



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:06 PM BST

PDB ID : 4AB2
EMDB ID: : EMD-1998
Title : ATP-triggered molecular mechanics of the chaperonin GroEL
Authors : Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.
Deposited on : 2011-12-06
Resolution : 8.50 Å(reported)
Based on PDB ID : 1OEL

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

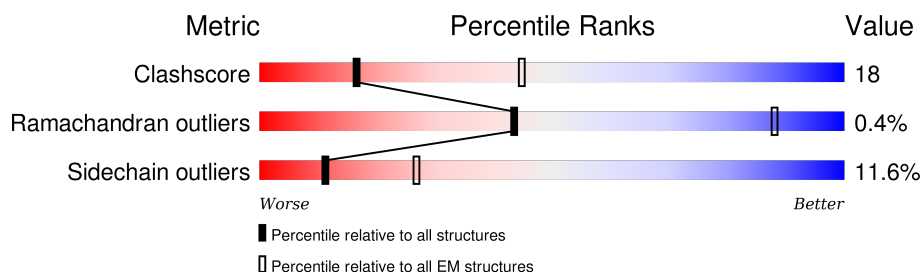
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	548	55% 29% 10% . .
1	B	548	55% 29% 10% . .
1	C	548	55% 29% 10% . .
1	D	548	56% 28% 10% . .
1	E	548	55% 29% 10% . .
1	F	548	55% 28% 10% . .
1	G	548	55% 29% 10% . .
1	H	548	57% 28% 9% . .
1	I	548	57% 28% 9% . .

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Mol	Chain	Length	Quality of chain
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	1528	-	-	X	-
4	PO4	B	1528	-	-	X	-
4	PO4	C	1528	-	-	X	-
4	PO4	D	1528	-	-	X	-
4	PO4	E	1528	-	-	X	-
4	PO4	F	1528	-	-	X	-
4	PO4	G	1528	-	-	X	-
4	PO4	H	1528	-	-	X	-
4	PO4	I	1528	-	-	X	-
4	PO4	J	1528	-	-	X	-
4	PO4	K	1528	-	-	X	-
4	PO4	L	1528	-	-	X	-
4	PO4	M	1528	-	-	X	-
4	PO4	N	1528	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 54474 atoms, of which 168 are hydrogens and 0 are deuteriums.

In the tables below, 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 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	B	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	C	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	D	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	E	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	F	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	G	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	H	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	I	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	J	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	K	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	L	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	M	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	N	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		

There are 14 discrepancies between the modelled and reference sequences:

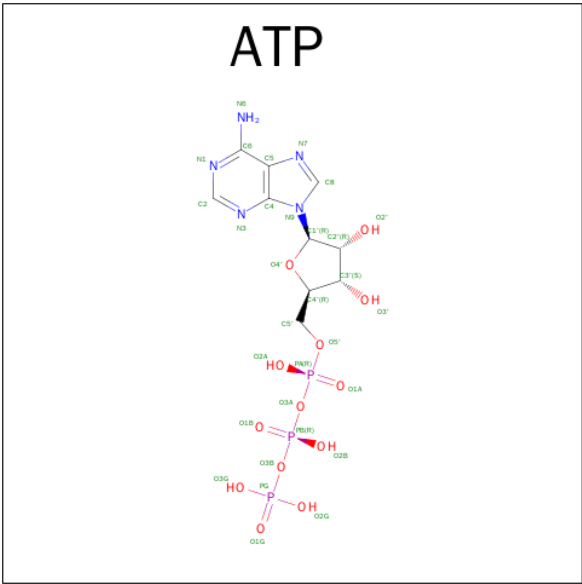
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
B	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
D	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
E	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
F	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
G	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
H	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
I	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
J	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
K	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
L	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
M	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
N	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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Mol	Chain	Residues	Atoms						AltConf
2	F	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	G	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	H	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	I	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	J	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	K	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	L	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	M	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	N	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

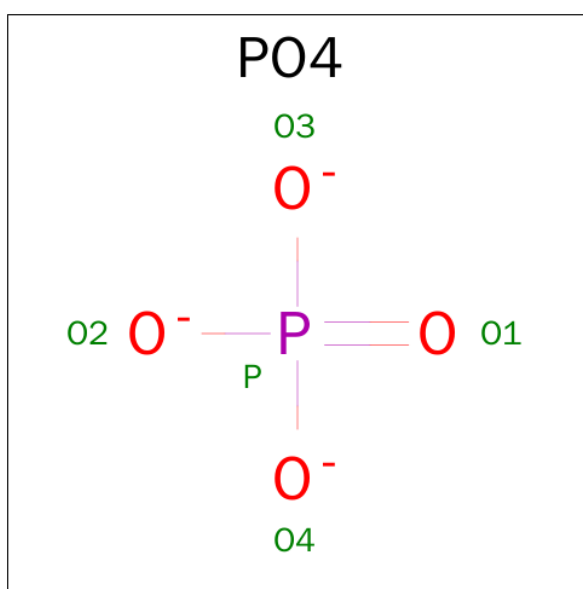
Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total 1	Mg 1	0
3	J	1	Total 1	Mg 1	0
3	D	1	Total 1	Mg 1	0
3	K	1	Total 1	Mg 1	0
3	E	1	Total 1	Mg 1	0
3	H	1	Total 1	Mg 1	0
3	B	1	Total 1	Mg 1	0
3	I	1	Total 1	Mg 1	0
3	C	1	Total 1	Mg 1	0
3	A	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	N	1	Total 1	Mg 1	0
3	L	1	Total 1	Mg 1	0
3	F	1	Total 1	Mg 1	0
3	M	1	Total 1	Mg 1	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	P 1	0
4	B	1	Total 1	P 1	0
4	C	1	Total 1	P 1	0
4	D	1	Total 1	P 1	0
4	E	1	Total 1	P 1	0
4	F	1	Total 1	P 1	0
4	G	1	Total 1	P 1	0

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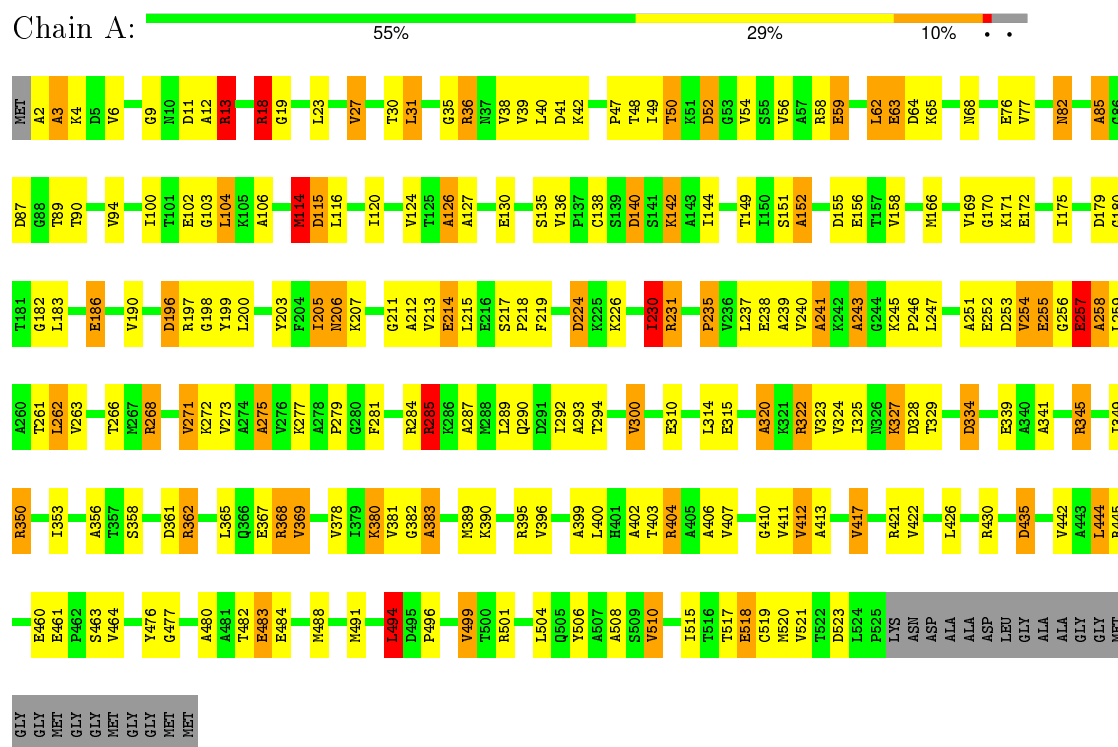
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Mol	Chain	Residues	Atoms		AltConf
4	H	1	Total 1	P 1	0
4	I	1	Total 1	P 1	0
4	J	1	Total 1	P 1	0
4	K	1	Total 1	P 1	0
4	L	1	Total 1	P 1	0
4	M	1	Total 1	P 1	0
4	N	1	Total 1	P 1	0

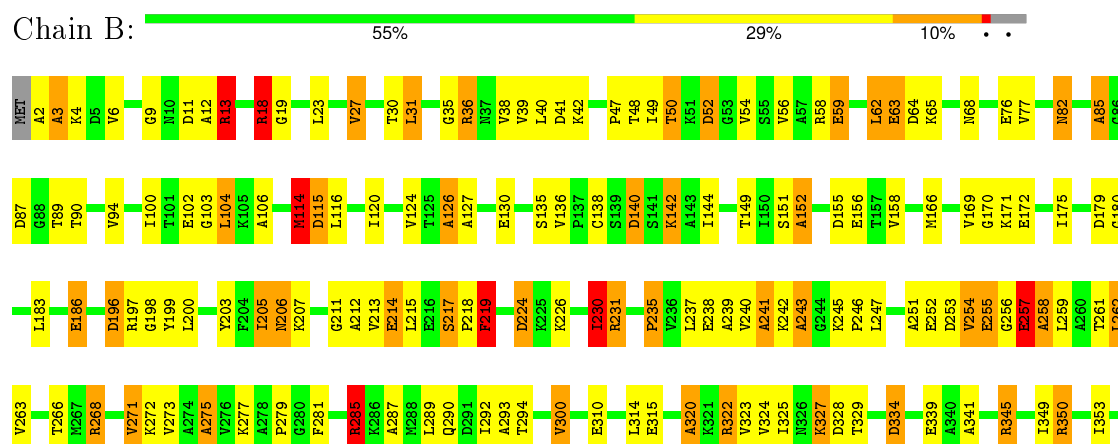
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 60 KDA CHAPERONIN

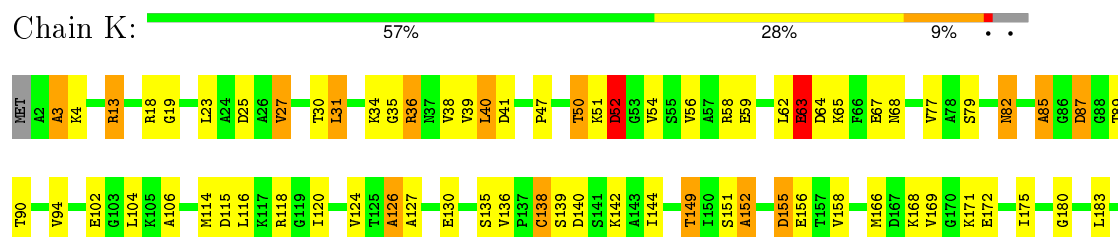


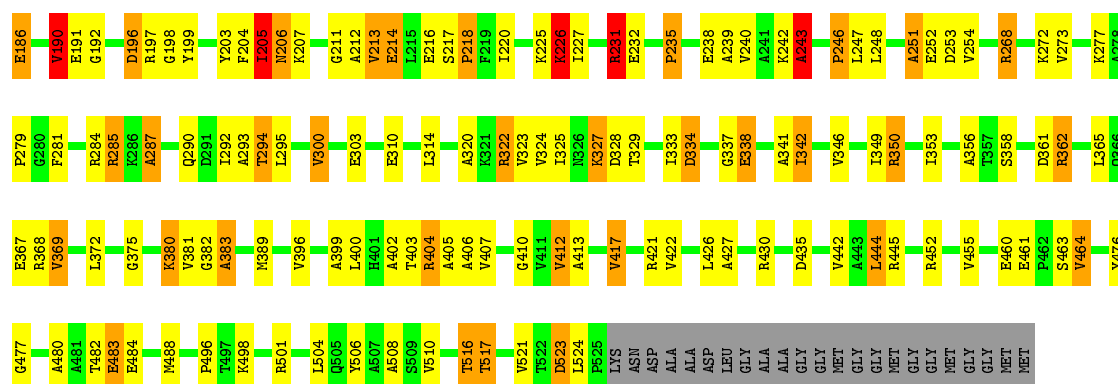
• Molecule 1: 60 KDA CHAPERONIN





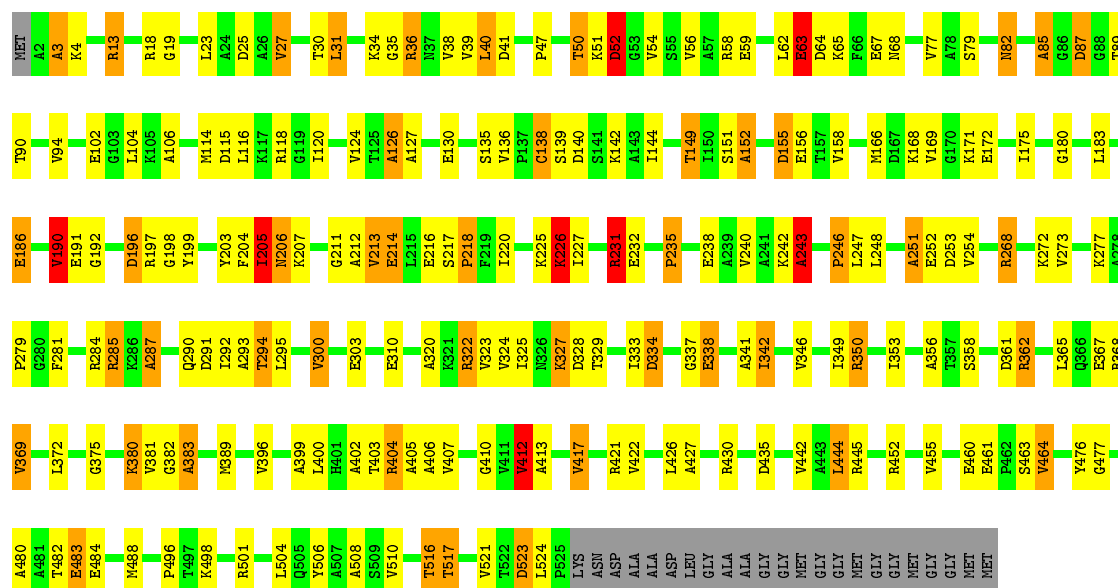






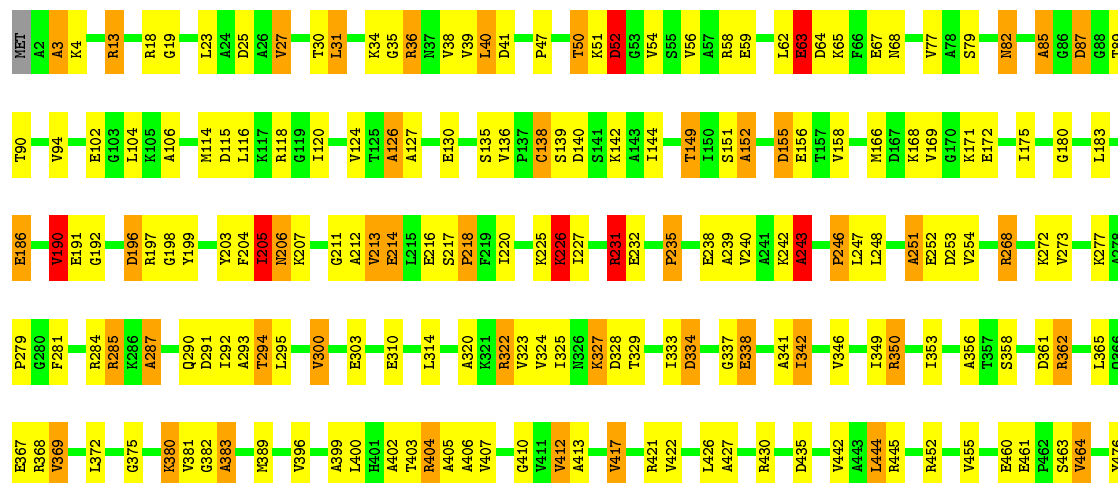
• Molecule 1: 60 KDA CHAPERONIN

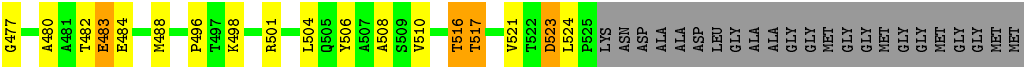
Chain L:



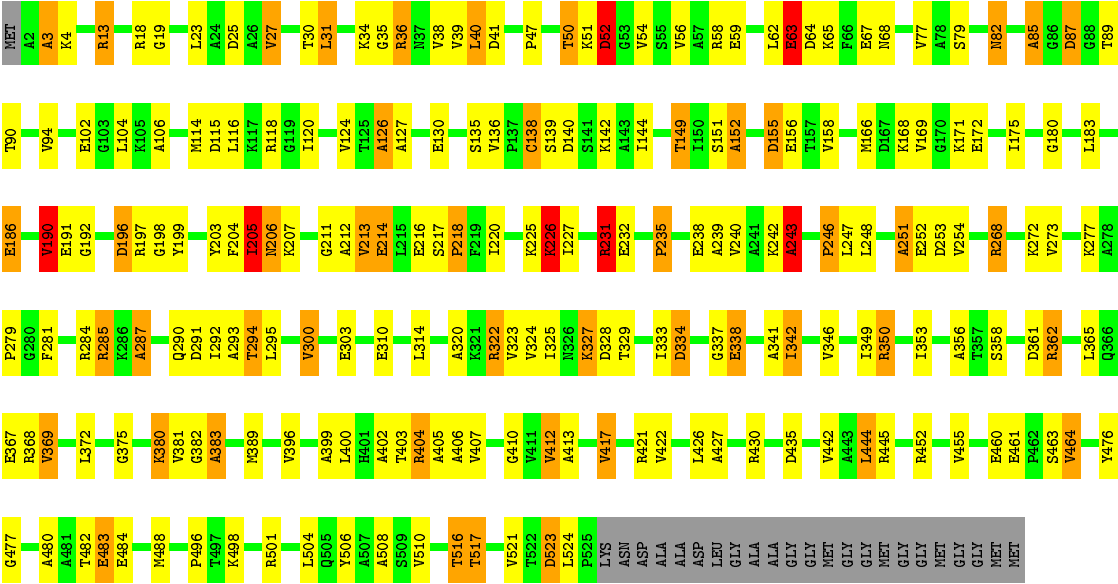
• Molecule 1: 60 KDA CHAPERONIN

Chain M:





• Molecule 1: 60 KDA CHAPERONIN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE WAS PHASE FLIPPED	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 4K CCD CAMERA	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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 > 2$	RMSZ	# $ Z > 2$
1	A	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	B	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	C	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	D	1.02	1/3873 (0.0%)	1.53	78/5229 (1.5%)
1	E	1.02	1/3873 (0.0%)	1.53	77/5229 (1.5%)
1	F	1.01	1/3873 (0.0%)	1.51	76/5229 (1.5%)
1	G	1.02	1/3873 (0.0%)	1.52	72/5229 (1.4%)
1	H	1.00	0/3873	1.45	72/5229 (1.4%)
1	I	1.00	0/3873	1.44	71/5229 (1.4%)
1	J	1.00	0/3873	1.45	74/5229 (1.4%)
1	K	1.00	0/3873	1.45	72/5229 (1.4%)
1	L	1.00	0/3873	1.45	74/5229 (1.4%)
1	M	1.00	0/3873	1.45	73/5229 (1.4%)
1	N	1.00	0/3873	1.45	73/5229 (1.4%)
All	All	1.01	7/54222 (0.0%)	1.49	1046/73206 (1.4%)

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	A	0	11
1	B	0	11
1	C	0	11
1	D	0	11
1	E	0	11
1	F	1	12
1	G	0	12
1	H	0	8
1	I	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	8
1	K	0	8
1	L	0	8
1	M	0	8
1	N	0	8
All	All	1	135

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	GLU	CA-CB	6.48	1.68	1.53
1	F	63	GLU	CA-CB	6.45	1.68	1.53
1	G	63	GLU	CA-CB	6.45	1.68	1.53
1	B	63	GLU	CA-CB	6.44	1.68	1.53
1	A	63	GLU	CA-CB	6.44	1.68	1.53
1	E	63	GLU	CA-CB	6.43	1.68	1.53
1	D	63	GLU	CA-CB	6.43	1.68	1.53

