



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:32 AM UTC

PDB ID : 4AB3 / pdb_00004ab3
EMDB ID : EMD-2003
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 initial model : 1OEL

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

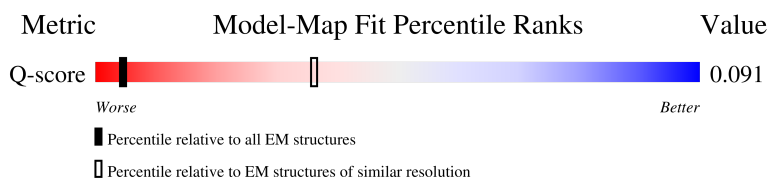
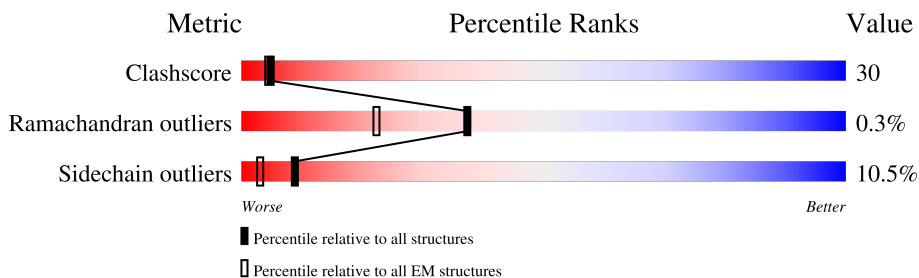
1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	328 (8.00 - 9.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	10% 52% 29% 12% • •
1	B	548	10% 52% 29% 12% • •
1	C	548	10% 51% 30% 11% • •
1	D	548	10% 51% 30% 11% • •

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Mol	Chain	Length	Quality of chain
1	E	548	
1	F	548	
1	G	548	
1	H	548	
1	I	548	
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
2	PO4	A	1525	-	-	X	-
2	PO4	B	1525	-	-	X	-
2	PO4	C	1525	-	-	X	-
2	PO4	D	1525	-	-	X	-
2	PO4	E	1525	-	-	X	-
2	PO4	F	1525	-	-	X	-
2	PO4	G	1525	-	-	X	-
2	PO4	H	1525	-	-	X	-
2	PO4	I	1525	-	-	X	-
2	PO4	J	1525	-	-	X	-
2	PO4	K	1525	-	-	X	-
2	PO4	L	1525	-	-	X	-
2	PO4	M	1525	-	-	X	-
2	PO4	N	1525	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 54293 atoms, of which 0 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
			3845	2391	664	770	20		
1	C	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	D	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	E	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	F	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	G	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	H	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	I	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	J	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	K	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	L	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	M	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	N	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		

There are 14 discrepancies between the modelled and reference sequences:

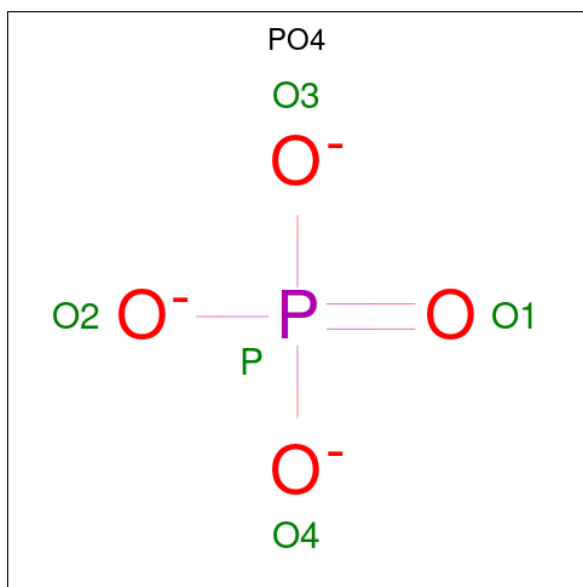
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

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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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total P 1 1	0
2	B	1	Total P 1 1	0
2	C	1	Total P 1 1	0
2	D	1	Total P 1 1	0
2	E	1	Total P 1 1	0

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

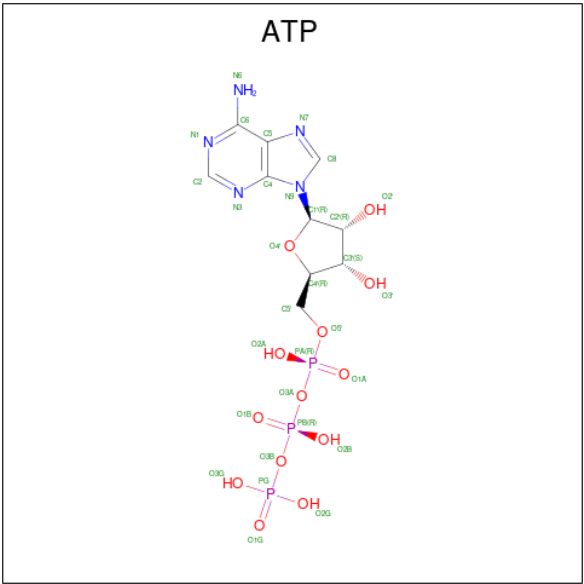
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	D	1	Total Mg 1 1	0
3	E	1	Total Mg 1 1	0
3	F	1	Total Mg 1 1	0
3	G	1	Total Mg 1 1	0
3	H	1	Total Mg 1 1	0
3	I	1	Total Mg 1 1	0
3	J	1	Total Mg 1 1	0

