: Chaperonin 60B1

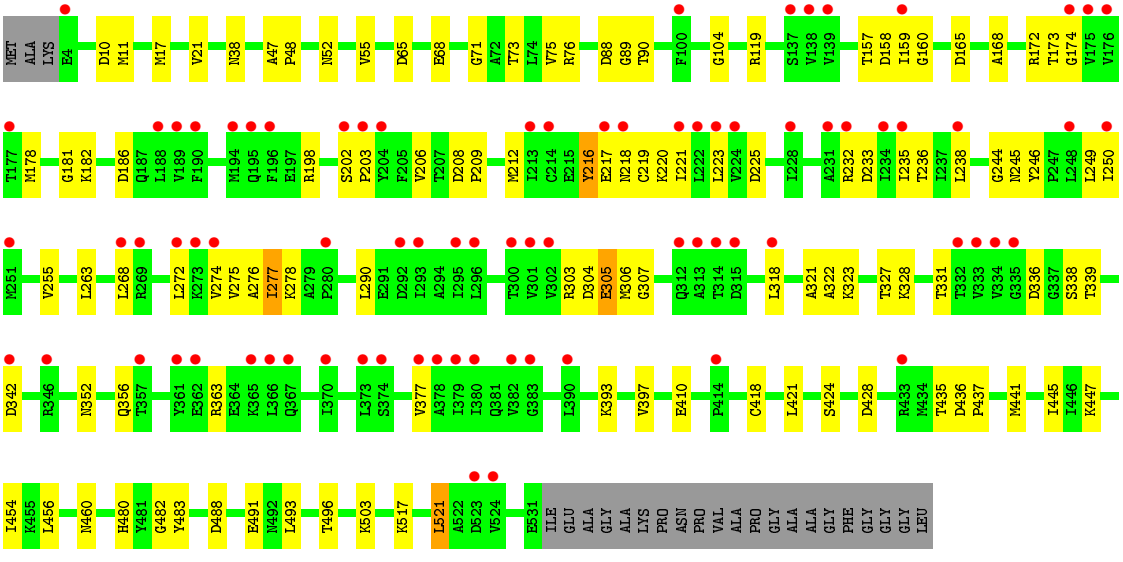
Chain L:



• Molecule 1: Chaperonin 60B1

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.50 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.275 , 0.325 0.283 , 0.324	Depositor DCC
R_{free} test set	1746 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	133.5	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 114.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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^2)	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.21	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(^{o})	Ideal(^{o})
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 (i)

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:205:PHE:HE2	1:E:267:LYS:HB3	1.00	0.81
1:E:251:MET:CG	1:E:277:ILE:CG2	2.55	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:327:THR:OG1	1:M:328:LYS:N	2.36	0.58
1:M:321:ALA:HA	1:M:336:ASP:HB3	1.84	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:17:MET:HA	1:K:68:GLU:HA	1.85	0.58
1:K:327:THR:OG1	1:K:328:LYS:N	2.35	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:277:ILE:HG22	1:B:326:ILE:CD1	2.38	0.54
1:B:278:LYS:CB	1:B:278:LYS:HZ2	2.21	0.54
1:D:483:TYR:OH	1:D:488:ASP:OD1	2.25	0.54
1:E:200:TYR:HB3	1:E:328:LYS:HA	1.90	0.54
1:E:202:SER:HB3	1:E:203:PRO:HA	1.89	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:421:LEU:HD11	1:K:454:ILE:HG21	1.91	0.53
1:K:424:SER:HB2	1:K:447:LYS:HD2	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:424:SER:HB2	1:G:447:LYS:HD2	1.92	0.51
1:G:40:VAL:HG22	1:G:50:ILE:HG22	1.92	0.51
1:H:483:TYR:OH	1:H:488:ASP:OD1	2.24	0.51
1:H:20:GLY:HA3	1:H:68:GLU:HB2	1.92	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:202:SER:OG	1:E:204:TYR:CB	2.58	0.50
1:E:137:SER:HB3	1:E:412:VAL:HG12	1.94	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:306:MET:HB2	1:N:307:GLY:HA2	1.96	0.48
1:N:21:VAL:HG13	1:N:75:VAL:HG21	1.95	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:303:ARG:HE	1:G:305:GLU:HB2	1.79	0.46
1:G:296:LEU:HG	1:G:343:VAL:HG22	1.97	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:65:ASP:HB3	1:H:68:GLU:HG2	1.97	0.46
1:H:78:ALA:HB2	1:H:515:VAL:HG11	1.98	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:104:GLY:HA3	1:D:520:LEU:HD21	1.96	0.46