All (1046) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	GLU	N-CA-CB	-18.59	77.15	110.60
1	F	63	GLU	N-CA-CB	-18.58	77.16	110.60
1	A	63	GLU	N-CA-CB	-18.58	77.16	110.60
1	C	63	GLU	N-CA-CB	-18.57	77.17	110.60
1	E	63	GLU	N-CA-CB	-18.57	77.17	110.60
1	B	63	GLU	N-CA-CB	-18.56	77.19	110.60
1	D	63	GLU	N-CA-CB	-18.55	77.21	110.60
1	C	231	ARG	NE-CZ-NH1	11.81	126.20	120.30
1	B	231	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	231	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	E	231	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	D	231	ARG	NE-CZ-NH1	11.65	126.12	120.30
1	M	383	ALA	N-CA-CB	11.58	126.31	110.10
1	N	383	ALA	N-CA-CB	11.58	126.31	110.10
1	K	383	ALA	N-CA-CB	11.57	126.30	110.10
1	H	383	ALA	N-CA-CB	11.56	126.28	110.10
1	I	383	ALA	N-CA-CB	11.55	126.27	110.10
1	J	383	ALA	N-CA-CB	11.54	126.25	110.10
1	L	383	ALA	N-CA-CB	11.53	126.24	110.10
1	C	383	ALA	N-CA-CB	11.18	125.75	110.10
1	D	383	ALA	N-CA-CB	11.17	125.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	383	ALA	N-CA-CB	11.17	125.74	110.10
1	G	383	ALA	N-CA-CB	11.17	125.74	110.10
1	F	383	ALA	N-CA-CB	11.16	125.73	110.10
1	B	114	MET	N-CA-CB	11.16	130.68	110.60
1	B	383	ALA	N-CA-CB	11.15	125.72	110.10
1	C	114	MET	N-CA-CB	11.15	130.67	110.60
1	A	114	MET	N-CA-CB	11.14	130.66	110.60
1	D	114	MET	N-CA-CB	11.14	130.66	110.60
1	E	114	MET	N-CA-CB	11.14	130.65	110.60
1	G	114	MET	N-CA-CB	11.14	130.65	110.60
1	F	114	MET	N-CA-CB	11.13	130.64	110.60
1	A	383	ALA	N-CA-CB	11.12	125.67	110.10
1	G	255	GLU	CB-CA-C	9.98	130.35	110.40
1	C	461	GLU	CB-CA-C	9.41	129.23	110.40
1	B	461	GLU	CB-CA-C	9.39	129.19	110.40
1	A	461	GLU	CB-CA-C	9.33	129.06	110.40
1	G	461	GLU	CB-CA-C	9.28	128.96	110.40
1	D	461	GLU	CB-CA-C	9.27	128.95	110.40
1	F	461	GLU	CB-CA-C	9.23	128.85	110.40
1	E	461	GLU	CB-CA-C	9.22	128.84	110.40
1	C	231	ARG	CB-CA-C	-9.21	91.99	110.40
1	E	231	ARG	CB-CA-C	-9.20	91.99	110.40
1	A	231	ARG	CB-CA-C	-9.19	92.02	110.40
1	B	231	ARG	CB-CA-C	-9.18	92.03	110.40
1	D	231	ARG	CB-CA-C	-9.17	92.06	110.40
1	I	51	LYS	N-CA-CB	9.01	126.82	110.60
1	H	51	LYS	N-CA-CB	9.01	126.81	110.60
1	J	51	LYS	N-CA-CB	9.01	126.81	110.60
1	M	51	LYS	N-CA-CB	9.01	126.81	110.60
1	K	51	LYS	N-CA-CB	9.01	126.81	110.60
1	L	51	LYS	N-CA-CB	8.99	126.78	110.60
1	N	51	LYS	N-CA-CB	8.98	126.76	110.60
1	N	231	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	J	231	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	H	231	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	M	231	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	L	231	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	K	231	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	N	87	ASP	CB-CG-OD2	8.54	125.98	118.30
1	H	18	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	H	87	ASP	CB-CG-OD2	8.50	125.95	118.30
1	K	87	ASP	CB-CG-OD2	8.47	125.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	87	ASP	CB-CG-OD2	8.42	125.88	118.30
1	M	87	ASP	CB-CG-OD2	8.41	125.87	118.30
1	L	87	ASP	CB-CG-OD2	8.41	125.87	118.30
1	M	115	ASP	CB-CA-C	8.40	127.21	110.40
1	H	115	ASP	CB-CA-C	8.40	127.20	110.40
1	I	115	ASP	CB-CA-C	8.40	127.20	110.40
1	M	18	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	L	115	ASP	CB-CA-C	8.40	127.19	110.40
1	J	115	ASP	CB-CA-C	8.39	127.18	110.40
1	N	115	ASP	CB-CA-C	8.38	127.16	110.40
1	K	115	ASP	CB-CA-C	8.38	127.15	110.40
1	J	18	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	N	18	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	K	18	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	E	3	ALA	N-CA-CB	-8.35	98.41	110.10
1	J	87	ASP	CB-CG-OD2	8.35	125.81	118.30
1	B	3	ALA	N-CA-CB	-8.34	98.43	110.10
1	F	3	ALA	N-CA-CB	-8.33	98.43	110.10
1	N	452	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	D	3	ALA	N-CA-CB	-8.32	98.45	110.10
1	A	3	ALA	N-CA-CB	-8.32	98.46	110.10
1	C	3	ALA	N-CA-CB	-8.31	98.46	110.10
1	L	18	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	G	3	ALA	N-CA-CB	-8.31	98.47	110.10
1	K	452	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	M	452	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	G	13	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	C	13	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	L	452	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	H	452	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	N	362	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	D	362	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	I	18	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	C	87	ASP	CB-CG-OD2	8.16	125.64	118.30
1	I	452	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	M	362	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	13	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	E	13	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	362	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	87	ASP	CB-CG-OD2	8.13	125.62	118.30
1	B	87	ASP	CB-CG-OD2	8.13	125.61	118.30
1	F	87	ASP	CB-CG-OD2	8.12	125.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	362	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	L	362	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	J	452	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	362	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	F	13	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	D	87	ASP	CB-CG-OD2	8.09	125.58	118.30
1	G	87	ASP	CB-CG-OD2	8.09	125.58	118.30
1	H	362	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	E	87	ASP	CB-CG-OD2	8.07	125.57	118.30
1	A	13	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	J	362	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	G	362	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	K	362	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	C	362	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	D	231	ARG	CA-CB-CG	8.03	131.06	113.40
1	E	362	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	13	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	231	ARG	CA-CB-CG	8.01	131.02	113.40
1	I	362	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	C	231	ARG	CA-CB-CG	7.98	130.96	113.40
1	F	404	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	231	ARG	CA-CB-CG	7.98	130.96	113.40
1	E	231	ARG	CA-CB-CG	7.98	130.95	113.40
1	A	285	ARG	CB-CA-C	-7.94	94.53	110.40
1	D	285	ARG	CB-CA-C	-7.93	94.53	110.40
1	B	285	ARG	CB-CA-C	-7.93	94.54	110.40
1	E	285	ARG	CB-CA-C	-7.92	94.55	110.40
1	F	285	ARG	CB-CA-C	-7.92	94.57	110.40
1	G	285	ARG	CB-CA-C	-7.91	94.59	110.40
1	C	404	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	404	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	D	230	ILE	CB-CA-C	-7.89	95.81	111.60
1	C	285	ARG	CB-CA-C	-7.89	94.62	110.40
1	D	404	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	G	404	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	E	230	ILE	CB-CA-C	-7.88	95.84	111.60
1	C	230	ILE	CB-CA-C	-7.88	95.84	111.60
1	B	230	ILE	CB-CA-C	-7.88	95.84	111.60
1	H	285	ARG	CB-CA-C	-7.87	94.67	110.40
1	K	285	ARG	CB-CA-C	-7.87	94.67	110.40
1	A	230	ILE	CB-CA-C	-7.86	95.88	111.60
1	F	257	GLU	CB-CA-C	7.86	126.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	285	ARG	CB-CA-C	-7.85	94.71	110.40
1	N	285	ARG	CB-CA-C	-7.84	94.73	110.40
1	E	404	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	I	285	ARG	CB-CA-C	-7.83	94.73	110.40
1	J	285	ARG	CB-CA-C	-7.83	94.74	110.40
1	L	285	ARG	CB-CA-C	-7.83	94.75	110.40
1	B	404	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	F	115	ASP	CB-CA-C	7.76	125.93	110.40
1	C	115	ASP	CB-CA-C	7.75	125.91	110.40
1	B	115	ASP	CB-CA-C	7.75	125.90	110.40
1	G	115	ASP	CB-CA-C	7.75	125.89	110.40
1	E	115	ASP	CB-CA-C	7.74	125.89	110.40
1	K	404	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	I	404	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	D	115	ASP	CB-CA-C	7.73	125.86	110.40
1	H	404	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	115	ASP	CB-CA-C	7.73	125.86	110.40
1	N	404	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	F	255	GLU	CB-CA-C	7.71	125.81	110.40
1	J	404	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	M	152	ALA	CB-CA-C	7.68	121.62	110.10
1	L	404	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	G	261	THR	N-CA-CB	7.65	124.84	110.30
1	K	152	ALA	CB-CA-C	7.65	121.58	110.10
1	I	152	ALA	CB-CA-C	7.64	121.57	110.10
1	N	152	ALA	CB-CA-C	7.64	121.57	110.10
1	L	152	ALA	CB-CA-C	7.64	121.55	110.10
1	H	152	ALA	CB-CA-C	7.63	121.54	110.10
1	J	152	ALA	CB-CA-C	7.62	121.53	110.10
1	C	104	LEU	CB-CA-C	7.58	124.61	110.20
1	E	104	LEU	CB-CA-C	7.58	124.61	110.20
1	G	104	LEU	CB-CA-C	7.58	124.59	110.20
1	D	104	LEU	CB-CA-C	7.57	124.58	110.20
1	F	104	LEU	CB-CA-C	7.57	124.57	110.20
1	A	104	LEU	CB-CA-C	7.56	124.57	110.20
1	B	104	LEU	CB-CA-C	7.55	124.55	110.20
1	M	404	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	J	34	LYS	CB-CA-C	7.55	125.50	110.40
1	L	34	LYS	CB-CA-C	7.54	125.47	110.40
1	I	34	LYS	CB-CA-C	7.54	125.47	110.40
1	M	34	LYS	CB-CA-C	7.53	125.47	110.40
1	H	34	LYS	CB-CA-C	7.53	125.45	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	34	LYS	CB-CA-C	7.53	125.45	110.40
1	N	34	LYS	CB-CA-C	7.51	125.42	110.40
1	A	285	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	F	203	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	E	285	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	F	3	ALA	CB-CA-C	-7.45	98.92	110.10
1	D	3	ALA	CB-CA-C	-7.45	98.93	110.10
1	B	3	ALA	CB-CA-C	-7.43	98.95	110.10
1	E	3	ALA	CB-CA-C	-7.43	98.95	110.10
1	G	3	ALA	CB-CA-C	-7.42	98.98	110.10
1	C	3	ALA	CB-CA-C	-7.41	98.98	110.10
1	A	3	ALA	CB-CA-C	-7.41	98.99	110.10
1	D	285	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	285	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	261	THR	N-CA-CB	7.35	124.27	110.30
1	G	285	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	261	THR	N-CA-CB	7.34	124.25	110.30
1	E	261	THR	N-CA-CB	7.34	124.25	110.30
1	C	285	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	261	THR	N-CA-CB	7.33	124.22	110.30
1	D	261	THR	N-CA-CB	7.32	124.21	110.30
1	N	85	ALA	N-CA-CB	-7.29	99.89	110.10
1	I	85	ALA	N-CA-CB	-7.29	99.90	110.10
1	K	85	ALA	N-CA-CB	-7.29	99.90	110.10
1	L	85	ALA	N-CA-CB	-7.28	99.90	110.10
1	J	85	ALA	N-CA-CB	-7.27	99.92	110.10
1	H	85	ALA	N-CA-CB	-7.27	99.92	110.10
1	M	85	ALA	N-CA-CB	-7.27	99.93	110.10
1	F	285	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	E	203	TYR	CB-CG-CD2	-7.18	116.69	121.00
1	F	261	THR	N-CA-CB	7.14	123.87	110.30
1	G	230	ILE	CB-CA-C	-7.11	97.38	111.60
1	G	203	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	C	152	ALA	CB-CA-C	7.10	120.75	110.10
1	A	203	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	G	152	ALA	CB-CA-C	7.08	120.72	110.10
1	E	152	ALA	CB-CA-C	7.08	120.71	110.10
1	F	152	ALA	CB-CA-C	7.08	120.71	110.10
1	B	203	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	A	152	ALA	CB-CA-C	7.06	120.69	110.10
1	B	152	ALA	CB-CA-C	7.06	120.69	110.10
1	C	203	TYR	CB-CG-CD2	-7.05	116.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	152	ALA	CB-CA-C	7.05	120.68	110.10
1	D	85	ALA	N-CA-CB	-7.01	100.28	110.10
1	D	58	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	F	85	ALA	N-CA-CB	-7.00	100.30	110.10
1	A	85	ALA	N-CA-CB	-6.99	100.31	110.10
1	E	85	ALA	N-CA-CB	-6.99	100.31	110.10
1	B	85	ALA	N-CA-CB	-6.99	100.31	110.10
1	D	203	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	C	85	ALA	N-CA-CB	-6.98	100.33	110.10
1	G	85	ALA	N-CA-CB	-6.98	100.33	110.10
1	E	58	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	L	13	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	M	13	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	N	13	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	K	13	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	G	58	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	H	13	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	58	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	B	58	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	J	13	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	58	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	M	523	ASP	CB-CG-OD1	6.87	124.48	118.30
1	F	58	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	I	523	ASP	CB-CG-OD1	6.85	124.46	118.30
1	H	523	ASP	CB-CG-OD1	6.84	124.46	118.30
1	I	353	ILE	CB-CA-C	-6.83	97.94	111.60
1	L	353	ILE	CB-CA-C	-6.83	97.94	111.60
1	L	523	ASP	CB-CG-OD1	6.83	124.44	118.30
1	M	353	ILE	CB-CA-C	-6.82	97.96	111.60
1	J	353	ILE	CB-CA-C	-6.82	97.96	111.60
1	E	482	THR	N-CA-CB	6.82	123.25	110.30
1	J	523	ASP	CB-CG-OD1	6.82	124.44	118.30
1	N	353	ILE	CB-CA-C	-6.82	97.97	111.60
1	H	353	ILE	CB-CA-C	-6.81	97.98	111.60
1	K	353	ILE	CB-CA-C	-6.81	97.98	111.60
1	A	482	THR	N-CA-CB	6.81	123.24	110.30
1	C	482	THR	N-CA-CB	6.81	123.24	110.30
1	B	482	THR	N-CA-CB	6.80	123.23	110.30
1	G	482	THR	N-CA-CB	6.80	123.22	110.30
1	K	367	GLU	CB-CA-C	-6.80	96.80	110.40
1	N	523	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	482	THR	N-CA-CB	6.79	123.20	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	523	ASP	CB-CG-OD1	6.79	124.41	118.30
1	J	367	GLU	CB-CA-C	-6.79	96.83	110.40
1	F	482	THR	N-CA-CB	6.78	123.18	110.30
1	N	367	GLU	CB-CA-C	-6.78	96.84	110.40
1	L	367	GLU	CB-CA-C	-6.77	96.85	110.40
1	M	367	GLU	CB-CA-C	-6.77	96.86	110.40
1	I	367	GLU	CB-CA-C	-6.77	96.86	110.40
1	H	367	GLU	CB-CA-C	-6.77	96.87	110.40
1	I	13	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	L	322	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	H	322	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	F	322	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	H	482	THR	N-CA-CB	6.71	123.05	110.30
1	L	482	THR	N-CA-CB	6.69	123.02	110.30
1	N	482	THR	N-CA-CB	6.69	123.01	110.30
1	A	322	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	M	482	THR	N-CA-CB	6.68	123.00	110.30
1	J	482	THR	N-CA-CB	6.68	122.99	110.30
1	K	482	THR	N-CA-CB	6.68	122.99	110.30
1	I	482	THR	N-CA-CB	6.66	122.95	110.30
1	M	322	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	E	322	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	F	203	TYR	CB-CG-CD1	6.64	124.99	121.00
1	J	322	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	255	GLU	CB-CA-C	6.62	123.65	110.40
1	K	322	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	322	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	D	255	GLU	CB-CA-C	6.62	123.63	110.40
1	C	322	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	255	GLU	CB-CA-C	6.61	123.62	110.40
1	C	255	GLU	CB-CA-C	6.61	123.61	110.40
1	C	444	LEU	CB-CA-C	-6.60	97.66	110.20
1	E	255	GLU	CB-CA-C	6.60	123.60	110.40
1	A	444	LEU	CB-CA-C	-6.59	97.68	110.20
1	B	444	LEU	CB-CA-C	-6.59	97.69	110.20
1	G	444	LEU	CB-CA-C	-6.59	97.68	110.20
1	E	444	LEU	CB-CA-C	-6.58	97.69	110.20
1	I	322	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	322	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	F	444	LEU	CB-CA-C	-6.58	97.70	110.20
1	D	444	LEU	CB-CA-C	-6.57	97.71	110.20
1	G	322	ARG	NE-CZ-NH1	6.57	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	THR	N-CA-CB	6.57	122.78	110.30
1	J	268	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	E	266	THR	N-CA-CB	6.56	122.77	110.30
1	E	417	VAL	CA-CB-CG2	-6.55	101.07	110.90
1	B	266	THR	N-CA-CB	6.55	122.75	110.30
1	F	417	VAL	CA-CB-CG2	-6.55	101.07	110.90
1	D	266	THR	N-CA-CB	6.55	122.75	110.30
1	H	417	VAL	CA-CB-CG2	-6.55	101.08	110.90
1	A	266	THR	N-CA-CB	6.55	122.74	110.30
1	K	417	VAL	CA-CB-CG2	-6.54	101.08	110.90
1	D	417	VAL	CA-CB-CG2	-6.54	101.09	110.90
1	I	417	VAL	CA-CB-CG2	-6.54	101.10	110.90
1	J	417	VAL	CA-CB-CG2	-6.54	101.10	110.90
1	D	353	ILE	CB-CA-C	-6.53	98.54	111.60
1	N	322	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	M	417	VAL	CA-CB-CG2	-6.52	101.12	110.90
1	B	417	VAL	CA-CB-CG2	-6.52	101.12	110.90
1	H	268	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	L	417	VAL	CA-CB-CG2	-6.51	101.13	110.90
1	B	353	ILE	CB-CA-C	-6.50	98.59	111.60
1	E	353	ILE	CB-CA-C	-6.50	98.60	111.60
1	G	417	VAL	CA-CB-CG2	-6.50	101.15	110.90
1	A	417	VAL	CA-CB-CG2	-6.50	101.15	110.90
1	C	417	VAL	CA-CB-CG2	-6.50	101.16	110.90
1	N	417	VAL	CA-CB-CG2	-6.49	101.16	110.90
1	G	353	ILE	CB-CA-C	-6.49	98.62	111.60
1	C	353	ILE	CB-CA-C	-6.48	98.64	111.60
1	D	257	GLU	CB-CA-C	6.48	123.36	110.40
1	A	257	GLU	CB-CA-C	6.48	123.36	110.40
1	A	353	ILE	CB-CA-C	-6.47	98.65	111.60
1	E	257	GLU	CB-CA-C	6.47	123.33	110.40
1	F	353	ILE	CB-CA-C	-6.47	98.67	111.60
1	C	257	GLU	CB-CA-C	6.46	123.33	110.40
1	B	257	GLU	CB-CA-C	6.46	123.33	110.40
1	D	268	ARG	CB-CA-C	6.45	123.30	110.40
1	C	268	ARG	CB-CA-C	6.45	123.30	110.40
1	E	268	ARG	CB-CA-C	6.43	123.27	110.40
1	A	268	ARG	CB-CA-C	6.43	123.27	110.40
1	F	268	ARG	CB-CA-C	6.43	123.27	110.40
1	M	268	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	268	ARG	CB-CA-C	6.43	123.26	110.40
1	D	63	GLU	CA-CB-CG	6.43	127.54	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	322	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	63	GLU	CA-CB-CG	6.42	127.52	113.40
1	B	63	GLU	CA-CB-CG	6.42	127.52	113.40
1	E	63	GLU	CA-CB-CG	6.42	127.51	113.40
1	N	268	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	G	268	ARG	CB-CA-C	6.41	123.21	110.40
1	F	63	GLU	CA-CB-CG	6.41	127.49	113.40
1	G	63	GLU	CA-CB-CG	6.41	127.49	113.40
1	C	63	GLU	CA-CB-CG	6.40	127.49	113.40
1	K	268	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	H	322	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	I	268	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	L	140	ASP	N-CA-CB	-6.37	99.14	110.60
1	J	140	ASP	N-CA-CB	-6.35	99.16	110.60
1	B	494	LEU	CB-CA-C	6.35	122.27	110.20
1	G	18	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	N	140	ASP	N-CA-CB	-6.35	99.17	110.60
1	K	140	ASP	N-CA-CB	-6.35	99.17	110.60
1	D	494	LEU	CB-CA-C	6.35	122.26	110.20
1	L	268	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	C	203	TYR	CB-CG-CD1	6.35	124.81	121.00
1	A	203	TYR	CB-CG-CD1	6.34	124.81	121.00
1	F	268	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	G	203	TYR	CB-CG-CD1	6.34	124.80	121.00
1	E	494	LEU	CB-CA-C	6.33	122.23	110.20
1	H	140	ASP	N-CA-CB	-6.33	99.20	110.60
1	G	494	LEU	CB-CA-C	6.33	122.23	110.20
1	F	494	LEU	CB-CA-C	6.33	122.22	110.20
1	I	140	ASP	N-CA-CB	-6.33	99.21	110.60
1	E	203	TYR	CB-CG-CD1	6.33	124.80	121.00
1	J	322	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	494	LEU	CB-CA-C	6.32	122.22	110.20
1	D	126	ALA	CB-CA-C	6.32	119.58	110.10
1	E	126	ALA	CB-CA-C	6.32	119.58	110.10
1	C	494	LEU	CB-CA-C	6.32	122.21	110.20
1	M	140	ASP	N-CA-CB	-6.32	99.22	110.60
1	F	126	ALA	CB-CA-C	6.32	119.58	110.10
1	C	126	ALA	CB-CA-C	6.32	119.57	110.10
1	A	126	ALA	CB-CA-C	6.31	119.56	110.10
1	B	126	ALA	CB-CA-C	6.31	119.56	110.10
1	M	322	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	G	126	ALA	CB-CA-C	6.31	119.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	203	TYR	CB-CG-CD1	6.29	124.77	121.00
1	G	341	ALA	N-CA-CB	6.24	118.84	110.10
1	B	341	ALA	N-CA-CB	6.24	118.83	110.10
1	B	18	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	341	ALA	N-CA-CB	6.23	118.82	110.10
1	G	268	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	K	322	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	I	322	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	N	322	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	341	ALA	N-CA-CB	6.21	118.80	110.10
1	F	341	ALA	N-CA-CB	6.21	118.80	110.10
1	E	341	ALA	N-CA-CB	6.20	118.78	110.10
1	D	203	TYR	CB-CG-CD1	6.20	124.72	121.00
1	C	341	ALA	N-CA-CB	6.19	118.76	110.10
1	E	18	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	F	18	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	G	243	ALA	N-CA-CB	6.17	118.74	110.10
1	D	18	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	18	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	H	58	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	K	3	ALA	CB-CA-C	6.13	119.30	110.10
1	I	3	ALA	CB-CA-C	6.12	119.27	110.10
1	M	3	ALA	CB-CA-C	6.11	119.27	110.10
1	L	3	ALA	CB-CA-C	6.11	119.27	110.10
1	M	190	VAL	CB-CA-C	6.11	123.00	111.40
1	I	190	VAL	CB-CA-C	6.10	122.99	111.40
1	N	3	ALA	CB-CA-C	6.10	119.25	110.10
1	J	190	VAL	CB-CA-C	6.09	122.98	111.40
1	H	3	ALA	CB-CA-C	6.09	119.24	110.10
1	H	190	VAL	CB-CA-C	6.09	122.97	111.40
1	J	3	ALA	CB-CA-C	6.09	119.23	110.10
1	L	190	VAL	CB-CA-C	6.09	122.97	111.40
1	N	190	VAL	CB-CA-C	6.08	122.95	111.40
1	K	190	VAL	CB-CA-C	6.08	122.94	111.40
1	K	510	VAL	CB-CA-C	-6.07	99.86	111.40
1	M	510	VAL	CB-CA-C	-6.07	99.86	111.40
1	N	510	VAL	CB-CA-C	-6.07	99.87	111.40
1	F	196	ASP	N-CA-CB	-6.06	99.69	110.60
1	J	243	ALA	N-CA-CB	6.06	118.58	110.10
1	L	510	VAL	CB-CA-C	-6.06	99.89	111.40
1	A	196	ASP	N-CA-CB	-6.06	99.70	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	510	VAL	CB-CA-C	-6.05	99.90	111.40
1	D	196	ASP	N-CA-CB	-6.05	99.71	110.60
1	H	510	VAL	CB-CA-C	-6.05	99.90	111.40
1	E	196	ASP	N-CA-CB	-6.05	99.71	110.60
1	J	510	VAL	CB-CA-C	-6.05	99.91	111.40
1	C	268	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	367	GLU	CB-CA-C	-6.04	98.33	110.40
1	G	196	ASP	N-CA-CB	-6.04	99.73	110.60
1	C	196	ASP	N-CA-CB	-6.04	99.74	110.60
1	D	367	GLU	CB-CA-C	-6.03	98.33	110.40
1	C	367	GLU	CB-CA-C	-6.03	98.34	110.40
1	F	367	GLU	CB-CA-C	-6.03	98.34	110.40
1	B	268	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	367	GLU	CB-CA-C	-6.02	98.36	110.40
1	B	196	ASP	N-CA-CB	-6.02	99.76	110.60
1	E	367	GLU	CB-CA-C	-6.01	98.37	110.40
1	G	367	GLU	CB-CA-C	-6.01	98.37	110.40
1	N	243	ALA	N-CA-CB	6.01	118.52	110.10
1	J	126	ALA	CB-CA-C	6.00	119.11	110.10
1	K	243	ALA	N-CA-CB	6.00	118.51	110.10
1	L	243	ALA	N-CA-CB	6.00	118.50	110.10
1	K	58	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	M	243	ALA	N-CA-CB	6.00	118.50	110.10
1	A	206	ASN	CA-CB-CG	5.99	126.59	113.40
1	I	243	ALA	N-CA-CB	5.99	118.49	110.10
1	E	206	ASN	CA-CB-CG	5.98	126.56	113.40
1	M	126	ALA	CB-CA-C	5.98	119.06	110.10
1	K	126	ALA	CB-CA-C	5.97	119.06	110.10
1	H	243	ALA	N-CA-CB	5.97	118.46	110.10
1	H	126	ALA	CB-CA-C	5.97	119.05	110.10
1	F	206	ASN	CA-CB-CG	5.96	126.52	113.40
1	N	126	ALA	CB-CA-C	5.96	119.05	110.10
1	I	126	ALA	CB-CA-C	5.96	119.04	110.10
1	D	206	ASN	CA-CB-CG	5.96	126.51	113.40
1	J	58	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	206	ASN	CA-CB-CG	5.96	126.50	113.40
1	L	126	ALA	CB-CA-C	5.95	119.03	110.10
1	L	58	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	N	196	ASP	N-CA-CB	-5.95	99.90	110.60
1	B	206	ASN	CA-CB-CG	5.94	126.47	113.40
1	J	196	ASP	N-CA-CB	-5.94	99.90	110.60
1	E	268	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	268	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	F	262	LEU	CB-CA-C	5.93	121.47	110.20
1	H	196	ASP	N-CA-CB	-5.92	99.95	110.60
1	I	58	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	E	380	LYS	N-CA-CB	-5.91	99.97	110.60
1	K	196	ASP	N-CA-CB	-5.91	99.97	110.60
1	J	139	SER	CB-CA-C	5.90	121.31	110.10
1	M	196	ASP	N-CA-CB	-5.90	99.97	110.60
1	L	139	SER	CB-CA-C	5.90	121.31	110.10
1	K	139	SER	CB-CA-C	5.90	121.31	110.10
1	C	320	ALA	CB-CA-C	5.90	118.94	110.10
1	B	320	ALA	CB-CA-C	5.89	118.94	110.10
1	I	139	SER	CB-CA-C	5.89	121.30	110.10
1	M	58	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	M	139	SER	CB-CA-C	5.89	121.30	110.10
1	N	139	SER	CB-CA-C	5.89	121.30	110.10
1	L	196	ASP	N-CA-CB	-5.89	100.00	110.60
1	F	320	ALA	CB-CA-C	5.89	118.93	110.10
1	H	203	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	I	196	ASP	N-CA-CB	-5.88	100.01	110.60
1	H	139	SER	CB-CA-C	5.88	121.28	110.10
1	D	380	LYS	N-CA-CB	-5.88	100.02	110.60
1	A	268	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	D	285	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	G	166	MET	CG-SD-CE	-5.87	90.80	100.20
1	E	320	ALA	CB-CA-C	5.87	118.91	110.10
1	G	380	LYS	N-CA-CB	-5.87	100.04	110.60
1	N	58	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	243	ALA	N-CA-CB	5.86	118.31	110.10
1	F	380	LYS	N-CA-CB	-5.86	100.06	110.60
1	B	380	LYS	N-CA-CB	-5.86	100.06	110.60
1	N	149	THR	N-CA-CB	5.86	121.43	110.30
1	I	149	THR	N-CA-CB	5.86	121.42	110.30
1	A	380	LYS	N-CA-CB	-5.85	100.08	110.60
1	C	166	MET	CG-SD-CE	-5.85	90.84	100.20
1	D	166	MET	CG-SD-CE	-5.85	90.84	100.20
1	A	166	MET	CG-SD-CE	-5.85	90.85	100.20
1	L	149	THR	N-CA-CB	5.85	121.41	110.30
1	B	315	GLU	CB-CA-C	5.84	122.09	110.40
1	E	315	GLU	CB-CA-C	5.84	122.09	110.40
1	K	149	THR	N-CA-CB	5.84	121.40	110.30
1	C	380	LYS	N-CA-CB	-5.84	100.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	ALA	CB-CA-C	5.84	118.86	110.10
1	E	166	MET	CG-SD-CE	-5.84	90.85	100.20
1	J	149	THR	N-CA-CB	5.84	121.40	110.30
1	B	166	MET	CG-SD-CE	-5.84	90.85	100.20
1	C	315	GLU	CB-CA-C	5.84	122.08	110.40
1	D	315	GLU	CB-CA-C	5.84	122.08	110.40
1	F	315	GLU	CB-CA-C	5.84	122.08	110.40
1	F	230	ILE	CA-CB-CG1	5.84	122.09	111.00
1	K	203	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	A	285	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	510	VAL	CB-CA-C	-5.83	100.33	111.40
1	A	510	VAL	CB-CA-C	-5.83	100.33	111.40
1	F	166	MET	CG-SD-CE	-5.83	90.88	100.20
1	E	285	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	H	149	THR	N-CA-CB	5.82	121.36	110.30
1	G	510	VAL	CB-CA-C	-5.82	100.34	111.40
1	F	510	VAL	CB-CA-C	-5.82	100.34	111.40
1	M	149	THR	N-CA-CB	5.82	121.36	110.30
1	C	510	VAL	CB-CA-C	-5.82	100.34	111.40
1	D	510	VAL	CB-CA-C	-5.82	100.35	111.40
1	B	285	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	J	168	LYS	N-CA-CB	-5.81	100.14	110.60
1	H	168	LYS	N-CA-CB	-5.81	100.15	110.60
1	A	320	ALA	CB-CA-C	5.81	118.81	110.10
1	E	510	VAL	CB-CA-C	-5.80	100.37	111.40
1	I	168	LYS	N-CA-CB	-5.80	100.16	110.60
1	I	190	VAL	CG1-CB-CG2	5.79	120.17	110.90
1	N	168	LYS	N-CA-CB	-5.78	100.19	110.60
1	I	203	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	L	190	VAL	CG1-CB-CG2	5.78	120.15	110.90
1	B	320	ALA	N-CA-CB	5.78	118.19	110.10
1	K	168	LYS	N-CA-CB	-5.78	100.20	110.60
1	K	190	VAL	CG1-CB-CG2	5.78	120.14	110.90
1	M	168	LYS	N-CA-CB	-5.78	100.20	110.60
1	F	320	ALA	N-CA-CB	5.77	118.18	110.10
1	J	203	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	M	190	VAL	CG1-CB-CG2	5.77	120.14	110.90
1	E	320	ALA	N-CA-CB	5.77	118.18	110.10
1	L	168	LYS	N-CA-CB	-5.77	100.22	110.60
1	F	36	ARG	CB-CA-C	5.76	121.93	110.40
1	F	285	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	M	203	TYR	CB-CG-CD2	-5.75	117.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	300	VAL	CB-CA-C	-5.75	100.47	111.40
1	J	190	VAL	CG1-CB-CG2	5.75	120.11	110.90
1	A	36	ARG	CB-CA-C	5.75	121.90	110.40
1	B	36	ARG	CB-CA-C	5.75	121.90	110.40
1	D	36	ARG	CB-CA-C	5.75	121.90	110.40
1	G	36	ARG	CB-CA-C	5.75	121.90	110.40
1	N	190	VAL	CG1-CB-CG2	5.75	120.10	110.90
1	C	320	ALA	N-CA-CB	5.75	118.15	110.10
1	D	320	ALA	N-CA-CB	5.75	118.15	110.10
1	E	36	ARG	CB-CA-C	5.75	121.89	110.40
1	B	300	VAL	CB-CA-C	-5.75	100.48	111.40
1	C	285	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	N	203	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	G	368	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	320	ALA	N-CA-CB	5.74	118.14	110.10
1	E	300	VAL	CB-CA-C	-5.74	100.50	111.40
1	K	138	CYS	N-CA-CB	5.74	120.93	110.60
1	C	36	ARG	CB-CA-C	5.74	121.87	110.40
1	A	87	ASP	OD1-CG-OD2	-5.74	112.40	123.30
1	H	190	VAL	CG1-CB-CG2	5.73	120.07	110.90
1	I	226	LYS	N-CA-CB	-5.73	100.29	110.60
1	A	300	VAL	CB-CA-C	-5.73	100.52	111.40
1	D	87	ASP	OD1-CG-OD2	-5.73	112.42	123.30
1	F	300	VAL	CB-CA-C	-5.73	100.52	111.40
1	L	203	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	87	ASP	OD1-CG-OD2	-5.72	112.43	123.30
1	E	87	ASP	OD1-CG-OD2	-5.72	112.44	123.30
1	F	87	ASP	OD1-CG-OD2	-5.72	112.44	123.30
1	G	300	VAL	CB-CA-C	-5.72	100.54	111.40
1	J	138	CYS	N-CA-CB	5.71	120.88	110.60
1	G	285	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	C	300	VAL	CB-CA-C	-5.70	100.56	111.40
1	M	138	CYS	N-CA-CB	5.70	120.86	110.60
1	L	138	CYS	N-CA-CB	5.70	120.86	110.60
1	I	138	CYS	N-CA-CB	5.70	120.85	110.60
1	N	36	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	G	87	ASP	OD1-CG-OD2	-5.69	112.49	123.30
1	H	138	CYS	N-CA-CB	5.69	120.84	110.60
1	N	138	CYS	N-CA-CB	5.69	120.84	110.60
1	J	226	LYS	N-CA-CB	-5.69	100.36	110.60
1	M	226	LYS	N-CA-CB	-5.69	100.36	110.60
1	C	87	ASP	OD1-CG-OD2	-5.69	112.50	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	226	LYS	N-CA-CB	-5.69	100.37	110.60
1	H	226	LYS	N-CA-CB	-5.68	100.37	110.60
1	H	166	MET	CG-SD-CE	-5.68	91.11	100.20
1	J	140	ASP	CB-CG-OD1	5.68	123.41	118.30
1	J	166	MET	CG-SD-CE	-5.67	91.12	100.20
1	I	166	MET	CG-SD-CE	-5.67	91.13	100.20
1	N	226	LYS	N-CA-CB	-5.67	100.39	110.60
1	N	140	ASP	CB-CG-OD1	5.67	123.40	118.30
1	M	140	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	315	GLU	CB-CA-C	5.66	121.73	110.40
1	J	517	THR	CA-CB-CG2	5.66	120.33	112.40
1	L	166	MET	CG-SD-CE	-5.66	91.14	100.20
1	K	226	LYS	N-CA-CB	-5.66	100.41	110.60
1	N	166	MET	CG-SD-CE	-5.66	91.15	100.20
1	H	517	THR	CA-CB-CG2	5.65	120.32	112.40
1	I	140	ASP	CB-CG-OD1	5.65	123.39	118.30
1	M	166	MET	CG-SD-CE	-5.65	91.16	100.20
1	H	87	ASP	OD1-CG-OD2	-5.65	112.57	123.30
1	K	140	ASP	CB-CG-OD1	5.65	123.38	118.30
1	K	166	MET	CG-SD-CE	-5.65	91.16	100.20
1	I	517	THR	CA-CB-CG2	5.64	120.30	112.40
1	K	87	ASP	OD1-CG-OD2	-5.64	112.58	123.30
1	I	36	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	N	87	ASP	OD1-CG-OD2	-5.64	112.59	123.30
1	E	271	VAL	CB-CA-C	-5.63	100.69	111.40
1	K	517	THR	CA-CB-CG2	5.63	120.28	112.40
1	B	271	VAL	CB-CA-C	-5.63	100.70	111.40
1	H	206	ASN	N-CA-CB	5.63	120.73	110.60
1	N	517	THR	CA-CB-CG2	5.63	120.28	112.40
1	L	87	ASP	OD1-CG-OD2	-5.63	112.61	123.30
1	L	517	THR	CA-CB-CG2	5.63	120.28	112.40
1	F	271	VAL	CB-CA-C	-5.63	100.71	111.40
1	K	206	ASN	N-CA-CB	5.63	120.73	110.60
1	I	87	ASP	OD1-CG-OD2	-5.62	112.61	123.30
1	F	11	ASP	CB-CA-C	5.62	121.64	110.40
1	M	206	ASN	N-CA-CB	5.62	120.71	110.60
1	H	140	ASP	CB-CG-OD1	5.61	123.35	118.30
1	M	517	THR	CA-CB-CG2	5.61	120.25	112.40
1	C	271	VAL	CB-CA-C	-5.61	100.74	111.40
1	D	271	VAL	CB-CA-C	-5.61	100.75	111.40
1	C	11	ASP	CB-CA-C	5.60	121.61	110.40
1	D	11	ASP	CB-CA-C	5.60	121.61	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	369	VAL	N-CA-CB	5.60	123.83	111.50
1	L	140	ASP	CB-CG-OD1	5.60	123.34	118.30
1	N	206	ASN	N-CA-CB	5.60	120.69	110.60
1	E	11	ASP	CB-CA-C	5.60	121.60	110.40
1	M	87	ASP	OD1-CG-OD2	-5.60	112.66	123.30
1	A	11	ASP	CB-CA-C	5.60	121.60	110.40
1	F	368	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	H	155	ASP	CB-CA-C	5.60	121.59	110.40
1	G	11	ASP	CB-CA-C	5.59	121.59	110.40
1	L	206	ASN	N-CA-CB	5.59	120.67	110.60
1	I	206	ASN	N-CA-CB	5.59	120.66	110.60
1	J	206	ASN	N-CA-CB	5.59	120.66	110.60
1	J	87	ASP	OD1-CG-OD2	-5.59	112.69	123.30
1	N	369	VAL	N-CA-CB	5.59	123.79	111.50
1	B	11	ASP	CB-CA-C	5.58	121.57	110.40
1	G	315	GLU	CB-CA-C	5.58	121.57	110.40
1	H	369	VAL	N-CA-CB	5.58	123.77	111.50
1	L	369	VAL	N-CA-CB	5.58	123.77	111.50
1	I	285	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	K	155	ASP	CB-CA-C	5.57	121.54	110.40
1	D	235	PRO	N-CA-CB	5.57	109.98	103.30
1	K	369	VAL	N-CA-CB	5.57	123.75	111.50
1	M	369	VAL	N-CA-CB	5.57	123.75	111.50
1	N	155	ASP	CB-CA-C	5.57	121.53	110.40
1	I	155	ASP	CB-CA-C	5.56	121.52	110.40
1	K	36	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	L	155	ASP	CB-CA-C	5.56	121.53	110.40
1	M	155	ASP	CB-CA-C	5.56	121.53	110.40
1	I	369	VAL	N-CA-CB	5.56	123.73	111.50
1	J	285	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	235	PRO	N-CA-CB	5.56	109.97	103.30
1	B	235	PRO	N-CA-CB	5.55	109.96	103.30
1	H	285	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	N	285	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	235	PRO	N-CA-CB	5.55	109.96	103.30
1	E	235	PRO	N-CA-CB	5.55	109.96	103.30
1	J	155	ASP	CB-CA-C	5.54	121.49	110.40
1	B	368	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	D	219	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	F	235	PRO	N-CA-CB	5.53	109.93	103.30
1	L	483	GLU	CB-CG-CD	5.52	129.11	114.20
1	A	368	ARG	NE-CZ-NH1	5.52	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	483	GLU	CB-CG-CD	5.52	129.09	114.20
1	B	501	ARG	N-CA-CB	-5.51	100.68	110.60
1	M	36	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	J	36	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	501	ARG	N-CA-CB	-5.51	100.69	110.60
1	K	483	GLU	CB-CG-CD	5.51	129.07	114.20
1	F	501	ARG	N-CA-CB	-5.50	100.69	110.60
1	H	483	GLU	CB-CG-CD	5.50	129.06	114.20
1	N	204	PHE	CB-CG-CD1	5.50	124.65	120.80
1	D	13	ARG	CD-NE-CZ	5.49	131.29	123.60
1	H	104	LEU	CB-CA-C	5.49	120.64	110.20
1	M	300	VAL	CB-CA-C	-5.49	100.96	111.40
1	N	483	GLU	CB-CG-CD	5.49	129.03	114.20
1	G	501	ARG	N-CA-CB	-5.49	100.71	110.60
1	I	483	GLU	CB-CG-CD	5.49	129.03	114.20
1	M	483	GLU	CB-CG-CD	5.49	129.03	114.20
1	L	104	LEU	CB-CA-C	5.49	120.62	110.20
1	H	204	PHE	CB-CG-CD1	5.48	124.64	120.80
1	N	104	LEU	CB-CA-C	5.48	120.62	110.20
1	I	104	LEU	CB-CA-C	5.48	120.61	110.20
1	I	300	VAL	CB-CA-C	-5.48	100.99	111.40
1	L	36	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	501	ARG	N-CA-CB	-5.48	100.74	110.60
1	B	27	VAL	CB-CA-C	5.47	121.80	111.40
1	H	300	VAL	CB-CA-C	-5.47	101.00	111.40
1	C	412	VAL	CB-CA-C	-5.47	101.00	111.40
1	K	104	LEU	CB-CA-C	5.47	120.60	110.20
1	M	104	LEU	CB-CA-C	5.47	120.60	110.20
1	C	501	ARG	N-CA-CB	-5.47	100.75	110.60
1	E	501	ARG	N-CA-CB	-5.47	100.75	110.60
1	J	104	LEU	CB-CA-C	5.47	120.59	110.20
1	N	300	VAL	CB-CA-C	-5.47	101.01	111.40
1	G	27	VAL	CB-CA-C	5.47	121.79	111.40
1	B	412	VAL	CB-CA-C	-5.46	101.02	111.40
1	J	204	PHE	CB-CG-CD1	5.46	124.62	120.80
1	A	483	GLU	N-CA-CB	5.46	120.43	110.60
1	E	412	VAL	CB-CA-C	-5.46	101.02	111.40
1	L	285	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	483	GLU	N-CA-CB	5.46	120.42	110.60
1	C	483	GLU	N-CA-CB	5.46	120.42	110.60
1	D	27	VAL	CB-CA-C	5.46	121.77	111.40
1	F	483	GLU	N-CA-CB	5.46	120.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	483	GLU	N-CA-CB	5.46	120.42	110.60
1	L	300	VAL	CB-CA-C	-5.46	101.03	111.40
1	D	483	GLU	N-CA-CB	5.46	120.42	110.60
1	F	27	VAL	CB-CA-C	5.46	121.76	111.40
1	E	27	VAL	CB-CA-C	5.45	121.76	111.40
1	H	36	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	J	300	VAL	CB-CA-C	-5.45	101.04	111.40
1	A	13	ARG	CD-NE-CZ	5.45	131.23	123.60
1	K	300	VAL	CB-CA-C	-5.45	101.04	111.40
1	A	412	VAL	CB-CA-C	-5.45	101.05	111.40
1	E	483	GLU	N-CA-CB	5.45	120.41	110.60
1	G	412	VAL	CB-CA-C	-5.45	101.05	111.40
1	A	27	VAL	CB-CA-C	5.44	121.74	111.40
1	C	27	VAL	CB-CA-C	5.44	121.74	111.40
1	C	294	THR	CA-CB-CG2	-5.44	104.79	112.40
1	E	368	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	F	412	VAL	CB-CA-C	-5.43	101.07	111.40
1	D	412	VAL	CB-CA-C	-5.43	101.08	111.40
1	G	275	ALA	CB-CA-C	5.43	118.25	110.10
1	K	285	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	I	204	PHE	CB-CG-CD1	5.43	124.60	120.80
1	F	275	ALA	CB-CA-C	5.43	118.24	110.10
1	B	13	ARG	CD-NE-CZ	5.42	131.19	123.60
1	M	204	PHE	CB-CG-CD1	5.42	124.59	120.80
1	E	294	THR	CA-CB-CG2	-5.42	104.82	112.40
1	B	294	THR	CA-CB-CG2	-5.41	104.82	112.40
1	F	13	ARG	CD-NE-CZ	5.41	131.18	123.60
1	D	294	THR	CA-CB-CG2	-5.41	104.83	112.40
1	C	219	PHE	CB-CG-CD2	-5.41	117.02	120.80
1	C	13	ARG	CD-NE-CZ	5.40	131.16	123.60
1	E	13	ARG	CD-NE-CZ	5.40	131.16	123.60
1	G	294	THR	CA-CB-CG2	-5.40	104.84	112.40
1	G	13	ARG	CD-NE-CZ	5.40	131.15	123.60
1	A	275	ALA	CB-CA-C	5.39	118.19	110.10
1	A	294	THR	CA-CB-CG2	-5.39	104.85	112.40
1	F	294	THR	CA-CB-CG2	-5.38	104.86	112.40
1	K	204	PHE	CB-CG-CD1	5.38	124.57	120.80
1	M	285	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	219	PHE	CB-CG-CD2	-5.38	117.04	120.80
1	C	368	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	275	ALA	CB-CA-C	5.38	118.17	110.10
1	A	59	GLU	CB-CA-C	5.38	121.15	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	K	284	ARG	CB-CA-C	-5.37	99.65	110.40
1	C	59	GLU	CB-CA-C	5.37	121.14	110.40
1	C	275	ALA	CB-CA-C	5.37	118.16	110.10
1	E	219	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	F	59	GLU	CB-CA-C	5.37	121.14	110.40
1	I	284	ARG	CB-CA-C	-5.37	99.66	110.40
1	D	368	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	L	338	GLU	CB-CA-C	5.37	121.14	110.40
1	B	275	ALA	CB-CA-C	5.37	118.15	110.10
1	G	59	GLU	CB-CA-C	5.37	121.13	110.40
1	H	284	ARG	CB-CA-C	-5.37	99.67	110.40
1	L	235	PRO	N-CA-CB	5.36	109.73	103.30
1	L	284	ARG	CB-CA-C	-5.36	99.67	110.40
1	B	59	GLU	CB-CA-C	5.36	121.12	110.40
1	D	275	ALA	CB-CA-C	5.36	118.14	110.10
1	G	334	ASP	CB-CG-OD1	5.36	123.12	118.30
1	M	338	GLU	CB-CA-C	5.36	121.12	110.40
1	N	284	ARG	CB-CA-C	-5.36	99.68	110.40
1	H	235	PRO	N-CA-CB	5.36	109.72	103.30
1	M	235	PRO	N-CA-CB	5.36	109.73	103.30
1	N	338	GLU	CB-CA-C	5.35	121.11	110.40
1	B	395	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	J	284	ARG	CB-CA-C	-5.35	99.70	110.40
1	K	338	GLU	CB-CA-C	5.35	121.10	110.40
1	K	483	GLU	N-CA-CB	5.35	120.23	110.60
1	I	338	GLU	CB-CA-C	5.35	121.10	110.40
1	M	284	ARG	CB-CA-C	-5.35	99.70	110.40
1	L	204	PHE	CB-CG-CD1	5.35	124.54	120.80
1	D	59	GLU	CB-CA-C	5.34	121.09	110.40
1	J	338	GLU	CB-CA-C	5.34	121.09	110.40
1	B	491	MET	CB-CA-C	5.34	121.08	110.40
1	D	491	MET	CB-CA-C	5.34	121.08	110.40
1	G	491	MET	CB-CA-C	5.34	121.08	110.40
1	I	483	GLU	N-CA-CB	5.34	120.21	110.60
1	M	483	GLU	N-CA-CB	5.34	120.21	110.60
1	N	483	GLU	N-CA-CB	5.34	120.21	110.60
1	E	59	GLU	CB-CA-C	5.34	121.08	110.40
1	C	491	MET	CB-CA-C	5.33	121.07	110.40
1	D	322	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	H	338	GLU	CB-CA-C	5.33	121.06	110.40
1	L	483	GLU	N-CA-CB	5.33	120.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	395	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	F	491	MET	CB-CA-C	5.32	121.04	110.40
1	B	345	ARG	CB-CA-C	5.32	121.04	110.40
1	G	345	ARG	CB-CA-C	5.32	121.04	110.40
1	I	444	LEU	CB-CA-C	-5.32	100.09	110.20
1	J	444	LEU	CB-CA-C	-5.32	100.09	110.20
1	F	219	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	J	235	PRO	CB-CA-C	5.32	125.29	112.00
1	K	235	PRO	CB-CA-C	5.32	125.29	112.00
1	C	395	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	E	491	MET	CB-CA-C	5.31	121.03	110.40
1	J	483	GLU	N-CA-CB	5.31	120.17	110.60
1	F	322	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	H	483	GLU	N-CA-CB	5.31	120.16	110.60
1	J	235	PRO	N-CA-CB	5.31	109.68	103.30
1	N	235	PRO	CB-CA-C	5.31	125.28	112.00
1	C	345	ARG	CB-CA-C	5.31	121.02	110.40
1	L	216	GLU	N-CA-CB	-5.31	101.04	110.60
1	A	491	MET	CB-CA-C	5.31	121.02	110.40
1	E	345	ARG	CB-CA-C	5.31	121.02	110.40
1	K	235	PRO	N-CA-CB	5.31	109.67	103.30
1	M	216	GLU	N-CA-CB	-5.31	101.05	110.60
1	A	345	ARG	CB-CA-C	5.30	121.01	110.40
1	F	345	ARG	CB-CA-C	5.30	121.01	110.40
1	M	235	PRO	CB-CA-C	5.30	125.26	112.00
1	N	67	GLU	CB-CA-C	5.30	121.01	110.40
1	N	235	PRO	N-CA-CB	5.30	109.67	103.30
1	N	444	LEU	CB-CA-C	-5.30	100.12	110.20
1	H	216	GLU	N-CA-CB	-5.30	101.05	110.60
1	N	27	VAL	CB-CA-C	5.30	121.47	111.40
1	N	216	GLU	N-CA-CB	-5.30	101.06	110.60
1	D	345	ARG	CB-CA-C	5.30	121.00	110.40
1	J	216	GLU	N-CA-CB	-5.29	101.07	110.60
1	J	218	PRO	N-CA-CB	5.29	109.65	103.30
1	H	235	PRO	CB-CA-C	5.29	125.22	112.00
1	L	235	PRO	CB-CA-C	5.29	125.22	112.00
1	B	334	ASP	CB-CG-OD1	5.29	123.06	118.30
1	G	395	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	I	216	GLU	N-CA-CB	-5.29	101.09	110.60
1	L	218	PRO	N-CA-CB	5.29	109.64	103.30
1	G	235	PRO	N-CA-CB	5.28	109.64	103.30
1	K	218	PRO	N-CA-CB	5.28	109.64	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	444	LEU	CB-CA-C	-5.28	100.16	110.20
1	K	216	GLU	N-CA-CB	-5.28	101.10	110.60
1	K	444	LEU	CB-CA-C	-5.28	100.17	110.20
1	N	218	PRO	N-CA-CB	5.28	109.63	103.30
1	M	67	GLU	CB-CA-C	5.28	120.95	110.40
1	L	67	GLU	CB-CA-C	5.27	120.95	110.40
1	K	67	GLU	CB-CA-C	5.27	120.95	110.40
1	M	218	PRO	N-CA-CB	5.27	109.63	103.30
1	M	444	LEU	CB-CA-C	-5.27	100.18	110.20
1	G	322	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	H	218	PRO	N-CA-CB	5.27	109.62	103.30
1	C	334	ASP	CB-CG-OD1	5.27	123.04	118.30
1	H	27	VAL	CB-CA-C	5.27	121.41	111.40
1	K	27	VAL	CB-CA-C	5.27	121.41	111.40
1	G	218	PRO	N-CA-CB	5.26	109.62	103.30
1	I	268	ARG	CB-CA-C	5.26	120.93	110.40
1	J	67	GLU	CB-CA-C	5.26	120.93	110.40
1	A	322	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	I	27	VAL	CB-CA-C	5.26	121.40	111.40
1	J	27	VAL	CB-CA-C	5.26	121.40	111.40
1	L	27	VAL	CB-CA-C	5.26	121.40	111.40
1	D	499	VAL	CA-CB-CG2	5.26	118.79	110.90
1	I	67	GLU	CB-CA-C	5.26	120.92	110.40
1	M	27	VAL	CB-CA-C	5.26	121.39	111.40
1	L	444	LEU	CB-CA-C	-5.26	100.21	110.20
1	I	501	ARG	N-CA-CB	-5.25	101.14	110.60
1	L	501	ARG	N-CA-CB	-5.25	101.15	110.60
1	N	501	ARG	N-CA-CB	-5.25	101.15	110.60
1	G	230	ILE	CA-CB-CG1	5.25	120.97	111.00
1	I	218	PRO	N-CA-CB	5.25	109.59	103.30
1	J	501	ARG	N-CA-CB	-5.25	101.16	110.60
1	M	501	ARG	N-CA-CB	-5.24	101.17	110.60
1	N	268	ARG	CB-CA-C	5.24	120.88	110.40
1	H	501	ARG	N-CA-CB	-5.24	101.18	110.60
1	K	268	ARG	CB-CA-C	5.24	120.87	110.40
1	L	268	ARG	CB-CA-C	5.24	120.87	110.40
1	A	334	ASP	CB-CG-OD1	5.23	123.01	118.30
1	F	395	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	499	VAL	CA-CB-CG2	5.23	118.74	110.90
1	F	499	VAL	CA-CB-CG2	5.23	118.74	110.90
1	H	67	GLU	CB-CA-C	5.23	120.85	110.40
1	M	268	ARG	CB-CA-C	5.23	120.85	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	G	499	VAL	CA-CB-CG2	5.22	118.73	110.90
1	H	203	TYR	CB-CG-CD1	5.22	124.13	121.00
1	K	501	ARG	N-CA-CB	-5.22	101.21	110.60
1	G	206	ASN	CA-CB-CG	5.22	124.88	113.40
1	I	380	LYS	N-CA-CB	-5.21	101.22	110.60
1	A	499	VAL	CA-CB-CG2	5.21	118.71	110.90
1	J	268	ARG	CB-CA-C	5.21	120.82	110.40
1	H	268	ARG	CB-CA-C	5.21	120.82	110.40
1	D	334	ASP	CB-CG-OD1	5.21	122.98	118.30
1	L	461	GLU	CB-CA-C	5.20	120.80	110.40
1	E	334	ASP	CB-CG-OD1	5.20	122.98	118.30
1	N	461	GLU	CB-CA-C	5.20	120.80	110.40
1	E	499	VAL	CA-CB-CG2	5.20	118.70	110.90
1	C	499	VAL	CA-CB-CG2	5.20	118.69	110.90
1	K	203	TYR	CB-CG-CD1	5.20	124.12	121.00
1	I	203	TYR	CB-CG-CD1	5.19	124.12	121.00
1	L	380	LYS	N-CA-CB	-5.19	101.26	110.60
1	K	461	GLU	CB-CA-C	5.19	120.78	110.40
1	I	284	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	K	380	LYS	N-CA-CB	-5.19	101.27	110.60
1	H	380	LYS	N-CA-CB	-5.18	101.27	110.60
1	I	235	PRO	CB-CA-C	5.18	124.96	112.00
1	M	461	GLU	CB-CA-C	5.18	120.76	110.40
1	F	334	ASP	CB-CG-OD1	5.18	122.96	118.30
1	F	369	VAL	CA-CB-CG2	5.18	118.67	110.90
1	M	380	LYS	N-CA-CB	-5.18	101.28	110.60
1	E	322	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	G	369	VAL	CA-CB-CG2	5.17	118.66	110.90
1	E	369	VAL	CA-CB-CG2	5.17	118.66	110.90
1	D	369	VAL	CA-CB-CG2	5.17	118.65	110.90
1	C	369	VAL	CA-CB-CG2	5.17	118.65	110.90
1	N	380	LYS	N-CA-CB	-5.17	101.30	110.60
1	J	380	LYS	N-CA-CB	-5.16	101.31	110.60
1	N	284	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	369	VAL	CA-CB-CG2	5.16	118.64	110.90
1	J	461	GLU	CB-CA-C	5.16	120.72	110.40
1	A	271	VAL	CB-CA-C	-5.16	101.60	111.40
1	F	310	GLU	N-CA-CB	-5.16	101.32	110.60
1	L	63	GLU	N-CA-CB	-5.16	101.31	110.60
1	E	62	LEU	CB-CA-C	5.16	120.00	110.20
1	G	179	ASP	N-CA-CB	-5.16	101.32	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	LEU	CB-CA-C	5.15	119.99	110.20
1	C	230	ILE	N-CA-CB	5.15	122.65	110.80
1	F	62	LEU	CB-CA-C	5.15	119.99	110.20
1	N	342	ILE	CB-CA-C	-5.15	101.30	111.60
1	B	369	VAL	CA-CB-CG2	5.15	118.63	110.90
1	M	203	TYR	CB-CG-CD1	5.15	124.09	121.00
1	K	52	ASP	N-CA-CB	5.15	119.86	110.60
1	G	369	VAL	N-CA-CB	5.14	122.82	111.50
1	K	342	ILE	CB-CA-C	-5.14	101.31	111.60
1	E	369	VAL	N-CA-CB	5.14	122.81	111.50
1	I	52	ASP	N-CA-CB	5.14	119.86	110.60
1	L	342	ILE	CB-CA-C	-5.14	101.31	111.60
1	D	62	LEU	CB-CA-C	5.14	119.97	110.20
1	L	203	TYR	CB-CG-CD1	5.14	124.08	121.00
1	M	342	ILE	CB-CA-C	-5.14	101.32	111.60
1	A	230	ILE	N-CA-CB	5.14	122.61	110.80
1	H	52	ASP	N-CA-CB	5.14	119.84	110.60
1	H	63	GLU	N-CA-CB	-5.14	101.35	110.60
1	J	63	GLU	N-CA-CB	-5.14	101.36	110.60
1	K	63	GLU	N-CA-CB	-5.14	101.35	110.60
1	H	342	ILE	CB-CA-C	-5.13	101.33	111.60
1	M	63	GLU	N-CA-CB	-5.13	101.36	110.60
1	N	203	TYR	CB-CG-CD1	5.13	124.08	121.00
1	G	62	LEU	CB-CA-C	5.13	119.95	110.20
1	N	63	GLU	N-CA-CB	-5.13	101.36	110.60
1	F	256	GLY	C-N-CA	5.13	134.53	121.70
1	C	322	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	G	271	VAL	CB-CA-C	-5.13	101.65	111.40
1	I	63	GLU	N-CA-CB	-5.13	101.37	110.60
1	A	231	ARG	N-CA-CB	5.13	119.83	110.60
1	B	369	VAL	N-CA-CB	5.13	122.78	111.50
1	E	230	ILE	N-CA-CB	5.13	122.59	110.80
1	F	369	VAL	N-CA-CB	5.13	122.78	111.50
1	K	251	ALA	N-CA-CB	-5.13	102.92	110.10
1	N	52	ASP	N-CA-CB	5.13	119.83	110.60
1	J	342	ILE	CB-CA-C	-5.13	101.34	111.60
1	L	205	ILE	CB-CA-C	5.13	121.85	111.60
1	A	369	VAL	N-CA-CB	5.12	122.77	111.50
1	C	369	VAL	N-CA-CB	5.12	122.77	111.50
1	D	369	VAL	N-CA-CB	5.12	122.77	111.50
1	N	251	ALA	N-CA-CB	-5.12	102.93	110.10
1	N	455	VAL	CB-CA-C	5.12	121.13	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ILE	N-CA-CB	5.12	122.58	110.80
1	I	342	ILE	CB-CA-C	-5.12	101.36	111.60
1	I	461	GLU	CB-CA-C	5.12	120.64	110.40
1	M	52	ASP	N-CA-CB	5.12	119.82	110.60
1	J	203	TYR	CB-CG-CD1	5.12	124.07	121.00
1	J	251	ALA	N-CA-CB	-5.12	102.93	110.10
1	B	62	LEU	CB-CA-C	5.12	119.92	110.20
1	C	62	LEU	CB-CA-C	5.12	119.93	110.20
1	L	251	ALA	N-CA-CB	-5.12	102.93	110.10
1	H	461	GLU	CB-CA-C	5.12	120.63	110.40
1	I	205	ILE	CB-CA-C	5.12	121.83	111.60
1	H	455	VAL	CB-CA-C	5.11	121.12	111.40
1	H	205	ILE	CB-CA-C	5.11	121.82	111.60
1	A	179	ASP	N-CA-CB	-5.11	101.40	110.60
1	D	230	ILE	N-CA-CB	5.11	122.55	110.80
1	I	251	ALA	N-CA-CB	-5.11	102.95	110.10
1	L	455	VAL	CB-CA-C	5.11	121.10	111.40
1	L	52	ASP	N-CA-CB	5.10	119.79	110.60
1	E	231	ARG	N-CA-CB	5.10	119.78	110.60
1	H	251	ALA	N-CA-CB	-5.10	102.96	110.10
1	J	52	ASP	N-CA-CB	5.10	119.78	110.60
1	N	205	ILE	CB-CA-C	5.10	121.81	111.60
1	M	205	ILE	CB-CA-C	5.10	121.80	111.60
1	B	179	ASP	N-CA-CB	-5.10	101.42	110.60
1	E	179	ASP	N-CA-CB	-5.10	101.42	110.60
1	M	455	VAL	CB-CA-C	5.09	121.08	111.40
1	C	179	ASP	N-CA-CB	-5.09	101.44	110.60
1	C	231	ARG	N-CA-CB	5.09	119.76	110.60
1	D	179	ASP	N-CA-CB	-5.09	101.44	110.60
1	G	284	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	J	205	ILE	CB-CA-C	5.09	121.78	111.60
1	K	205	ILE	CB-CA-C	5.09	121.77	111.60
1	M	251	ALA	N-CA-CB	-5.09	102.98	110.10
1	J	455	VAL	CB-CA-C	5.08	121.06	111.40
1	D	395	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	284	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	K	455	VAL	CB-CA-C	5.08	121.06	111.40
1	D	231	ARG	N-CA-CB	5.08	119.74	110.60
1	M	287	ALA	CB-CA-C	5.08	117.72	110.10
1	J	287	ALA	CB-CA-C	5.08	117.71	110.10
1	N	287	ALA	CB-CA-C	5.07	117.71	110.10
1	A	284	ARG	NE-CZ-NH1	5.07	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	ASP	N-CA-CB	-5.07	101.47	110.60
1	L	284	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	231	ARG	N-CA-CB	5.07	119.72	110.60
1	G	258	ALA	N-CA-CB	5.07	117.19	110.10
1	I	455	VAL	CB-CA-C	5.07	121.03	111.40
1	I	287	ALA	CB-CA-C	5.06	117.69	110.10
1	H	287	ALA	CB-CA-C	5.06	117.69	110.10
1	L	287	ALA	CB-CA-C	5.06	117.68	110.10
1	M	284	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	K	287	ALA	CB-CA-C	5.05	117.67	110.10
1	D	284	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	J	284	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	13	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	F	411	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	J	412	VAL	CB-CA-C	-5.01	101.88	111.40
1	C	155	ASP	CB-CA-C	5.00	120.41	110.40
1	L	412	VAL	CB-CA-C	-5.00	101.89	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	257	GLU	CA