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

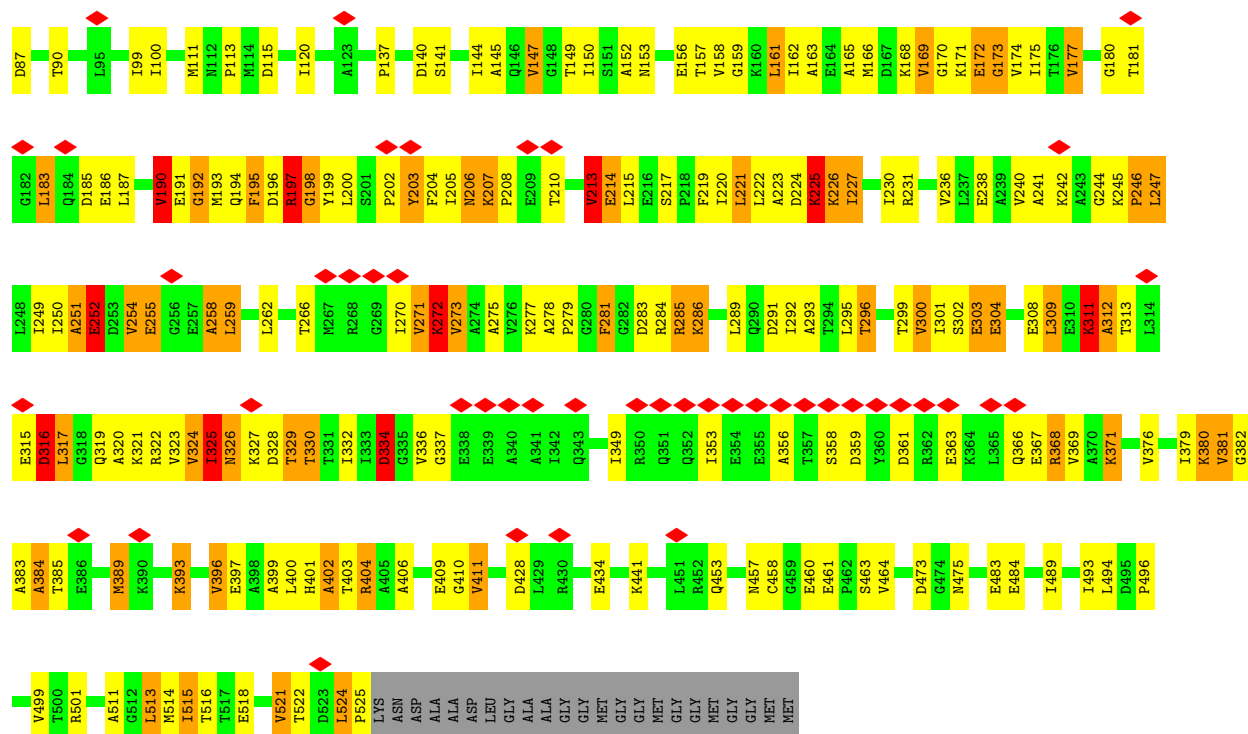


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

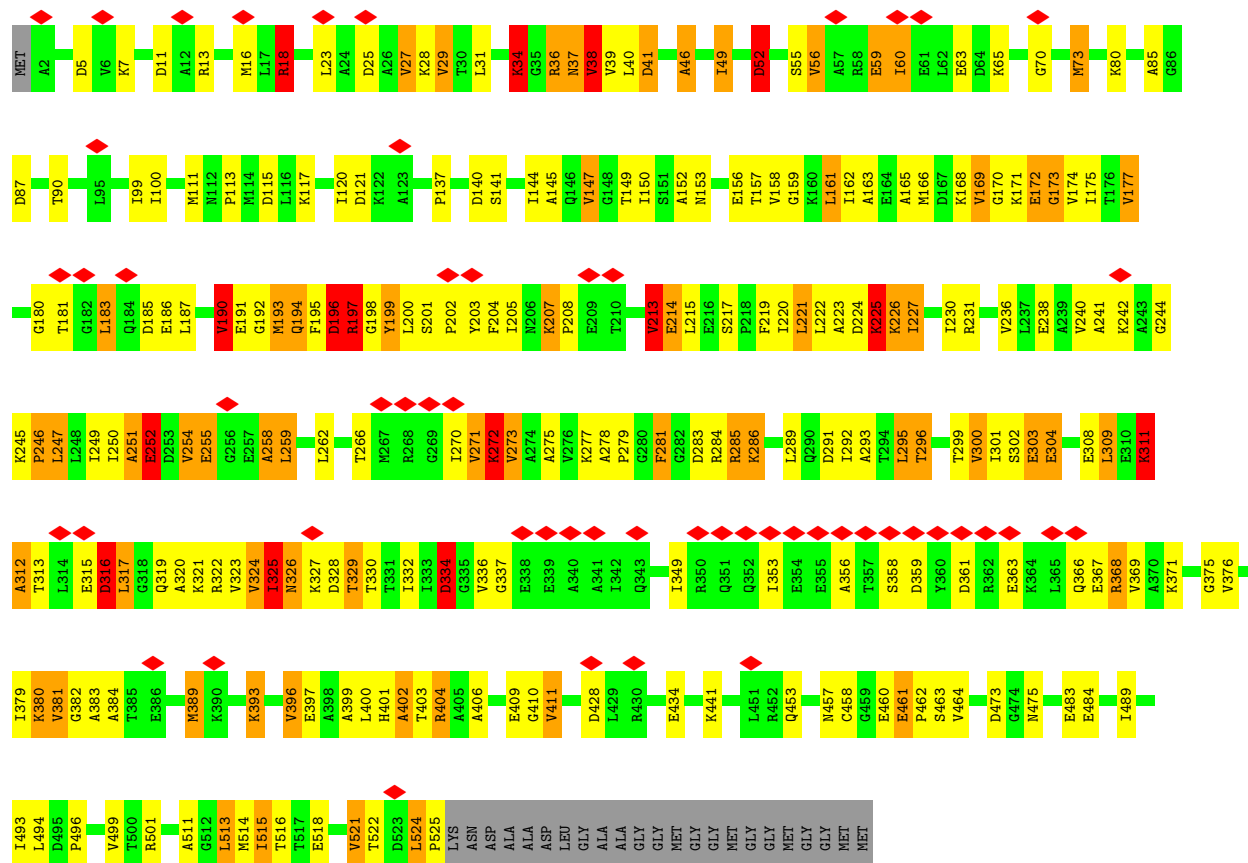
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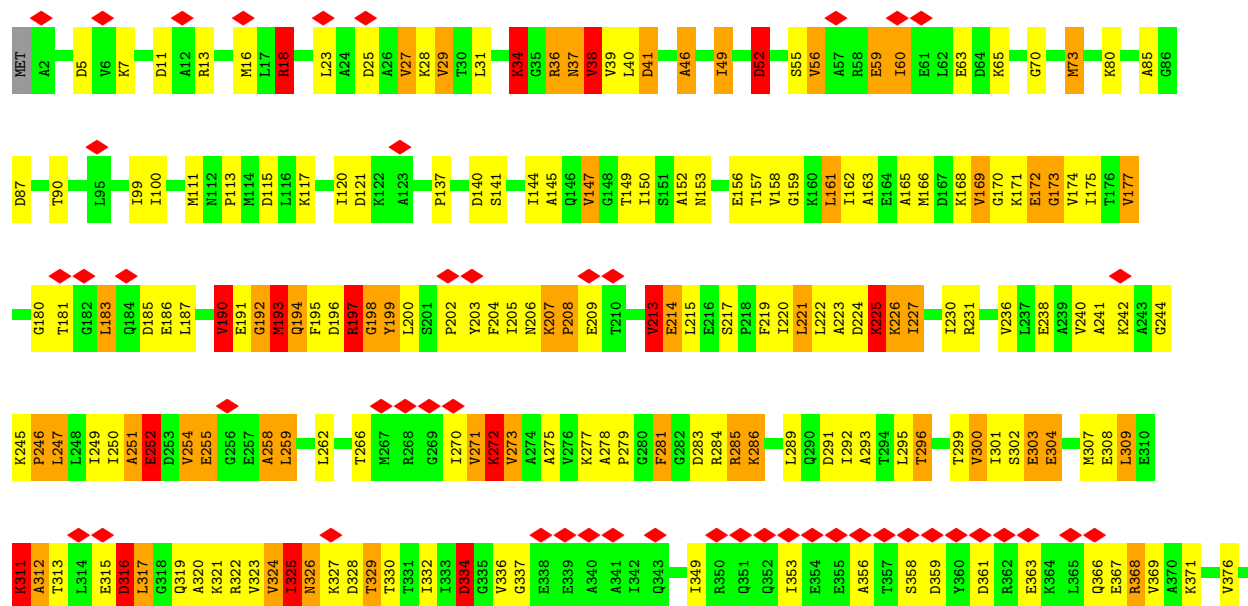
Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total 31	C 10	N 5	O 13	P 3	0
4	I	1	Total 31	C 10	N 5	O 13	P 3	0
4	J	1	Total 31	C 10	N 5	O 13	P 3	0
4	K	1	Total 31	C 10	N 5	O 13	P 3	0
4	L	1	Total 31	C 10	N 5	O 13	P 3	0
4	M	1	Total 31	C 10	N 5	O 13	P 3	0
4	N	1	Total 31	C 10	N 5	O 13	P 3	0