1:D:334:VAL:HG23	1:D:377:VAL:HG21	1.91	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:17:MET:HB2	1:A:71:GLY:HA3	1.98	0.45
1:A:306:MET:HB2	1:A:307:GLY:HA2	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:104:GLY:HA3	1:G:520:LEU:HD21	1.97	0.45
1:G:157:THR:OG1	1:G:158:ASP:N	2.47	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:205:PHE:C	1:E:206:VAL:CG2	2.85	0.43
1:E:205:PHE:CD1	1:E:267:LYS:HG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:THR:OG1	1:E:328:LYS:N	2.46	0.43
1:E:193:GLY:HA3	1:E:377:VAL:HB	1.99	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:23:LYS:HD3	1:H:23:LYS:HA	1.89	0.42
1:H:193:GLY:HA3	1:H:377:VAL:HB	2.02	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:221:ILE:HG13	1:E:319:GLY:O	2.19	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: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:436:ASP:OD1	1:F:436:ASP:N	2.50	0.41
1:F:24:LEU:HD11	1:F:76:ARG:HG3	2.01	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:104:GLY:HA3	1:I:520:LEU:HD21	2.02	0.40
1:I:194:MET:HE1	1:I:373:LEU:HA	2.03	0.40
1:I:225:ASP:HB3	1:I:290:LEU:HD21	2.03	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:432:ARG:HD3	1:D:432:ARG:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:VAL:HG21	1:D:517:LYS:HG3	2.02	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/552 (95%)	480 (91%)	40 (8%)	6 (1%)	17	65
1	B	526/552 (95%)	473 (90%)	46 (9%)	7 (1%)	15	61
1	C	526/552 (95%)	479 (91%)	40 (8%)	7 (1%)	15	61
1	D	526/552 (95%)	479 (91%)	42 (8%)	5 (1%)	19	66
1	E	526/552 (95%)	472 (90%)	40 (8%)	14 (3%)	6	48
1	F	526/552 (95%)	480 (91%)	42 (8%)	4 (1%)	24	70
1	G	526/552 (95%)	483 (92%)	37 (7%)	6 (1%)	17	65
1	H	526/552 (95%)	478 (91%)	43 (8%)	5 (1%)	19	66
1	I	526/552 (95%)	482 (92%)	39 (7%)	5 (1%)	19	66
1	J	526/552 (95%)	480 (91%)	42 (8%)	4 (1%)	24	70
1	K	526/552 (95%)	478 (91%)	43 (8%)	5 (1%)	19	66
1	L	526/552 (95%)	478 (91%)	43 (8%)	5 (1%)	19	66
1	M	526/552 (95%)	475 (90%)	47 (9%)	4 (1%)	24	70
1	N	526/552 (95%)	480 (91%)	42 (8%)	4 (1%)	24	70
All	All	7364/7728 (95%)	6697 (91%)	586 (8%)	81 (1%)	17	65

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 (i)

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%)	55 83
1	B	433/445 (97%)	424 (98%)	9 (2%)	61 86
1	C	433/445 (97%)	424 (98%)	9 (2%)	61 86
1	D	433/445 (97%)	422 (98%)	11 (2%)	55 83