All (135) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	241	ALA	Peptide
1	A	245	LYS	Peptide
1	A	256	GLY	Peptide
1	A	285	ARG	Sidechain
1	A	345	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	404	ARG	Sidechain
1	A	445	ARG	Sidechain
1	B	18	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	241	ALA	Peptide
1	B	245	LYS	Peptide
1	B	256	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	285	ARG	Sidechain
1	B	345	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	445	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	241	ALA	Peptide
1	C	245	LYS	Peptide
1	C	256	GLY	Peptide
1	C	285	ARG	Sidechain
1	C	345	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	445	ARG	Sidechain
1	D	18	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	241	ALA	Peptide
1	D	245	LYS	Peptide
1	D	256	GLY	Peptide
1	D	285	ARG	Sidechain
1	D	345	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	404	ARG	Sidechain
1	D	445	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	197	ARG	Sidechain
1	E	241	ALA	Peptide
1	E	245	LYS	Peptide
1	E	256	GLY	Peptide
1	E	285	ARG	Sidechain
1	E	345	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	362	ARG	Sidechain
1	E	404	ARG	Sidechain
1	E	445	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	197	ARG	Sidechain
1	F	231	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	241	ALA	Peptide
1	F	245	LYS	Peptide
1	F	255	GLU	Peptide
1	F	285	ARG	Sidechain
1	F	345	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	362	ARG	Sidechain
1	F	404	ARG	Sidechain
1	F	445	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	197	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	241	ALA	Peptide
1	G	244	GLY	Peptide
1	G	256	GLY	Peptide
1	G	285	ARG	Sidechain
1	G	345	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	404	ARG	Sidechain
1	G	445	ARG	Sidechain
1	H	118	ARG	Sidechain
1	H	13	ARG	Sidechain
1	H	197	ARG	Sidechain
1	H	231	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	362	ARG	Sidechain
1	H	404	ARG	Sidechain
1	H	445	ARG	Sidechain
1	I	118	ARG	Sidechain
1	I	13	ARG	Sidechain
1	I	197	ARG	Sidechain
1	I	231	ARG	Sidechain
1	I	350	ARG	Sidechain
1	I	362	ARG	Sidechain
1	I	404	ARG	Sidechain
1	I	445	ARG	Sidechain
1	J	118	ARG	Sidechain
1	J	13	ARG	Sidechain
1	J	197	ARG	Sidechain
1	J	231	ARG	Sidechain
1	J	350	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	J	362	ARG	Sidechain
1	J	404	ARG	Sidechain
1	J	445	ARG	Sidechain
1	K	118	ARG	Sidechain
1	K	13	ARG	Sidechain
1	K	197	ARG	Sidechain
1	K	231	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	404	ARG	Sidechain
1	K	445	ARG	Sidechain
1	L	118	ARG	Sidechain
1	L	13	ARG	Sidechain
1	L	197	ARG	Sidechain
1	L	231	ARG	Sidechain
1	L	350	ARG	Sidechain
1	L	362	ARG	Sidechain
1	L	404	ARG	Sidechain
1	L	445	ARG	Sidechain
1	M	118	ARG	Sidechain
1	M	13	ARG	Sidechain
1	M	197	ARG	Sidechain
1	M	231	ARG	Sidechain
1	M	350	ARG	Sidechain
1	M	362	ARG	Sidechain
1	M	404	ARG	Sidechain
1	M	445	ARG	Sidechain
1	N	118	ARG	Sidechain
1	N	13	ARG	Sidechain
1	N	197	ARG	Sidechain
1	N	231	ARG	Sidechain
1	N	350	ARG	Sidechain
1	N	362	ARG	Sidechain
1	N	404	ARG	Sidechain
1	N	445	ARG	Sidechain

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	3846	0	3970	181	0
1	B	3846	0	3970	181	0
1	C	3846	0	3970	179	0
1	D	3846	0	3970	181	0
1	E	3846	0	3970	182	0
1	F	3846	0	3970	183	0
1	G	3846	0	3970	182	0
1	H	3846	0	3970	127	0
1	I	3846	0	3970	129	0
1	J	3846	0	3970	128	0
1	K	3846	0	3970	127	0
1	L	3846	0	3970	125	0
1	M	3846	0	3970	127	0
1	N	3846	0	3970	128	0
2	A	31	12	12	3	0
2	B	31	12	12	3	0
2	C	31	12	12	3	0
2	D	31	12	12	3	0
2	E	31	12	12	3	0
2	F	31	12	12	3	0
2	G	31	12	12	3	0
2	H	31	12	12	3	0
2	I	31	12	12	3	0
2	J	31	12	12	3	0
2	K	31	12	12	3	0
2	L	31	12	12	3	0
2	M	31	12	12	3	0
2	N	31	12	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	1	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	4	0
4	C	1	0	0	4	0
4	D	1	0	0	4	0
4	E	1	0	0	4	0
4	F	1	0	0	4	0
4	G	1	0	0	4	0
4	H	1	0	0	4	0
4	I	1	0	0	4	0
4	J	1	0	0	4	0
4	K	1	0	0	4	0
4	L	1	0	0	4	0
4	M	1	0	0	4	0
4	N	1	0	0	4	0
All	All	54306	168	55748	2023	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 18.