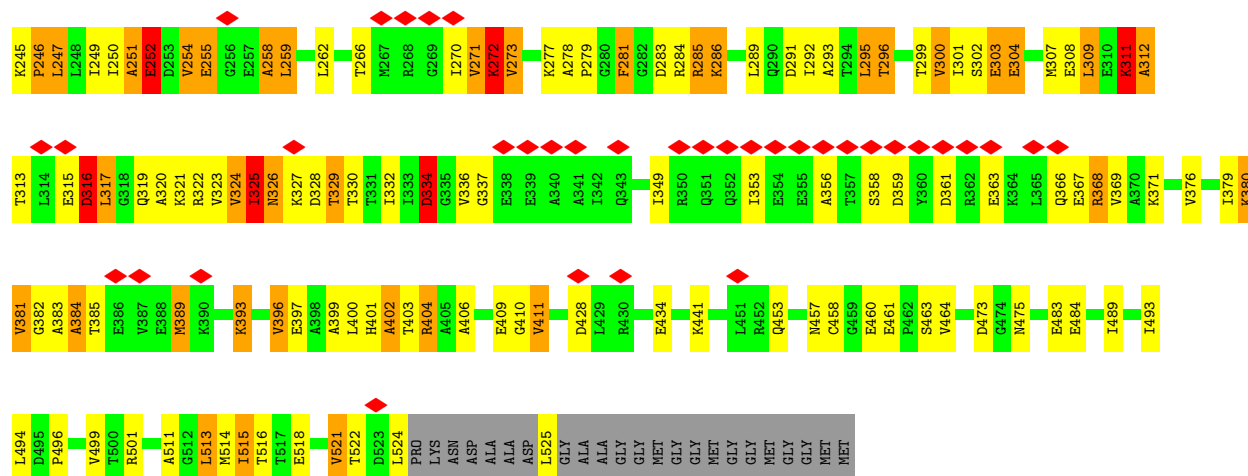


• Molecule 1: 60 KDA CHAPERONIN

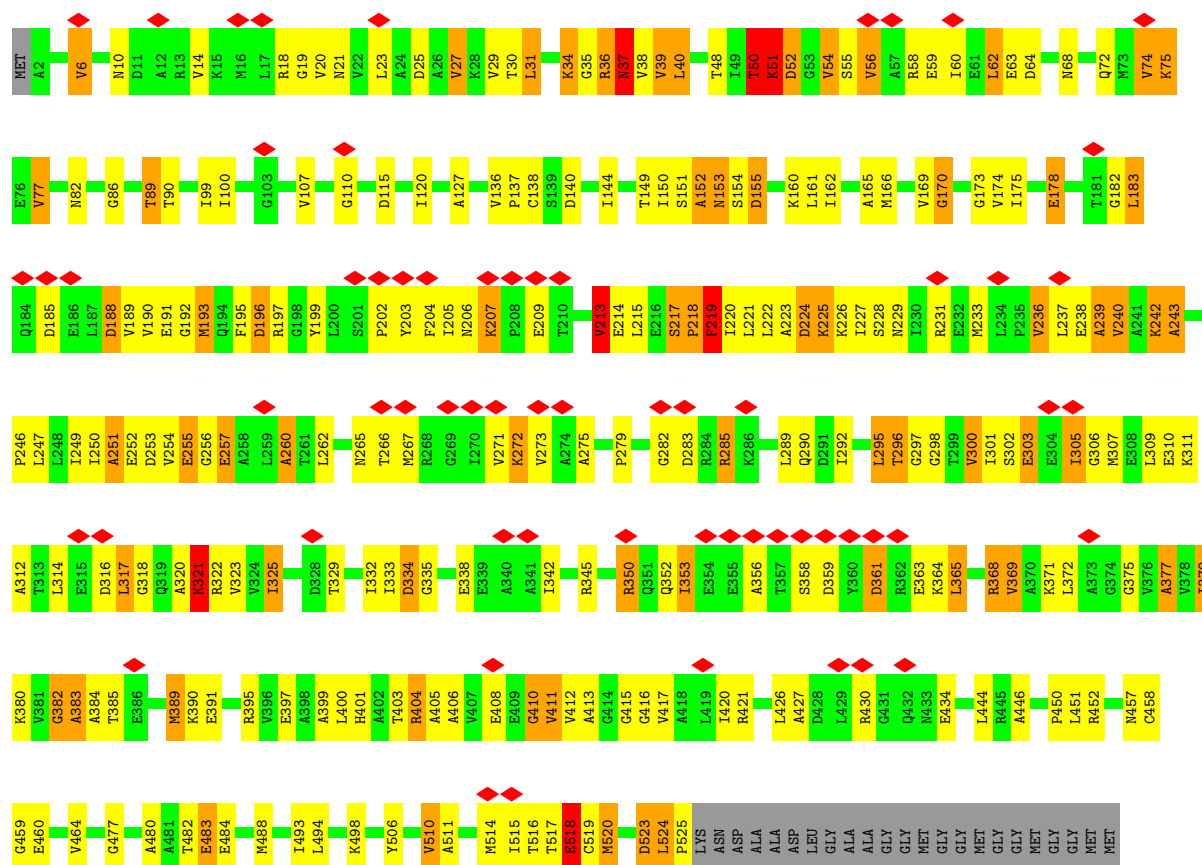


Chain D:

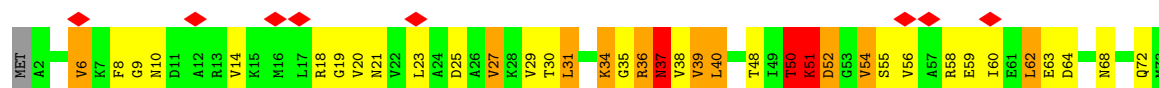




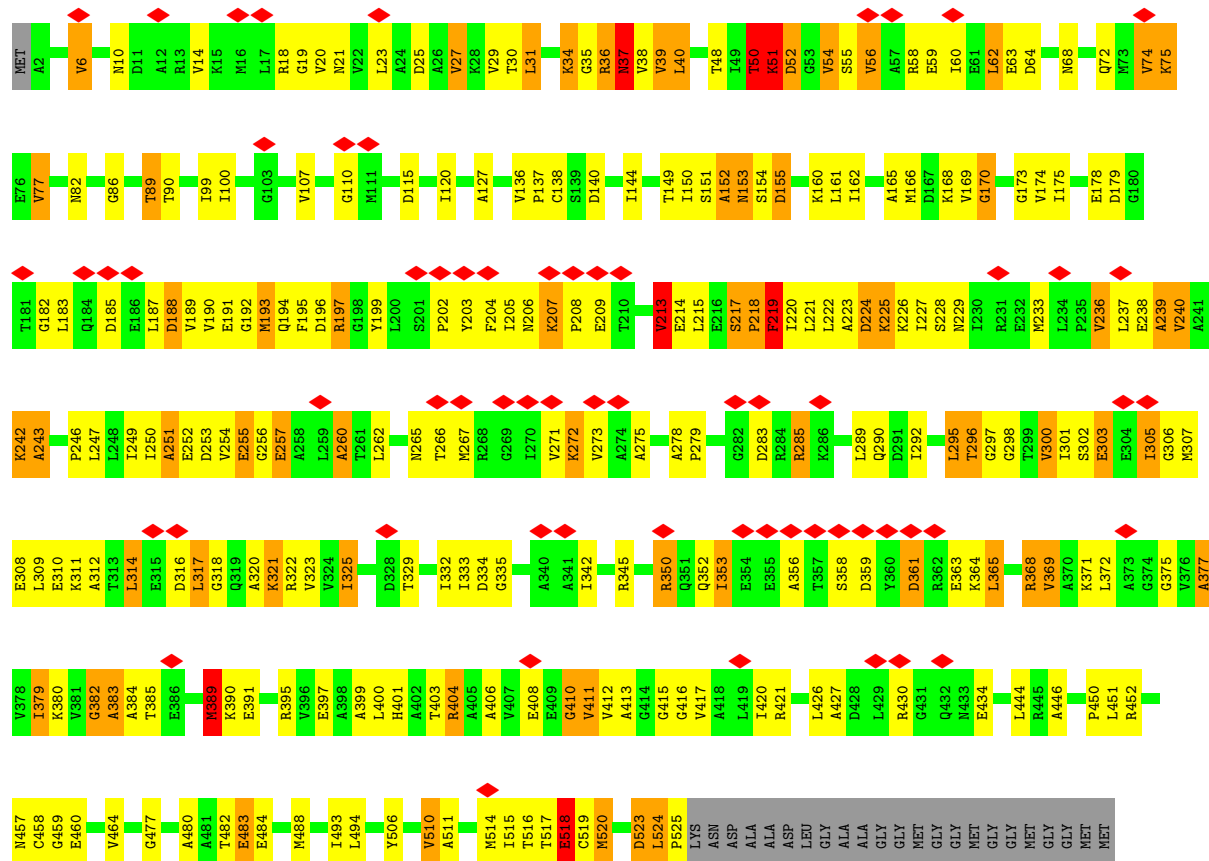
• Molecule 1: 60 KDA CHAPERONIN



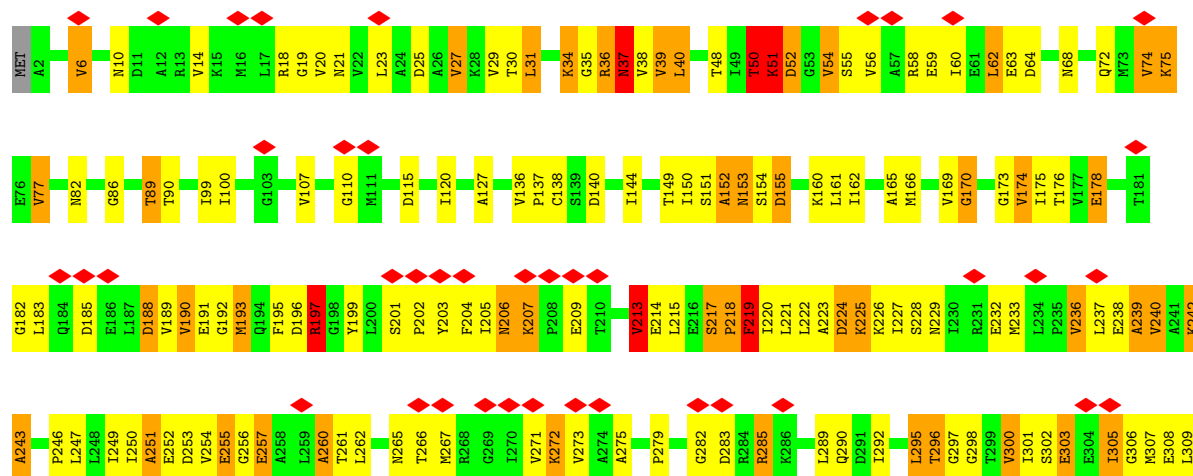
• Molecule 1: 60 KDA CHAPERONIN



- Molecule 1: 60 KDA CHAPERONIN



Chain K: 11% 49% 33% 13% . .







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	15000	Depositor
Resolution determination method	Not provided	
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	148500	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	2.147	Depositor
Minimum map value	-1.318	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	387.84, 387.84, 387.84	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.02, 2.02, 2.02	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, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.15	10/3873 (0.3%)	1.93	146/5229 (2.8%)
1	B	1.18	10/3872 (0.3%)	1.93	149/5227 (2.9%)
1	C	1.17	10/3872 (0.3%)	1.93	144/5227 (2.8%)
1	D	1.18	11/3872 (0.3%)	1.93	148/5227 (2.8%)
1	E	1.19	11/3872 (0.3%)	1.94	148/5227 (2.8%)
1	F	1.19	12/3872 (0.3%)	1.94	146/5227 (2.8%)
1	G	1.19	10/3872 (0.3%)	1.98	157/5227 (3.0%)
1	H	1.49	5/3872 (0.1%)	2.02	112/5227 (2.1%)
1	I	1.49	4/3872 (0.1%)	2.02	118/5227 (2.3%)
1	J	1.49	4/3872 (0.1%)	2.02	112/5227 (2.1%)
1	K	1.50	6/3872 (0.2%)	2.02	112/5227 (2.1%)
1	L	1.50	6/3872 (0.2%)	2.04	122/5227 (2.3%)
1	M	1.49	5/3872 (0.1%)	2.01	115/5227 (2.2%)
1	N	1.56	13/3872 (0.3%)	2.09	129/5227 (2.5%)
All	All	1.35	117/54209 (0.2%)	1.99	1858/73180 (2.5%)