1	E	433/445 (97%)	410 (95%)	23 (5%)	28 69
1	F	433/445 (97%)	422 (98%)	11 (2%)	55 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	433/445 (97%)	421 (97%)	12 (3%)	51 81
1	H	433/445 (97%)	421 (97%)	12 (3%)	51 81
1	I	433/445 (97%)	420 (97%)	13 (3%)	48 80
1	J	433/445 (97%)	422 (98%)	11 (2%)	55 83
1	K	433/445 (97%)	424 (98%)	9 (2%)	61 86
1	L	433/445 (97%)	420 (97%)	13 (3%)	48 80
1	M	433/445 (97%)	421 (97%)	12 (3%)	51 81
1	N	433/445 (97%)	425 (98%)	8 (2%)	66 88
All	All	6062/6230 (97%)	5898 (97%)	164 (3%)	52 82

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	A	528/552 (95%)	0.40	47 (8%) 12 7	64, 175, 274, 319	0
1	B	528/552 (95%)	0.39	36 (6%) 20 12	49, 165, 283, 325	0
1	C	528/552 (95%)	0.39	39 (7%) 17 11	50, 166, 284, 318	0
1	D	528/552 (95%)	0.30	34 (6%) 23 13	55, 153, 262, 292	0
1	E	528/552 (95%)	0.28	25 (4%) 35 23	26, 159, 234, 301	0
1	F	528/552 (95%)	0.40	34 (6%) 23 13	69, 184, 271, 303	0
1	G	528/552 (95%)	0.55	52 (9%) 10 6	55, 193, 280, 315	0
1	H	528/552 (95%)	0.43	43 (8%) 15 9	57, 182, 288, 319	0
1	I	528/552 (95%)	0.53	63 (11%) 6 5	57, 192, 299, 325	0
1	J	528/552 (95%)	0.51	58 (10%) 7 5	84, 203, 315, 369	0
1	K	528/552 (95%)	0.64	69 (13%) 5 4	71, 189, 307, 340	0
1	L	528/552 (95%)	0.70	72 (13%) 4 3	70, 185, 310, 357	0
1	M	528/552 (95%)	0.70	80 (15%) 3 2	81, 207, 326, 366	0
1	N	528/552 (95%)	0.64	59 (11%) 7 5	77, 194, 294, 335	0
All	All	7392/7728 (95%)	0.49	711 (9%) 10 6	26, 178, 296, 369	0

All (711) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	302	VAL	18.9
1	C	302	VAL	12.1
1	G	316	ALA	10.3
1	L	225	ASP	9.8
1	M	362	GLU	9.3
1	B	302	VAL	8.6
1	G	312	GLN	8.6
1	H	302	VAL	8.3

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Mol	Chain	Res	Type	RSRZ
1	K	194	MET	8.1
1	I	384	ALA	7.9
1	L	301	VAL	7.8
1	M	195	GLN	7.6
1	N	313	ALA	7.4
1	N	186	ASP	7.3
1	E	272	LEU	7.3
1	F	308	VAL	7.2
1	B	315	ASP	7.2
1	L	223	LEU	7.2
1	K	300	THR	7.2
1	D	302	VAL	7.1
1	F	307	GLY	7.1
1	N	312	GLN	7.1
1	M	194	MET	7.0
1	G	311	GLU	7.0
1	L	312	GLN	7.0
1	G	300	THR	6.9
1	M	177	THR	6.9
1	K	316	ALA	6.8
1	L	231	ALA	6.7
1	G	315	ASP	6.7
1	J	302	VAL	6.7
1	K	195	GLN	6.7
1	N	302	VAL	6.7
1	H	312	GLN	6.6
1	A	312	GLN	6.3
1	G	225	ASP	6.3
1	A	302	VAL	6.3
1	N	276	ALA	6.2
1	L	275	VAL	6.2
1	L	248	LEU	6.2
1	A	300	THR	6.1
1	N	190	PHE	6.1
1	N	195	GLN	6.1
1	F	306	MET	6.0