All (2023) 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:3:ALA:HA	1:F:63:GLU:CA	1.69	1.23
1:D:3:ALA:HA	1:E:63:GLU:CA	1.69	1.22
1:F:3:ALA:HA	1:G:63:GLU:CA	1.69	1.22
1:C:3:ALA:HA	1:D:63:GLU:CA	1.69	1.22
1:N:30:THR:HA	1:N:35:GLY:HA3	1.22	1.21
1:A:63:GLU:CA	1:G:3:ALA:HA	1.69	1.20
1:B:3:ALA:HA	1:C:63:GLU:CA	1.69	1.20
1:A:3:ALA:HA	1:B:63:GLU:CA	1.69	1.20
1:H:30:THR:HA	1:H:35:GLY:HA3	1.23	1.17
1:M:30:THR:HA	1:M:35:GLY:HA3	1.22	1.16
1:I:30:THR:HA	1:I:35:GLY:HA3	1.22	1.14
1:J:30:THR:HA	1:J:35:GLY:HA3	1.22	1.12
1:L:30:THR:HA	1:L:35:GLY:HA3	1.23	1.11
1:K:30:THR:HA	1:K:35:GLY:HA3	1.23	1.10
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.44	1.00
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.44	1.00
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.43	1.00
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.44	1.00
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.44	1.00
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.44	0.99
1:F:3:ALA:CA	1:G:63:GLU:HA	1.93	0.99
1:A:3:ALA:CA	1:B:63:GLU:HA	1.93	0.99
1:E:3:ALA:CA	1:F:63:GLU:HA	1.93	0.99
1:D:3:ALA:CA	1:E:63:GLU:HA	1.93	0.98
1:A:63:GLU:HA	1:G:3:ALA:CA	1.93	0.98
1:B:3:ALA:CA	1:C:63:GLU:HA	1.93	0.98
1:C:3:ALA:CA	1:D:63:GLU:HA	1.93	0.98
1:B:3:ALA:HA	1:C:63:GLU:HA	1.46	0.97
1:A:3:ALA:HA	1:B:63:GLU:HA	1.46	0.97
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.47	0.95
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.47	0.95
1:E:3:ALA:HA	1:F:63:GLU:HA	1.45	0.95
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.47	0.95
1:D:3:ALA:HA	1:E:63:GLU:HA	1.46	0.94
1:A:63:GLU:HA	1:G:3:ALA:HA	1.46	0.94
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.47	0.94
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.47	0.94
1:C:3:ALA:HA	1:D:63:GLU:HA	1.46	0.93
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.47	0.93
1:F:3:ALA:HA	1:G:63:GLU:HA	1.46	0.92
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.47	0.92
1:F:30:THR:HA	1:F:35:GLY:HA3	1.52	0.92
1:G:30:THR:HA	1:G:35:GLY:HA3	1.52	0.91
1:C:30:THR:HA	1:C:35:GLY:HA3	1.52	0.91
1:B:30:THR:HA	1:B:35:GLY:HA3	1.51	0.90
1:A:3:ALA:CA	1:B:63:GLU:CA	2.49	0.90
1:E:30:THR:HA	1:E:35:GLY:HA3	1.52	0.90
1:A:63:GLU:CA	1:G:3:ALA:CA	2.49	0.90
1:B:3:ALA:CA	1:C:63:GLU:CA	2.49	0.89
1:D:30:THR:HA	1:D:35:GLY:HA3	1.52	0.89
1:A:30:THR:HA	1:A:35:GLY:HA3	1.52	0.89
1:F:3:ALA:CA	1:G:63:GLU:CA	2.49	0.89
1:E:3:ALA:CA	1:F:63:GLU:CA	2.49	0.88
1:C:3:ALA:CA	1:D:63:GLU:CA	2.49	0.87
1:D:3:ALA:CA	1:E:63:GLU:CA	2.49	0.87
1:K:30:THR:CA	1:K:35:GLY:HA3	2.07	0.85
1:J:30:THR:CA	1:J:35:GLY:HA3	2.07	0.84
1:I:30:THR:CA	1:I:35:GLY:HA3	2.07	0.84
1:H:30:THR:CA	1:H:35:GLY:HA3	2.07	0.82
1:E:3:ALA:HA	1:F:63:GLU:C	2.00	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:ALA:HA	1:G:63:GLU:C	2.00	0.82
1:A:63:GLU:C	1:G:3:ALA:HA	2.00	0.82
1:N:30:THR:CA	1:N:35:GLY:HA3	2.07	0.81
1:A:3:ALA:HA	1:B:63:GLU:C	2.00	0.81
1:D:3:ALA:HA	1:E:63:GLU:C	2.00	0.81
1:B:3:ALA:HA	1:C:63:GLU:C	2.00	0.81
1:J:39:VAL:HB	1:K:517:THR:HG23	1.62	0.81
1:M:30:THR:CA	1:M:35:GLY:HA3	2.07	0.81
1:C:3:ALA:HA	1:D:63:GLU:C	2.00	0.80
1:K:39:VAL:HB	1:L:517:THR:HG23	1.62	0.80
1:I:39:VAL:HB	1:J:517:THR:HG23	1.62	0.80
1:H:517:THR:HG23	1:N:39:VAL:HB	1.62	0.80
1:D:183:LEU:O	1:D:382:GLY:HA3	1.82	0.80
1:B:183:LEU:O	1:B:382:GLY:HA3	1.82	0.80
1:C:183:LEU:O	1:C:382:GLY:HA3	1.82	0.80
1:A:183:LEU:O	1:A:382:GLY:HA3	1.82	0.80
1:H:39:VAL:HB	1:I:517:THR:HG23	1.62	0.80
1:D:138:CYS:N	1:D:410:GLY:HA2	1.97	0.79
1:E:183:LEU:O	1:E:382:GLY:HA3	1.82	0.79
1:G:183:LEU:O	1:G:382:GLY:HA3	1.82	0.79
1:L:39:VAL:HB	1:M:517:THR:HG23	1.62	0.79
1:E:138:CYS:N	1:E:410:GLY:HA2	1.97	0.79
1:L:30:THR:CA	1:L:35:GLY:HA3	2.07	0.79
1:J:183:LEU:O	1:J:382:GLY:HA3	1.83	0.79
1:K:183:LEU:O	1:K:382:GLY:HA3	1.83	0.79
1:F:183:LEU:O	1:F:382:GLY:HA3	1.82	0.79
1:C:138:CYS:N	1:C:410:GLY:HA2	1.97	0.79
1:C:240:VAL:HA	1:C:243:ALA:HB3	1.65	0.79
1:D:240:VAL:HA	1:D:243:ALA:HB3	1.65	0.79
1:B:240:VAL:HA	1:B:243:ALA:HB3	1.65	0.79
1:G:138:CYS:N	1:G:410:GLY:HA2	1.97	0.78
1:A:138:CYS:N	1:A:410:GLY:HA2	1.97	0.78
1:D:127:ALA:HB2	1:D:426:LEU:HD11	1.65	0.78
1:B:138:CYS:N	1:B:410:GLY:HA2	1.97	0.78
1:C:127:ALA:HB2	1:C:426:LEU:HD11	1.65	0.78
1:F:138:CYS:N	1:F:410:GLY:HA2	1.97	0.78
1:M:39:VAL:HB	1:N:517:THR:HG23	1.62	0.78
1:A:127:ALA:HB2	1:A:426:LEU:HD11	1.65	0.78
1:M:183:LEU:O	1:M:382:GLY:HA3	1.83	0.78
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.66	0.78
1:E:240:VAL:HA	1:E:243:ALA:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:LEU:O	1:I:382:GLY:HA3	1.83	0.78
1:N:183:LEU:O	1:N:382:GLY:HA3	1.83	0.78
1:F:127:ALA:HB2	1:F:426:LEU:HD11	1.65	0.78
1:F:240:VAL:HA	1:F:243:ALA:HB3	1.65	0.77
1:G:127:ALA:HB2	1:G:426:LEU:HD11	1.65	0.77
1:J:85:ALA:O	1:J:402:ALA:HA	1.85	0.77
1:K:85:ALA:O	1:K:402:ALA:HA	1.84	0.77
1:H:183:LEU:O	1:H:382:GLY:HA3	1.83	0.77
1:L:183:LEU:O	1:L:382:GLY:HA3	1.83	0.77
1:L:85:ALA:O	1:L:402:ALA:HA	1.85	0.77
1:N:85:ALA:O	1:N:402:ALA:HA	1.85	0.77
1:I:85:ALA:O	1:I:402:ALA:HA	1.85	0.77
1:B:214:GLU:HA	1:B:323:VAL:O	1.85	0.77
1:M:85:ALA:O	1:M:402:ALA:HA	1.84	0.77
1:E:214:GLU:HA	1:E:323:VAL:O	1.85	0.77
1:F:214:GLU:HA	1:F:323:VAL:O	1.85	0.77
1:H:85:ALA:O	1:H:402:ALA:HA	1.85	0.77
2:A:1525:ATP:O1A	4:A:1528:PO4:P	2.44	0.77
1:A:214:GLU:HA	1:A:323:VAL:O	1.85	0.77
2:B:1525:ATP:O1G	4:B:1528:PO4:P	2.43	0.76
2:C:1526:ATP:O1G	4:C:1528:PO4:P	2.44	0.76
2:E:1525:ATP:O1A	4:E:1528:PO4:P	2.43	0.76
1:G:214:GLU:HA	1:G:323:VAL:O	1.85	0.76
1:D:214:GLU:HA	1:D:323:VAL:O	1.85	0.76
2:B:1525:ATP:O1A	4:B:1528:PO4:P	2.43	0.76
1:C:214:GLU:HA	1:C:323:VAL:O	1.85	0.76
2:F:1525:ATP:O1A	4:F:1528:PO4:P	2.43	0.76
2:G:1525:ATP:O1A	4:G:1528:PO4:P	2.43	0.76
1:B:127:ALA:HB2	1:B:426:LEU:HD11	1.65	0.76
1:D:4:LYS:H	1:E:63:GLU:HB2	1.51	0.76
2:D:1525:ATP:O1G	4:D:1528:PO4:P	2.44	0.76
1:E:4:LYS:H	1:F:63:GLU:HB2	1.51	0.76
1:F:4:LYS:H	1:G:63:GLU:HB2	1.51	0.76
1:C:4:LYS:H	1:D:63:GLU:HB2	1.51	0.76
2:D:1525:ATP:O1A	4:D:1528:PO4:P	2.43	0.75
2:A:1525:ATP:O1G	4:A:1528:PO4:P	2.44	0.75
1:H:480:ALA:O	1:H:483:GLU:HG2	1.86	0.75
1:B:4:LYS:H	1:C:63:GLU:HB2	1.51	0.75
1:A:4:LYS:H	1:B:63:GLU:HB2	1.51	0.75
2:G:1525:ATP:O1G	4:G:1528:PO4:P	2.44	0.75
1:I:480:ALA:O	1:I:483:GLU:HG2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1525:ATP:O1G	4:F:1528:PO4:P	2.44	0.75
1:L:480:ALA:O	1:L:483:GLU:HG2	1.86	0.75
1:A:63:GLU:HB2	1:G:4:LYS:H	1.51	0.75
1:H:138:CYS:N	1:H:410:GLY:HA2	2.02	0.75
1:I:138:CYS:N	1:I:410:GLY:HA2	2.02	0.75
2:E:1525:ATP:O1G	4:E:1528:PO4:P	2.44	0.75
1:K:138:CYS:N	1:K:410:GLY:HA2	2.02	0.75
1:J:480:ALA:O	1:J:483:GLU:HG2	1.86	0.75
1:N:480:ALA:O	1:N:483:GLU:HG2	1.86	0.75
2:C:1526:ATP:O1A	4:C:1528:PO4:P	2.43	0.74
1:A:206:ASN:HB2	1:A:213:VAL:HA	1.69	0.74
1:C:206:ASN:HB2	1:C:213:VAL:HA	1.69	0.74
1:B:206:ASN:HB2	1:B:213:VAL:HA	1.70	0.74
1:N:127:ALA:HB2	1:N:426:LEU:HD11	1.70	0.74
1:N:138:CYS:N	1:N:410:GLY:HA2	2.02	0.74
1:J:138:CYS:N	1:J:410:GLY:HA2	2.02	0.74
1:M:480:ALA:O	1:M:483:GLU:HG2	1.86	0.74
1:I:198:GLY:HA2	1:I:327:LYS:O	1.88	0.74
1:J:198:GLY:HA2	1:J:327:LYS:O	1.88	0.74
1:K:480:ALA:O	1:K:483:GLU:HG2	1.86	0.74
1:M:198:GLY:HA2	1:M:327:LYS:O	1.88	0.74
1:H:127:ALA:HB2	1:H:426:LEU:HD11	1.70	0.74
1:K:198:GLY:HA2	1:K:327:LYS:O	1.88	0.74
1:L:138:CYS:N	1:L:410:GLY:HA2	2.02	0.74
1:L:127:ALA:HB2	1:L:426:LEU:HD11	1.70	0.74
1:D:206:ASN:HB2	1:D:213:VAL:HA	1.69	0.73
1:I:127:ALA:HB2	1:I:426:LEU:HD11	1.70	0.73
1:K:127:ALA:HB2	1:K:426:LEU:HD11	1.70	0.73
1:I:191:GLU:O	1:I:334:ASP:HA	1.89	0.73
1:G:206:ASN:HB2	1:G:213:VAL:HA	1.70	0.73
1:G:255:GLU:HB2	1:G:258:ALA:HB3	1.70	0.73
1:H:198:GLY:HA2	1:H:327:LYS:O	1.88	0.73
1:H:191:GLU:O	1:H:334:ASP:HA	1.89	0.73
1:F:206:ASN:HB2	1:F:213:VAL:HA	1.69	0.73
1:M:138:CYS:N	1:M:410:GLY:HA2	2.02	0.73
1:J:191:GLU:O	1:J:334:ASP:HA	1.89	0.73
1:J:127:ALA:HB2	1:J:426:LEU:HD11	1.70	0.73
2:K:1527:ATP:O1G	4:K:1528:PO4:P	2.47	0.73
1:L:198:GLY:HA2	1:L:327:LYS:O	1.88	0.72
1:N:198:GLY:HA2	1:N:327:LYS:O	1.88	0.72
2:M:1527:ATP:O1G	4:M:1528:PO4:P	2.47	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:GLU:O	1:N:334:ASP:HA	1.89	0.72
1:E:4:LYS:H	1:F:63:GLU:CB	2.03	0.72
1:A:4:LYS:H	1:B:63:GLU:CB	2.03	0.72
1:M:127:ALA:HB2	1:M:426:LEU:HD11	1.70	0.72
2:H:1527:ATP:O1G	4:H:1528:PO4:P	2.47	0.72
1:D:198:GLY:HA2	1:D:327:LYS:O	1.90	0.72
1:E:206:ASN:HB2	1:E:213:VAL:HA	1.69	0.72
2:J:1526:ATP:O1G	4:J:1528:PO4:P	2.47	0.72
1:F:4:LYS:H	1:G:63:GLU:CB	2.03	0.72
1:G:198:GLY:HA2	1:G:327:LYS:O	1.90	0.72
1:L:191:GLU:O	1:L:334:ASP:HA	1.88	0.72
2:I:1525:ATP:O1G	4:I:1528:PO4:P	2.47	0.72
2:L:1527:ATP:O1G	4:L:1528:PO4:P	2.47	0.72
1:A:198:GLY:HA2	1:A:327:LYS:O	1.90	0.72
1:C:4:LYS:H	1:D:63:GLU:CB	2.03	0.72
1:K:191:GLU:O	1:K:334:ASP:HA	1.89	0.72
1:C:198:GLY:HA2	1:C:327:LYS:O	1.90	0.72
1:M:191:GLU:O	1:M:334:ASP:HA	1.89	0.72
1:A:63:GLU:CB	1:G:4:LYS:H	2.03	0.72
1:B:2:ALA:O	1:C:63:GLU:HA	1.90	0.72
2:H:1527:ATP:O1A	4:H:1528:PO4:P	2.48	0.72
2:N:1527:ATP:O1G	4:N:1528:PO4:P	2.47	0.72
1:E:198:GLY:HA2	1:E:327:LYS:O	1.90	0.72
1:D:4:LYS:H	1:E:63:GLU:CB	2.03	0.72
1:F:2:ALA:O	1:G:63:GLU:HA	1.90	0.71
1:A:63:GLU:HA	1:G:2:ALA:O	1.90	0.71
1:A:2:ALA:O	1:B:63:GLU:HA	1.90	0.71
2:M:1527:ATP:O1A	4:M:1528:PO4:P	2.48	0.71
2:K:1527:ATP:O1A	4:K:1528:PO4:P	2.48	0.71
2:J:1526:ATP:O1A	4:J:1528:PO4:P	2.48	0.71
1:L:214:GLU:HA	1:L:323:VAL:O	1.91	0.71
1:M:199:TYR:CD2	1:M:205:ILE:HD11	2.25	0.71
1:I:199:TYR:CD2	1:I:205:ILE:HD11	2.25	0.71
1:J:38:VAL:HB	1:J:56:VAL:HG22	1.71	0.71
1:K:38:VAL:HB	1:K:56:VAL:HG22	1.71	0.71
1:J:199:TYR:CD2	1:J:205:ILE:HD11	2.25	0.71
1:N:199:TYR:CD2	1:N:205:ILE:HD11	2.25	0.71
2:N:1527:ATP:O1A	4:N:1528:PO4:P	2.48	0.71
1:N:214:GLU:HA	1:N:323:VAL:O	1.91	0.71
1:H:214:GLU:HA	1:H:323:VAL:O	1.90	0.71
1:D:2:ALA:O	1:E:63:GLU:HA	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:VAL:HB	1:H:56:VAL:HG22	1.71	0.71
2:I:1525:ATP:O1A	4:I:1528:PO4:P	2.48	0.71
1:I:214:GLU:HA	1:I:323:VAL:O	1.91	0.71
1:K:214:GLU:HA	1:K:323:VAL:O	1.91	0.71
1:E:2:ALA:O	1:F:63:GLU:HA	1.90	0.70
1:B:4:LYS:H	1:C:63:GLU:CB	2.03	0.70
1:A:243:ALA:HA	1:G:258:ALA:HA	1.72	0.70
2:L:1527:ATP:O1A	4:L:1528:PO4:P	2.48	0.70
1:B:198:GLY:HA2	1:B:327:LYS:O	1.90	0.70
1:H:199:TYR:CD2	1:H:205:ILE:HD11	2.25	0.70
1:L:199:TYR:CD2	1:L:205:ILE:HD11	2.26	0.70
1:A:39:VAL:HB	1:G:517:THR:HG23	1.73	0.70
1:N:38:VAL:HB	1:N:56:VAL:HG22	1.71	0.70
1:I:38:VAL:HB	1:I:56:VAL:HG22	1.72	0.70
1:L:38:VAL:HB	1:L:56:VAL:HG22	1.71	0.70
1:K:199:TYR:CD2	1:K:205:ILE:HD11	2.25	0.70
1:F:517:THR:HG23	1:G:39:VAL:HB	1.73	0.70
1:F:198:GLY:HA2	1:F:327:LYS:O	1.90	0.70
1:J:214:GLU:HA	1:J:323:VAL:O	1.91	0.70
1:M:214:GLU:HA	1:M:323:VAL:O	1.91	0.70
1:E:517:THR:HG23	1:F:39:VAL:HB	1.73	0.70
1:A:517:THR:HG23	1:B:39:VAL:HB	1.73	0.69
1:C:2:ALA:O	1:D:63:GLU:HA	1.90	0.69
1:M:38:VAL:HB	1:M:56:VAL:HG22	1.71	0.69
1:C:517:THR:HG23	1:D:39:VAL:HB	1.73	0.69
1:I:30:THR:HA	1:I:35:GLY:CA	2.14	0.69
1:D:517:THR:HG23	1:E:39:VAL:HB	1.73	0.69
1:B:517:THR:HG23	1:C:39:VAL:HB	1.73	0.68
1:A:240:VAL:HA	1:A:243:ALA:HB3	1.75	0.68
1:H:30:THR:HA	1:H:35:GLY:CA	2.14	0.68
1:J:30:THR:HA	1:J:35:GLY:CA	2.14	0.68
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.76	0.68
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.76	0.68
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.76	0.67
1:D:199:TYR:CD2	1:D:205:ILE:HD11	2.30	0.67
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.30	0.67
1:L:30:THR:HA	1:L:35:GLY:CA	2.14	0.67
1:E:199:TYR:CD2	1:E:205:ILE:HD11	2.30	0.67
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.76	0.67
1:C:41:ASP:HA	1:C:47:PRO:HB3	1.77	0.67
1:K:30:THR:HA	1:K:35:GLY:CA	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ASP:HA	1:D:47:PRO:HB3	1.77	0.67
1:N:287:ALA:HB1	1:N:368:ARG:CZ	2.25	0.67
1:H:287:ALA:HB1	1:H:368:ARG:CZ	2.25	0.67
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.76	0.67
1:B:41:ASP:HA	1:B:47:PRO:HB3	1.77	0.67
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.30	0.67
1:K:287:ALA:HB1	1:K:368:ARG:CZ	2.25	0.67
1:M:287:ALA:HB1	1:M:368:ARG:CZ	2.25	0.67
1:I:287:ALA:HB1	1:I:368:ARG:CZ	2.25	0.67
1:F:199:TYR:CD2	1:F:205:ILE:HD11	2.30	0.67
1:L:287:ALA:HB1	1:L:368:ARG:CZ	2.25	0.67
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.76	0.67
1:J:287:ALA:HB1	1:J:368:ARG:CZ	2.25	0.67
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.76	0.66
1:A:41:ASP:HA	1:A:47:PRO:HB3	1.77	0.66
1:I:39:VAL:CB	1:J:517:THR:HG23	2.26	0.66
1:E:41:ASP:HA	1:E:47:PRO:HB3	1.77	0.66
1:L:27:VAL:HG12	1:L:90:THR:CG2	2.25	0.66
1:M:27:VAL:HG12	1:M:90:THR:CG2	2.25	0.66
1:J:39:VAL:CB	1:K:517:THR:HG23	2.26	0.66
1:L:39:VAL:CB	1:M:517:THR:HG23	2.26	0.66
1:I:3:ALA:HB3	1:I:524:LEU:HB3	1.78	0.66
1:H:3:ALA:HB3	1:H:524:LEU:HB3	1.78	0.66
1:F:41:ASP:HA	1:F:47:PRO:HB3	1.77	0.66
1:M:30:THR:HA	1:M:35:GLY:CA	2.14	0.66
1:N:27:VAL:HG12	1:N:90:THR:CG2	2.25	0.66
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.30	0.66
1:G:41:ASP:HA	1:G:47:PRO:HB3	1.77	0.66
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.30	0.65
1:D:251:ALA:O	1:D:277:LYS:HA	1.96	0.65
1:G:251:ALA:O	1:G:277:LYS:HA	1.96	0.65
1:E:251:ALA:O	1:E:277:LYS:HA	1.96	0.65
1:H:517:THR:HG23	1:N:39:VAL:CB	2.26	0.65
1:J:3:ALA:HB3	1:J:524:LEU:HB3	1.77	0.65
1:K:27:VAL:HG12	1:K:90:THR:CG2	2.25	0.65
1:K:39:VAL:CB	1:L:517:THR:HG23	2.26	0.65
1:H:39:VAL:CB	1:I:517:THR:HG23	2.26	0.65
1:F:251:ALA:O	1:F:277:LYS:HA	1.96	0.65
1:C:251:ALA:O	1:C:277:LYS:HA	1.96	0.65
1:B:251:ALA:O	1:B:277:LYS:HA	1.96	0.65
1:M:39:VAL:CB	1:N:517:THR:HG23	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:SER:HA	1:G:412:VAL:HG12	1.79	0.65
1:A:251:ALA:O	1:A:277:LYS:HA	1.96	0.65
1:A:200:LEU:HD13	1:A:254:VAL:HG11	1.80	0.64
1:B:200:LEU:HD13	1:B:254:VAL:HG11	1.79	0.64
1:H:27:VAL:HG12	1:H:90:THR:CG2	2.25	0.64
1:G:218:PRO:HG2	1:G:320:ALA:HB3	1.78	0.64
1:A:135:SER:HA	1:A:412:VAL:HG12	1.79	0.64
1:M:3:ALA:HB3	1:M:524:LEU:HB3	1.78	0.64
1:F:135:SER:HA	1:F:412:VAL:HG12	1.80	0.64
1:N:3:ALA:HB3	1:N:524:LEU:HB3	1.78	0.64
1:N:30:THR:HA	1:N:35:GLY:CA	2.14	0.64
1:K:3:ALA:HB3	1:K:524:LEU:HB3	1.78	0.64
1:A:130:GLU:HB3	1:A:422:VAL:HG12	1.80	0.64
1:D:135:SER:HA	1:D:412:VAL:HG12	1.79	0.64
1:E:135:SER:HA	1:E:412:VAL:HG12	1.80	0.64
1:F:130:GLU:HB3	1:F:422:VAL:HG12	1.80	0.64
1:G:130:GLU:HB3	1:G:422:VAL:HG12	1.80	0.64
1:L:3:ALA:HB3	1:L:524:LEU:HB3	1.78	0.64
1:F:200:LEU:HD13	1:F:254:VAL:HG11	1.80	0.64
1:C:200:LEU:HD13	1:C:254:VAL:HG11	1.80	0.64
1:D:138:CYS:HB3	1:D:407:VAL:HA	1.81	0.63
1:B:130:GLU:HB3	1:B:422:VAL:HG12	1.80	0.63
1:D:50:THR:HG21	1:D:56:VAL:HA	1.80	0.63
1:C:135:SER:HA	1:C:412:VAL:HG12	1.79	0.63
1:C:50:THR:HG21	1:C:56:VAL:HA	1.80	0.63
1:E:52:ASP:O	1:E:56:VAL:HG23	1.98	0.63
1:E:200:LEU:HD13	1:E:254:VAL:HG11	1.80	0.63
1:D:27:VAL:HG12	1:D:90:THR:CG2	2.26	0.63
1:E:130:GLU:HB3	1:E:422:VAL:HG12	1.80	0.63
1:A:52:ASP:O	1:A:56:VAL:HG23	1.98	0.63
1:E:138:CYS:HB3	1:E:407:VAL:HA	1.81	0.63
1:D:200:LEU:HD13	1:D:254:VAL:HG11	1.80	0.63
1:J:27:VAL:HG12	1:J:90:THR:CG2	2.25	0.63
1:E:50:THR:HG21	1:E:56:VAL:HA	1.80	0.63
1:B:135:SER:HA	1:B:412:VAL:HG12	1.80	0.63
1:G:52:ASP:O	1:G:56:VAL:HG23	1.98	0.63
1:C:138:CYS:HB3	1:C:407:VAL:HA	1.81	0.63
1:D:52:ASP:O	1:D:56:VAL:HG23	1.98	0.63
1:D:3:ALA:C	1:E:63:GLU:HA	2.19	0.63
1:C:3:ALA:C	1:D:63:GLU:HA	2.19	0.63
1:F:138:CYS:HB3	1:F:407:VAL:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLU:HB3	1:C:422:VAL:HG12	1.80	0.62
1:B:52:ASP:O	1:B:56:VAL:HG23	1.98	0.62
1:A:50:THR:HG21	1:A:56:VAL:HA	1.80	0.62
1:B:50:THR:HG21	1:B:56:VAL:HA	1.80	0.62
1:D:130:GLU:HB3	1:D:422:VAL:HG12	1.80	0.62
1:G:200:LEU:HD13	1:G:254:VAL:HG11	1.81	0.62
1:I:180:GLY:HA2	1:I:380:LYS:HB3	1.82	0.62
1:B:3:ALA:C	1:C:63:GLU:HA	2.19	0.62
1:G:50:THR:HG21	1:G:56:VAL:HA	1.80	0.62
1:F:50:THR:HG21	1:F:56:VAL:HA	1.80	0.62
1:H:180:GLY:HA2	1:H:380:LYS:HB3	1.82	0.62
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.82	0.62
1:E:3:ALA:C	1:F:63:GLU:HA	2.19	0.62
1:G:138:CYS:HB3	1:G:407:VAL:HA	1.81	0.62
1:C:52:ASP:O	1:C:56:VAL:HG23	1.98	0.62
1:F:52:ASP:O	1:F:56:VAL:HG23	1.98	0.62
1:N:180:GLY:HA2	1:N:380:LYS:HB3	1.82	0.62
1:E:27:VAL:HG12	1:E:90:THR:CG2	2.26	0.62
1:B:138:CYS:HB3	1:B:407:VAL:HA	1.81	0.62
1:A:138:CYS:HB3	1:A:407:VAL:HA	1.81	0.61
1:I:27:VAL:HG12	1:I:90:THR:CG2	2.25	0.61
1:K:180:GLY:HA2	1:K:380:LYS:HB3	1.82	0.61
1:E:54:VAL:HG13	1:E:89:THR:HG21	1.83	0.61
1:D:54:VAL:HG13	1:D:89:THR:HG21	1.83	0.61
1:M:149:THR:HA	1:M:152:ALA:HB3	1.83	0.61
1:G:240:VAL:HG11	1:G:247:LEU:HD22	1.83	0.61
1:C:54:VAL:HG13	1:C:89:THR:HG21	1.83	0.61
1:G:257:GLU:CD	1:G:257:GLU:H	2.03	0.61
1:J:149:THR:HA	1:J:152:ALA:HB3	1.83	0.61
1:F:54:VAL:HG13	1:F:89:THR:HG21	1.83	0.61
1:F:3:ALA:C	1:G:63:GLU:HA	2.19	0.61
1:A:3:ALA:C	1:B:63:GLU:HA	2.19	0.61
1:F:149:THR:HA	1:F:152:ALA:HB3	1.83	0.61
1:M:180:GLY:HA2	1:M:380:LYS:HB3	1.82	0.61
1:A:63:GLU:HA	1:G:3:ALA:C	2.19	0.61
1:F:27:VAL:HG12	1:F:90:THR:CG2	2.26	0.61
1:H:149:THR:HA	1:H:152:ALA:HB3	1.83	0.61
1:I:149:THR:HA	1:I:152:ALA:HB3	1.83	0.61
1:E:149:THR:HA	1:E:152:ALA:HB3	1.83	0.61
1:M:52:ASP:OD1	4:M:1528:PO4:P	2.59	0.61
1:L:149:THR:HA	1:L:152:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:149:THR:HA	1:N:152:ALA:HB3	1.83	0.61
1:D:149:THR:HA	1:D:152:ALA:HB3	1.83	0.61
1:H:426:LEU:HB2	1:H:444:LEU:HD22	1.83	0.60
1:C:149:THR:HA	1:C:152:ALA:HB3	1.83	0.60
1:I:426:LEU:HB2	1:I:444:LEU:HD22	1.83	0.60
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.84	0.60
1:K:40:LEU:HD13	1:K:41:ASP:O	2.01	0.60
1:C:218:PRO:HG2	1:C:320:ALA:HB3	1.84	0.60
1:J:426:LEU:HB2	1:J:444:LEU:HD22	1.83	0.60
1:L:52:ASP:OD1	4:L:1528:PO4:P	2.59	0.60
1:K:149:THR:HA	1:K:152:ALA:HB3	1.83	0.60
1:H:52:ASP:OD1	4:H:1528:PO4:P	2.59	0.60
1:B:54:VAL:HG13	1:B:89:THR:HG21	1.83	0.60
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.84	0.60
1:N:52:ASP:OD1	4:N:1528:PO4:P	2.59	0.60
1:E:464:VAL:HG22	1:L:464:VAL:HG22	1.83	0.60
1:L:40:LEU:HD13	1:L:41:ASP:O	2.02	0.60
1:L:180:GLY:HA2	1:L:380:LYS:HB3	1.82	0.60
1:G:54:VAL:HG13	1:G:89:THR:HG21	1.83	0.60
1:N:426:LEU:HB2	1:N:444:LEU:HD22	1.83	0.60
1:K:426:LEU:HB2	1:K:444:LEU:HD22	1.83	0.60
1:H:3:ALA:O	1:H:523:ASP:HA	2.02	0.60
1:B:217:SER:HA	1:B:320:ALA:O	2.02	0.60
1:J:40:LEU:HD13	1:J:41:ASP:O	2.02	0.60
1:G:149:THR:HA	1:G:152:ALA:HB3	1.83	0.60
1:F:218:PRO:HG2	1:F:320:ALA:HB3	1.84	0.60
1:I:52:ASP:OD1	4:I:1528:PO4:P	2.59	0.60
1:I:3:ALA:O	1:I:523:ASP:HA	2.02	0.60
1:D:218:PRO:HG2	1:D:320:ALA:HB3	1.84	0.60
1:A:54:VAL:HG13	1:A:89:THR:HG21	1.83	0.60
1:G:27:VAL:HG12	1:G:90:THR:CG2	2.26	0.60
1:B:31:LEU:HA	4:B:1528:PO4:P	2.42	0.60
1:I:40:LEU:HD13	1:I:41:ASP:O	2.02	0.60
1:H:40:LEU:HD13	1:H:41:ASP:O	2.02	0.60
1:D:31:LEU:HA	4:D:1528:PO4:P	2.42	0.59
1:L:426:LEU:HB2	1:L:444:LEU:HD22	1.83	0.59
1:F:464:VAL:HG22	1:M:464:VAL:HG22	1.83	0.59
1:E:218:PRO:HG2	1:E:320:ALA:HB3	1.84	0.59
1:F:31:LEU:HA	4:F:1528:PO4:P	2.42	0.59
1:E:31:LEU:HA	4:E:1528:PO4:P	2.42	0.59
1:E:31:LEU:CB	1:E:90:THR:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:CB	1:D:90:THR:HG21	2.32	0.59
1:J:52:ASP:OD1	4:J:1528:PO4:P	2.59	0.59
1:E:186:GLU:H	1:E:380:LYS:HB2	1.67	0.59
1:N:3:ALA:O	1:N:523:ASP:HA	2.02	0.59
1:B:40:LEU:HD11	1:B:59:GLU:O	2.03	0.59
1:A:149:THR:HA	1:A:152:ALA:HB3	1.83	0.59
1:B:149:THR:HA	1:B:152:ALA:HB3	1.83	0.59
1:F:40:LEU:HD11	1:F:59:GLU:O	2.03	0.59
1:K:130:GLU:HB3	1:K:422:VAL:HG12	1.83	0.59
1:G:31:LEU:HA	4:G:1528:PO4:P	2.42	0.59
1:A:27:VAL:HG12	1:A:90:THR:CG2	2.26	0.59
1:B:186:GLU:H	1:B:380:LYS:HB2	1.67	0.59
1:C:38:VAL:HB	1:C:56:VAL:HG22	1.84	0.59
1:C:40:LEU:HD11	1:C:59:GLU:O	2.02	0.59
1:J:130:GLU:HB3	1:J:422:VAL:HG12	1.83	0.59
1:M:40:LEU:HD13	1:M:41:ASP:O	2.02	0.59
1:L:3:ALA:O	1:L:523:ASP:HA	2.02	0.59
1:E:40:LEU:HD11	1:E:59:GLU:O	2.03	0.59
1:J:235:PRO:HB2	1:J:310:GLU:HA	1.85	0.59
1:C:31:LEU:HA	4:C:1528:PO4:P	2.42	0.59
1:M:426:LEU:HB2	1:M:444:LEU:HD22	1.83	0.59
1:H:235:PRO:HB2	1:H:310:GLU:HA	1.85	0.59
1:K:52:ASP:OD1	4:K:1528:PO4:P	2.59	0.59
1:K:3:ALA:O	1:K:523:ASP:HA	2.02	0.59
1:D:464:VAL:HG22	1:K:464:VAL:HG22	1.83	0.59
1:G:212:ALA:HA	1:G:325:ILE:O	2.03	0.59
1:L:130:GLU:HB3	1:L:422:VAL:HG12	1.83	0.59
1:B:27:VAL:HG12	1:B:90:THR:CG2	2.26	0.59
2:N:1527:ATP:PG	4:N:1528:PO4:P	3.01	0.59
1:E:38:VAL:HB	1:E:56:VAL:HG22	1.85	0.59
1:G:38:VAL:HB	1:G:56:VAL:HG22	1.85	0.59
1:B:38:VAL:HB	1:B:56:VAL:HG22	1.85	0.59
1:F:38:VAL:HB	1:F:56:VAL:HG22	1.85	0.59
1:C:464:VAL:HG22	1:J:464:VAL:HG22	1.84	0.59
1:N:235:PRO:HB2	1:N:310:GLU:HA	1.85	0.59
1:N:40:LEU:HD13	1:N:41:ASP:O	2.02	0.59
1:F:31:LEU:CB	1:F:90:THR:HG21	2.32	0.59
1:A:31:LEU:CB	1:A:90:THR:HG21	2.32	0.59
2:J:1526:ATP:PG	4:J:1528:PO4:P	3.01	0.59
1:G:186:GLU:H	1:G:380:LYS:HB2	1.67	0.59
1:A:38:VAL:HB	1:A:56:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD11	1:D:59:GLU:O	2.03	0.59
1:I:130:GLU:HB3	1:I:422:VAL:HG12	1.84	0.59
1:A:40:LEU:HD11	1:A:59:GLU:O	2.03	0.59
1:D:38:VAL:HB	1:D:56:VAL:HG22	1.85	0.59
1:E:217:SER:HA	1:E:320:ALA:O	2.02	0.59
1:F:230:ILE:HG22	1:F:263:VAL:HG23	1.84	0.59
1:G:464:VAL:HG22	1:N:464:VAL:HG22	1.84	0.59
1:G:31:LEU:CB	1:G:90:THR:HG21	2.33	0.59
2:M:1527:ATP:PG	4:M:1528:PO4:P	3.01	0.59
1:D:217:SER:HA	1:D:320:ALA:O	2.02	0.59
1:N:130:GLU:HB3	1:N:422:VAL:HG12	1.83	0.59
1:G:40:LEU:HD11	1:G:59:GLU:O	2.03	0.59
1:I:30:THR:HG21	1:I:56:VAL:HG21	1.85	0.58
1:D:212:ALA:HA	1:D:325:ILE:O	2.03	0.58
2:K:1527:ATP:PG	4:K:1528:PO4:P	3.01	0.58
2:H:1527:ATP:PG	4:H:1528:PO4:P	3.01	0.58
1:J:3:ALA:O	1:J:523:ASP:HA	2.02	0.58
1:M:3:ALA:O	1:M:523:ASP:HA	2.02	0.58
1:B:31:LEU:CB	1:B:90:THR:HG21	2.33	0.58
1:A:212:ALA:HA	1:A:325:ILE:O	2.03	0.58
1:K:235:PRO:HB2	1:K:310:GLU:HA	1.85	0.58
1:N:30:THR:HG21	1:N:56:VAL:HG21	1.85	0.58
1:A:31:LEU:HA	4:A:1528:PO4:P	2.42	0.58
1:B:519:CYS:O	1:C:39:VAL:O	2.21	0.58
1:A:230:ILE:CG2	1:A:263:VAL:HA	2.34	0.58
1:M:235:PRO:HB2	1:M:310:GLU:HA	1.85	0.58
2:L:1527:ATP:PG	4:L:1528:PO4:P	3.01	0.58
1:F:186:GLU:H	1:F:380:LYS:HB2	1.67	0.58
1:D:186:GLU:H	1:D:380:LYS:HB2	1.67	0.58
1:A:186:GLU:H	1:A:380:LYS:HB2	1.67	0.58
1:C:85:ALA:O	1:C:402:ALA:HA	2.03	0.58
1:D:85:ALA:O	1:D:402:ALA:HA	2.04	0.58
1:B:464:VAL:HG22	1:I:464:VAL:HG22	1.84	0.58
1:M:130:GLU:HB3	1:M:422:VAL:HG12	1.83	0.58
1:C:186:GLU:H	1:C:380:LYS:HB2	1.67	0.58
1:C:217:SER:HA	1:C:320:ALA:O	2.02	0.58
1:F:217:SER:HA	1:F:320:ALA:O	2.02	0.58
1:E:230:ILE:CG2	1:E:263:VAL:HA	2.34	0.58
1:H:130:GLU:HB3	1:H:422:VAL:HG12	1.83	0.58
1:B:230:ILE:CG2	1:B:263:VAL:HA	2.34	0.58
1:H:30:THR:HG21	1:H:56:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:CB	1:C:90:THR:HG21	2.32	0.58
1:B:212:ALA:HA	1:B:325:ILE:O	2.03	0.58
1:E:169:VAL:HG11	1:E:175:ILE:HG12	1.86	0.58
1:D:169:VAL:HG11	1:D:175:ILE:HG12	1.85	0.58
1:J:30:THR:HG21	1:J:56:VAL:HG21	1.85	0.58
1:F:212:ALA:HA	1:F:325:ILE:O	2.03	0.58
1:E:212:ALA:HA	1:E:325:ILE:O	2.03	0.58
2:I:1525:ATP:PG	4:I:1528:PO4:P	3.01	0.58
1:M:279:PRO:HG3	1:M:292:ILE:HD11	1.85	0.58
1:C:230:ILE:CG2	1:C:263:VAL:HA	2.34	0.58
1:G:169:VAL:HG11	1:G:175:ILE:CG1	2.34	0.58
1:D:169:VAL:HG11	1:D:175:ILE:CG1	2.34	0.58
1:J:279:PRO:HG3	1:J:292:ILE:HD11	1.85	0.58
1:N:251:ALA:O	1:N:277:LYS:HA	2.04	0.58
1:L:235:PRO:HB2	1:L:310:GLU:HA	1.85	0.58
1:E:519:CYS:O	1:F:39:VAL:O	2.21	0.58
1:N:279:PRO:HG3	1:N:292:ILE:HD11	1.86	0.58
1:F:169:VAL:HG11	1:F:175:ILE:CG1	2.34	0.58
1:D:4:LYS:N	1:E:63:GLU:CA	2.67	0.57
1:C:4:LYS:N	1:D:63:GLU:CA	2.67	0.57
1:B:4:LYS:N	1:C:63:GLU:CA	2.67	0.57
1:A:4:LYS:N	1:B:63:GLU:CA	2.67	0.57
1:M:30:THR:HG21	1:M:56:VAL:HG21	1.85	0.57
1:C:212:ALA:HA	1:C:325:ILE:O	2.03	0.57
1:G:217:SER:HA	1:G:320:ALA:O	2.04	0.57
1:E:169:VAL:HG11	1:E:175:ILE:CG1	2.34	0.57
1:C:169:VAL:HG11	1:C:175:ILE:CG1	2.34	0.57
1:K:251:ALA:O	1:K:277:LYS:HA	2.04	0.57
1:A:464:VAL:HG22	1:H:464:VAL:HG22	1.84	0.57
1:G:85:ALA:O	1:G:402:ALA:HA	2.04	0.57
1:I:279:PRO:HG3	1:I:292:ILE:HD11	1.85	0.57
1:A:519:CYS:O	1:B:39:VAL:O	2.21	0.57
1:H:251:ALA:O	1:H:277:LYS:HA	2.04	0.57
1:A:85:ALA:O	1:A:402:ALA:HA	2.04	0.57
1:F:4:LYS:N	1:G:63:GLU:CA	2.67	0.57
1:A:169:VAL:HG11	1:A:175:ILE:HG12	1.86	0.57
1:D:519:CYS:O	1:E:39:VAL:O	2.21	0.57
1:F:169:VAL:HG11	1:F:175:ILE:HG12	1.86	0.57
1:B:85:ALA:O	1:B:402:ALA:HA	2.04	0.57
1:F:85:ALA:O	1:F:402:ALA:HA	2.03	0.57
1:F:519:CYS:O	1:G:39:VAL:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:VAL:HG11	1:C:175:ILE:HG12	1.85	0.57
1:A:169:VAL:HG11	1:A:175:ILE:CG1	2.34	0.57
1:D:230:ILE:CG2	1:D:263:VAL:HA	2.34	0.57
1:K:279:PRO:HG3	1:K:292:ILE:HD11	1.85	0.57
1:L:279:PRO:HG3	1:L:292:ILE:HD11	1.85	0.57
1:E:4:LYS:N	1:F:63:GLU:CA	2.67	0.57
1:A:63:GLU:CA	1:G:4:LYS:N	2.67	0.57
1:K:30:THR:HG21	1:K:56:VAL:HG21	1.85	0.57
1:C:519:CYS:O	1:D:39:VAL:O	2.21	0.57
1:G:169:VAL:HG11	1:G:175:ILE:HG12	1.85	0.57
1:G:230:ILE:CG2	1:G:263:VAL:HA	2.35	0.57
1:L:251:ALA:O	1:L:277:LYS:HA	2.04	0.57
1:J:251:ALA:O	1:J:277:LYS:HA	2.04	0.57
1:M:251:ALA:O	1:M:277:LYS:HA	2.04	0.57
1:L:30:THR:HG21	1:L:56:VAL:HG21	1.85	0.57
1:A:39:VAL:O	1:G:519:CYS:O	2.21	0.57
1:I:251:ALA:O	1:I:277:LYS:HA	2.04	0.57
1:E:85:ALA:O	1:E:402:ALA:HA	2.04	0.57
1:H:212:ALA:HA	1:H:325:ILE:O	2.05	0.57
1:I:235:PRO:HB2	1:I:310:GLU:HA	1.87	0.57
1:H:279:PRO:HG3	1:H:292:ILE:HD11	1.85	0.57
1:M:212:ALA:HA	1:M:325:ILE:O	2.05	0.56
1:B:169:VAL:HG11	1:B:175:ILE:CG1	2.34	0.56
1:C:27:VAL:HG12	1:C:90:THR:CG2	2.26	0.56
1:A:127:ALA:N	1:A:426:LEU:HD21	2.21	0.56
1:G:12:ALA:HB2	1:G:520:MET:H	1.71	0.56
1:C:127:ALA:N	1:C:426:LEU:HD21	2.20	0.56
1:B:169:VAL:HG11	1:B:175:ILE:HG12	1.86	0.56
1:F:12:ALA:HB2	1:F:520:MET:H	1.71	0.56
1:N:212:ALA:HA	1:N:325:ILE:O	2.05	0.56
1:F:127:ALA:N	1:F:426:LEU:HD21	2.20	0.56
1:G:127:ALA:N	1:G:426:LEU:HD21	2.20	0.56
1:A:12:ALA:HB2	1:A:520:MET:H	1.71	0.56
1:C:151:SER:CB	1:C:399:ALA:HA	2.36	0.56
1:J:212:ALA:HA	1:J:325:ILE:O	2.06	0.56
1:K:212:ALA:HA	1:K:325:ILE:O	2.05	0.56
1:A:151:SER:CB	1:A:399:ALA:HA	2.36	0.56
1:E:12:ALA:HB2	1:E:520:MET:H	1.70	0.56
1:C:240:VAL:HG11	1:C:247:LEU:HD22	1.88	0.56
1:D:127:ALA:N	1:D:426:LEU:HD21	2.20	0.56
1:F:240:VAL:HG11	1:F:247:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:ILE:H	1:H:251:ALA:HB1	1.71	0.56
1:D:240:VAL:HG11	1:D:247:LEU:HD22	1.88	0.56
1:B:127:ALA:N	1:B:426:LEU:HD21	2.20	0.56
1:I:212:ALA:HA	1:I:325:ILE:O	2.05	0.56
1:B:12:ALA:HB2	1:B:520:MET:H	1.71	0.56
1:D:12:ALA:HB2	1:D:520:MET:H	1.70	0.56
1:E:240:VAL:HG11	1:E:247:LEU:HD22	1.88	0.56
1:F:151:SER:CB	1:F:399:ALA:HA	2.36	0.56
1:C:12:ALA:HB2	1:C:520:MET:H	1.70	0.56
1:E:151:SER:CB	1:E:399:ALA:HA	2.36	0.56
1:B:240:VAL:HG11	1:B:247:LEU:HD22	1.88	0.56
1:G:240:VAL:O	1:G:271:VAL:HG21	2.06	0.56
1:G:151:SER:CB	1:G:399:ALA:HA	2.36	0.56
1:J:138:CYS:CB	1:J:407:VAL:HA	2.36	0.55
1:J:151:SER:CB	1:J:399:ALA:HA	2.36	0.55
1:H:31:LEU:CB	1:H:90:THR:HG21	2.37	0.55
1:M:516:THR:O	1:M:517:THR:HB	2.06	0.55
1:L:138:CYS:CB	1:L:407:VAL:HA	2.37	0.55
1:N:138:CYS:CB	1:N:407:VAL:HA	2.36	0.55
1:N:227:ILE:H	1:N:251:ALA:HB1	1.71	0.55
1:M:227:ILE:H	1:M:251:ALA:HB1	1.71	0.55
1:D:151:SER:CB	1:D:399:ALA:HA	2.36	0.55
1:L:212:ALA:HA	1:L:325:ILE:O	2.05	0.55
1:I:31:LEU:CB	1:I:90:THR:HG21	2.37	0.55
1:B:151:SER:CB	1:B:399:ALA:HA	2.36	0.55
1:E:127:ALA:N	1:E:426:LEU:HD21	2.21	0.55
1:K:138:CYS:CB	1:K:407:VAL:HA	2.36	0.55
1:L:151:SER:CB	1:L:399:ALA:HA	2.36	0.55
1:N:31:LEU:CB	1:N:90:THR:HG21	2.37	0.55
1:H:138:CYS:CB	1:H:407:VAL:HA	2.36	0.55
1:M:138:CYS:CB	1:M:407:VAL:HA	2.36	0.55
1:L:227:ILE:H	1:L:251:ALA:HB1	1.71	0.55
1:M:151:SER:CB	1:M:399:ALA:HA	2.36	0.55
1:I:151:SER:CB	1:I:399:ALA:HA	2.36	0.55
1:N:516:THR:O	1:N:517:THR:HB	2.06	0.55
1:J:227:ILE:H	1:J:251:ALA:HB1	1.71	0.55
1:M:196:ASP:HA	1:M:329:THR:HA	1.89	0.55
1:H:151:SER:CB	1:H:399:ALA:HA	2.36	0.55
1:L:516:THR:O	1:L:517:THR:HB	2.06	0.54
1:I:227:ILE:H	1:I:251:ALA:HB1	1.71	0.54
1:J:196:ASP:HA	1:J:329:THR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:151:SER:CB	1:N:399:ALA:HA	2.36	0.54
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.37	0.54
1:K:151:SER:CB	1:K:399:ALA:HA	2.36	0.54
1:N:196:ASP:HA	1:N:329:THR:HA	1.89	0.54
1:K:196:ASP:HA	1:K:329:THR:HA	1.90	0.54
1:D:4:LYS:H	1:E:63:GLU:CA	2.21	0.54
1:A:4:LYS:H	1:B:63:GLU:CA	2.21	0.54
1:L:144:ILE:HG23	1:L:403:THR:CG2	2.38	0.54
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.37	0.54
1:J:31:LEU:CB	1:J:90:THR:HG21	2.37	0.54
1:I:516:THR:O	1:I:517:THR:HB	2.06	0.54
1:M:144:ILE:HG23	1:M:403:THR:CG2	2.38	0.54
1:I:144:ILE:HG23	1:I:403:THR:CG2	2.38	0.54
1:K:31:LEU:CB	1:K:90:THR:HG21	2.37	0.54
1:L:196:ASP:HA	1:L:329:THR:HA	1.89	0.54
1:L:31:LEU:CB	1:L:90:THR:HG21	2.37	0.54
1:J:516:THR:O	1:J:517:THR:HB	2.06	0.54
1:A:206:ASN:CB	1:A:213:VAL:HA	2.37	0.54
1:H:196:ASP:HA	1:H:329:THR:HA	1.89	0.54
1:K:144:ILE:HG23	1:K:403:THR:CG2	2.38	0.54
1:F:4:LYS:H	1:G:63:GLU:CA	2.21	0.54
1:K:227:ILE:H	1:K:251:ALA:HB1	1.71	0.54
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.38	0.54
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.37	0.54
1:C:4:LYS:H	1:D:63:GLU:CA	2.21	0.54
1:F:31:LEU:HB2	1:F:90:THR:HG21	1.89	0.54
1:K:516:THR:O	1:K:517:THR:HB	2.06	0.54
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.37	0.54
1:J:144:ILE:HG23	1:J:403:THR:CG2	2.38	0.54
1:A:63:GLU:CA	1:G:4:LYS:H	2.21	0.54
1:A:255:GLU:HB2	1:A:258:ALA:HB3	1.90	0.54
1:I:138:CYS:CB	1:I:407:VAL:HA	2.37	0.54
1:E:12:ALA:HB2	1:E:520:MET:N	2.23	0.54
1:I:196:ASP:HA	1:I:329:THR:HA	1.89	0.54
1:B:4:LYS:H	1:C:63:GLU:CA	2.21	0.54
1:E:31:LEU:HB2	1:E:90:THR:HG21	1.89	0.54
1:M:31:LEU:CB	1:M:90:THR:HG21	2.37	0.54
1:H:349:ILE:HG22	1:H:369:VAL:HG13	1.90	0.54
1:G:12:ALA:HB2	1:G:520:MET:N	2.23	0.54
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.37	0.54
1:H:218:PRO:HG2	1:H:320:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:PRO:HG2	1:I:320:ALA:HB3	1.90	0.53
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.37	0.53
1:N:144:ILE:HG23	1:N:403:THR:CG2	2.38	0.53
1:B:255:GLU:HB2	1:B:258:ALA:HB3	1.90	0.53
1:N:218:PRO:HG2	1:N:320:ALA:HB3	1.90	0.53
1:M:349:ILE:HG22	1:M:369:VAL:HG13	1.90	0.53
1:G:31:LEU:HB2	1:G:90:THR:HG21	1.89	0.53
1:N:349:ILE:HG22	1:N:369:VAL:HG13	1.91	0.53