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	19
1	B	0	18
1	C	0	18
1	D	0	18
1	E	0	19
1	F	0	19
1	G	0	18
1	H	1	13
1	I	1	14

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	1	14
1	K	1	15
1	L	1	14
1	M	1	14
1	N	1	18
All	All	7	231

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	LYS	C-N	-19.82	1.07	1.33
1	A	7	LYS	C-N	-19.82	1.07	1.33
1	E	7	LYS	C-N	-19.82	1.07	1.33
1	G	7	LYS	C-N	-19.82	1.07	1.33
1	B	7	LYS	C-N	-19.81	1.07	1.33
1	D	7	LYS	C-N	-19.81	1.07	1.33
1	F	7	LYS	C-N	-19.81	1.07	1.33
1	L	518	GLU	CA-CB	19.16	1.83	1.53
1	M	518	GLU	CA-CB	19.16	1.83	1.53
1	H	518	GLU	CA-CB	19.15	1.83	1.53
1	J	518	GLU	CA-CB	19.15	1.83	1.53
1	K	518	GLU	CA-CB	19.15	1.83	1.53
1	I	518	GLU	CA-CB	19.13	1.83	1.53
1	C	213	VAL	C-N	-19.12	1.08	1.33
1	N	518	GLU	CA-CB	19.11	1.83	1.53
1	D	213	VAL	C-N	-19.09	1.08	1.33
1	F	213	VAL	C-N	-19.08	1.08	1.33
1	G	213	VAL	C-N	-19.08	1.08	1.33
1	B	213	VAL	C-N	-19.08	1.08	1.33
1	E	213	VAL	C-N	-19.07	1.08	1.33
1	N	208	PRO	CA-C	17.14	1.76	1.52
1	D	11	ASP	C-N	13.47	1.52	1.33
1	G	11	ASP	C-N	13.46	1.52	1.33
1	A	11	ASP	C-N	13.45	1.52	1.33
1	B	11	ASP	C-N	13.45	1.52	1.33
1	E	11	ASP	C-N	13.44	1.52	1.33
1	F	11	ASP	C-N	13.44	1.52	1.33
1	C	11	ASP	C-N	13.44	1.52	1.33
1	C	230	ILE	C-N	13.32	1.50	1.33
1	G	230	ILE	C-N	13.32	1.50	1.33
1	F	230	ILE	C-N	13.31	1.50	1.33
1	D	230	ILE	C-N	13.31	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	ILE	C-N	13.31	1.50	1.33
1	B	230	ILE	C-N	13.31	1.50	1.33
1	E	230	ILE	C-N	13.31	1.50	1.33
1	N	208	PRO	C-N	12.78	1.53	1.33
1	G	200	LEU	CA-C	-12.53	1.44	1.52
1	B	513	LEU	C-N	-11.52	1.18	1.33
1	E	513	LEU	C-N	-11.49	1.18	1.33
1	A	513	LEU	C-N	-11.47	1.19	1.33
1	F	513	LEU	C-N	-11.47	1.19	1.33
1	C	513	LEU	C-N	-11.46	1.19	1.33
1	G	513	LEU	C-N	-11.45	1.19	1.33
1	N	207	LYS	CA-CB	11.44	1.71	1.53
1	D	513	LEU	C-N	-11.43	1.19	1.33
1	B	518	GLU	C-N	-10.19	1.19	1.33
1	F	518	GLU	C-N	-10.15	1.19	1.33
1	A	518	GLU	C-N	-10.14	1.19	1.33
1	C	518	GLU	C-N	-10.14	1.19	1.33
1	E	518	GLU	C-N	-10.14	1.19	1.33
1	G	518	GLU	C-N	-10.14	1.19	1.33
1	D	518	GLU	C-N	-10.12	1.19	1.33
1	B	52	ASP	C-N	-9.21	1.20	1.33
1	A	52	ASP	C-N	-9.16	1.20	1.33
1	E	52	ASP	C-N	-9.16	1.20	1.33
1	D	52	ASP	C-N	-9.15	1.20	1.33
1	F	52	ASP	C-N	-9.15	1.20	1.33
1	C	52	ASP	C-N	-9.14	1.20	1.33
1	G	52	ASP	C-N	-9.13	1.20	1.33
1	H	242	LYS	CA-CB	9.00	1.67	1.53
1	K	242	LYS	CA-CB	8.87	1.67	1.53
1	K	206	ASN	CA-C	-8.42	1.49	1.53
1	L	206	ASN	CA-C	-8.30	1.49	1.53
1	K	240	VAL	CA-CB	-7.68	1.44	1.54
1	H	240	VAL	CA-CB	-7.67	1.44	1.54
1	J	240	VAL	CA-CB	-7.67	1.44	1.54
1	N	240	VAL	CA-CB	-7.67	1.44	1.54
1	I	240	VAL	CA-CB	-7.65	1.45	1.54
1	M	240	VAL	CA-CB	-7.63	1.45	1.54
1	L	240	VAL	CA-CB	-7.62	1.45	1.54
1	N	208	PRO	N-CA	7.24	1.56	1.47
1	E	381	VAL	CA-CB	-7.00	1.46	1.54
1	G	381	VAL	CA-CB	-6.98	1.46	1.54
1	C	381	VAL	CA-CB	-6.96	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	381	VAL	CA-CB	-6.95	1.46	1.54
1	A	381	VAL	CA-CB	-6.94	1.46	1.54
1	B	381	VAL	CA-CB	-6.93	1.46	1.54
1	F	381	VAL	CA-CB	-6.92	1.46	1.54
1	N	207	LYS	CE-NZ	6.87	1.70	1.49
1	N	207	LYS	CB-CG	6.83	1.73	1.52
1	M	242	LYS	CA-CB	6.44	1.63	1.53
1	N	207	LYS	CG-CD	6.33	1.71	1.52
1	A	193	MET	C-N	6.31	1.42	1.33
1	D	193	MET	C-N	6.30	1.42	1.33
1	E	193	MET	C-N	6.26	1.41	1.33
1	F	193	MET	C-N	5.87	1.42	1.33
1	F	198	GLY	CA-C	5.81	1.56	1.52
1	N	207	LYS	CD-CE	5.69	1.69	1.52
1	N	207	LYS	CA-C	5.61	1.59	1.52
1	L	206	ASN	N-CA	-5.56	1.42	1.46
1	F	29	VAL	C-N	5.41	1.41	1.33
1	A	29	VAL	C-N	5.40	1.41	1.33
1	D	29	VAL	C-N	5.40	1.41	1.33
1	C	29	VAL	C-N	5.38	1.41	1.33
1	B	29	VAL	C-N	5.38	1.41	1.33
1	E	29	VAL	C-N	5.37	1.41	1.33
1	G	29	VAL	C-N	5.37	1.41	1.33
1	N	217	SER	CA-CB	5.19	1.56	1.52
1	K	217	SER	CA-CB	5.18	1.56	1.52
1	I	217	SER	CA-CB	5.15	1.56	1.52
1	J	217	SER	CA-CB	5.14	1.56	1.52
1	M	217	SER	CA-CB	5.12	1.56	1.52
1	H	217	SER	CA-CB	5.12	1.56	1.52
1	E	524	LEU	C-N	-5.10	1.26	1.34
1	N	207	LYS	N-CA	-5.08	1.39	1.46
1	L	524	LEU	C-N	-5.07	1.26	1.34
1	L	217	SER	CA-CB	5.07	1.56	1.52
1	C	524	LEU	C-N	-5.07	1.26	1.34
1	I	524	LEU	C-N	-5.07	1.26	1.34
1	M	524	LEU	C-N	-5.06	1.26	1.34
1	D	524	LEU	C-N	-5.06	1.26	1.34
1	B	524	LEU	C-N	-5.05	1.26	1.34
1	H	524	LEU	C-N	-5.05	1.26	1.34
1	K	524	LEU	C-N	-5.04	1.26	1.34
1	J	524	LEU	C-N	-5.03	1.26	1.34
1	A	524	LEU	C-N	-5.03	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	524	LEU	C-N	-5.03	1.26	1.34