1	N	275	VAL	6.0
1	L	274	VAL	5.9
1	L	311	GLU	5.9
1	I	271	THR	5.9
1	J	292	ASP	5.9
1	K	315	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	L	316	ALA	5.8
1	L	276	ALA	5.8
1	K	235	ILE	5.8
1	B	356	GLN	5.8
1	C	356	GLN	5.8
1	L	224	VAL	5.7
1	L	255	VAL	5.7
1	J	316	ALA	5.7
1	J	315	ASP	5.6
1	B	303	ARG	5.6
1	J	194	MET	5.6
1	J	358	ASP	5.5
1	N	314	THR	5.5
1	M	235	ILE	5.4
1	J	303	ARG	5.4
1	L	195	GLN	5.4
1	C	335	GLY	5.4
1	M	335	GLY	5.4
1	A	270	GLY	5.4
1	A	359	GLN	5.4
1	B	277	ILE	5.4
1	F	343	VAL	5.3
1	F	433	ARG	5.3
1	L	247	PRO	5.2
1	N	188	LEU	5.2
1	C	531	GLU	5.2
1	C	336	ASP	5.2
1	E	271	THR	5.2
1	J	273	LYS	5.2
1	M	231	ALA	5.2
1	G	246	TYR	5.2
1	G	195	GLN	5.1
1	A	301	VAL	5.1
1	J	246	TYR	5.1
1	J	225	ASP	5.1
1	I	176	VAL	5.0
1	M	334	VAL	5.0
1	M	313	ALA	5.0
1	I	251	MET	5.0
1	A	195	GLN	5.0
1	L	194	MET	5.0
1	K	301	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	335	GLY	5.0
1	K	302	VAL	4.9
1	M	361	TYR	4.9
1	M	333	VAL	4.9
1	M	366	LEU	4.9
1	L	303	ARG	4.9
1	E	186	ASP	4.8
1	B	316	ALA	4.8
1	M	223	LEU	4.8
1	B	359	GLN	4.8
1	A	194	MET	4.7
1	B	255	VAL	4.7
1	J	255	VAL	4.7
1	F	4	GLU	4.7
1	M	379	ILE	4.6
1	G	226	LYS	4.6
1	D	154	GLY	4.6
1	F	186	ASP	4.6
1	F	316	ALA	4.6
1	I	383	GLY	4.6
1	N	315	ASP	4.6
1	M	175	VAL	4.6
1	J	300	THR	4.5
1	M	176	VAL	4.5
1	J	272	LEU	4.5
1	I	291	GLU	4.5
1	M	272	LEU	4.5
1	N	271	THR	4.5
1	F	312	GLN	4.5
1	I	496	THR	4.5
1	H	352	ASN	4.5
1	N	370	ILE	4.5
1	J	304	ASP	4.4
1	N	422	ARG	4.4
1	K	434	MET	4.4
1	K	171	GLY	4.4
1	H	239	GLU	4.4
1	L	235	ILE	4.4
1	H	232	ARG	4.4
1	K	335	GLY	4.4
1	L	315	ASP	4.4
1	M	280	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	K	317	VAL	4.4
1	F	309	SER	4.3
1	C	259	ALA	4.3
1	G	270	GLY	4.3
1	M	312	GLN	4.3
1	C	308	VAL	4.2
1	N	531	GLU	4.2
1	K	312	GLN	4.2
1	B	361	TYR	4.2
1	I	316	ALA	4.2
1	G	147	ASN	4.2
1	N	235	ILE	4.2
1	H	248	LEU	4.2
1	I	246	TYR	4.2
1	H	223	LEU	4.2
1	I	223	LEU	4.1
1	J	301	VAL	4.1
1	N	270	GLY	4.1
1	G	245	ASN	4.1
1	C	227	LYS	4.1
1	M	302	VAL	4.1
1	E	359	GLN	4.1
1	J	343	VAL	4.1
1	L	250	ILE	4.1
1	N	274	VAL	4.0
1	A	338	SER	4.0
1	J	357	THR	4.0
1	G	377	VAL	4.0
1	M	4	GLU	4.0
1	L	226	LYS	4.0
1	E	196	PHE	4.0
1	M	189	VAL	4.0
1	J	368	GLU	4.0
1	A	311	GLU	4.0
1	G	366	LEU	3.9
1	M	217	GLU	3.9
1	A	482	GLY	3.9
1	H	224	VAL	3.9
1	B	232	ARG	3.9
1	G	357	THR	3.9
1	M	314	THR	3.9
1	L	270	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	L	356	GLN	3.9