1:I:349:ILE:HG22	1:I:369:VAL:HG13	1.91	0.53
1:H:516:THR:O	1:H:517:THR:HB	2.06	0.53
1:B:206:ASN:CB	1:B:213:VAL:HA	2.37	0.53
1:N:217:SER:HA	1:N:320:ALA:O	2.09	0.53
1:L:349:ILE:HG22	1:L:369:VAL:HG13	1.90	0.53
1:D:31:LEU:HB2	1:D:90:THR:HG21	1.89	0.53
1:J:217:SER:HA	1:J:320:ALA:O	2.09	0.53
1:I:206:ASN:HB2	1:I:213:VAL:HA	1.90	0.53
1:E:4:LYS:H	1:F:63:GLU:CA	2.21	0.53
1:F:258:ALA:HA	1:G:242:LYS:CA	2.39	0.53
1:K:349:ILE:HG22	1:K:369:VAL:HG13	1.90	0.53
1:A:217:SER:HA	1:A:320:ALA:O	2.08	0.53
1:F:12:ALA:HB2	1:F:520:MET:N	2.23	0.53
1:J:218:PRO:HG2	1:J:320:ALA:HB3	1.90	0.53
1:L:206:ASN:HB2	1:L:213:VAL:HA	1.90	0.53
1:C:31:LEU:HB2	1:C:90:THR:HG21	1.89	0.53
1:B:31:LEU:HB2	1:B:90:THR:HG21	1.89	0.53
1:J:206:ASN:HB2	1:J:213:VAL:HA	1.90	0.53
1:C:206:ASN:CB	1:C:213:VAL:HA	2.37	0.53
1:F:41:ASP:HA	1:F:47:PRO:CB	2.39	0.53
1:D:12:ALA:HB2	1:D:520:MET:N	2.23	0.53
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.37	0.53
1:J:142:LYS:H	1:J:142:LYS:HD2	1.74	0.53
1:C:255:GLU:HB2	1:C:258:ALA:HB3	1.90	0.52
1:D:255:GLU:HB2	1:D:258:ALA:HB3	1.90	0.52
1:H:206:ASN:HB2	1:H:213:VAL:HA	1.90	0.52
1:M:206:ASN:HB2	1:M:213:VAL:HA	1.90	0.52
1:C:12:ALA:HB2	1:C:520:MET:N	2.23	0.52
1:J:349:ILE:HG22	1:J:369:VAL:HG13	1.91	0.52
1:M:106:ALA:CB	1:M:116:LEU:HD21	2.39	0.52
1:N:106:ALA:CB	1:N:116:LEU:HD21	2.40	0.52
1:H:106:ALA:CB	1:H:116:LEU:HD21	2.40	0.52
1:M:218:PRO:HG2	1:M:320:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:217:SER:HA	1:M:320:ALA:O	2.09	0.52
1:A:41:ASP:HA	1:A:47:PRO:CB	2.39	0.52
1:L:142:LYS:H	1:L:142:LYS:HD2	1.74	0.52
1:M:142:LYS:H	1:M:142:LYS:HD2	1.75	0.52
1:K:106:ALA:CB	1:K:116:LEU:HD21	2.40	0.52
1:D:172:GLU:H	1:D:172:GLU:CD	2.12	0.52
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.89	0.52
1:K:217:SER:HA	1:K:320:ALA:O	2.09	0.52
1:A:12:ALA:HB2	1:A:520:MET:N	2.23	0.52
1:K:206:ASN:HB2	1:K:213:VAL:HA	1.90	0.52
1:F:255:GLU:HB2	1:F:258:ALA:HB3	1.91	0.52
1:H:142:LYS:H	1:H:142:LYS:HD2	1.74	0.52
1:E:255:GLU:HB2	1:E:258:ALA:HB3	1.90	0.52
1:L:217:SER:HA	1:L:320:ALA:O	2.09	0.52
1:H:217:SER:HA	1:H:320:ALA:O	2.09	0.52
1:D:41:ASP:HA	1:D:47:PRO:CB	2.39	0.52
1:G:254:VAL:HG23	1:G:259:LEU:HB3	1.92	0.52
1:K:142:LYS:HD2	1:K:142:LYS:H	1.75	0.52
1:I:217:SER:HA	1:I:320:ALA:O	2.09	0.52
1:K:218:PRO:HG2	1:K:320:ALA:HB3	1.90	0.52
1:A:169:VAL:HG13	1:A:170:GLY:O	2.10	0.52
1:J:106:ALA:CB	1:J:116:LEU:HD21	2.40	0.52
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.40	0.52
1:L:106:ALA:CB	1:L:116:LEU:HD21	2.40	0.52
1:F:206:ASN:HB2	1:F:213:VAL:CB	2.40	0.52
1:A:254:VAL:HG23	1:A:259:LEU:HB3	1.91	0.52
1:L:427:ALA:HA	1:L:444:LEU:HD11	1.92	0.52
1:B:254:VAL:HG23	1:B:259:LEU:HB3	1.91	0.52
1:N:206:ASN:HB2	1:N:213:VAL:HA	1.90	0.52
1:B:12:ALA:HB2	1:B:520:MET:N	2.23	0.52
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.40	0.52
1:B:172:GLU:CD	1:B:172:GLU:H	2.12	0.52
1:M:427:ALA:HA	1:M:444:LEU:HD11	1.92	0.52
1:C:41:ASP:HA	1:C:47:PRO:CB	2.39	0.52
1:J:226:LYS:HA	1:J:253:ASP:H	1.75	0.52
1:E:172:GLU:CD	1:E:172:GLU:H	2.12	0.52
1:B:206:ASN:HB2	1:B:213:VAL:CB	2.40	0.52
1:D:206:ASN:CB	1:D:213:VAL:HA	2.37	0.52
1:F:206:ASN:CB	1:F:213:VAL:HA	2.37	0.52
1:E:206:ASN:HB2	1:E:213:VAL:CB	2.40	0.52
1:C:180:GLY:HA3	1:C:381:VAL:O	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:VAL:HG13	1:G:170:GLY:O	2.10	0.52
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.40	0.52
1:I:226:LYS:HA	1:I:253:ASP:H	1.75	0.52
1:M:226:LYS:HA	1:M:253:ASP:H	1.75	0.52
1:N:142:LYS:H	1:N:142:LYS:HD2	1.75	0.52
1:K:427:ALA:HA	1:K:444:LEU:HD11	1.92	0.51
1:B:169:VAL:HG13	1:B:170:GLY:O	2.10	0.51
1:I:190:VAL:HG13	1:I:333:ILE:O	2.10	0.51
1:C:172:GLU:H	1:C:172:GLU:CD	2.12	0.51
1:N:427:ALA:HA	1:N:444:LEU:HD11	1.92	0.51
1:H:427:ALA:HA	1:H:444:LEU:HD11	1.92	0.51
1:G:206:ASN:CB	1:G:213:VAL:HA	2.37	0.51
1:A:199:TYR:CE2	1:A:327:LYS:HB3	2.46	0.51
1:B:180:GLY:HA3	1:B:381:VAL:O	2.10	0.51
1:N:190:VAL:HG13	1:N:333:ILE:O	2.10	0.51
1:L:190:VAL:HG13	1:L:333:ILE:O	2.10	0.51
1:L:218:PRO:HG2	1:L:320:ALA:HB3	1.90	0.51
1:D:180:GLY:HA3	1:D:381:VAL:O	2.10	0.51
1:F:257:GLU:HG2	1:F:258:ALA:H	1.75	0.51
1:M:190:VAL:HG13	1:M:333:ILE:O	2.10	0.51
1:K:190:VAL:HG13	1:K:333:ILE:O	2.10	0.51
1:L:417:VAL:HG21	1:L:477:GLY:HA3	1.91	0.51
1:J:190:VAL:HG13	1:J:333:ILE:O	2.10	0.51
1:G:199:TYR:CE2	1:G:327:LYS:HB3	2.46	0.51
1:K:417:VAL:HG21	1:K:477:GLY:HA3	1.91	0.51
1:M:417:VAL:HG21	1:M:477:GLY:HA3	1.91	0.51
1:D:206:ASN:HB2	1:D:213:VAL:CB	2.40	0.51
1:I:127:ALA:N	1:I:426:LEU:HD21	2.26	0.51
1:B:199:TYR:CE2	1:B:327:LYS:HB3	2.46	0.51
1:E:169:VAL:HG13	1:E:170:GLY:O	2.10	0.51
1:F:169:VAL:HG13	1:F:170:GLY:O	2.10	0.51
1:C:169:VAL:HG13	1:C:170:GLY:O	2.10	0.51
1:J:417:VAL:HG21	1:J:477:GLY:HA3	1.91	0.51
1:K:226:LYS:HA	1:K:253:ASP:H	1.75	0.51
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.40	0.51
1:L:247:LEU:O	1:L:273:VAL:HA	2.11	0.51
1:C:206:ASN:HB2	1:C:213:VAL:CB	2.40	0.51
1:H:226:LYS:HA	1:H:253:ASP:H	1.75	0.51
1:N:417:VAL:HG21	1:N:477:GLY:HA3	1.91	0.51
1:H:190:VAL:HG13	1:H:333:ILE:O	2.10	0.51
1:B:258:ALA:HA	1:C:243:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:ALA:N	1:H:426:LEU:HD21	2.26	0.51
1:J:127:ALA:N	1:J:426:LEU:HD21	2.26	0.51
1:F:199:TYR:CE2	1:F:327:LYS:HB3	2.46	0.51
1:E:254:VAL:HG23	1:E:259:LEU:HB3	1.91	0.51
1:D:169:VAL:HG13	1:D:170:GLY:O	2.10	0.51
1:N:226:LYS:HA	1:N:253:ASP:H	1.75	0.51
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.40	0.51
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.40	0.51
1:H:417:VAL:HG21	1:H:477:GLY:HA3	1.91	0.51
1:F:172:GLU:H	1:F:172:GLU:CD	2.12	0.51
1:N:127:ALA:N	1:N:426:LEU:HD21	2.26	0.51
1:G:206:ASN:HB2	1:G:213:VAL:CB	2.41	0.51
1:A:240:VAL:HG11	1:A:247:LEU:HD22	1.92	0.51
1:A:240:VAL:O	1:A:271:VAL:HG21	2.11	0.51
1:M:127:ALA:N	1:M:426:LEU:HD21	2.26	0.51
1:B:41:ASP:HA	1:B:47:PRO:CB	2.39	0.51
1:C:254:VAL:HG23	1:C:259:LEU:HB3	1.91	0.51
1:A:218:PRO:HA	1:A:246:PRO:O	2.10	0.51
1:I:106:ALA:CB	1:I:116:LEU:HD21	2.40	0.51
1:B:293:ALA:HB2	1:B:300:VAL:CG2	2.41	0.51
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.40	0.51
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.41	0.51
1:I:417:VAL:HG21	1:I:477:GLY:HA3	1.91	0.51
1:L:127:ALA:N	1:L:426:LEU:HD21	2.26	0.51
1:I:427:ALA:HA	1:I:444:LEU:HD11	1.93	0.51
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.41	0.51
1:A:258:ALA:HA	1:B:243:ALA:HA	1.93	0.51
1:A:206:ASN:HB2	1:A:213:VAL:CB	2.40	0.51
1:K:127:ALA:N	1:K:426:LEU:HD21	2.26	0.51
1:C:199:TYR:CE2	1:C:327:LYS:HB3	2.46	0.51
1:G:180:GLY:HA3	1:G:381:VAL:O	2.10	0.51
1:D:254:VAL:HG23	1:D:259:LEU:HB3	1.91	0.51
1:E:406:ALA:HB2	1:E:496:PRO:HG3	1.93	0.51
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.41	0.51
1:I:142:LYS:H	1:I:142:LYS:HD2	1.75	0.51
1:D:4:LYS:N	1:E:63:GLU:HA	2.26	0.50
1:F:4:LYS:N	1:G:63:GLU:HA	2.26	0.50
1:C:4:LYS:N	1:D:63:GLU:HA	2.26	0.50
1:J:427:ALA:HA	1:J:444:LEU:HD11	1.93	0.50
1:F:180:GLY:HA3	1:F:381:VAL:O	2.11	0.50
1:A:180:GLY:HA3	1:A:381:VAL:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ASP:HA	1:E:47:PRO:CB	2.39	0.50
1:G:41:ASP:HA	1:G:47:PRO:CB	2.39	0.50
1:L:124:VAL:HG21	1:L:508:ALA:CB	2.41	0.50
1:K:247:LEU:O	1:K:273:VAL:HA	2.11	0.50
1:G:172:GLU:H	1:G:172:GLU:CD	2.12	0.50
1:A:172:GLU:H	1:A:172:GLU:CD	2.12	0.50
1:E:206:ASN:CB	1:E:213:VAL:HA	2.37	0.50
1:E:180:GLY:HA3	1:E:381:VAL:O	2.11	0.50
1:H:247:LEU:O	1:H:273:VAL:HA	2.11	0.50
1:J:124:VAL:HG21	1:J:508:ALA:CB	2.41	0.50
1:M:247:LEU:O	1:M:273:VAL:HA	2.11	0.50
1:B:196:ASP:HA	1:B:329:THR:HA	1.94	0.50
1:D:106:ALA:CB	1:D:116:LEU:HD21	2.42	0.50
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.41	0.50
1:I:247:LEU:O	1:I:273:VAL:HA	2.11	0.50
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.41	0.50
1:C:258:ALA:HA	1:D:243:ALA:HA	1.92	0.50
1:C:106:ALA:CB	1:C:116:LEU:HD21	2.42	0.50
1:J:138:CYS:HB2	1:J:407:VAL:HA	1.94	0.50
1:D:199:TYR:CE2	1:D:327:LYS:HB3	2.46	0.50
1:C:496:PRO:HB2	1:C:499:VAL:HG13	1.93	0.50
1:D:406:ALA:HB2	1:D:496:PRO:HG3	1.94	0.50
1:I:138:CYS:HB2	1:I:407:VAL:HA	1.94	0.50
1:J:40:LEU:O	1:J:47:PRO:HB2	2.12	0.50
1:N:349:ILE:HG23	1:N:365:LEU:HD13	1.93	0.50
1:L:226:LYS:HA	1:L:253:ASP:H	1.75	0.50
1:H:293:ALA:HB2	1:H:300:VAL:CG2	2.42	0.50
1:C:31:LEU:HB3	1:C:90:THR:HG21	1.94	0.50
2:B:1525:ATP:PG	4:B:1528:PO4:P	3.10	0.50
1:N:293:ALA:HB2	1:N:300:VAL:CG2	2.42	0.50
1:J:293:ALA:HB2	1:J:300:VAL:CG2	2.42	0.50
1:L:293:ALA:HB2	1:L:300:VAL:CG2	2.42	0.50
1:G:106:ALA:CB	1:G:116:LEU:HD21	2.42	0.50
2:D:1525:ATP:PG	4:D:1528:PO4:P	3.10	0.50
1:E:199:TYR:CE2	1:E:327:LYS:HB3	2.46	0.50
1:I:40:LEU:O	1:I:47:PRO:HB2	2.12	0.50
1:E:262:LEU:HB2	1:F:242:LYS:HA	1.94	0.50
1:H:349:ILE:HG23	1:H:365:LEU:HD13	1.93	0.50
1:D:496:PRO:HB2	1:D:499:VAL:HG13	1.93	0.50
1:B:496:PRO:HB2	1:B:499:VAL:HG13	1.93	0.50
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.41	0.50
1:F:406:ALA:HB2	1:F:496:PRO:HG3	1.93	0.50
1:E:4:LYS:N	1:F:63:GLU:HA	2.26	0.50
1:B:4:LYS:N	1:C:63:GLU:HA	2.26	0.50
2:C:1526:ATP:PG	4:C:1528:PO4:P	3.10	0.50
2:E:1525:ATP:PG	4:E:1528:PO4:P	3.10	0.50
1:E:258:ALA:HA	1:F:243:ALA:HA	1.93	0.50
1:N:124:VAL:HG21	1:N:508:ALA:CB	2.41	0.50
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.41	0.50
1:A:196:ASP:HA	1:A:329:THR:HA	1.94	0.50
1:N:247:LEU:O	1:N:273:VAL:HA	2.11	0.50
1:C:196:ASP:HA	1:C:329:THR:HA	1.94	0.50
1:K:293:ALA:HB2	1:K:300:VAL:CG2	2.42	0.50
1:J:247:LEU:O	1:J:273:VAL:HA	2.11	0.50
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.94	0.49
1:C:126:ALA:HB3	1:C:426:LEU:HD22	1.94	0.49
1:D:258:ALA:HA	1:E:243:ALA:HA	1.93	0.49
1:B:262:LEU:HB2	1:C:242:LYS:HA	1.94	0.49
1:D:262:LEU:HB2	1:E:242:LYS:HA	1.94	0.49
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.94	0.49
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.42	0.49
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.94	0.49
1:G:293:ALA:HB2	1:G:300:VAL:CG2	2.41	0.49
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.94	0.49
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.94	0.49
1:D:126:ALA:HB3	1:D:426:LEU:HD22	1.94	0.49
1:B:126:ALA:HB3	1:B:426:LEU:HD22	1.95	0.49
1:K:40:LEU:O	1:K:47:PRO:HB2	2.12	0.49
1:C:262:LEU:HB2	1:D:242:LYS:HA	1.94	0.49
1:M:349:ILE:HG23	1:M:365:LEU:HD13	1.93	0.49
1:C:293:ALA:HB2	1:C:300:VAL:CG2	2.41	0.49
1:F:106:ALA:CB	1:F:116:LEU:HD21	2.42	0.49
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.95	0.49
1:A:106:ALA:CB	1:A:116:LEU:HD21	2.42	0.49
1:G:496:PRO:HB2	1:G:499:VAL:HG13	1.93	0.49
1:A:126:ALA:HB3	1:A:426:LEU:HD22	1.94	0.49
1:N:186:GLU:H	1:N:380:LYS:HB2	1.77	0.49
1:A:262:LEU:HB2	1:B:242:LYS:HA	1.94	0.49
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.93	0.49
1:E:106:ALA:CB	1:E:116:LEU:HD21	2.42	0.49
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.94	0.49
1:J:356:ALA:HB1	1:J:361:ASP:HB2	1.95	0.49
1:A:496:PRO:HB2	1:A:499:VAL:HG13	1.93	0.49
1:I:172:GLU:CD	1:I:172:GLU:H	2.15	0.49
2:F:1525:ATP:PG	4:F:1528:PO4:P	3.10	0.49
1:A:31:LEU:HB3	1:A:90:THR:HG21	1.94	0.49
1:F:496:PRO:HB2	1:F:499:VAL:HG13	1.93	0.49
1:L:356:ALA:HB1	1:L:361:ASP:HB2	1.95	0.49
1:G:349:ILE:HG22	1:G:369:VAL:HG13	1.95	0.49
1:A:349:ILE:HG22	1:A:369:VAL:HG13	1.94	0.49
1:E:196:ASP:HA	1:E:329:THR:HA	1.93	0.49
1:A:63:GLU:HA	1:G:4:LYS:N	2.26	0.49
1:E:126:ALA:HB3	1:E:426:LEU:HD22	1.94	0.49
1:H:186:GLU:H	1:H:380:LYS:HB2	1.77	0.49
1:K:356:ALA:HB1	1:K:361:ASP:HB2	1.95	0.49
1:F:349:ILE:HG22	1:F:369:VAL:HG13	1.95	0.49
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.41	0.49
1:M:293:ALA:HB2	1:M:300:VAL:CG2	2.42	0.49
1:D:349:ILE:HG22	1:D:369:VAL:HG13	1.95	0.49
1:D:31:LEU:HB3	1:D:90:THR:HG21	1.94	0.49
1:K:138:CYS:HB2	1:K:407:VAL:HA	1.94	0.49
1:H:40:LEU:O	1:H:47:PRO:HB2	2.12	0.49
1:L:349:ILE:HG23	1:L:365:LEU:HD13	1.93	0.49
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.93	0.49
1:D:237:LEU:O	1:D:241:ALA:N	2.46	0.49
1:K:172:GLU:CD	1:K:172:GLU:H	2.15	0.49
1:J:172:GLU:H	1:J:172:GLU:CD	2.15	0.49
1:E:31:LEU:HB3	1:E:90:THR:HG21	1.94	0.49
2:A:1525:ATP:PG	4:A:1528:PO4:P	3.10	0.49
1:B:82:ASN:HB2	1:B:89:THR:HG23	1.95	0.49
1:L:40:LEU:O	1:L:47:PRO:HB2	2.12	0.49
1:L:186:GLU:H	1:L:380:LYS:HB2	1.77	0.49
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.93	0.49
1:I:293:ALA:HB2	1:I:300:VAL:CG2	2.42	0.49
1:N:31:LEU:HB2	1:N:90:THR:HG21	1.94	0.49
1:I:31:LEU:HB2	1:I:90:THR:HG21	1.95	0.49
1:H:31:LEU:HB2	1:H:90:THR:HG21	1.95	0.49
1:I:349:ILE:HG23	1:I:365:LEU:HD13	1.93	0.49
1:L:190:VAL:HG11	1:L:333:ILE:HG23	1.94	0.49
1:H:190:VAL:HG11	1:H:333:ILE:HG23	1.95	0.49
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:337:GLY:HA3	1:H:342:ILE:HD11	1.94	0.49
1:M:356:ALA:HB1	1:M:361:ASP:HB2	1.95	0.49
1:B:349:ILE:HG22	1:B:369:VAL:HG13	1.94	0.49
1:I:337:GLY:HA3	1:I:342:ILE:HD11	1.94	0.49
1:C:349:ILE:HG22	1:C:369:VAL:HG13	1.94	0.49
1:N:172:GLU:CD	1:N:172:GLU:H	2.15	0.49
2:G:1525:ATP:PG	4:G:1528:PO4:P	3.10	0.49
1:K:186:GLU:H	1:K:380:LYS:HB2	1.77	0.49
1:A:82:ASN:HB2	1:A:89:THR:HG23	1.95	0.49
1:J:349:ILE:HG23	1:J:365:LEU:HD13	1.93	0.49
1:C:237:LEU:O	1:C:241:ALA:N	2.46	0.49
1:H:138:CYS:HB2	1:H:407:VAL:HA	1.94	0.49
1:I:199:TYR:CE2	1:I:327:LYS:HB3	2.48	0.49
1:H:199:TYR:CE2	1:H:327:LYS:HB3	2.48	0.49
1:C:82:ASN:HB2	1:C:89:THR:HG23	1.95	0.49
1:I:190:VAL:HG11	1:I:333:ILE:HG23	1.95	0.49
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.94	0.49
1:E:114:MET:CB	1:F:36:ARG:HD2	2.43	0.49
1:F:196:ASP:HA	1:F:329:THR:HA	1.94	0.49
1:A:281:PHE:CA	1:A:285:ARG:HB2	2.43	0.49
1:A:138:CYS:CB	1:A:407:VAL:HA	2.43	0.48
1:G:126:ALA:HB3	1:G:426:LEU:HD22	1.94	0.48
1:F:254:VAL:HG23	1:F:259:LEU:HB2	1.95	0.48
1:L:337:GLY:HA3	1:L:342:ILE:HD11	1.94	0.48
1:D:196:ASP:HA	1:D:329:THR:HA	1.94	0.48
1:I:356:ALA:HB1	1:I:361:ASP:HB2	1.95	0.48
1:A:36:ARG:HD2	1:G:114:MET:CB	2.43	0.48
1:D:3:ALA:HA	1:E:63:GLU:CB	2.42	0.48
1:G:138:CYS:CB	1:G:407:VAL:HA	2.43	0.48
1:N:199:TYR:CE2	1:N:327:LYS:HB3	2.48	0.48
1:J:180:GLY:HA3	1:J:381:VAL:O	2.14	0.48
1:N:180:GLY:HA3	1:N:381:VAL:O	2.14	0.48
1:N:40:LEU:O	1:N:47:PRO:HB2	2.12	0.48
1:E:230:ILE:HG12	1:E:262:LEU:HD12	1.95	0.48
1:G:229:ASN:ND2	1:G:230:ILE:H	2.10	0.48
1:K:349:ILE:HG23	1:K:365:LEU:HD13	1.93	0.48
1:A:411:VAL:HG12	1:A:494:LEU:HB2	1.95	0.48
1:F:114:MET:CB	1:G:36:ARG:HD2	2.43	0.48
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.94	0.48
1:E:237:LEU:O	1:E:241:ALA:N	2.46	0.48
1:A:4:LYS:N	1:B:63:GLU:HA	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:LEU:HB2	1:K:90:THR:HG21	1.94	0.48
1:B:138:CYS:CB	1:B:407:VAL:HA	2.43	0.48
1:N:138:CYS:HB2	1:N:407:VAL:HA	1.94	0.48
1:K:180:GLY:HA3	1:K:381:VAL:O	2.14	0.48
1:M:40:LEU:O	1:M:47:PRO:HB2	2.12	0.48
1:C:411:VAL:HG12	1:C:494:LEU:HB2	1.95	0.48
1:D:411:VAL:HG12	1:D:494:LEU:HB2	1.96	0.48
1:G:411:VAL:HG12	1:G:494:LEU:HB2	1.95	0.48
1:N:337:GLY:HA3	1:N:342:ILE:HD11	1.94	0.48
1:J:337:GLY:HA3	1:J:342:ILE:HD11	1.94	0.48
1:G:31:LEU:HB3	1:G:90:THR:HG21	1.94	0.48
1:L:31:LEU:HB2	1:L:90:THR:HG21	1.95	0.48
1:M:199:TYR:CE2	1:M:327:LYS:HB3	2.48	0.48
1:M:205:ILE:HD12	1:M:211:GLY:O	2.13	0.48
1:L:138:CYS:HB2	1:L:407:VAL:HA	1.94	0.48
1:I:186:GLU:H	1:I:380:LYS:HB2	1.77	0.48
1:J:186:GLU:H	1:J:380:LYS:HB2	1.77	0.48
1:F:258:ALA:HA	1:G:242:LYS:C	2.34	0.48
1:E:411:VAL:HG12	1:E:494:LEU:HB2	1.96	0.48
1:F:281:PHE:CA	1:F:285:ARG:HB2	2.43	0.48
1:N:356:ALA:HB1	1:N:361:ASP:HB2	1.95	0.48
1:M:337:GLY:HA3	1:M:342:ILE:HD11	1.94	0.48
1:J:31:LEU:HB2	1:J:90:THR:HG21	1.94	0.48
1:G:183:LEU:C	1:G:382:GLY:HA3	2.34	0.48
1:C:138:CYS:CB	1:C:407:VAL:HA	2.43	0.48
1:N:205:ILE:HD12	1:N:211:GLY:O	2.13	0.48
1:G:218:PRO:HA	1:G:246:PRO:O	2.13	0.48
1:I:180:GLY:HA3	1:I:381:VAL:O	2.14	0.48
1:M:190:VAL:HG11	1:M:333:ILE:HG23	1.95	0.48
1:K:190:VAL:HG11	1:K:333:ILE:HG23	1.95	0.48
1:F:411:VAL:HG12	1:F:494:LEU:HB2	1.96	0.48
1:G:196:ASP:HA	1:G:329:THR:HA	1.93	0.48
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.95	0.48
1:H:356:ALA:HB1	1:H:361:ASP:HB2	1.95	0.48
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.95	0.48
1:L:172:GLU:CD	1:L:172:GLU:H	2.15	0.48
1:C:257:GLU:CD	1:C:257:GLU:H	2.17	0.48
1:D:240:VAL:O	1:D:271:VAL:HG21	2.14	0.48
1:A:257:GLU:H	1:A:257:GLU:CD	2.17	0.48
1:K:199:TYR:CE2	1:K:327:LYS:HB3	2.48	0.48
1:K:205:ILE:HD12	1:K:211:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:205:ILE:HD12	1:L:211:GLY:O	2.13	0.48
1:L:199:TYR:CE2	1:L:327:LYS:HB3	2.48	0.48
1:F:200:LEU:CD1	1:F:254:VAL:HG11	2.44	0.48
1:D:230:ILE:HG12	1:D:262:LEU:HD12	1.95	0.48
1:D:281:PHE:CA	1:D:285:ARG:HB2	2.43	0.48
1:A:114:MET:CB	1:B:36:ARG:HD2	2.43	0.48
1:B:114:MET:CB	1:C:36:ARG:HD2	2.43	0.48
1:M:31:LEU:HB2	1:M:90:THR:HG21	1.95	0.48
1:D:257:GLU:H	1:D:257:GLU:CD	2.17	0.48
1:H:205:ILE:HD12	1:H:211:GLY:O	2.13	0.48
1:M:138:CYS:HB2	1:M:407:VAL:HA	1.94	0.48
1:A:200:LEU:CD1	1:A:254:VAL:HG11	2.44	0.48
1:L:180:GLY:HA3	1:L:381:VAL:O	2.14	0.48
1:E:281:PHE:CA	1:E:285:ARG:HB2	2.43	0.48
1:B:281:PHE:CA	1:B:285:ARG:HB2	2.43	0.48
1:A:23:LEU:O	1:A:27:VAL:HG23	2.14	0.48
1:F:183:LEU:C	1:F:382:GLY:HA3	2.34	0.48
1:F:138:CYS:CB	1:F:407:VAL:HA	2.43	0.48
1:E:82:ASN:HB2	1:E:89:THR:HG23	1.95	0.48
1:F:82:ASN:HB2	1:F:89:THR:HG23	1.95	0.48
1:B:230:ILE:HG12	1:B:262:LEU:HD12	1.95	0.48
1:N:190:VAL:HG11	1:N:333:ILE:HG23	1.95	0.48
1:B:411:VAL:HG12	1:B:494:LEU:HB2	1.96	0.48
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.95	0.48
1:B:219:PHE:CE2	1:B:314:LEU:HD22	2.49	0.48
1:F:219:PHE:CE2	1:F:314:LEU:HD22	2.49	0.48
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.95	0.48
1:A:115:ASP:HB2	1:A:435:ASP:HB2	1.96	0.48
1:M:172:GLU:H	1:M:172:GLU:CD	2.15	0.48
1:H:172:GLU:H	1:H:172:GLU:CD	2.15	0.48
1:E:3:ALA:HA	1:F:63:GLU:CB	2.42	0.48
1:D:138:CYS:CB	1:D:407:VAL:HA	2.43	0.48
1:D:426:LEU:HB2	1:D:444:LEU:HD22	1.96	0.48
1:F:426:LEU:HB2	1:F:444:LEU:HD22	1.96	0.48
1:J:199:TYR:CE2	1:J:327:LYS:HB3	2.48	0.48
1:J:190:VAL:HG11	1:J:333:ILE:HG23	1.95	0.48
1:A:237:LEU:O	1:A:241:ALA:N	2.46	0.48
1:I:54:VAL:HG13	1:I:89:THR:HG21	1.96	0.48
1:C:281:PHE:CA	1:C:285:ARG:HB2	2.43	0.48
1:D:224:ASP:HA	1:D:289:LEU:CD1	2.44	0.48
1:E:219:PHE:CE2	1:E:314:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:LYS:HD3	1:F:523:ASP:HA	1.95	0.48
1:C:3:ALA:HA	1:D:63:GLU:CB	2.42	0.48
1:G:4:LYS:HD3	1:G:523:ASP:HA	1.95	0.48
1:B:136:VAL:O	1:B:410:GLY:HA3	2.14	0.48
1:C:426:LEU:HB2	1:C:444:LEU:HD22	1.96	0.48
1:E:240:VAL:O	1:E:271:VAL:HG21	2.14	0.48
1:E:224:ASP:HA	1:E:289:LEU:CD1	2.44	0.48
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.96	0.48
1:C:219:PHE:CE2	1:C:314:LEU:HD22	2.49	0.48
1:K:337:GLY:HA3	1:K:342:ILE:HD11	1.94	0.48
1:G:19:GLY:HA2	1:G:62:LEU:HD13	1.96	0.48
1:C:4:LYS:HD3	1:C:523:ASP:HA	1.95	0.47
1:C:23:LEU:O	1:C:27:VAL:HG23	2.14	0.47
1:D:23:LEU:O	1:D:27:VAL:HG23	2.14	0.47
1:A:183:LEU:C	1:A:382:GLY:HA3	2.34	0.47
1:C:240:VAL:O	1:C:271:VAL:HG21	2.14	0.47
1:E:257:GLU:H	1:E:257:GLU:CD	2.17	0.47
1:F:228:SER:O	1:F:258:ALA:HB1	2.14	0.47
1:C:114:MET:CB	1:D:36:ARG:HD2	2.43	0.47
1:D:114:MET:CB	1:E:36:ARG:HD2	2.43	0.47
1:C:224:ASP:HA	1:C:289:LEU:CD1	2.44	0.47
1:J:54:VAL:HG13	1:J:89:THR:HG21	1.96	0.47
1:C:115:ASP:HB2	1:C:435:ASP:HB2	1.96	0.47
1:B:224:ASP:HA	1:B:289:LEU:CD1	2.44	0.47
1:A:19:GLY:HA2	1:A:62:LEU:HD13	1.96	0.47
1:A:4:LYS:HD3	1:A:523:ASP:HA	1.95	0.47
1:E:23:LEU:O	1:E:27:VAL:HG23	2.14	0.47
1:E:138:CYS:CB	1:E:407:VAL:HA	2.43	0.47
1:B:257:GLU:CD	1:B:257:GLU:H	2.17	0.47
1:E:426:LEU:HB2	1:E:444:LEU:HD22	1.96	0.47
1:F:126:ALA:HB3	1:F:426:LEU:HD22	1.95	0.47
1:G:82:ASN:HB2	1:G:89:THR:HG23	1.95	0.47
1:B:115:ASP:HB2	1:B:435:ASP:HB2	1.96	0.47
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.96	0.47
1:G:115:ASP:HB2	1:G:435:ASP:HB2	1.96	0.47
1:D:219:PHE:CE2	1:D:314:LEU:HD22	2.49	0.47
1:A:224:ASP:HA	1:A:289:LEU:CD1	2.44	0.47
1:E:4:LYS:HD3	1:E:523:ASP:HA	1.95	0.47
1:L:31:LEU:HB3	1:L:90:THR:HG21	1.96	0.47
1:A:136:VAL:O	1:A:410:GLY:HA3	2.14	0.47
1:F:240:VAL:O	1:F:271:VAL:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:LEU:HB2	1:G:444:LEU:HD22	1.96	0.47
1:N:126:ALA:HB3	1:N:426:LEU:HD22	1.97	0.47
1:B:200:LEU:CD1	1:B:254:VAL:HG11	2.44	0.47
1:M:180:GLY:HA3	1:M:381:VAL:O	2.14	0.47
1:B:152:ALA:HB1	1:B:155:ASP:O	2.15	0.47
1:B:237:LEU:O	1:B:241:ALA:N	2.46	0.47
1:F:237:LEU:O	1:F:241:ALA:N	2.46	0.47
1:G:281:PHE:CA	1:G:285:ARG:HB2	2.43	0.47
1:F:19:GLY:HA2	1:F:62:LEU:HD13	1.96	0.47
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.95	0.47
1:D:4:LYS:HD3	1:D:523:ASP:HA	1.95	0.47
1:B:23:LEU:O	1:B:27:VAL:HG23	2.14	0.47
1:G:23:LEU:O	1:G:27:VAL:HG23	2.14	0.47
1:K:31:LEU:HB3	1:K:90:THR:HG21	1.97	0.47
1:B:183:LEU:C	1:B:382:GLY:HA3	2.34	0.47
1:B:426:LEU:HB2	1:B:444:LEU:HD22	1.96	0.47
1:E:151:SER:HB3	1:E:399:ALA:HA	1.97	0.47
1:B:281:PHE:HA	1:B:285:ARG:HB2	1.96	0.47
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.96	0.47
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.95	0.47
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.44	0.47
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.96	0.47
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.44	0.47
1:F:206:ASN:HB2	1:F:213:VAL:HB	1.96	0.47
1:H:180:GLY:HA3	1:H:381:VAL:O	2.14	0.47
1:D:82:ASN:HB2	1:D:89:THR:HG23	1.95	0.47
1:M:186:GLU:H	1:M:380:LYS:HB2	1.77	0.47
1:C:230:ILE:HG12	1:C:262:LEU:HD12	1.95	0.47
1:K:213:VAL:HG13	1:K:325:ILE:HB	1.97	0.47
1:D:279:PRO:HG3	1:D:292:ILE:HD11	1.97	0.47
1:F:287:ALA:HB1	1:F:368:ARG:CZ	2.44	0.47
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.44	0.47
1:B:19:GLY:HA2	1:B:62:LEU:HD13	1.96	0.47
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.44	0.47
1:A:426:LEU:HB2	1:A:444:LEU:HD22	1.96	0.47
1:C:152:ALA:HB1	1:C:155:ASP:O	2.14	0.47
1:A:230:ILE:HG12	1:A:262:LEU:HD12	1.95	0.47
1:H:213:VAL:HG13	1:H:325:ILE:HB	1.97	0.47
1:C:281:PHE:HA	1:C:285:ARG:HB2	1.96	0.47
1:F:224:ASP:HA	1:F:289:LEU:CD1	2.44	0.47
1:B:4:LYS:HD3	1:B:523:ASP:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:LEU:HB3	1:J:90:THR:HG21	1.97	0.47
1:C:183:LEU:C	1:C:382:GLY:HA3	2.34	0.47
1:G:136:VAL:O	1:G:410:GLY:HA3	2.14	0.47
1:F:136:VAL:O	1:F:410:GLY:HA3	2.14	0.47
1:B:206:ASN:HB2	1:B:213:VAL:HB	1.96	0.47
1:I:205:ILE:HD12	1:I:211:GLY:O	2.13	0.47
1:J:205:ILE:HD12	1:J:211:GLY:O	2.13	0.47
1:M:126:ALA:HB3	1:M:426:LEU:HD22	1.97	0.47
1:M:152:ALA:HB1	1:M:155:ASP:HB3	1.97	0.47
1:N:213:VAL:HG13	1:N:325:ILE:HB	1.97	0.47
1:J:213:VAL:HG13	1:J:325:ILE:HB	1.97	0.47
1:I:213:VAL:HG13	1:I:325:ILE:HB	1.97	0.47
1:L:213:VAL:HG13	1:L:325:ILE:HB	1.97	0.47
1:L:54:VAL:HG13	1:L:89:THR:HG21	1.96	0.47
1:D:115:ASP:HB2	1:D:435:ASP:HB2	1.96	0.47
1:C:279:PRO:HG3	1:C:292:ILE:HD11	1.97	0.47
1:H:54:VAL:HG13	1:H:89:THR:HG21	1.96	0.47
1:F:115:ASP:HB2	1:F:435:ASP:HB2	1.96	0.47
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.95	0.47
1:A:4:LYS:HZ2	1:A:523:ASP:CG	2.18	0.47
1:H:126:ALA:HB3	1:H:426:LEU:HD22	1.97	0.47
1:N:152:ALA:HB1	1:N:155:ASP:HB3	1.97	0.47
1:F:151:SER:HB3	1:F:399:ALA:HA	1.97	0.47
1:A:281:PHE:HA	1:A:285:ARG:HB2	1.96	0.47
1:D:281:PHE:HA	1:D:285:ARG:HB2	1.96	0.47
1:E:279:PRO:HG3	1:E:292:ILE:HD11	1.97	0.47
1:M:31:LEU:HB3	1:M:90:THR:HG21	1.97	0.47
1:E:136:VAL:O	1:E:410:GLY:HA3	2.14	0.47
1:B:240:VAL:O	1:B:271:VAL:HG21	2.14	0.47
1:F:152:ALA:HB1	1:F:155:ASP:O	2.14	0.47
1:E:12:ALA:HB3	1:E:518:GLU:O	2.15	0.47
1:D:12:ALA:HB3	1:D:518:GLU:O	2.15	0.47
1:G:224:ASP:HA	1:G:289:LEU:CD1	2.44	0.47
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.96	0.47
1:C:136:VAL:O	1:C:410:GLY:HA3	2.14	0.47
1:A:206:ASN:HB2	1:A:213:VAL:HB	1.97	0.47
1:G:206:ASN:HB2	1:G:213:VAL:HB	1.97	0.47
1:L:152:ALA:HB1	1:L:155:ASP:HB3	1.97	0.47
1:B:218:PRO:HA	1:B:246:PRO:O	2.15	0.47
1:K:152:ALA:HB1	1:K:155:ASP:HB3	1.97	0.47
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:ALA:HB1	1:E:368:ARG:CZ	2.44	0.47
1:E:19:GLY:HA2	1:E:62:LEU:HD13	1.96	0.47
1:C:206:ASN:HB2	1:C:213:VAL:HB	1.96	0.46
1:D:200:LEU:CD1	1:D:254:VAL:HG11	2.44	0.46
1:C:12:ALA:HB3	1:C:518:GLU:O	2.16	0.46
1:D:183:LEU:C	1:D:382:GLY:HA3	2.34	0.46
1:D:136:VAL:O	1:D:410:GLY:HA3	2.14	0.46
1:G:255:GLU:HB3	1:G:257:GLU:HG2	1.96	0.46
1:E:206:ASN:HB2	1:E:213:VAL:HB	1.97	0.46
1:E:152:ALA:HB1	1:E:155:ASP:O	2.14	0.46
1:C:218:PRO:HA	1:C:246:PRO:O	2.15	0.46
1:A:152:ALA:HB1	1:A:155:ASP:O	2.14	0.46
1:B:12:ALA:HB3	1:B:518:GLU:O	2.15	0.46
1:C:19:GLY:HA2	1:C:62:LEU:HD13	1.96	0.46
1:K:54:VAL:HG13	1:K:89:THR:HG21	1.96	0.46
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.97	0.46
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.96	0.46
1:M:54:VAL:HG13	1:M:89:THR:HG21	1.96	0.46
1:I:31:LEU:HB3	1:I:90:THR:HG21	1.97	0.46
1:G:151:SER:HB3	1:G:399:ALA:HA	1.97	0.46
1:H:151:SER:HB3	1:H:399:ALA:HA	1.98	0.46
1:E:281:PHE:HA	1:E:285:ARG:HB2	1.96	0.46
1:E:115:ASP:HB2	1:E:435:ASP:HB2	1.96	0.46
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.97	0.46
1:G:152:ALA:HB1	1:G:155:ASP:O	2.15	0.46
1:D:151:SER:HB3	1:D:399:ALA:HA	1.97	0.46
1:G:281:PHE:HA	1:G:285:ARG:HB2	1.96	0.46
1:D:19:GLY:HA2	1:D:62:LEU:HD13	1.96	0.46
1:F:3:ALA:HA	1:G:63:GLU:CB	2.42	0.46
1:B:3:ALA:HA	1:C:63:GLU:CB	2.42	0.46
1:F:23:LEU:O	1:F:27:VAL:HG23	2.14	0.46
1:D:206:ASN:HB2	1:D:213:VAL:HB	1.97	0.46
1:M:213:VAL:HG13	1:M:325:ILE:HB	1.97	0.46
1:A:120:ILE:O	1:A:124:VAL:HG23	2.16	0.46
1:J:120:ILE:O	1:J:124:VAL:HG23	2.16	0.46
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.97	0.46
1:K:346:VAL:HG22	1:K:372:LEU:HD13	1.98	0.46
1:G:279:PRO:HG3	1:G:292:ILE:HD11	1.96	0.46
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.96	0.46
1:E:183:LEU:C	1:E:382:GLY:HA3	2.34	0.46
1:D:206:ASN:HB2	1:D:213:VAL:CA	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:152:ALA:HB1	1:J:155:ASP:HB3	1.97	0.46
1:I:151:SER:HB3	1:I:399:ALA:HA	1.97	0.46
1:B:120:ILE:O	1:B:124:VAL:HG23	2.16	0.46
1:E:120:ILE:O	1:E:124:VAL:HG23	2.16	0.46
1:B:114:MET:H	1:C:36:ARG:HG3	1.80	0.46
1:F:235:PRO:HB2	1:F:310:GLU:HA	1.97	0.46
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.97	0.46
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.97	0.46
1:D:152:ALA:HB1	1:D:155:ASP:O	2.14	0.46
1:F:12:ALA:HB3	1:F:518:GLU:O	2.15	0.46
1:A:151:SER:HB3	1:A:399:ALA:HA	1.97	0.46
1:B:151:SER:HB3	1:B:399:ALA:HA	1.97	0.46
1:G:120:ILE:O	1:G:124:VAL:HG23	2.16	0.46
1:L:120:ILE:O	1:L:124:VAL:HG23	2.16	0.46
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.46	0.46
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.46	0.46
1:N:54:VAL:HG13	1:N:89:THR:HG21	1.96	0.46
1:G:102:GLU:HB2	1:G:442:VAL:HG13	1.97	0.46
1:B:279:PRO:HG3	1:B:292:ILE:HD11	1.97	0.46
1:D:4:LYS:HZ2	1:D:523:ASP:CG	2.18	0.46
1:H:38:VAL:HG21	1:H:56:VAL:HG13	1.98	0.46
1:J:126:ALA:HB3	1:J:426:LEU:HD22	1.97	0.46
1:H:152:ALA:HB1	1:H:155:ASP:HB3	1.97	0.46
1:F:218:PRO:HA	1:F:246:PRO:O	2.15	0.46
1:L:151:SER:HB3	1:L:399:ALA:HA	1.97	0.46
1:F:281:PHE:HA	1:F:285:ARG:HB2	1.96	0.46
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.46	0.46
1:I:406:ALA:HB2	1:I:496:PRO:HG3	1.97	0.46
1:J:406:ALA:HB2	1:J:496:PRO:HG3	1.97	0.46
1:L:346:VAL:HG22	1:L:372:LEU:HD13	1.98	0.46
1:N:38:VAL:HG21	1:N:56:VAL:HG13	1.98	0.46
1:E:90:THR:HG22	1:E:94:VAL:HG23	1.98	0.46
1:D:90:THR:HG22	1:D:94:VAL:HG23	1.98	0.46
1:C:240:VAL:HA	1:C:243:ALA:CB	2.43	0.46
1:K:126:ALA:HB3	1:K:426:LEU:HD22	1.97	0.46
1:B:205:ILE:HD12	1:B:211:GLY:O	2.16	0.46
1:C:200:LEU:CD1	1:C:254:VAL:HG11	2.44	0.46
1:J:152:ALA:HB1	1:J:155:ASP:CA	2.46	0.46
1:K:152:ALA:HB1	1:K:155:ASP:CA	2.46	0.46
1:E:218:PRO:HA	1:E:246:PRO:O	2.15	0.46
1:A:12:ALA:HB3	1:A:518:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:O	1:D:124:VAL:HG23	2.16	0.46
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.46	0.46
1:N:158:VAL:HG22	1:N:396:VAL:HG22	1.98	0.46
1:E:102:GLU:HB2	1:E:442:VAL:HG13	1.97	0.46
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.97	0.46
1:C:205:ILE:HD12	1:C:211:GLY:O	2.16	0.46
1:I:152:ALA:HB1	1:I:155:ASP:CA	2.46	0.46
1:D:218:PRO:HA	1:D:246:PRO:O	2.15	0.46
1:G:230:ILE:HG21	1:G:263:VAL:HA	1.97	0.46
1:C:120:ILE:O	1:C:124:VAL:HG23	2.16	0.46
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.46	0.46
1:B:235:PRO:HB2	1:B:310:GLU:HA	1.98	0.46
1:N:31:LEU:HB3	1:N:90:THR:HG21	1.97	0.45
1:D:240:VAL:HA	1:D:243:ALA:CB	2.43	0.45
1:L:126:ALA:HB3	1:L:426:LEU:HD22	1.97	0.45
1:L:152:ALA:HB1	1:L:155:ASP:CA	2.46	0.45
1:J:151:SER:HB3	1:J:399:ALA:HA	1.97	0.45
1:F:120:ILE:O	1:F:124:VAL:HG23	2.16	0.45
1:N:120:ILE:O	1:N:124:VAL:HG23	2.16	0.45
1:F:114:MET:H	1:G:36:ARG:HG3	1.80	0.45
1:A:235:PRO:HB2	1:A:310:GLU:HA	1.98	0.45
1:D:102:GLU:HB2	1:D:442:VAL:HG13	1.97	0.45
1:C:140:ASP:CG	1:C:142:LYS:HZ3	2.20	0.45
1:A:279:PRO:HG3	1:A:292:ILE:HD11	1.97	0.45
1:H:31:LEU:HB3	1:H:90:THR:HG21	1.96	0.45
1:N:151:SER:HB3	1:N:399:ALA:HA	1.97	0.45
1:I:120:ILE:O	1:I:124:VAL:HG23	2.16	0.45
1:K:120:ILE:O	1:K:124:VAL:HG23	2.16	0.45
1:M:120:ILE:O	1:M:124:VAL:HG23	2.16	0.45
1:H:120:ILE:O	1:H:124:VAL:HG23	2.16	0.45
1:H:158:VAL:HG22	1:H:396:VAL:HG22	1.98	0.45
1:I:126:ALA:HB3	1:I:426:LEU:HD22	1.97	0.45
1:A:205:ILE:HD12	1:A:211:GLY:O	2.16	0.45
1:C:151:SER:HB3	1:C:399:ALA:HA	1.97	0.45
1:K:151:SER:HB3	1:K:399:ALA:HA	1.97	0.45
1:N:240:VAL:HG21	1:N:247:LEU:HD22	1.98	0.45
1:A:36:ARG:HG3	1:G:114:MET:H	1.80	0.45
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.46	0.45
1:M:346:VAL:HG22	1:M:372:LEU:HD13	1.98	0.45
1:M:158:VAL:HG22	1:M:396:VAL:HG22	1.98	0.45
1:B:206:ASN:HB2	1:B:213:VAL:CA	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:VAL:O	1:D:324:VAL:HA	2.17	0.45
1:E:206:ASN:HB2	1:E:213:VAL:CA	2.43	0.45
1:H:152:ALA:HB1	1:H:155:ASP:CA	2.46	0.45
1:N:152:ALA:HB1	1:N:155:ASP:CA	2.46	0.45
1:A:114:MET:H	1:B:36:ARG:HG3	1.80	0.45
1:I:102:GLU:HB2	1:I:442:VAL:HG13	1.99	0.45
1:G:237:LEU:O	1:G:241:ALA:N	2.50	0.45
1:B:102:GLU:HB2	1:B:442:VAL:HG13	1.98	0.45
1:J:346:VAL:HG22	1:J:372:LEU:HD13	1.98	0.45
1:M:406:ALA:HB2	1:M:496:PRO:HG3	1.97	0.45
1:F:90:THR:HG22	1:F:94:VAL:HG23	1.98	0.45
1:G:90:THR:HG22	1:G:94:VAL:HG23	1.98	0.45
1:A:90:THR:HG22	1:A:94:VAL:HG23	1.98	0.45
1:C:213:VAL:O	1:C:324:VAL:HA	2.17	0.45