All (1858) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	242	LYS	N-CA-CB	-26.85	69.85	109.85
1	H	242	LYS	N-CA-CB	-26.53	70.32	109.85
1	J	518	GLU	N-CA-CB	25.43	146.95	110.07
1	L	518	GLU	N-CA-CB	25.41	146.92	110.07
1	I	518	GLU	N-CA-CB	25.40	146.89	110.07
1	K	518	GLU	N-CA-CB	25.38	146.87	110.07
1	H	518	GLU	N-CA-CB	25.36	146.84	110.07
1	N	518	GLU	N-CA-CB	25.34	146.81	110.07
1	M	518	GLU	N-CA-CB	25.34	146.81	110.07
1	L	242	LYS	CB-CA-C	24.98	149.86	109.89
1	J	242	LYS	CB-CA-C	24.38	148.90	109.89
1	N	242	LYS	CB-CA-C	24.37	148.88	109.89
1	I	242	LYS	CB-CA-C	24.33	148.81	109.89
1	J	518	GLU	CB-CA-C	-23.48	73.80	110.90
1	K	518	GLU	CB-CA-C	-23.47	73.82	110.90
1	M	518	GLU	CB-CA-C	-23.46	73.83	110.90
1	L	518	GLU	CB-CA-C	-23.46	73.84	110.90
1	I	518	GLU	CB-CA-C	-23.44	73.86	110.90
1	N	518	GLU	CB-CA-C	-23.44	73.87	110.90
1	H	518	GLU	CB-CA-C	-23.42	73.89	110.90
1	I	243	ALA	CB-CA-C	-23.11	75.83	110.50
1	L	243	ALA	CB-CA-C	-23.11	75.83	110.50
1	N	243	ALA	CB-CA-C	-23.11	75.84	110.50
1	J	243	ALA	CB-CA-C	-23.10	75.85	110.50
1	H	243	ALA	CB-CA-C	-23.09	75.86	110.50
1	K	243	ALA	CB-CA-C	-23.07	75.90	110.50
1	M	243	ALA	CB-CA-C	-23.05	75.93	110.50
1	M	242	LYS	N-CA-CB	-21.14	78.36	109.85
1	G	199	TYR	CA-C-N	-19.18	98.62	121.64
1	G	199	TYR	C-N-CA	-19.18	98.62	121.64
1	N	260	ALA	N-CA-CB	17.24	135.47	110.12
1	J	242	LYS	N-CA-CB	-17.14	84.31	109.85
1	I	242	LYS	N-CA-CB	-17.12	84.35	109.85
1	N	242	LYS	N-CA-CB	-17.10	84.37	109.85
1	D	518	GLU	CA-C-N	16.82	150.05	122.29
1	D	518	GLU	C-N-CA	16.82	150.05	122.29
1	C	518	GLU	CA-C-N	16.82	150.04	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	518	GLU	C-N-CA	16.82	150.04	122.29
1	E	518	GLU	CA-C-N	16.82	150.04	122.29
1	E	518	GLU	C-N-CA	16.82	150.04	122.29
1	F	518	GLU	CA-C-N	16.82	150.04	122.29
1	F	518	GLU	C-N-CA	16.82	150.04	122.29
1	A	518	GLU	CA-C-N	16.81	150.03	122.29
1	A	518	GLU	C-N-CA	16.81	150.03	122.29
1	G	518	GLU	CA-C-N	16.81	150.03	122.29
1	G	518	GLU	C-N-CA	16.81	150.03	122.29
1	B	518	GLU	CA-C-N	16.79	150.00	122.29
1	B	518	GLU	C-N-CA	16.79	150.00	122.29
1	M	260	ALA	N-CA-CB	16.78	134.79	110.12
1	L	242	LYS	N-CA-CB	-16.66	85.02	109.85
1	C	7	LYS	CA-C-N	-16.52	95.93	122.36
1	C	7	LYS	C-N-CA	-16.52	95.93	122.36
1	A	7	LYS	CA-C-N	-16.50	95.96	122.36
1	A	7	LYS	C-N-CA	-16.50	95.96	122.36
1	E	7	LYS	CA-C-N	-16.50	95.96	122.36
1	E	7	LYS	C-N-CA	-16.50	95.96	122.36
1	G	7	LYS	CA-C-N	-16.49	95.97	122.36
1	G	7	LYS	C-N-CA	-16.49	95.97	122.36
1	B	7	LYS	CA-C-N	-16.49	95.98	122.36
1	B	7	LYS	C-N-CA	-16.49	95.98	122.36
1	C	518	GLU	O-C-N	-16.48	104.29	122.09
1	D	7	LYS	CA-C-N	-16.48	95.99	122.36
1	D	7	LYS	C-N-CA	-16.48	95.99	122.36
1	F	7	LYS	CA-C-N	-16.48	95.99	122.36
1	F	7	LYS	C-N-CA	-16.48	95.99	122.36
1	E	518	GLU	O-C-N	-16.47	104.30	122.09
1	G	518	GLU	O-C-N	-16.46	104.31	122.09
1	F	518	GLU	O-C-N	-16.45	104.32	122.09
1	A	518	GLU	O-C-N	-16.45	104.32	122.09
1	D	518	GLU	O-C-N	-16.44	104.33	122.09
1	J	260	ALA	N-CA-CB	16.41	134.24	110.12
1	B	518	GLU	O-C-N	-16.40	104.37	122.09
1	H	260	ALA	N-CA-CB	16.40	134.23	110.12
1	K	260	ALA	N-CA-CB	16.39	134.22	110.12
1	E	29	VAL	O-C-N	16.34	138.66	121.83
1	G	29	VAL	O-C-N	16.34	138.66	121.83
1	A	29	VAL	O-C-N	16.31	138.63	121.83
1	F	29	VAL	O-C-N	16.31	138.63	121.83
1	C	29	VAL	O-C-N	16.31	138.63	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	VAL	O-C-N	16.30	138.62	121.83
1	D	29	VAL	O-C-N	16.30	138.62	121.83
1	N	208	PRO	CA-C-N	-15.54	98.31	122.08
1	N	208	PRO	C-N-CA	-15.54	98.31	122.08
1	H	242	LYS	CA-CB-CG	15.35	144.79	114.10
1	K	242	LYS	CA-CB-CG	14.96	144.03	114.10
1	N	208	PRO	N-CA-C	14.36	142.06	112.47