1	H	377	VAL	3.9
1	B	274	VAL	3.8
1	E	531	GLU	3.8
1	H	235	ILE	3.8
1	M	234	ILE	3.8
1	N	277	ILE	3.8
1	G	370	ILE	3.8
1	I	224	VAL	3.8
1	B	203	PRO	3.8
1	D	477	ASP	3.8
1	K	255	VAL	3.8
1	K	147	ASN	3.8
1	A	390	LEU	3.8
1	L	263	LEU	3.8
1	B	251	MET	3.8
1	F	178	MET	3.8
1	J	274	VAL	3.8
1	D	433	ARG	3.7
1	K	216	TYR	3.7
1	L	271	THR	3.7
1	N	356	GLN	3.7
1	K	248	LEU	3.7
1	C	301	VAL	3.7
1	G	378	ALA	3.7
1	J	333	VAL	3.7
1	J	270	GLY	3.7
1	N	317	VAL	3.7
1	H	204	TYR	3.7
1	H	531	GLU	3.7
1	M	370	ILE	3.7
1	D	349	GLN	3.7
1	L	273	LYS	3.7
1	H	274	VAL	3.7
1	L	378	ALA	3.7
1	J	156	ASN	3.6
1	L	269	ARG	3.6
1	L	334	VAL	3.6
1	M	238	LEU	3.6
1	J	155	GLY	3.6
1	F	305	GLU	3.6
1	C	228	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	302	VAL	3.6
1	L	264	VAL	3.6
1	L	222	LEU	3.6
1	N	497	GLY	3.6
1	N	316	ALA	3.6
1	M	390	LEU	3.6
1	K	234	ILE	3.6
1	D	350	ILE	3.6
1	K	178	MET	3.6
1	M	202	SER	3.6
1	J	271	THR	3.6
1	L	379	ILE	3.6
1	E	195	GLN	3.6
1	G	196	PHE	3.5
1	K	277	ILE	3.5
1	F	315	ASP	3.5
1	J	342	ASP	3.5
1	G	335	GLY	3.5
1	M	296	LEU	3.5
1	I	292	ASP	3.5
1	I	335	GLY	3.5
1	N	366	LEU	3.5
1	L	353	LEU	3.5
1	M	269	ARG	3.5
1	A	352	ASN	3.5
1	H	335	GLY	3.5
1	N	332	THR	3.5
1	M	274	VAL	3.5
1	L	335	GLY	3.5
1	K	318	LEU	3.5
1	L	272	LEU	3.4
1	K	247	PRO	3.4
1	A	362	GLU	3.4
1	I	175	VAL	3.4
1	L	333	VAL	3.4
1	H	238	LEU	3.4
1	M	378	ALA	3.4
1	E	335	GLY	3.4
1	L	260	LEU	3.4
1	K	176	VAL	3.4
1	D	361	TYR	3.4
1	A	361	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	194	MET	3.4
1	A	235	ILE	3.4
1	N	269	ARG	3.4
1	F	255	VAL	3.4
1	C	307	GLY	3.3
1	I	194	MET	3.3
1	K	377	VAL	3.3
1	M	292	ASP	3.3
1	N	206	VAL	3.3
1	M	251	MET	3.3
1	I	315	ASP	3.3
1	H	350	ILE	3.3
1	N	234	ILE	3.3
1	H	271	THR	3.3
1	L	343	VAL	3.3
1	G	277	ILE	3.3
1	N	355	MET	3.3
1	B	477	ASP	3.3
1	H	225	ASP	3.3
1	K	186	ASP	3.3
1	K	260	LEU	3.3
1	A	350	ILE	3.3
1	I	272	LEU	3.2
1	D	312	GLN	3.2
1	K	261	ALA	3.2
1	M	300	THR	3.2
1	C	287	SER	3.2
1	B	140	GLN	3.2
1	L	234	ILE	3.2
1	L	204	TYR	3.2
1	M	213	ILE	3.2
1	G	215	GLU	3.2
1	G	352	ASN	3.2
1	M	221	ILE	3.2
1	E	357	THR	3.2
1	H	291	GLU	3.2
1	B	317	VAL	3.2
1	H	280	PRO	3.2
1	N	481	TYR	3.2
1	K	336	ASP	3.2
1	N	263	LEU	3.2
1	K	262	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	362	GLU	3.1
1	K	239	GLU	3.1
1	M	232	ARG	3.1
1	G	213	ILE	3.1
1	I	280	PRO	3.1
1	K	343	VAL	3.1
1	M	523	ASP	3.1
1	G	390	LEU	3.1