1:E:205:ILE:HD12	1:E:211:GLY:O	2.16	0.45
1:F:205:ILE:HD12	1:F:211:GLY:O	2.16	0.45
1:I:152:ALA:HB1	1:I:155:ASP:HB3	1.97	0.45
1:M:151:SER:HB3	1:M:399:ALA:HA	1.97	0.45
1:J:240:VAL:HG21	1:J:247:LEU:HD22	1.98	0.45
1:C:114:MET:H	1:D:36:ARG:HG3	1.81	0.45
1:D:114:MET:H	1:E:36:ARG:HG3	1.81	0.45
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.46	0.45
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.97	0.45
1:J:102:GLU:HB2	1:J:442:VAL:HG13	1.99	0.45
1:H:102:GLU:HB2	1:H:442:VAL:HG13	1.99	0.45
1:F:279:PRO:HG3	1:F:292:ILE:HD11	1.97	0.45
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.97	0.45
1:N:406:ALA:HB2	1:N:496:PRO:HG3	1.97	0.45
1:C:90:THR:HG22	1:C:94:VAL:HG23	1.98	0.45
1:A:206:ASN:HB2	1:A:213:VAL:CA	2.43	0.45
1:G:12:ALA:HB3	1:G:518:GLU:O	2.15	0.45
1:K:240:VAL:HG21	1:K:247:LEU:HD22	1.98	0.45
1:H:240:VAL:HG21	1:H:247:LEU:HD22	1.98	0.45
1:F:102:GLU:HB2	1:F:442:VAL:HG13	1.97	0.45
1:K:406:ALA:HB2	1:K:496:PRO:HG3	1.97	0.45
1:N:102:GLU:HB2	1:N:442:VAL:HG13	1.99	0.45
1:G:213:VAL:O	1:G:324:VAL:HA	2.16	0.45
1:F:206:ASN:HB2	1:F:213:VAL:CA	2.43	0.45
1:E:200:LEU:CD1	1:E:254:VAL:HG11	2.44	0.45
1:H:406:ALA:HB2	1:H:496:PRO:HG3	1.97	0.45
1:K:158:VAL:HG22	1:K:396:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:PRO:HB2	1:E:310:GLU:HA	1.98	0.45
1:B:240:VAL:HA	1:B:243:ALA:CB	2.43	0.45
1:G:255:GLU:HB3	1:G:258:ALA:H	1.81	0.45
1:D:205:ILE:HD12	1:D:211:GLY:O	2.16	0.45
1:G:205:ILE:HD12	1:G:211:GLY:O	2.16	0.45
1:K:102:GLU:HB2	1:K:442:VAL:HG13	1.99	0.45
1:J:158:VAL:HG22	1:J:396:VAL:HG22	1.98	0.45
1:J:64:ASP:O	1:J:68:ASN:HB2	2.17	0.45
1:I:346:VAL:HG22	1:I:372:LEU:HD13	1.98	0.45
1:H:346:VAL:HG22	1:H:372:LEU:HD13	1.98	0.45
1:K:199:TYR:CD2	1:K:327:LYS:HA	2.52	0.45
1:F:213:VAL:O	1:F:324:VAL:HA	2.17	0.45
1:B:39:VAL:HG22	1:B:49:ILE:HG23	1.99	0.45
1:G:200:LEU:CD1	1:G:254:VAL:HG11	2.45	0.45
1:I:281:PHE:HA	1:I:285:ARG:HB2	1.99	0.45
1:M:192:GLY:O	1:M:375:GLY:HA2	2.17	0.45
1:L:406:ALA:HB2	1:L:496:PRO:HG3	1.97	0.45
1:A:63:GLU:CB	1:G:3:ALA:HA	2.42	0.45
1:A:3:ALA:HA	1:B:63:GLU:CB	2.42	0.45
1:M:38:VAL:HG21	1:M:56:VAL:HG13	1.98	0.45
1:I:38:VAL:HG21	1:I:56:VAL:HG13	1.98	0.45
1:K:23:LEU:O	1:K:27:VAL:HG23	2.17	0.45
1:M:23:LEU:O	1:M:27:VAL:HG23	2.17	0.45
1:I:23:LEU:O	1:I:27:VAL:HG23	2.17	0.45
1:E:213:VAL:O	1:E:324:VAL:HA	2.17	0.45
1:M:240:VAL:HG21	1:M:247:LEU:HD22	1.98	0.45
1:G:140:ASP:CG	1:G:142:LYS:HZ3	2.20	0.45
1:N:64:ASP:O	1:N:68:ASN:HB2	2.17	0.45
1:M:175:ILE:HD12	1:M:400:LEU:CD1	2.47	0.45
1:N:192:GLY:O	1:N:375:GLY:HA2	2.17	0.45
1:C:102:GLU:HB2	1:C:442:VAL:HG13	1.97	0.45
1:M:64:ASP:O	1:M:68:ASN:HB2	2.17	0.45
1:B:90:THR:HG22	1:B:94:VAL:HG23	1.98	0.44
1:B:213:VAL:O	1:B:324:VAL:HA	2.17	0.44
1:M:152:ALA:HB1	1:M:155:ASP:CA	2.46	0.44
1:E:114:MET:H	1:F:36:ARG:HG3	1.81	0.44
1:L:175:ILE:HD12	1:L:400:LEU:CD1	2.47	0.44
1:C:235:PRO:HB2	1:C:310:GLU:HA	1.98	0.44
1:J:175:ILE:HD12	1:J:400:LEU:CD1	2.47	0.44
1:D:140:ASP:CG	1:D:142:LYS:HZ3	2.20	0.44
1:D:235:PRO:HB2	1:D:310:GLU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:PHE:HA	1:H:285:ARG:HB2	1.99	0.44
1:J:199:TYR:CD2	1:J:327:LYS:HA	2.53	0.44
1:F:215:LEU:HD22	1:F:246:PRO:HB2	1.99	0.44
1:C:231:ARG:O	1:C:235:PRO:HD2	2.18	0.44
1:M:102:GLU:HB2	1:M:442:VAL:HG13	1.99	0.44
1:L:192:GLY:O	1:L:375:GLY:HA2	2.17	0.44
1:H:64:ASP:O	1:H:68:ASN:HB2	2.17	0.44
1:K:220:ILE:HD12	1:K:248:LEU:HD23	2.00	0.44
1:K:90:THR:HG22	1:K:94:VAL:HG23	1.99	0.44
1:C:39:VAL:HG22	1:C:49:ILE:HG23	1.99	0.44
1:J:349:ILE:HG23	1:J:365:LEU:CD1	2.48	0.44
1:L:240:VAL:HG21	1:L:247:LEU:HD22	1.98	0.44
1:J:192:GLY:O	1:J:375:GLY:HA2	2.17	0.44
1:G:235:PRO:HB2	1:G:310:GLU:HA	1.99	0.44
1:K:64:ASP:O	1:K:68:ASN:HB2	2.17	0.44
1:J:220:ILE:HD12	1:J:248:LEU:HD23	2.00	0.44
1:N:346:VAL:HG22	1:N:372:LEU:HD13	1.98	0.44
1:N:281:PHE:HA	1:N:285:ARG:HB2	1.99	0.44
1:F:4:LYS:HZ2	1:F:523:ASP:CG	2.21	0.44
1:J:38:VAL:HG21	1:J:56:VAL:HG13	1.98	0.44
1:L:23:LEU:O	1:L:27:VAL:HG23	2.17	0.44
1:J:90:THR:HG22	1:J:94:VAL:HG23	1.99	0.44
1:C:206:ASN:HB2	1:C:213:VAL:CA	2.43	0.44
1:L:41:ASP:HB2	1:M:521:VAL:O	2.17	0.44
1:D:215:LEU:HD22	1:D:246:PRO:HB2	1.99	0.44
1:H:521:VAL:O	1:N:41:ASP:HB2	2.18	0.44
1:A:230:ILE:HG22	1:A:263:VAL:HG22	1.99	0.44
1:E:230:ILE:HG22	1:E:263:VAL:HG22	1.99	0.44
1:F:257:GLU:HA	1:G:243:ALA:C	2.38	0.44
1:H:82:ASN:HB2	1:H:89:THR:HG23	1.99	0.44
1:B:231:ARG:O	1:B:235:PRO:HD2	2.18	0.44
1:A:231:ARG:O	1:A:235:PRO:HD2	2.18	0.44
1:D:231:ARG:O	1:D:235:PRO:HD2	2.18	0.44
1:A:213:VAL:O	1:A:324:VAL:HA	2.17	0.44
1:C:215:LEU:HD22	1:C:246:PRO:HB2	1.99	0.44
1:D:230:ILE:HG22	1:D:263:VAL:HG22	1.99	0.44
1:M:106:ALA:HB1	1:M:116:LEU:HD21	2.00	0.44
1:N:106:ALA:HB1	1:N:116:LEU:HD21	2.00	0.44
1:L:106:ALA:HB1	1:L:116:LEU:HD21	2.00	0.44
1:A:349:ILE:HG23	1:A:365:LEU:CD1	2.48	0.44
1:L:413:ALA:HB1	1:L:488:MET:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:281:PHE:HA	1:J:285:ARG:HB2	1.99	0.44
1:B:140:ASP:CG	1:B:142:LYS:HZ3	2.21	0.44
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.99	0.44
1:M:413:ALA:HB1	1:M:488:MET:HB2	2.00	0.44
1:I:192:GLY:O	1:I:375:GLY:HA2	2.17	0.44
1:L:38:VAL:HG21	1:L:56:VAL:HG13	1.98	0.44
1:K:38:VAL:HG21	1:K:56:VAL:HG13	1.98	0.44
1:E:240:VAL:HA	1:E:243:ALA:CB	2.43	0.44
1:E:255:GLU:HB3	1:E:257:GLU:HG2	2.00	0.44
1:M:199:TYR:CD2	1:M:327:LYS:HA	2.52	0.44
1:L:199:TYR:CD2	1:L:327:LYS:HA	2.53	0.44
1:F:230:ILE:HG21	1:F:262:LEU:C	2.38	0.44
1:M:349:ILE:HG23	1:M:365:LEU:CD1	2.48	0.44
1:H:106:ALA:HB1	1:H:116:LEU:HD21	2.00	0.44
1:I:240:VAL:HG21	1:I:247:LEU:HD22	1.98	0.44
1:K:175:ILE:HD12	1:K:400:LEU:CD1	2.48	0.44
1:I:158:VAL:HG22	1:I:396:VAL:HG22	1.98	0.44
1:H:23:LEU:O	1:H:27:VAL:HG23	2.17	0.44
1:A:255:GLU:HB3	1:A:257:GLU:HG2	2.00	0.44
1:I:199:TYR:CD2	1:I:327:LYS:HA	2.52	0.44
1:N:199:TYR:CD2	1:N:327:LYS:HA	2.53	0.44
1:M:152:ALA:HB1	1:M:155:ASP:O	2.18	0.44
1:H:41:ASP:HB2	1:I:521:VAL:O	2.18	0.44
1:B:230:ILE:HG22	1:B:263:VAL:HG22	1.99	0.44
1:E:9:GLY:HA2	1:E:518:GLU:O	2.18	0.44
1:H:349:ILE:HG23	1:H:365:LEU:CD1	2.48	0.44
1:E:349:ILE:HG23	1:E:365:LEU:CD1	2.48	0.44
1:I:82:ASN:HB2	1:I:89:THR:HG23	1.99	0.44
1:L:281:PHE:HA	1:L:285:ARG:HB2	1.99	0.44
1:I:413:ALA:HB1	1:I:488:MET:HB2	2.00	0.44
1:B:6:VAL:HG22	1:B:521:VAL:HG13	2.00	0.44
1:J:413:ALA:HB1	1:J:488:MET:HB2	2.00	0.44
1:N:23:LEU:O	1:N:27:VAL:HG23	2.17	0.44
1:G:206:ASN:HB2	1:G:213:VAL:CA	2.44	0.44
1:A:39:VAL:HG22	1:A:49:ILE:HG23	1.99	0.44
1:I:152:ALA:HB1	1:I:155:ASP:O	2.18	0.44
1:E:246:PRO:HB3	1:E:272:LYS:HB2	2.00	0.44
1:M:41:ASP:HB2	1:N:521:VAL:O	2.17	0.44
1:A:9:GLY:HA2	1:A:518:GLU:O	2.18	0.44
1:I:349:ILE:HG23	1:I:365:LEU:CD1	2.48	0.44
1:J:417:VAL:HG13	1:J:476:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:220:ILE:HD12	1:L:248:LEU:HD23	2.00	0.44
1:K:192:GLY:O	1:K:375:GLY:HA2	2.17	0.44
1:K:281:PHE:HA	1:K:285:ARG:HB2	1.99	0.44
1:I:220:ILE:HD12	1:I:248:LEU:HD23	2.00	0.44
1:M:281:PHE:HA	1:M:285:ARG:HB2	1.99	0.44
1:H:175:ILE:HD12	1:H:400:LEU:CD1	2.48	0.44
1:L:158:VAL:HG22	1:L:396:VAL:HG22	1.98	0.44
1:L:136:VAL:O	1:L:410:GLY:HA3	2.18	0.44
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.48	0.44
1:F:246:PRO:HB3	1:F:272:LYS:HB2	2.00	0.44
1:C:230:ILE:HG22	1:C:263:VAL:HG22	1.99	0.44
1:C:9:GLY:HA2	1:C:518:GLU:O	2.18	0.44
1:F:349:ILE:HG23	1:F:365:LEU:CD1	2.48	0.44
1:C:349:ILE:HG23	1:C:365:LEU:CD1	2.48	0.44
1:K:413:ALA:HB1	1:K:488:MET:HB2	2.00	0.44
1:H:199:TYR:CD2	1:H:327:LYS:HA	2.52	0.43
1:J:152:ALA:HB1	1:J:155:ASP:O	2.18	0.43
1:G:152:ALA:HB1	1:G:155:ASP:CA	2.48	0.43
1:F:175:ILE:HD12	1:F:400:LEU:CD1	2.48	0.43
1:K:349:ILE:HG23	1:K:365:LEU:CD1	2.48	0.43
1:K:417:VAL:HG13	1:K:476:TYR:O	2.18	0.43
1:B:349:ILE:HG23	1:B:365:LEU:CD1	2.48	0.43
1:N:82:ASN:HB2	1:N:89:THR:HG23	1.99	0.43
1:E:231:ARG:O	1:E:235:PRO:HD2	2.18	0.43
1:H:192:GLY:O	1:H:375:GLY:HA2	2.17	0.43
1:N:90:THR:HG22	1:N:94:VAL:HG23	1.99	0.43
1:F:39:VAL:HG22	1:F:49:ILE:HG23	1.99	0.43
1:E:215:LEU:HD22	1:E:246:PRO:HB2	1.99	0.43
1:A:152:ALA:HB1	1:A:155:ASP:CA	2.48	0.43
1:B:152:ALA:HB1	1:B:155:ASP:CA	2.48	0.43
1:G:349:ILE:HG23	1:G:365:LEU:CD1	2.48	0.43
1:L:338:GLU:HB3	1:L:341:ALA:HB3	2.00	0.43
1:N:338:GLU:HB3	1:N:341:ALA:HB3	2.00	0.43
1:C:6:VAL:HG22	1:C:521:VAL:HG13	2.00	0.43
1:C:13:ARG:HH11	1:C:13:ARG:HG3	1.84	0.43
1:M:90:THR:HG22	1:M:94:VAL:HG23	1.99	0.43
1:N:136:VAL:O	1:N:410:GLY:HA3	2.18	0.43
1:J:136:VAL:O	1:J:410:GLY:HA3	2.18	0.43
1:D:199:TYR:CD2	1:D:327:LYS:HA	2.54	0.43
1:C:199:TYR:CD2	1:C:327:LYS:HA	2.54	0.43
1:E:39:VAL:HG22	1:E:49:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:VAL:HG23	1:G:259:LEU:CB	2.49	0.43
1:L:152:ALA:HB1	1:L:155:ASP:O	2.18	0.43
1:K:41:ASP:HB2	1:L:521:VAL:O	2.17	0.43
1:K:152:ALA:HB1	1:K:155:ASP:O	2.18	0.43
1:I:41:ASP:HB2	1:J:521:VAL:O	2.18	0.43
1:E:175:ILE:HD12	1:E:400:LEU:CD1	2.48	0.43
1:D:9:GLY:HA2	1:D:518:GLU:O	2.18	0.43
1:L:417:VAL:HG13	1:L:476:TYR:O	2.18	0.43
1:L:295:LEU:HA	1:L:342:ILE:HG12	2.00	0.43
1:N:175:ILE:HD12	1:N:400:LEU:CD1	2.47	0.43
1:E:140:ASP:CG	1:E:142:LYS:HZ3	2.22	0.43
1:A:480:ALA:O	1:A:483:GLU:HG2	2.19	0.43
1:I:90:THR:HG22	1:I:94:VAL:HG23	1.99	0.43
1:J:23:LEU:O	1:J:27:VAL:HG23	2.17	0.43
1:H:90:THR:HG22	1:H:94:VAL:HG23	1.99	0.43
1:D:255:GLU:HB3	1:D:257:GLU:HG2	2.00	0.43
1:E:199:TYR:CD2	1:E:327:LYS:HA	2.53	0.43
1:B:199:TYR:CD2	1:B:327:LYS:HA	2.53	0.43
1:F:199:TYR:CD2	1:F:327:LYS:HA	2.53	0.43
1:F:9:GLY:HA2	1:F:518:GLU:O	2.18	0.43
1:B:9:GLY:HA2	1:B:518:GLU:O	2.18	0.43
1:L:349:ILE:HG23	1:L:365:LEU:CD1	2.48	0.43
1:L:82:ASN:HB2	1:L:89:THR:HG23	1.99	0.43
1:M:82:ASN:HB2	1:M:89:THR:HG23	1.99	0.43
1:M:338:GLU:HB3	1:M:341:ALA:HB3	2.00	0.43
1:H:413:ALA:HB1	1:H:488:MET:HB2	2.00	0.43
1:E:480:ALA:O	1:E:483:GLU:HG2	2.19	0.43
1:L:64:ASP:O	1:L:68:ASN:HB2	2.17	0.43
1:F:77:VAL:HG12	1:F:506:TYR:HB3	2.01	0.43
1:N:413:ALA:HB1	1:N:488:MET:HB2	2.00	0.43
1:B:255:GLU:HB3	1:B:257:GLU:HG2	2.00	0.43
1:C:240:VAL:CA	1:C:243:ALA:HB3	2.43	0.43
1:K:136:VAL:O	1:K:410:GLY:HA3	2.18	0.43
1:B:215:LEU:HD22	1:B:246:PRO:HB2	1.99	0.43
1:J:41:ASP:HB2	1:K:521:VAL:O	2.17	0.43
1:D:246:PRO:HB3	1:D:272:LYS:HB2	2.00	0.43
1:H:417:VAL:HG13	1:H:476:TYR:O	2.18	0.43
1:I:106:ALA:HB1	1:I:116:LEU:HD21	2.00	0.43
1:D:349:ILE:HG23	1:D:365:LEU:CD1	2.48	0.43
1:G:231:ARG:O	1:G:235:PRO:HD2	2.18	0.43
1:I:64:ASP:O	1:I:68:ASN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:ILE:HD12	1:I:400:LEU:CD1	2.47	0.43
1:J:405:ALA:HB1	1:J:498:LYS:HD2	2.01	0.43
1:K:405:ALA:HB1	1:K:498:LYS:HD2	2.00	0.43
1:C:77:VAL:HG12	1:C:506:TYR:HB3	2.01	0.43
1:L:90:THR:HG22	1:L:94:VAL:HG23	1.99	0.43
1:D:39:VAL:HG22	1:D:49:ILE:HG23	1.99	0.43
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.48	0.43
1:C:246:PRO:HB3	1:C:272:LYS:HB2	2.00	0.43
1:B:152:ALA:HB1	1:B:155:ASP:HB3	2.01	0.43
1:D:175:ILE:HD12	1:D:400:LEU:CD1	2.48	0.43
1:G:9:GLY:HA2	1:G:518:GLU:O	2.18	0.43
1:N:349:ILE:HG23	1:N:365:LEU:CD1	2.48	0.43
1:K:106:ALA:HB1	1:K:116:LEU:HD21	2.00	0.43
1:I:417:VAL:HG13	1:I:476:TYR:O	2.18	0.43
1:K:295:LEU:HA	1:K:342:ILE:HG12	2.00	0.43
1:A:140:ASP:CG	1:A:142:LYS:HZ3	2.22	0.43
1:G:77:VAL:HG12	1:G:506:TYR:HB3	2.01	0.43
1:F:480:ALA:O	1:F:483:GLU:HG2	2.19	0.43
1:F:152:ALA:HB1	1:F:155:ASP:HB3	2.01	0.43
1:H:152:ALA:HB1	1:H:155:ASP:O	2.18	0.43
1:G:175:ILE:HD12	1:G:400:LEU:CD1	2.48	0.43
1:J:240:VAL:HA	1:J:243:ALA:HB3	2.01	0.43
1:J:82:ASN:HB2	1:J:89:THR:HG23	1.99	0.43
1:A:6:VAL:HG22	1:A:521:VAL:HG13	2.00	0.43
1:K:338:GLU:HB3	1:K:341:ALA:HB3	2.00	0.43
1:C:4:LYS:HZ2	1:C:523:ASP:CG	2.21	0.43
1:C:255:GLU:HB3	1:C:257:GLU:HG2	2.00	0.43
1:L:218:PRO:HG2	1:L:323:VAL:HG23	2.00	0.43
1:K:218:PRO:HG2	1:K:323:VAL:HG23	2.01	0.43
1:N:152:ALA:HB1	1:N:155:ASP:O	2.18	0.43
1:G:152:ALA:HB1	1:G:155:ASP:HB3	2.01	0.43
1:A:152:ALA:HB1	1:A:155:ASP:HB3	2.01	0.43
1:B:175:ILE:HD12	1:B:400:LEU:CD1	2.48	0.43
1:N:417:VAL:HG13	1:N:476:TYR:O	2.18	0.43
1:N:405:ALA:HB1	1:N:498:LYS:HD2	2.00	0.43
1:D:480:ALA:O	1:D:483:GLU:HG2	2.18	0.43
1:H:338:GLU:HB3	1:H:341:ALA:HB3	2.00	0.43
1:D:77:VAL:HG12	1:D:506:TYR:HB3	2.01	0.43
1:E:77:VAL:HG12	1:E:506:TYR:HB3	2.01	0.43
1:M:220:ILE:HD12	1:M:248:LEU:HD23	2.00	0.43
1:G:39:VAL:HG22	1:G:49:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:213:VAL:O	1:K:324:VAL:HA	2.19	0.43
1:K:240:VAL:HA	1:K:243:ALA:HB3	2.01	0.43
1:G:417:VAL:HG13	1:G:476:TYR:O	2.19	0.43
1:N:281:PHE:CA	1:N:285:ARG:HB2	2.49	0.43
1:C:480:ALA:O	1:C:483:GLU:HG2	2.19	0.43
1:I:405:ALA:HB1	1:I:498:LYS:HD2	2.00	0.43
1:B:426:LEU:HB2	1:B:444:LEU:CD2	2.49	0.43
1:A:243:ALA:HA	1:G:258:ALA:CA	2.46	0.43
1:G:199:TYR:CD2	1:G:327:LYS:HA	2.53	0.43
1:E:152:ALA:HB1	1:E:155:ASP:HB3	2.01	0.43
1:E:230:ILE:HG21	1:E:263:VAL:HA	2.00	0.43
1:H:206:ASN:HB2	1:H:213:VAL:CB	2.49	0.43
1:K:206:ASN:HB2	1:K:213:VAL:CB	2.49	0.43
1:L:213:VAL:O	1:L:324:VAL:HA	2.19	0.43
1:M:417:VAL:HG13	1:M:476:TYR:O	2.18	0.43
1:E:417:VAL:HG13	1:E:476:TYR:O	2.19	0.43
1:B:77:VAL:HG12	1:B:506:TYR:HB3	2.01	0.43
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.83	0.43
1:H:220:ILE:HD12	1:H:248:LEU:HD23	2.00	0.43
1:E:6:VAL:HG22	1:E:521:VAL:HG13	2.00	0.43
1:B:356:ALA:HB1	1:B:361:ASP:HB2	2.01	0.43
1:C:356:ALA:HB1	1:C:361:ASP:HB2	2.01	0.43
1:D:6:VAL:HG22	1:D:521:VAL:HG13	2.00	0.43
1:B:13:ARG:HH11	1:B:13:ARG:HG3	1.84	0.43
1:D:240:VAL:CA	1:D:243:ALA:HB3	2.43	0.42
1:E:426:LEU:HB2	1:E:444:LEU:CD2	2.49	0.42
1:J:218:PRO:HG2	1:J:323:VAL:HG23	2.00	0.42
1:M:218:PRO:HG2	1:M:323:VAL:HG23	2.00	0.42
1:C:152:ALA:HB1	1:C:155:ASP:HB3	2.01	0.42
1:N:251:ALA:HB3	1:N:254:VAL:HG23	2.02	0.42
1:A:175:ILE:HD12	1:A:400:LEU:CD1	2.48	0.42
1:J:206:ASN:HB2	1:J:213:VAL:CB	2.49	0.42
1:H:295:LEU:HA	1:H:342:ILE:HG12	2.00	0.42
1:K:82:ASN:HB2	1:K:89:THR:HG23	1.99	0.42
1:F:417:VAL:HG13	1:F:476:TYR:O	2.19	0.42
1:F:231:ARG:O	1:F:235:PRO:HD2	2.18	0.42
1:H:281:PHE:CA	1:H:285:ARG:HB2	2.49	0.42
1:K:281:PHE:CA	1:K:285:ARG:HB2	2.49	0.42
1:I:405:ALA:HB1	1:I:498:LYS:CD	2.49	0.42
1:B:413:ALA:HB1	1:B:488:MET:HB2	2.01	0.42
1:L:405:ALA:HB1	1:L:498:LYS:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:480:ALA:O	1:G:483:GLU:HG2	2.19	0.42
1:G:13:ARG:HG3	1:G:13:ARG:HH11	1.83	0.42
1:C:426:LEU:HB2	1:C:444:LEU:CD2	2.49	0.42
1:H:136:VAL:O	1:H:410:GLY:HA3	2.18	0.42
1:A:199:TYR:CD2	1:A:327:LYS:HA	2.53	0.42
1:N:218:PRO:HG2	1:N:323:VAL:HG23	2.00	0.42
1:C:215:LEU:O	1:C:322:ARG:HA	2.19	0.42
1:A:215:LEU:O	1:A:322:ARG:HA	2.19	0.42
1:A:230:ILE:HG21	1:A:263:VAL:HA	2.00	0.42
1:H:251:ALA:HB3	1:H:254:VAL:HG23	2.02	0.42
1:I:251:ALA:HB3	1:I:254:VAL:HG23	2.02	0.42
1:M:295:LEU:HA	1:M:342:ILE:HG12	2.00	0.42
1:C:114:MET:HB3	1:D:36:ARG:HD2	2.01	0.42
1:C:417:VAL:HG13	1:C:476:TYR:O	2.19	0.42
1:I:281:PHE:CA	1:I:285:ARG:HB2	2.49	0.42
1:M:281:PHE:CA	1:M:285:ARG:HB2	2.49	0.42
1:F:6:VAL:HG22	1:F:521:VAL:HG13	2.00	0.42
1:C:413:ALA:HB1	1:C:488:MET:HB2	2.01	0.42
1:G:215:LEU:O	1:G:322:ARG:HA	2.19	0.42
1:E:13:ARG:HG3	1:E:13:ARG:HH11	1.83	0.42
1:M:405:ALA:HB1	1:M:498:LYS:CD	2.49	0.42
1:B:240:VAL:CA	1:B:243:ALA:HB3	2.43	0.42
1:A:426:LEU:HB2	1:A:444:LEU:CD2	2.49	0.42
1:M:206:ASN:HB2	1:M:213:VAL:CB	2.49	0.42
1:I:206:ASN:HB2	1:I:213:VAL:CB	2.49	0.42
1:H:294:THR:HB	1:H:342:ILE:HA	2.01	0.42
1:I:295:LEU:HA	1:I:342:ILE:HG12	2.00	0.42
1:N:294:THR:HB	1:N:342:ILE:HA	2.01	0.42
1:N:405:ALA:HB1	1:N:498:LYS:CD	2.49	0.42
1:M:405:ALA:HB1	1:M:498:LYS:HD2	2.00	0.42
1:A:77:VAL:HG12	1:A:506:TYR:HB3	2.01	0.42
1:N:220:ILE:HD12	1:N:248:LEU:HD23	2.00	0.42
1:D:64:ASP:O	1:D:68:ASN:HB2	2.20	0.42
1:D:356:ALA:HB1	1:D:361:ASP:HB2	2.01	0.42
1:M:136:VAL:O	1:M:410:GLY:HA3	2.18	0.42
1:H:218:PRO:HG2	1:H:323:VAL:HG23	2.00	0.42
1:D:152:ALA:HB1	1:D:155:ASP:HB3	2.01	0.42
1:B:215:LEU:O	1:B:322:ARG:HA	2.19	0.42
1:B:246:PRO:HB3	1:B:272:LYS:HB2	2.00	0.42
1:D:215:LEU:O	1:D:322:ARG:HA	2.19	0.42
1:E:215:LEU:O	1:E:322:ARG:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HG21	1:B:263:VAL:HA	2.00	0.42
1:C:230:ILE:HG21	1:C:263:VAL:HA	2.00	0.42
1:G:230:ILE:HG22	1:G:263:VAL:HG22	2.01	0.42
1:M:251:ALA:HB3	1:M:254:VAL:HG23	2.01	0.42
1:N:206:ASN:HB2	1:N:213:VAL:CB	2.50	0.42
1:L:206:ASN:HB2	1:L:213:VAL:CB	2.49	0.42
1:K:87:ASP:CG	1:K:151:SER:HA	2.40	0.42
1:L:240:VAL:HA	1:L:243:ALA:HB3	2.01	0.42
1:B:114:MET:HB3	1:C:36:ARG:HD2	2.01	0.42
1:G:6:VAL:HG22	1:G:521:VAL:HG13	2.00	0.42
1:B:64:ASP:O	1:B:68:ASN:HB2	2.20	0.42
1:A:13:ARG:HG3	1:A:13:ARG:HH11	1.83	0.42
1:G:4:LYS:HZ2	1:G:523:ASP:CG	2.23	0.42
1:J:183:LEU:C	1:J:382:GLY:HA3	2.40	0.42
1:K:183:LEU:C	1:K:382:GLY:HA3	2.40	0.42
1:F:240:VAL:HA	1:F:243:ALA:CB	2.43	0.42
1:I:218:PRO:HG2	1:I:323:VAL:HG23	2.00	0.42
1:E:152:ALA:HB1	1:E:155:ASP:CA	2.48	0.42
1:C:175:ILE:HD12	1:C:400:LEU:CD1	2.48	0.42
1:J:251:ALA:HB3	1:J:254:VAL:HG23	2.02	0.42
1:D:106:ALA:HB1	1:D:116:LEU:HD21	2.02	0.42
1:I:240:VAL:HA	1:I:243:ALA:HB3	2.01	0.42
1:N:295:LEU:HA	1:N:342:ILE:HG12	2.00	0.42
1:B:417:VAL:HG13	1:B:476:TYR:O	2.19	0.42
1:L:281:PHE:CA	1:L:285:ARG:HB2	2.49	0.42
1:G:506:TYR:O	1:G:510:VAL:HG23	2.20	0.42
1:H:405:ALA:HB1	1:H:498:LYS:HD2	2.00	0.42
1:N:77:VAL:HG12	1:N:506:TYR:HB3	2.02	0.42
1:I:338:GLU:HB3	1:I:341:ALA:HB3	2.00	0.42
1:J:77:VAL:HG12	1:J:506:TYR:HB3	2.02	0.42
1:I:19:GLY:HA2	1:I:62:LEU:CD1	2.50	0.42
1:G:64:ASP:O	1:G:68:ASN:HB2	2.20	0.42
1:F:426:LEU:HB2	1:F:444:LEU:CD2	2.50	0.42
1:I:136:VAL:O	1:I:410:GLY:HA3	2.18	0.42
1:A:40:LEU:HG	1:A:59:GLU:HB3	2.02	0.42
1:D:230:ILE:HG21	1:D:263:VAL:HA	2.00	0.42
1:M:87:ASP:CG	1:M:151:SER:HA	2.40	0.42
1:D:506:TYR:O	1:D:510:VAL:HG23	2.20	0.42
1:H:19:GLY:HA2	1:H:62:LEU:CD1	2.50	0.42
1:J:338:GLU:HB3	1:J:341:ALA:HB3	2.00	0.42
1:M:19:GLY:HA2	1:M:62:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ALA:HB1	1:A:488:MET:HB2	2.01	0.42
1:L:218:PRO:HA	1:L:246:PRO:O	2.20	0.42
1:C:200:LEU:HD22	1:C:254:VAL:HG11	2.01	0.42
1:J:213:VAL:O	1:J:324:VAL:HA	2.19	0.42
1:M:240:VAL:HA	1:M:243:ALA:HB3	2.01	0.42
1:I:294:THR:HB	1:I:342:ILE:HA	2.01	0.42
1:F:506:TYR:O	1:F:510:VAL:HG23	2.20	0.42
1:J:405:ALA:HB1	1:J:498:LYS:CD	2.49	0.42
1:B:480:ALA:O	1:B:483:GLU:HG2	2.19	0.42
1:E:4:LYS:HZ2	1:E:523:ASP:CG	2.23	0.42
1:D:426:LEU:HB2	1:D:444:LEU:CD2	2.49	0.42
1:G:426:LEU:HB2	1:G:444:LEU:CD2	2.49	0.42
1:N:218:PRO:HA	1:N:246:PRO:O	2.20	0.42
1:J:218:PRO:HA	1:J:246:PRO:O	2.20	0.42
1:H:213:VAL:CG1	1:H:325:ILE:HB	2.50	0.42
1:N:213:VAL:CG1	1:N:325:ILE:HB	2.50	0.42
1:I:213:VAL:O	1:I:324:VAL:HA	2.19	0.42
1:D:417:VAL:HG13	1:D:476:TYR:O	2.19	0.42
1:I:19:GLY:HA2	1:I:62:LEU:HD13	2.02	0.42
1:M:77:VAL:HG12	1:M:506:TYR:HB3	2.02	0.42
1:N:19:GLY:HA2	1:N:62:LEU:CD1	2.50	0.42
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.50	0.42
1:I:50:THR:HG21	1:I:59:GLU:HG2	2.01	0.42
1:B:200:LEU:HD22	1:B:254:VAL:HG11	2.01	0.42
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.48	0.42
1:G:40:LEU:HG	1:G:59:GLU:HB3	2.02	0.42
1:H:213:VAL:O	1:H:324:VAL:HA	2.19	0.42
1:M:213:VAL:O	1:M:324:VAL:HA	2.19	0.42
1:F:114:MET:HB3	1:G:36:ARG:HD2	2.01	0.42
1:A:114:MET:HB3	1:B:36:ARG:HD2	2.01	0.42
1:A:417:VAL:HG13	1:A:476:TYR:O	2.19	0.42
1:H:77:VAL:HG12	1:H:506:TYR:HB3	2.02	0.42
1:L:19:GLY:HA2	1:L:62:LEU:CD1	2.50	0.42
1:B:103:GLY:HA3	1:B:515:ILE:HG12	2.02	0.42
1:A:103:GLY:HA3	1:A:515:ILE:HG12	2.02	0.42
1:K:19:GLY:HA2	1:K:62:LEU:CD1	2.50	0.42
1:F:64:ASP:O	1:F:68:ASN:HB2	2.19	0.42
1:N:50:THR:HG21	1:N:59:GLU:HG2	2.02	0.42
1:J:517:THR:O	1:J:517:THR:HG22	2.20	0.42
1:I:517:THR:HG22	1:I:517:THR:O	2.20	0.42
1:E:247:LEU:O	1:E:273:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:LEU:C	1:I:382:GLY:HA3	2.40	0.42
1:A:200:LEU:HD22	1:A:254:VAL:HG11	2.01	0.42
1:D:200:LEU:HD22	1:D:254:VAL:HG11	2.01	0.42
1:F:215:LEU:O	1:F:322:ARG:HA	2.19	0.42
1:B:40:LEU:HG	1:B:59:GLU:HB3	2.02	0.42
1:J:213:VAL:CG1	1:J:325:ILE:HB	2.50	0.42
1:J:87:ASP:CG	1:J:151:SER:HA	2.40	0.42
1:I:87:ASP:CG	1:I:151:SER:HA	2.40	0.42
1:H:87:ASP:CG	1:H:151:SER:HA	2.40	0.42
1:N:240:VAL:HA	1:N:243:ALA:HB3	2.01	0.42
1:B:106:ALA:HB1	1:B:116:LEU:HD21	2.02	0.42
1:E:114:MET:HB3	1:F:36:ARG:HD2	2.01	0.42
1:K:383:ALA:HB3	1:K:389:MET:N	2.35	0.42
1:L:383:ALA:HB3	1:L:389:MET:N	2.35	0.42
1:C:506:TYR:O	1:C:510:VAL:HG23	2.20	0.42
1:A:239:ALA:HB1	1:A:314:LEU:HG	2.02	0.42
1:A:356:ALA:HB1	1:A:361:ASP:HB2	2.01	0.42
1:I:77:VAL:HG12	1:I:506:TYR:HB3	2.02	0.42
1:F:13:ARG:HH11	1:F:13:ARG:HG3	1.83	0.42
1:A:64:ASP:O	1:A:68:ASN:HB2	2.20	0.42
1:F:200:LEU:CD1	1:F:275:ALA:HB3	2.50	0.41
1:G:200:LEU:HD22	1:G:254:VAL:HG11	2.00	0.41
1:L:251:ALA:HB3	1:L:254:VAL:HG23	2.02	0.41
1:I:213:VAL:CG1	1:I:325:ILE:HB	2.50	0.41
1:K:294:THR:HB	1:K:342:ILE:HA	2.01	0.41
1:D:114:MET:HB3	1:E:36:ARG:HD2	2.01	0.41
1:D:100:ILE:O	1:D:104:LEU:HG	2.20	0.41
1:J:19:GLY:HA2	1:J:62:LEU:HD13	2.02	0.41
1:E:64:ASP:O	1:E:68:ASN:HB2	2.19	0.41
1:L:517:THR:HG22	1:L:517:THR:O	2.20	0.41
1:F:213:VAL:CG1	1:F:325:ILE:HB	2.50	0.41
1:K:218:PRO:HA	1:K:246:PRO:O	2.20	0.41
1:C:40:LEU:HD21	1:C:59:GLU:C	2.41	0.41
1:K:251:ALA:HB3	1:K:254:VAL:HG23	2.02	0.41
1:C:106:ALA:HB1	1:C:116:LEU:HD21	2.02	0.41
1:A:349:ILE:HG23	1:A:365:LEU:HD13	2.02	0.41
1:J:295:LEU:HA	1:J:342:ILE:HG12	2.00	0.41
1:M:294:THR:HB	1:M:342:ILE:HA	2.01	0.41
1:A:506:TYR:O	1:A:510:VAL:HG23	2.20	0.41
1:H:19:GLY:HA2	1:H:62:LEU:HD13	2.02	0.41
1:C:103:GLY:HA3	1:C:515:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:GLY:HA3	1:G:515:ILE:HG12	2.02	0.41
1:D:413:ALA:HB1	1:D:488:MET:HB2	2.01	0.41
1:J:63:GLU:HB3	1:K:4:LYS:O	2.21	0.41
1:K:77:VAL:HG12	1:K:506:TYR:HB3	2.02	0.41
1:M:50:THR:HG21	1:M:59:GLU:HG2	2.02	0.41
1:C:213:VAL:CG1	1:C:325:ILE:HB	2.50	0.41
1:D:40:LEU:HD21	1:D:59:GLU:C	2.41	0.41
1:L:87:ASP:CG	1:L:151:SER:HA	2.40	0.41
1:J:106:ALA:HB1	1:J:116:LEU:HD21	2.00	0.41
1:B:411:VAL:HG13	1:B:496:PRO:HA	2.02	0.41
1:A:106:ALA:HB1	1:A:116:LEU:HD21	2.02	0.41
1:E:106:ALA:HB1	1:E:116:LEU:HD21	2.02	0.41
1:L:294:THR:HB	1:L:342:ILE:HA	2.01	0.41
1:K:383:ALA:HB3	1:K:389:MET:CA	2.51	0.41
1:M:383:ALA:HB3	1:M:389:MET:N	2.35	0.41
1:J:383:ALA:HB3	1:J:389:MET:N	2.35	0.41
1:E:506:TYR:O	1:E:510:VAL:HG23	2.20	0.41
1:E:100:ILE:O	1:E:104:LEU:HG	2.21	0.41
1:C:64:ASP:O	1:C:68:ASN:HB2	2.20	0.41
1:J:50:THR:HG21	1:J:59:GLU:HG2	2.02	0.41
1:I:63:GLU:HB3	1:J:4:LYS:O	2.21	0.41
1:G:220:ILE:HD12	1:G:248:LEU:HD23	2.02	0.41
1:K:63:GLU:HB3	1:L:4:LYS:O	2.21	0.41
1:G:190:VAL:HB	1:G:378:VAL:HG23	2.02	0.41
1:F:413:ALA:HB1	1:F:488:MET:HB2	2.01	0.41
1:F:247:LEU:O	1:F:273:VAL:HA	2.20	0.41
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.50	0.41
1:E:200:LEU:CD1	1:E:275:ALA:HB3	2.50	0.41
1:E:200:LEU:HD22	1:E:254:VAL:HG11	2.01	0.41
1:G:247:LEU:O	1:G:273:VAL:HA	2.20	0.41
1:B:40:LEU:HD21	1:B:59:GLU:C	2.41	0.41
1:F:40:LEU:HG	1:F:59:GLU:HB3	2.02	0.41
1:K:213:VAL:CG1	1:K:325:ILE:HB	2.50	0.41
1:N:87:ASP:CG	1:N:151:SER:HA	2.40	0.41
1:N:417:VAL:CG2	1:N:477:GLY:HA3	2.50	0.41
1:C:411:VAL:HG13	1:C:496:PRO:HA	2.02	0.41
1:N:383:ALA:HB3	1:N:389:MET:CA	2.51	0.41
1:I:383:ALA:HB3	1:I:389:MET:N	2.35	0.41
1:J:281:PHE:CA	1:J:285:ARG:HB2	2.49	0.41
1:K:405:ALA:HB1	1:K:498:LYS:CD	2.49	0.41
1:B:506:TYR:O	1:B:510:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:405:ALA:HB1	1:L:498:LYS:CD	2.49	0.41
1:K:19:GLY:HA2	1:K:62:LEU:HD13	2.02	0.41
1:J:135:SER:HA	1:J:412:VAL:HG12	2.03	0.41
1:H:517:THR:HG22	1:H:517:THR:O	2.20	0.41
1:I:218:PRO:HA	1:I:246:PRO:O	2.20	0.41
1:M:213:VAL:CG1	1:M:325:ILE:HB	2.50	0.41
1:I:417:VAL:CG2	1:I:477:GLY:HA3	2.50	0.41
1:H:240:VAL:HA	1:H:243:ALA:HB3	2.01	0.41
1:M:383:ALA:HB3	1:M:389:MET:CA	2.50	0.41
1:J:383:ALA:HB3	1:J:389:MET:CA	2.51	0.41
1:L:383:ALA:HB3	1:L:389:MET:CA	2.51	0.41
1:N:135:SER:HA	1:N:412:VAL:HG12	2.03	0.41
1:C:226:LYS:HB2	1:C:253:ASP:O	2.20	0.41
1:E:413:ALA:HB1	1:E:488:MET:HB2	2.01	0.41
1:M:63:GLU:HB3	1:N:4:LYS:O	2.21	0.41
1:N:517:THR:HG22	1:N:517:THR:O	2.20	0.41
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.51	0.41
1:M:218:PRO:HA	1:M:246:PRO:O	2.20	0.41
1:M:106:ALA:HB3	1:M:116:LEU:HD21	2.03	0.41
1:K:106:ALA:HB3	1:K:116:LEU:HD21	2.03	0.41
1:J:106:ALA:HB3	1:J:116:LEU:HD21	2.03	0.41
1:I:106:ALA:HB3	1:I:116:LEU:HD21	2.03	0.41
1:G:106:ALA:HB1	1:G:116:LEU:HD21	2.02	0.41
1:B:349:ILE:HG23	1:B:365:LEU:HD13	2.02	0.41
1:H:405:ALA:HB1	1:H:498:LYS:CD	2.49	0.41
1:F:100:ILE:O	1:F:104:LEU:HG	2.21	0.41
1:H:135:SER:HA	1:H:412:VAL:HG12	2.03	0.41
1:F:190:VAL:HB	1:F:378:VAL:HG23	2.02	0.41
1:F:140:ASP:CG	1:F:142:LYS:HZ3	2.23	0.41
1:G:413:ALA:HB1	1:G:488:MET:HB2	2.01	0.41
1:K:517:THR:HG22	1:K:517:THR:O	2.20	0.41
1:A:200:LEU:CD1	1:A:275:ALA:HB3	2.50	0.41
1:G:200:LEU:CD1	1:G:275:ALA:HB3	2.50	0.41
1:E:40:LEU:HG	1:E:59:GLU:HB3	2.02	0.41
1:M:417:VAL:CG2	1:M:477:GLY:HA3	2.51	0.41
1:G:349:ILE:HG23	1:G:365:LEU:HD13	2.02	0.41
1:A:36:ARG:HD2	1:G:114:MET:HB3	2.01	0.41
1:J:294:THR:HB	1:J:342:ILE:HA	2.01	0.41
1:N:383:ALA:HB3	1:N:389:MET:N	2.35	0.41
1:E:239:ALA:HB1	1:E:314:LEU:HG	2.03	0.41
1:D:239:ALA:HB1	1:D:314:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ASP:CB	1:F:435:ASP:HB2	2.51	0.41
1:C:100:ILE:O	1:C:104:LEU:HG	2.21	0.41
1:E:356:ALA:HB1	1:E:361:ASP:HB2	2.01	0.41
1:H:239:ALA:HB1	1:H:314:LEU:HG	2.02	0.41
1:I:135:SER:HA	1:I:412:VAL:HG12	2.03	0.41
1:K:50:THR:HG21	1:K:59:GLU:HG2	2.02	0.41
1:L:50:THR:HG21	1:L:59:GLU:HG2	2.02	0.41
1:L:77:VAL:HG12	1:L:506:TYR:HB3	2.02	0.41
1:E:40:LEU:HD21	1:E:59:GLU:C	2.41	0.41
1:F:106:ALA:HB1	1:F:116:LEU:HD21	2.02	0.41
1:D:115:ASP:CB	1:D:435:ASP:HB2	2.51	0.41
1:N:239:ALA:HB1	1:N:314:LEU:HG	2.02	0.41
1:E:190:VAL:HB	1:E:378:VAL:HG23	2.02	0.41
1:A:226:LYS:HB2	1:A:253:ASP:O	2.20	0.41
1:G:356:ALA:HB1	1:G:361:ASP:HB2	2.01	0.41
1:K:135:SER:HA	1:K:412:VAL:HG12	2.03	0.41
1:L:63:GLU:HB3	1:M:4:LYS:O	2.20	0.41
1:H:50:THR:HG21	1:H:59:GLU:HG2	2.01	0.41
1:M:517:THR:HG22	1:M:517:THR:O	2.20	0.41
1:D:247:LEU:O	1:D:273:VAL:HA	2.20	0.41
1:H:183:LEU:C	1:H:382:GLY:HA3	2.40	0.41
1:A:247:LEU:O	1:A:273:VAL:HA	2.20	0.41
1:H:218:PRO:HA	1:H:246:PRO:O	2.20	0.41
1:B:200:LEU:CD1	1:B:275:ALA:HB3	2.50	0.41
1:D:200:LEU:CD1	1:D:275:ALA:HB3	2.50	0.41
1:A:215:LEU:HD22	1:A:246:PRO:HB2	2.02	0.41
1:G:40:LEU:HD21	1:G:59:GLU:C	2.41	0.41
1:N:213:VAL:O	1:N:324:VAL:HA	2.19	0.41
1:L:213:VAL:CG1	1:L:325:ILE:HB	2.50	0.41
1:H:291:ASP:OD1	1:H:349:ILE:HD11	2.21	0.41
1:M:291:ASP:OD1	1:M:349:ILE:HD11	2.21	0.41
1:I:291:ASP:OD1	1:I:349:ILE:HD11	2.21	0.41
1:N:291:ASP:OD1	1:N:349:ILE:HD11	2.21	0.41
1:H:106:ALA:HB3	1:H:116:LEU:HD21	2.03	0.41
1:H:417:VAL:CG2	1:H:477:GLY:HA3	2.50	0.41
1:A:411:VAL:HG13	1:A:496:PRO:HA	2.02	0.41
1:F:349:ILE:HG23	1:F:365:LEU:HD13	2.02	0.41
1:B:239:ALA:HB1	1:B:314:LEU:HG	2.03	0.41
1:F:239:ALA:HB1	1:F:314:LEU:HG	2.03	0.41
1:B:115:ASP:CB	1:B:435:ASP:HB2	2.51	0.41
1:G:115:ASP:CB	1:G:435:ASP:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:383:ALA:HB3	1:I:389:MET:CA	2.51	0.41
1:H:383:ALA:HB3	1:H:389:MET:N	2.35	0.41
1:E:115:ASP:CB	1:E:435:ASP:HB2	2.51	0.41
1:F:77:VAL:CB	1:F:510:VAL:HG22	2.51	0.41
1:D:13:ARG:HB2	1:D:104:LEU:HD22	2.03	0.41
1:F:356:ALA:HB1	1:F:361:ASP:HB2	2.01	0.41
1:H:4:LYS:O	1:N:63:GLU:HB3	2.20	0.41
1:D:103:GLY:HA3	1:D:515:ILE:HG12	2.02	0.41
1:E:226:LYS:HB2	1:E:253:ASP:O	2.20	0.41
1:G:100:ILE:O	1:G:104:LEU:HG	2.20	0.41
1:M:239:ALA:HB1	1:M:314:LEU:HG	2.02	0.41
1:M:135:SER:HA	1:M:412:VAL:HG12	2.03	0.41
1:L:135:SER:HA	1:L:412:VAL:HG12	2.03	0.41
1:H:63:GLU:HB3	1:I:4:LYS:O	2.21	0.41
1:B:100:ILE:O	1:B:104:LEU:HG	2.20	0.41
1:K:239:ALA:HB1	1:K:314:LEU:HG	2.02	0.41
1:B:247:LEU:O	1:B:273:VAL:HA	2.20	0.41
1:C:200:LEU:CD1	1:C:275:ALA:HB3	2.50	0.41
1:G:240:VAL:HG21	1:G:247:LEU:HD22	2.03	0.41
1:C:40:LEU:HG	1:C:59:GLU:HB3	2.02	0.41
1:D:40:LEU:HG	1:D:59:GLU:HB3	2.02	0.41
1:E:411:VAL:HG13	1:E:496:PRO:HA	2.02	0.41
1:E:349:ILE:HG23	1:E:365:LEU:HD13	2.02	0.41
1:E:13:ARG:HB2	1:E:104:LEU:HD22	2.03	0.41
1:N:19:GLY:HA2	1:N:62:LEU:HD13	2.02	0.41
1:L:19:GLY:HA2	1:L:62:LEU:HD13	2.02	0.41
1:B:226:LYS:HB2	1:B:253:ASP:O	2.20	0.41
1:C:190:VAL:HB	1:C:378:VAL:HG23	2.02	0.41
1:A:100:ILE:O	1:A:104:LEU:HG	2.21	0.41
1:E:240:VAL:CA	1:E:243:ALA:HB3	2.43	0.40
1:A:40:LEU:HD21	1:A:59:GLU:C	2.41	0.40
1:C:239:ALA:HB1	1:C:314:LEU:HG	2.03	0.40
1:J:239:ALA:HB1	1:J:314:LEU:HG	2.02	0.40
1:A:190:VAL:HB	1:A:378:VAL:HG23	2.03	0.40
1:A:213:VAL:CG1	1:A:325:ILE:HB	2.50	0.40
1:N:231:ARG:O	1:N:235:PRO:HD2	2.21	0.40
1:N:106:ALA:HB3	1:N:116:LEU:HD21	2.03	0.40
1:F:411:VAL:HG13	1:F:496:PRO:HA	2.02	0.40
1:C:349:ILE:HG23	1:C:365:LEU:HD13	2.02	0.40
1:A:36:ARG:HD2	1:G:114:MET:HB2	2.04	0.40
1:G:226:LYS:HB2	1:G:253:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:239:ALA:HB1	1:I:314:LEU:HG	2.03	0.40
1:A:182:GLY:O	1:A:382:GLY:HA2	2.22	0.40
1:C:247:LEU:O	1:C:273:VAL:HA	2.20	0.40
1:F:137:PRO:HA	1:F:410:GLY:HA3	2.04	0.40
1:F:254:VAL:HG23	1:F:259:LEU:CB	2.51	0.40
1:M:231:ARG:O	1:M:235:PRO:HD2	2.21	0.40
1:D:383:ALA:HB3	1:D:389:MET:CA	2.52	0.40
1:D:383:ALA:HB3	1:D:389:MET:N	2.36	0.40
1:G:77:VAL:CB	1:G:510:VAL:HG22	2.52	0.40
1:B:77:VAL:CB	1:B:510:VAL:HG22	2.51	0.40
1:D:213:VAL:CG1	1:D:325:ILE:HB	2.51	0.40
1:B:378:VAL:HG11	1:B:380:LYS:HZ2	1.86	0.40
1:F:200:LEU:HD22	1:F:254:VAL:HG11	2.02	0.40
1:F:169:VAL:HG11	1:F:175:ILE:HG13	2.04	0.40
1:I:144:ILE:HG23	1:I:403:THR:HG21	2.04	0.40
1:L:106:ALA:HB3	1:L:116:LEU:HD21	2.03	0.40
1:K:417:VAL:CG2	1:K:477:GLY:HA3	2.51	0.40
1:D:411:VAL:HG13	1:D:496:PRO:HA	2.02	0.40
1:G:411:VAL:CG1	1:G:494:LEU:HB2	2.52	0.40
1:A:77:VAL:CB	1:A:510:VAL:HG22	2.52	0.40
1:E:103:GLY:HA3	1:E:515:ILE:HG12	2.02	0.40
1:G:262:LEU:HA	1:G:262:LEU:HD12	1.98	0.40
1:E:137:PRO:HA	1:E:410:GLY:HA3	2.04	0.40
1:G:138:CYS:CA	1:G:410:GLY:HA2	2.52	0.40
1:F:138:CYS:CA	1:F:410:GLY:HA2	2.52	0.40
1:A:246:PRO:HB3	1:A:272:LYS:HB2	2.03	0.40
1:F:40:LEU:HD21	1:F:59:GLU:C	2.41	0.40
1:J:231:ARG:O	1:J:235:PRO:HD2	2.21	0.40
1:J:144:ILE:HG23	1:J:403:THR:HG21	2.04	0.40
1:L:291:ASP:OD1	1:L:349:ILE:HD11	2.21	0.40
1:D:349:ILE:HG23	1:D:365:LEU:HD13	2.02	0.40
1:F:114:MET:HB2	1:G:36:ARG:HD2	2.04	0.40
1:A:114:MET:HB2	1:B:36:ARG:HD2	2.04	0.40
1:A:115:ASP:CB	1:A:435:ASP:HB2	2.51	0.40
1:F:13:ARG:HB2	1:F:104:LEU:HD22	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 PDB entries followed by that with respect to all EM entries.