1	K	213	VAL	O-C-N	-14.13	110.25	122.97
1	N	213	VAL	O-C-N	-14.10	110.28	122.97
1	I	213	VAL	O-C-N	-14.10	110.28	122.97
1	J	213	VAL	O-C-N	-14.10	110.28	122.97
1	L	213	VAL	O-C-N	-14.10	110.28	122.97
1	F	29	VAL	CA-C-N	-14.09	101.08	120.38
1	F	29	VAL	C-N-CA	-14.09	101.08	120.38
1	A	29	VAL	CA-C-N	-14.08	101.09	120.38
1	A	29	VAL	C-N-CA	-14.08	101.09	120.38
1	B	29	VAL	CA-C-N	-14.08	101.09	120.38
1	B	29	VAL	C-N-CA	-14.08	101.09	120.38
1	C	29	VAL	CA-C-N	-14.06	101.11	120.38
1	C	29	VAL	C-N-CA	-14.06	101.11	120.38
1	D	29	VAL	CA-C-N	-14.06	101.12	120.38
1	D	29	VAL	C-N-CA	-14.06	101.12	120.38
1	E	29	VAL	CA-C-N	-14.06	101.12	120.38
1	E	29	VAL	C-N-CA	-14.06	101.12	120.38
1	G	29	VAL	CA-C-N	-14.06	101.12	120.38
1	G	29	VAL	C-N-CA	-14.06	101.12	120.38
1	H	213	VAL	O-C-N	-14.06	110.32	122.97
1	M	213	VAL	O-C-N	-14.03	110.34	122.97
1	M	242	LYS	CB-CA-C	13.98	132.26	109.89
1	I	260	ALA	N-CA-CB	13.97	130.65	110.12
1	L	260	ALA	N-CA-CB	13.93	130.60	110.12
1	K	153	ASN	CA-CB-CG	12.58	125.18	112.60
1	I	153	ASN	CA-CB-CG	12.57	125.17	112.60
1	L	153	ASN	CA-CB-CG	12.57	125.17	112.60
1	H	153	ASN	CA-CB-CG	12.56	125.16	112.60
1	J	153	ASN	CA-CB-CG	12.54	125.14	112.60
1	M	153	ASN	CA-CB-CG	12.53	125.13	112.60
1	N	153	ASN	CA-CB-CG	12.52	125.12	112.60
1	I	37	ASN	N-CA-CB	12.43	128.07	110.17
1	M	37	ASN	N-CA-CB	12.40	128.03	110.17
1	H	37	ASN	N-CA-CB	12.40	128.03	110.17
1	J	37	ASN	N-CA-CB	12.40	128.03	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	37	ASN	N-CA-CB	12.40	128.03	110.17
1	N	37	ASN	N-CA-CB	12.40	128.03	110.17
1	L	37	ASN	N-CA-CB	12.39	128.01	110.17
1	D	41	ASP	N-CA-CB	12.37	127.99	110.17
1	I	260	ALA	CB-CA-C	-12.37	90.27	110.79
1	C	41	ASP	N-CA-CB	12.36	127.96	110.17
1	L	260	ALA	CB-CA-C	-12.35	90.28	110.79
1	B	41	ASP	N-CA-CB	12.35	127.95	110.17
1	E	41	ASP	N-CA-CB	12.34	127.95	110.17
1	A	41	ASP	N-CA-CB	12.34	127.94	110.17
1	G	41	ASP	N-CA-CB	12.34	127.94	110.17
1	F	41	ASP	N-CA-CB	12.33	127.93	110.17
1	E	56	VAL	CB-CA-C	-12.27	95.94	112.02
1	G	56	VAL	CB-CA-C	-12.26	95.96	112.02
1	A	56	VAL	CB-CA-C	-12.25	95.97	112.02
1	D	56	VAL	CB-CA-C	-12.25	95.97	112.02
1	F	56	VAL	CB-CA-C	-12.24	95.98	112.02
1	C	56	VAL	CB-CA-C	-12.24	95.98	112.02
1	B	56	VAL	CB-CA-C	-12.23	95.99	112.02
1	B	230	ILE	O-C-N	12.03	133.54	121.87
1	D	230	ILE	O-C-N	12.02	133.53	121.87
1	A	230	ILE	O-C-N	12.02	133.53	121.87
1	F	230	ILE	O-C-N	12.00	133.51	121.87
1	E	230	ILE	O-C-N	12.00	133.51	121.87
1	G	230	ILE	O-C-N	12.00	133.51	121.87
1	C	230	ILE	O-C-N	11.99	133.50	121.87
1	C	7	LYS	O-C-N	11.96	139.14	123.11
1	G	7	LYS	O-C-N	11.94	139.11	123.11
1	A	7	LYS	O-C-N	11.94	139.11	123.11
1	E	7	LYS	O-C-N	11.93	139.10	123.11
1	B	7	LYS	O-C-N	11.92	139.08	123.11
1	K	242	LYS	CB-CA-C	11.91	128.95	109.89
1	F	7	LYS	O-C-N	11.90	139.05	123.11
1	D	7	LYS	O-C-N	11.89	139.04	123.11
1	L	77	VAL	CB-CA-C	-11.74	96.94	111.97
1	K	77	VAL	CB-CA-C	-11.74	96.95	111.97
1	N	77	VAL	CB-CA-C	-11.74	96.95	111.97
1	I	77	VAL	CB-CA-C	-11.73	96.95	111.97
1	J	77	VAL	CB-CA-C	-11.73	96.96	111.97
1	H	77	VAL	CB-CA-C	-11.72	96.97	111.97
1	M	77	VAL	CB-CA-C	-11.71	96.98	111.97
1	G	213	VAL	O-C-N	11.64	136.27	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	213	VAL	O-C-N	11.64	136.27	123.00
1	E	213	VAL	O-C-N	11.63	136.26	123.00
1	C	213	VAL	O-C-N	11.63	136.26	123.00
1	H	242	LYS	CB-CA-C	11.62	128.48	109.89
1	B	213	VAL	O-C-N	11.62	136.25	123.00
1	D	213	VAL	O-C-N	11.58	136.20	123.00
1	D	39	VAL	O-C-N	11.43	134.80	123.14
1	F	39	VAL	O-C-N	11.40	134.77	123.14
1	N	207	LYS	CB-CG-CD	11.40	137.51	111.30
1	A	39	VAL	O-C-N	11.37	134.74	123.14
1	B	39	VAL	O-C-N	11.37	134.74	123.14
1	G	39	VAL	O-C-N	11.37	134.74	123.14