1	I	356	GLN	3.1
1	G	272	LEU	3.1
1	A	224	VAL	3.1
1	K	172	ARG	3.1
1	K	193	GLY	3.1
1	A	303	ARG	3.1
1	N	251	MET	3.1
1	C	258	GLU	3.1
1	N	196	PHE	3.1
1	B	228	ILE	3.1
1	F	377	VAL	3.1
1	A	225	ASP	3.1
1	I	277	ILE	3.1
1	G	271	THR	3.1
1	J	186	ASP	3.0
1	C	226	LYS	3.0
1	B	384	ALA	3.0
1	C	290	LEU	3.0
1	D	4	GLU	3.0
1	D	301	VAL	3.0
1	J	305	GLU	3.0
1	J	223	LEU	3.0
1	H	251	MET	3.0
1	J	193	GLY	3.0
1	N	176	VAL	3.0
1	L	317	VAL	3.0
1	I	225	ASP	3.0
1	A	339	THR	3.0
1	N	382	VAL	3.0
1	A	335	GLY	3.0
1	L	186	ASP	3.0
1	M	273	LYS	3.0
1	K	376	GLY	3.0
1	A	497	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	302	VAL	3.0
1	I	276	ALA	3.0
1	M	204	TYR	3.0
1	J	245	ASN	3.0
1	J	269	ARG	2.9
1	J	308	VAL	2.9
1	K	274	VAL	2.9
1	L	519	PHE	2.9
1	I	370	ILE	2.9
1	F	192	GLU	2.9
1	I	289	TYR	2.9
1	J	247	PRO	2.9
1	N	223	LEU	2.9
1	G	168	ALA	2.9
1	I	287	SER	2.9
1	K	353	LEU	2.9
1	J	334	VAL	2.9
1	N	303	ARG	2.9
1	I	193	GLY	2.9
1	I	140	GLN	2.9
1	G	259	ALA	2.9
1	C	343	VAL	2.8
1	I	255	VAL	2.8
1	K	238	LEU	2.8
1	B	357	THR	2.8
1	M	218	ASN	2.8
1	A	196	PHE	2.8
1	H	387	GLU	2.8
1	A	234	ILE	2.8
1	D	155	GLY	2.8
1	E	370	ILE	2.8
1	F	204	TYR	2.8
1	L	232	ARG	2.8
1	E	356	GLN	2.8
1	H	287	SER	2.8
1	N	125	VAL	2.8
1	M	174	GLY	2.8
1	M	248	LEU	2.8
1	F	313	ALA	2.8
1	L	357	THR	2.8
1	N	296	LEU	2.8
1	J	188	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	373	LEU	2.8
1	J	509	MET	2.7
1	G	477	ASP	2.7
1	G	223	LEU	2.7
1	A	495	GLU	2.7
1	I	192	GLU	2.7
1	J	433	ARG	2.7
1	G	4	GLU	2.7
1	K	306	MET	2.7
1	E	188	LEU	2.7
1	B	234	ILE	2.7
1	C	315	ASP	2.7
1	D	186	ASP	2.7
1	F	225	ASP	2.7
1	C	334	VAL	2.7
1	L	277	ILE	2.7
1	H	364	GLU	2.7
1	I	190	PHE	2.7
1	B	433	ARG	2.7
1	I	406	ALA	2.7
1	M	203	PRO	2.7
1	M	382	VAL	2.7
1	A	271	THR	2.7
1	I	263	LEU	2.7
1	I	377	VAL	2.7
1	D	203	PRO	2.7
1	E	437	PRO	2.7
1	M	214	CYS	2.7
1	B	4	GLU	2.7
1	F	269	ARG	2.7
1	F	346	ARG	2.7
1	M	100	PHE	2.7
1	G	224	VAL	2.7
1	B	304	ASP	2.7
1	I	284	GLU	2.7
1	K	249	LEU	2.7
1	L	325	THR	2.7
1	M	301	VAL	2.7
1	H	366	LEU	2.7
1	L	332	THR	2.7
1	B	478	ARG	2.6
1	N	255	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	377	VAL	2.6
1	H	176	VAL	2.6
1	A	306	MET	2.6
1	F	247	PRO	2.6
1	N	272	LEU	2.6
1	L	251	MET	2.6
1	J	296	LEU	2.6
1	E	194	MET	2.6
1	A	384	ALA	2.6
1	E	490	PHE	2.6
1	D	287	SER	2.6
1	F	292	ASP	2.6
1	J	309	SER	2.6
1	C	377	VAL	2.6
1	M	159	ILE	2.6
1	I	177	THR	2.6
1	H	193	GLY	2.6