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	522/548 (95%)	516 (99%)	4 (1%)	2 (0%)	39	80
1	B	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	C	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	D	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	E	522/548 (95%)	515 (99%)	4 (1%)	3 (1%)	30	74
1	F	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	30	74
1	G	522/548 (95%)	518 (99%)	3 (1%)	1 (0%)	52	86
1	H	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	I	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	J	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	K	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	L	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	M	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	N	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
All	All	7308/7672 (95%)	7239 (99%)	37 (0%)	32 (0%)	43	80

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLU
1	B	257	GLU
1	C	257	GLU
1	D	257	GLU
1	E	257	GLU
1	F	257	GLU
1	G	257	GLU
1	H	243	ALA
1	I	243	ALA

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Mol	Chain	Res	Type
1	J	243	ALA
1	K	243	ALA
1	L	243	ALA
1	M	243	ALA
1	N	243	ALA
1	H	516	THR
1	I	516	THR
1	J	516	THR
1	K	516	THR
1	L	516	THR
1	M	516	THR
1	N	516	THR
1	A	258	ALA
1	B	258	ALA
1	C	258	ALA
1	D	258	ALA
1	E	258	ALA
1	B	243	ALA
1	C	243	ALA
1	D	243	ALA
1	E	243	ALA
1	F	243	ALA
1	F	258	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	B	402/414 (97%)	356 (89%)	46 (11%)	7	33
1	C	402/414 (97%)	356 (89%)	46 (11%)	7	33
1	D	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	E	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	F	402/414 (97%)	356 (89%)	46 (11%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	H	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	I	402/414 (97%)	355 (88%)	47 (12%)	7	32
1	J	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	K	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	L	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	M	402/414 (97%)	354 (88%)	48 (12%)	6	31
1	N	402/414 (97%)	354 (88%)	48 (12%)	6	31
All	All	5628/5796 (97%)	4975 (88%)	653 (12%)	11	32