1	G	176	VAL	2.6
1	I	215	GLU	2.6
1	J	154	GLY	2.6
1	L	249	LEU	2.6
1	A	275	VAL	2.6
1	F	187	GLN	2.6
1	K	251	MET	2.6
1	M	196	PHE	2.6
1	A	255	VAL	2.6
1	D	276	ALA	2.6
1	L	300	THR	2.6
1	I	195	GLN	2.6
1	I	203	PRO	2.6
1	G	337	GLY	2.6
1	M	315	ASP	2.6
1	A	251	MET	2.6
1	K	334	VAL	2.6
1	N	187	GLN	2.5
1	G	243	ARG	2.5
1	E	366	LEU	2.5
1	B	350	ILE	2.5
1	N	413	VAL	2.5
1	K	225	ASP	2.5
1	L	354	GLN	2.5
1	A	223	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	493	LEU	2.5
1	F	350	ILE	2.5
1	G	247	PRO	2.5
1	J	227	LYS	2.5
1	K	293	ILE	2.5
1	D	303	ARG	2.5
1	J	239	GLU	2.5
1	L	177	THR	2.5
1	L	478	ARG	2.5
1	L	530	LYS	2.5
1	A	276	ALA	2.5
1	A	366	LEU	2.5
1	I	269	ARG	2.5
1	B	282	PHE	2.5
1	D	273	LYS	2.5
1	E	148	VAL	2.5
1	B	342	ASP	2.5
1	L	230	THR	2.5
1	E	334	VAL	2.5
1	I	189	VAL	2.5
1	E	349	GLN	2.5
1	D	353	LEU	2.5
1	I	301	VAL	2.5
1	M	222	LEU	2.5
1	D	213	ILE	2.5
1	L	176	VAL	2.5
1	A	360	ASP	2.5
1	B	186	ASP	2.5
1	J	336	ASP	2.5
1	I	290	LEU	2.4
1	E	394	LYS	2.4
1	C	222	LEU	2.4
1	D	360	ASP	2.4
1	J	254	GLU	2.4
1	F	176	VAL	2.4
1	M	377	VAL	2.4
1	A	370	ILE	2.4
1	A	496	THR	2.4
1	C	361	TYR	2.4
1	M	365	LYS	2.4
1	M	318	LEU	2.4
1	H	301	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	358	ASP	2.4
1	N	232	ARG	2.4
1	D	255	VAL	2.4
1	K	433	ARG	2.4
1	D	316	ALA	2.4
1	F	100	PHE	2.4
1	I	355	MET	2.4
1	I	168	ALA	2.4
1	A	423	LEU	2.4
1	N	334	VAL	2.4
1	H	63	LEU	2.4
1	H	353	LEU	2.4
1	I	228	ILE	2.4
1	M	380	ILE	2.4
1	G	282	PHE	2.4
1	B	377	VAL	2.4
1	L	346	ARG	2.4
1	N	519	PHE	2.4
1	K	228	ILE	2.4
1	G	244	GLY	2.4
1	J	312	GLN	2.4
1	D	313	ALA	2.4
1	N	248	LEU	2.4
1	H	311	GLU	2.4
1	C	316	ALA	2.4
1	K	285	ARG	2.4
1	D	370	ILE	2.4
1	M	433	ARG	2.4
1	N	414	PRO	2.4
1	K	432	ARG	2.4
1	M	383	GLY	2.4
1	K	177	THR	2.4
1	A	284	GLU	2.4
1	B	311	GLU	2.4
1	G	299	GLY	2.4
1	K	303	ARG	2.4
1	I	275	VAL	2.3
1	I	321	ALA	2.3
1	H	192	GLU	2.3
1	C	352	ASN	2.3
1	H	252	ALA	2.3
1	I	4	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	374	SER	2.3
1	D	246	TYR	2.3
1	E	362	GLU	2.3
1	D	342	ASP	2.3
1	K	204	TYR	2.3
1	J	138	VAL	2.3
1	C	195	GLN	2.3
1	M	357	THR	2.3
1	D	232	ARG	2.3
1	N	300	THR	2.3
1	C	357	THR	2.3
1	K	289	TYR	2.3
1	J	189	VAL	2.3
1	N	335	GLY	2.3
1	L	355	MET	2.3
1	B	204	TYR	2.3
1	C	224	VAL	2.3
1	H	373	LEU	2.3
1	F	252	ALA	2.3
1	K	276	ALA	2.3
1	M	295	ILE	2.3
1	C	176	VAL	2.3
1	J	248	LEU	2.3
1	L	414	PRO	2.3
1	M	268	LEU	2.3
1	N	201	THR	2.3
1	M	342	ASP	2.3
1	B	272	LEU	2.3
1	C	274	VAL	2.3
1	I	352	ASN	2.3
1	I	531	GLU	2.3
1	H	433	ARG	2.3
1	K	372	ARG	2.3
1	M	190	PHE	2.3
1	D	318	LEU	2.3
1	H	270	GLY	2.3
1	G	188	LEU	2.3
1	C	246	TYR	2.3
1	D	356	GLN	2.2
1	L	359	GLN	2.2
1	A	167	MET	2.2
1	E	251	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	323	LYS	2.2
1	G	350	ILE	2.2
1	J	259	ALA	2.2
1	M	524	VAL	2.2
1	K	332	THR	2.2
1	K	370	ILE	2.2
1	N	299	GLY	2.2
1	M	367	GLN	2.2
1	A	238	LEU	2.2
1	J	370	ILE	2.2
1	C	215	GLU	2.2
1	J	228	ILE	2.2
1	M	224	VAL	2.2
1	L	261	ALA	2.2
1	C	314	THR	2.2
1	G	88	ASP	2.2
1	K	509	MET	2.2
1	K	227	LYS	2.2
1	M	414	PRO	2.2
1	N	374	SER	2.2
1	H	221	ILE	2.2
1	L	418	CYS	2.2
1	K	371	ALA	2.2
1	N	331	THR	2.2
1	G	374	SER	2.2
1	M	139	VAL	2.2
1	B	355	MET	2.2
1	G	369	ARG	2.2
1	C	251	MET	2.2
1	C	255	VAL	2.2
1	C	362	GLU	2.2
1	M	188	LEU	2.2
1	H	190	PHE	2.2
1	N	165	ASP	2.2
1	M	332	THR	2.2
1	I	334	VAL	2.2
1	C	192	GLU	2.2
1	B	276	ALA	2.1
1	H	222	LEU	2.1
1	I	281	GLY	2.1
1	I	288	SER	2.1
1	F	281	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	156	ASN	2.1
1	G	292	ASP	2.1
1	E	406	ALA	2.1
1	G	178	MET	2.1
1	H	334	VAL	2.1
1	M	346	ARG	2.1
1	M	228	ILE	2.1
1	A	317	VAL	2.1
1	C	248	LEU	2.1
1	G	60	GLU	2.1
1	J	307	GLY	2.1
1	J	366	LEU	2.1
1	L	504	VAL	2.1
1	I	519	PHE	2.1
1	M	293	ILE	2.1
1	N	260	LEU	2.1
1	G	301	VAL	2.1
1	M	250	ILE	2.1
1	J	280	PRO	2.1
1	J	377	VAL	2.1
1	K	210	GLU	2.1
1	M	138	VAL	2.1
1	I	318	LEU	2.1
1	K	254	GLU	2.1
1	L	238	LEU	2.1
1	N	361	TYR	2.1
1	C	235	ILE	2.1
1	C	312	GLN	2.1
1	K	175	VAL	2.1
1	K	357	THR	2.1
1	L	265	VAL	2.1
1	L	531	GLU	2.1
1	K	259	ALA	2.1
1	D	228	ILE	2.1
1	H	379	ILE	2.1
1	I	317	VAL	2.1
1	L	366	LEU	2.1
1	I	379	ILE	2.1
1	A	357	THR	2.1
1	G	164	SER	2.0
1	M	137	SER	2.0
1	G	314	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	335	GLY	2.0
1	I	490	PHE	2.0
1	C	221	ILE	2.0
1	K	252	ALA	2.0
1	J	332	THR	2.0
1	K	422	ARG	2.0
1	F	274	VAL	2.0
1	B	195	GLN	2.0
1	F	280	PRO	2.0
1	I	259	ALA	2.0
1	A	222	LEU	2.0
1	I	188	LEU	2.0
1	L	189	VAL	2.0
1	L	308	VAL	2.0
1	K	190	PHE	2.0
1	I	154	GLY	2.0
1	D	509	MET	2.0
1	I	235	ILE	2.0
1	F	96	LEU	2.0
1	K	308	VAL	2.0
1	F	342	ASP	2.0
1	N	498	ILE	2.0
1	D	346	ARG	2.0
1	L	350	ILE	2.0
1	A	232	ARG	2.0
1	D	434	MET	2.0
1	E	358	ASP	2.0
1	G	327	THR	2.0
1	H	339	THR	2.0
1	K	237	ILE	2.0
1	K	246	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.