All (653) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	18	ARG
1	A	31	LEU
1	A	42	LYS
1	A	48	THR
1	A	50	THR
1	A	52	ASP
1	A	65	LYS
1	A	76	GLU
1	A	82	ASN
1	A	114	MET
1	A	140	ASP
1	A	142	LYS
1	A	156	GLU
1	A	171	LYS
1	A	186	GLU
1	A	205	ILE
1	A	207	LYS
1	A	214	GLU
1	A	219	PHE
1	A	224	ASP
1	A	230	ILE
1	A	238	GLU
1	A	252	GLU
1	A	254	VAL
1	A	257	GLU

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Mol	Chain	Res	Type
1	A	262	LEU
1	A	268	ARG
1	A	290	GLN
1	A	327	LYS
1	A	328	ASP
1	A	334	ASP
1	A	339	GLU
1	A	350	ARG
1	A	358	SER
1	A	390	LYS
1	A	421	ARG
1	A	430	ARG
1	A	435	ASP
1	A	460	GLU
1	A	463	SER
1	A	484	GLU
1	A	494	LEU
1	A	504	LEU
1	A	518	GLU
1	B	13	ARG
1	B	18	ARG
1	B	31	LEU
1	B	42	LYS
1	B	48	THR
1	B	50	THR
1	B	52	ASP
1	B	65	LYS
1	B	76	GLU
1	B	82	ASN
1	B	114	MET
1	B	140	ASP
1	B	142	LYS
1	B	156	GLU
1	B	171	LYS
1	B	186	GLU
1	B	205	ILE
1	B	207	LYS
1	B	214	GLU
1	B	217	SER
1	B	219	PHE
1	B	224	ASP
1	B	230	ILE

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Mol	Chain	Res	Type
1	B	238	GLU
1	B	252	GLU
1	B	254	VAL
1	B	257	GLU
1	B	262	LEU
1	B	268	ARG
1	B	290	GLN
1	B	327	LYS
1	B	328	ASP
1	B	334	ASP
1	B	339	GLU
1	B	350	ARG
1	B	358	SER
1	B	390	LYS
1	B	421	ARG
1	B	430	ARG
1	B	435	ASP
1	B	460	GLU
1	B	463	SER
1	B	484	GLU
1	B	494	LEU
1	B	504	LEU
1	B	518	GLU
1	C	13	ARG
1	C	18	ARG
1	C	31	LEU
1	C	42	LYS
1	C	48	THR
1	C	50	THR
1	C	52	ASP
1	C	65	LYS
1	C	76	GLU
1	C	82	ASN
1	C	114	MET
1	C	140	ASP
1	C	142	LYS
1	C	156	GLU
1	C	171	LYS
1	C	186	GLU
1	C	205	ILE
1	C	207	LYS
1	C	214	GLU

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Mol	Chain	Res	Type
1	C	217	SER
1	C	219	PHE
1	C	224	ASP
1	C	230	ILE
1	C	238	GLU
1	C	252	GLU
1	C	254	VAL
1	C	257	GLU
1	C	262	LEU
1	C	268	ARG
1	C	290	GLN
1	C	327	LYS
1	C	328	ASP
1	C	334	ASP
1	C	339	GLU
1	C	350	ARG
1	C	358	SER
1	C	390	LYS
1	C	421	ARG
1	C	430	ARG
1	C	435	ASP
1	C	460	GLU
1	C	463	SER
1	C	484	GLU
1	C	494	LEU
1	C	504	LEU
1	C	518	GLU
1	D	13	ARG
1	D	18	ARG
1	D	31	LEU
1	D	42	LYS
1	D	48	THR
1	D	50	THR
1	D	52	ASP
1	D	65	LYS
1	D	76	GLU
1	D	82	ASN
1	D	114	MET
1	D	140	ASP
1	D	142	LYS
1	D	156	GLU
1	D	171	LYS

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Mol	Chain	Res	Type
1	D	186	GLU
1	D	205	ILE
1	D	207	LYS
1	D	214	GLU
1	D	217	SER
1	D	219	PHE
1	D	224	ASP
1	D	230	ILE
1	D	238	GLU
1	D	252	GLU
1	D	254	VAL
1	D	257	GLU
1	D	262	LEU
1	D	268	ARG
1	D	290	GLN
1	D	327	LYS
1	D	328	ASP
1	D	334	ASP
1	D	339	GLU
1	D	350	ARG
1	D	358	SER
1	D	390	LYS
1	D	421	ARG
1	D	430	ARG
1	D	460	GLU
1	D	463	SER
1	D	484	GLU
1	D	494	LEU
1	D	504	LEU
1	D	518	GLU
1	E	13	ARG
1	E	18	ARG
1	E	31	LEU
1	E	42	LYS
1	E	48	THR
1	E	50	THR
1	E	52	ASP
1	E	65	LYS
1	E	76	GLU
1	E	82	ASN
1	E	114	MET
1	E	140	ASP

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Mol	Chain	Res	Type
1	E	142	LYS
1	E	156	GLU
1	E	171	LYS
1	E	186	GLU
1	E	205	ILE
1	E	207	LYS
1	E	214	GLU
1	E	217	SER
1	E	219	PHE
1	E	224	ASP
1	E	230	ILE
1	E	238	GLU
1	E	252	GLU
1	E	254	VAL
1	E	257	GLU
1	E	262	LEU
1	E	268	ARG
1	E	290	GLN
1	E	327	LYS
1	E	328	ASP
1	E	334	ASP
1	E	339	GLU
1	E	350	ARG
1	E	358	SER
1	E	390	LYS
1	E	421	ARG
1	E	430	ARG
1	E	460	GLU
1	E	463	SER
1	E	484	GLU
1	E	494	LEU
1	E	504	LEU
1	E	518	GLU
1	F	13	ARG
1	F	18	ARG
1	F	31	LEU
1	F	42	LYS
1	F	48	THR
1	F	50	THR
1	F	52	ASP
1	F	65	LYS
1	F	76	GLU

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Mol	Chain	Res	Type
1	F	82	ASN
1	F	114	MET
1	F	140	ASP
1	F	142	LYS
1	F	156	GLU
1	F	171	LYS
1	F	186	GLU
1	F	205	ILE
1	F	207	LYS
1	F	214	GLU
1	F	217	SER
1	F	219	PHE
1	F	224	ASP
1	F	231	ARG
1	F	232	GLU
1	F	238	GLU
1	F	252	GLU
1	F	254	VAL
1	F	257	GLU
1	F	268	ARG
1	F	290	GLN
1	F	327	LYS
1	F	328	ASP
1	F	334	ASP
1	F	339	GLU
1	F	350	ARG
1	F	358	SER
1	F	390	LYS
1	F	421	ARG
1	F	430	ARG
1	F	435	ASP
1	F	460	GLU
1	F	463	SER
1	F	484	GLU
1	F	494	LEU
1	F	504	LEU
1	F	518	GLU
1	G	13	ARG
1	G	18	ARG
1	G	31	LEU
1	G	42	LYS
1	G	48	THR

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Mol	Chain	Res	Type
1	G	50	THR
1	G	52	ASP
1	G	65	LYS
1	G	76	GLU
1	G	82	ASN
1	G	114	MET
1	G	140	ASP
1	G	142	LYS
1	G	156	GLU
1	G	171	LYS
1	G	186	GLU
1	G	205	ILE
1	G	207	LYS
1	G	214	GLU
1	G	216	GLU
1	G	224	ASP
1	G	230	ILE
1	G	240	VAL
1	G	242	LYS
1	G	252	GLU
1	G	254	VAL
1	G	257	GLU
1	G	268	ARG
1	G	290	GLN
1	G	327	LYS
1	G	328	ASP
1	G	334	ASP
1	G	339	GLU
1	G	350	ARG
1	G	358	SER
1	G	390	LYS
1	G	421	ARG
1	G	430	ARG
1	G	435	ASP
1	G	460	GLU
1	G	463	SER
1	G	484	GLU
1	G	494	LEU
1	G	504	LEU
1	G	518	GLU
1	H	25	ASP
1	H	31	LEU

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Mol	Chain	Res	Type
1	H	36	ARG
1	H	40	LEU
1	H	50	THR
1	H	52	ASP
1	H	63	GLU
1	H	65	LYS
1	H	79	SER
1	H	82	ASN
1	H	114	MET
1	H	156	GLU
1	H	169	VAL
1	H	171	LYS
1	H	186	GLU
1	H	190	VAL
1	H	205	ILE
1	H	207	LYS
1	H	213	VAL
1	H	214	GLU
1	H	225	LYS
1	H	226	LYS
1	H	231	ARG
1	H	232	GLU
1	H	238	GLU
1	H	242	LYS
1	H	246	PRO
1	H	252	GLU
1	H	268	ARG
1	H	272	LYS
1	H	290	GLN
1	H	294	THR
1	H	303	GLU
1	H	322	ARG
1	H	327	LYS
1	H	328	ASP
1	H	334	ASP
1	H	350	ARG
1	H	358	SER
1	H	412	VAL
1	H	421	ARG
1	H	430	ARG
1	H	435	ASP
1	H	460	GLU

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Mol	Chain	Res	Type
1	H	463	SER
1	H	464	VAL
1	H	484	GLU
1	H	504	LEU
1	I	25	ASP
1	I	31	LEU
1	I	36	ARG
1	I	40	LEU
1	I	50	THR
1	I	52	ASP
1	I	63	GLU
1	I	65	LYS
1	I	79	SER
1	I	82	ASN
1	I	114	MET
1	I	156	GLU
1	I	169	VAL
1	I	171	LYS
1	I	186	GLU
1	I	190	VAL
1	I	205	ILE
1	I	207	LYS
1	I	213	VAL
1	I	214	GLU
1	I	225	LYS
1	I	226	LYS
1	I	231	ARG
1	I	238	GLU
1	I	242	LYS
1	I	246	PRO
1	I	252	GLU
1	I	268	ARG
1	I	272	LYS
1	I	290	GLN
1	I	294	THR
1	I	303	GLU
1	I	322	ARG
1	I	327	LYS
1	I	328	ASP
1	I	334	ASP
1	I	350	ARG
1	I	358	SER

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Mol	Chain	Res	Type
1	I	412	VAL
1	I	421	ARG
1	I	430	ARG
1	I	435	ASP
1	I	460	GLU
1	I	463	SER
1	I	464	VAL
1	I	484	GLU
1	I	504	LEU
1	J	25	ASP
1	J	31	LEU
1	J	36	ARG
1	J	40	LEU
1	J	50	THR
1	J	52	ASP
1	J	63	GLU
1	J	65	LYS
1	J	79	SER
1	J	82	ASN
1	J	114	MET
1	J	156	GLU
1	J	169	VAL
1	J	171	LYS
1	J	186	GLU
1	J	190	VAL
1	J	205	ILE
1	J	207	LYS
1	J	213	VAL
1	J	214	GLU
1	J	225	LYS
1	J	226	LYS
1	J	231	ARG
1	J	232	GLU
1	J	238	GLU
1	J	242	LYS
1	J	246	PRO
1	J	252	GLU
1	J	268	ARG
1	J	272	LYS
1	J	290	GLN
1	J	294	THR
1	J	303	GLU

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Mol	Chain	Res	Type
1	J	322	ARG
1	J	327	LYS
1	J	328	ASP
1	J	334	ASP
1	J	350	ARG
1	J	358	SER
1	J	412	VAL
1	J	421	ARG
1	J	430	ARG
1	J	435	ASP
1	J	460	GLU
1	J	463	SER
1	J	464	VAL
1	J	484	GLU
1	J	504	LEU
1	K	25	ASP
1	K	31	LEU
1	K	36	ARG
1	K	40	LEU
1	K	50	THR
1	K	52	ASP
1	K	63	GLU
1	K	65	LYS
1	K	79	SER
1	K	82	ASN
1	K	114	MET
1	K	156	GLU
1	K	169	VAL
1	K	171	LYS
1	K	186	GLU
1	K	190	VAL
1	K	205	ILE
1	K	207	LYS
1	K	213	VAL
1	K	214	GLU
1	K	225	LYS
1	K	226	LYS
1	K	231	ARG
1	K	232	GLU
1	K	238	GLU
1	K	242	LYS
1	K	246	PRO

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Mol	Chain	Res	Type
1	K	252	GLU
1	K	268	ARG
1	K	272	LYS
1	K	290	GLN
1	K	294	THR
1	K	303	GLU
1	K	322	ARG
1	K	327	LYS
1	K	328	ASP
1	K	334	ASP
1	K	350	ARG
1	K	358	SER
1	K	412	VAL
1	K	421	ARG
1	K	430	ARG
1	K	435	ASP
1	K	460	GLU
1	K	463	SER
1	K	464	VAL
1	K	484	GLU
1	K	504	LEU
1	L	25	ASP
1	L	31	LEU
1	L	36	ARG
1	L	40	LEU
1	L	50	THR
1	L	52	ASP
1	L	63	GLU
1	L	65	LYS
1	L	79	SER
1	L	82	ASN
1	L	114	MET
1	L	156	GLU
1	L	169	VAL
1	L	171	LYS
1	L	186	GLU
1	L	190	VAL
1	L	205	ILE
1	L	207	LYS
1	L	213	VAL
1	L	214	GLU
1	L	225	LYS

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Mol	Chain	Res	Type
1	L	226	LYS
1	L	231	ARG
1	L	232	GLU
1	L	238	GLU
1	L	242	LYS
1	L	246	PRO
1	L	252	GLU
1	L	268	ARG
1	L	272	LYS
1	L	290	GLN
1	L	294	THR
1	L	303	GLU
1	L	322	ARG
1	L	327	LYS
1	L	328	ASP
1	L	334	ASP
1	L	350	ARG
1	L	358	SER
1	L	412	VAL
1	L	421	ARG
1	L	430	ARG
1	L	435	ASP
1	L	460	GLU
1	L	463	SER
1	L	464	VAL
1	L	484	GLU
1	L	504	LEU
1	M	25	ASP
1	M	31	LEU
1	M	36	ARG
1	M	40	LEU
1	M	50	THR
1	M	52	ASP
1	M	63	GLU
1	M	65	LYS
1	M	79	SER
1	M	82	ASN
1	M	114	MET
1	M	156	GLU
1	M	169	VAL
1	M	171	LYS
1	M	186	GLU

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Mol	Chain	Res	Type
1	M	190	VAL
1	M	205	ILE
1	M	207	LYS
1	M	213	VAL
1	M	214	GLU
1	M	225	LYS
1	M	226	LYS
1	M	231	ARG
1	M	232	GLU
1	M	238	GLU
1	M	242	LYS
1	M	246	PRO
1	M	252	GLU
1	M	268	ARG
1	M	272	LYS
1	M	290	GLN
1	M	294	THR
1	M	303	GLU
1	M	322	ARG
1	M	327	LYS
1	M	328	ASP
1	M	334	ASP
1	M	350	ARG
1	M	358	SER
1	M	412	VAL
1	M	421	ARG
1	M	430	ARG
1	M	435	ASP
1	M	460	GLU
1	M	463	SER
1	M	464	VAL
1	M	484	GLU
1	M	504	LEU
1	N	25	ASP
1	N	31	LEU
1	N	36	ARG
1	N	40	LEU
1	N	50	THR
1	N	52	ASP
1	N	63	GLU
1	N	65	LYS
1	N	79	SER

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Mol	Chain	Res	Type
1	N	82	ASN
1	N	114	MET
1	N	156	GLU
1	N	169	VAL
1	N	171	LYS
1	N	186	GLU
1	N	190	VAL
1	N	205	ILE
1	N	207	LYS
1	N	213	VAL
1	N	214	GLU
1	N	225	LYS
1	N	226	LYS
1	N	231	ARG
1	N	232	GLU
1	N	238	GLU
1	N	242	LYS
1	N	246	PRO
1	N	252	GLU
1	N	268	ARG
1	N	272	LYS
1	N	290	GLN
1	N	294	THR
1	N	303	GLU
1	N	322	ARG
1	N	327	LYS
1	N	328	ASP
1	N	334	ASP
1	N	350	ARG
1	N	358	SER
1	N	412	VAL
1	N	421	ARG
1	N	430	ARG
1	N	435	ASP
1	N	460	GLU
1	N	463	SER
1	N	464	VAL
1	N	484	GLU
1	N	504	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	453	GLN
1	B	229	ASN
1	B	453	GLN
1	C	229	ASN
1	C	453	GLN
1	D	229	ASN
1	D	453	GLN
1	E	229	ASN
1	E	453	GLN
1	F	453	GLN
1	G	453	GLN
1	H	453	GLN
1	I	453	GLN
1	J	453	GLN
1	K	453	GLN
1	L	453	GLN
1	M	453	GLN
1	N	453	GLN

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 ⓘ

Of 42 ligands modelled in this entry, 14 are monoatomic and 14 are modelled with single atom - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	A	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	B	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	C	1526	3	26,33,33	0.73	0	26,52,52	1.14	3 (11%)
2	ATP	D	1525	3	26,33,33	0.73	0	26,52,52	1.14	3 (11%)
2	ATP	E	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	F	1525	3	26,33,33	0.72	0	26,52,52	1.14	3 (11%)
2	ATP	G	1525	3	26,33,33	0.73	0	26,52,52	1.14	3 (11%)
2	ATP	H	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)
2	ATP	I	1525	3	26,33,33	0.72	0	26,52,52	1.11	4 (15%)
2	ATP	J	1526	3	26,33,33	0.72	0	26,52,52	1.11	3 (11%)
2	ATP	K	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)
2	ATP	L	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)
2	ATP	M	1527	3	26,33,33	0.72	0	26,52,52	1.11	4 (15%)
2	ATP	N	1527	3	26,33,33	0.71	0	26,52,52	1.11	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	B	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	C	1526	3	-	0/18/38/38	0/3/3/3
2	ATP	D	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	E	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	F	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	G	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	H	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	I	1525	3	-	0/18/38/38	0/3/3/3
2	ATP	J	1526	3	-	0/18/38/38	0/3/3/3
2	ATP	K	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	L	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	M	1527	3	-	0/18/38/38	0/3/3/3
2	ATP	N	1527	3	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1525	ATP	C5'-C4'-C3'	-2.53	105.40	115.20
2	F	1525	ATP	C5'-C4'-C3'	-2.53	105.43	115.20
2	D	1525	ATP	C5'-C4'-C3'	-2.52	105.45	115.20
2	G	1525	ATP	C5'-C4'-C3'	-2.52	105.46	115.20
2	C	1526	ATP	C5'-C4'-C3'	-2.52	105.47	115.20
2	E	1525	ATP	C5'-C4'-C3'	-2.51	105.47	115.20
2	A	1525	ATP	C5'-C4'-C3'	-2.51	105.48	115.20
2	H	1527	ATP	C5'-C4'-C3'	-2.49	105.56	115.20
2	N	1527	ATP	C5'-C4'-C3'	-2.49	105.56	115.20
2	M	1527	ATP	C5'-C4'-C3'	-2.49	105.57	115.20
2	J	1526	ATP	C5'-C4'-C3'	-2.49	105.57	115.20
2	L	1527	ATP	C5'-C4'-C3'	-2.49	105.57	115.20
2	K	1527	ATP	C5'-C4'-C3'	-2.49	105.58	115.20
2	I	1525	ATP	C5'-C4'-C3'	-2.49	105.58	115.20
2	L	1527	ATP	O2G-PG-O1G	2.00	117.16	110.63
2	K	1527	ATP	O2G-PG-O1G	2.01	117.20	110.63
2	I	1525	ATP	O2G-PG-O1G	2.01	117.20	110.63
2	H	1527	ATP	O2G-PG-O1G	2.02	117.22	110.63
2	M	1527	ATP	O2G-PG-O1G	2.02	117.23	110.63
2	N	1527	ATP	O2G-PG-O1G	2.03	117.27	110.63
2	F	1525	ATP	O2A-PA-O3A	2.08	114.20	105.27
2	B	1525	ATP	O2A-PA-O3A	2.09	114.21	105.27
2	D	1525	ATP	O2A-PA-O3A	2.09	114.21	105.27
2	A	1525	ATP	O2A-PA-O3A	2.09	114.23	105.27
2	E	1525	ATP	O2A-PA-O3A	2.09	114.23	105.27
2	C	1526	ATP	O2A-PA-O3A	2.09	114.24	105.27
2	G	1525	ATP	O2A-PA-O3A	2.11	114.31	105.27
2	H	1527	ATP	O3G-PG-O2G	2.13	115.27	107.44
2	I	1525	ATP	O3G-PG-O2G	2.14	115.28	107.44
2	M	1527	ATP	O3G-PG-O2G	2.14	115.28	107.44
2	L	1527	ATP	O3G-PG-O2G	2.14	115.30	107.44
2	N	1527	ATP	O3G-PG-O2G	2.15	115.33	107.44
2	J	1526	ATP	O3G-PG-O2G	2.15	115.35	107.44
2	K	1527	ATP	O3G-PG-O2G	2.16	115.36	107.44
2	F	1525	ATP	O3G-PG-O2G	2.25	115.71	107.44
2	I	1525	ATP	O2A-PA-O3A	2.25	114.92	105.27
2	K	1527	ATP	O2A-PA-O3A	2.25	114.92	105.27
2	L	1527	ATP	O2A-PA-O3A	2.25	114.92	105.27
2	D	1525	ATP	O3G-PG-O2G	2.25	115.72	107.44
2	G	1525	ATP	O3G-PG-O2G	2.26	115.73	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1525	ATP	O3G-PG-O2G	2.26	115.73	107.44
2	J	1526	ATP	O2A-PA-O3A	2.26	114.95	105.27
2	E	1525	ATP	O3G-PG-O2G	2.26	115.74	107.44
2	B	1525	ATP	O3G-PG-O2G	2.27	115.78	107.44
2	M	1527	ATP	O2A-PA-O3A	2.27	115.00	105.27
2	H	1527	ATP	O2A-PA-O3A	2.27	115.01	105.27
2	C	1526	ATP	O3G-PG-O2G	2.28	115.80	107.44
2	N	1527	ATP	O2A-PA-O3A	2.28	115.03	105.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1525	ATP	3	0
2	B	1525	ATP	3	0
2	C	1526	ATP	3	0
2	D	1525	ATP	3	0
2	E	1525	ATP	3	0
2	F	1525	ATP	3	0
2	G	1525	ATP	3	0
2	H	1527	ATP	3	0
2	I	1525	ATP	3	0
2	J	1526	ATP	3	0
2	K	1527	ATP	3	0
2	L	1527	ATP	3	0
2	M	1527	ATP	3	0
2	N	1527	ATP	3	0

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.