1	C	39	VAL	O-C-N	11.36	134.72	123.14
1	E	39	VAL	O-C-N	11.34	134.71	123.14
1	D	225	LYS	N-CA-CB	10.99	125.97	110.26
1	B	225	LYS	N-CA-CB	10.98	125.97	110.26
1	G	225	LYS	N-CA-CB	10.98	125.96	110.26
1	E	225	LYS	N-CA-CB	10.98	125.96	110.26
1	A	225	LYS	N-CA-CB	10.98	125.96	110.26
1	C	225	LYS	N-CA-CB	10.96	125.94	110.26
1	F	225	LYS	N-CA-CB	10.96	125.94	110.26
1	C	359	ASP	CA-CB-CG	-10.85	101.75	112.60
1	G	359	ASP	CA-CB-CG	-10.85	101.75	112.60
1	F	359	ASP	CA-CB-CG	-10.83	101.77	112.60
1	A	359	ASP	CA-CB-CG	-10.82	101.78	112.60
1	E	214	GLU	CB-CA-C	-10.82	90.71	109.65
1	D	359	ASP	CA-CB-CG	-10.82	101.78	112.60
1	E	359	ASP	CA-CB-CG	-10.82	101.78	112.60
1	N	52	ASP	CA-CB-CG	-10.82	101.78	112.60
1	B	359	ASP	CA-CB-CG	-10.82	101.78	112.60
1	D	214	GLU	CB-CA-C	-10.82	90.72	109.65
1	F	214	GLU	CB-CA-C	-10.82	90.72	109.65
1	K	52	ASP	CA-CB-CG	-10.82	101.78	112.60
1	M	52	ASP	CA-CB-CG	-10.82	101.78	112.60
1	H	52	ASP	CA-CB-CG	-10.81	101.79	112.60
1	B	214	GLU	CB-CA-C	-10.80	90.74	109.65
1	G	214	GLU	CB-CA-C	-10.80	90.74	109.65
1	C	214	GLU	CB-CA-C	-10.79	90.76	109.65
1	L	52	ASP	CA-CB-CG	-10.79	101.81	112.60
1	J	52	ASP	CA-CB-CG	-10.78	101.82	112.60
1	I	52	ASP	CA-CB-CG	-10.77	101.83	112.60
1	N	219	PHE	N-CA-CB	10.66	127.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	219	PHE	N-CA-CB	10.61	127.42	110.23
1	L	219	PHE	N-CA-CB	10.55	127.31	110.23
1	I	219	PHE	N-CA-CB	10.54	127.30	110.23
1	J	260	ALA	CB-CA-C	-10.54	93.30	110.79
1	M	219	PHE	N-CA-CB	10.54	127.30	110.23
1	H	260	ALA	CB-CA-C	-10.53	93.31	110.79
1	J	219	PHE	N-CA-CB	10.53	127.28	110.23
1	K	260	ALA	CB-CA-C	-10.51	93.35	110.79
1	H	219	PHE	N-CA-CB	10.50	127.23	110.23
1	A	214	GLU	CB-CA-C	-10.48	90.73	109.70
1	A	518	GLU	N-CA-CB	10.45	125.22	110.07
1	C	461	GLU	CB-CA-C	10.39	120.46	110.17
1	E	518	GLU	N-CA-CB	10.39	125.14	110.07
1	B	461	GLU	CB-CA-C	10.38	120.44	110.17
1	C	518	GLU	N-CA-CB	10.37	125.11	110.07
1	G	518	GLU	N-CA-CB	10.34	125.07	110.07
1	F	518	GLU	N-CA-CB	10.34	125.07	110.07
1	D	518	GLU	N-CA-CB	10.34	125.06	110.07
1	B	518	GLU	N-CA-CB	10.33	125.05	110.07
1	D	461	GLU	CB-CA-C	10.32	120.39	110.17
1	A	461	GLU	CB-CA-C	10.31	120.38	110.17
1	M	260	ALA	CB-CA-C	-10.27	93.74	110.79
1	E	461	GLU	CB-CA-C	10.22	120.29	110.17
1	E	213	VAL	CA-C-N	-10.21	105.17	122.33
1	E	213	VAL	C-N-CA	-10.21	105.17	122.33
1	F	213	VAL	CA-C-N	-10.21	105.18	122.33
1	F	213	VAL	C-N-CA	-10.21	105.18	122.33
1	G	461	GLU	CB-CA-C	10.20	120.27	110.17
1	B	213	VAL	CA-C-N	-10.19	105.21	122.33
1	B	213	VAL	C-N-CA	-10.19	105.21	122.33
1	G	213	VAL	CA-C-N	-10.19	105.21	122.33
1	G	213	VAL	C-N-CA	-10.19	105.21	122.33
1	L	115	ASP	CB-CA-C	10.18	127.69	110.79
1	N	115	ASP	CB-CA-C	10.18	127.68	110.79
1	C	213	VAL	CA-C-N	-10.17	105.24	122.33
1	C	213	VAL	C-N-CA	-10.17	105.24	122.33
1	I	115	ASP	CB-CA-C	10.17	127.68	110.79
1	D	213	VAL	CA-C-N	-10.17	105.24	122.33
1	D	213	VAL	C-N-CA	-10.17	105.24	122.33
1	H	115	ASP	CB-CA-C	10.17	127.67	110.79
1	K	115	ASP	CB-CA-C	10.17	127.67	110.79
1	J	115	ASP	CB-CA-C	10.16	127.66	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	115	ASP	CB-CA-C	10.16	127.66	110.79
1	F	461	GLU	CB-CA-C	10.15	120.22	110.17
1	L	257	GLU	N-CA-CB	-10.05	95.44	110.01
1	N	207	LYS	CA-CB-CG	9.98	134.07	114.10
1	N	310	GLU	CB-CA-C	-9.95	94.28	110.79
1	H	310	GLU	CB-CA-C	-9.94	94.29	110.79
1	K	310	GLU	CB-CA-C	-9.94	94.30	110.79
1	M	310	GLU	CB-CA-C	-9.88	94.39	110.79
1	J	310	GLU	CB-CA-C	-9.87	94.40	110.79
1	L	310	GLU	CB-CA-C	-9.87	94.41	110.79
1	I	310	GLU	CB-CA-C	-9.81	94.50	110.79
1	N	260	ALA	CB-CA-C	-9.74	94.62	110.79
1	L	401	HIS	CA-CB-CG	9.66	123.46	113.80
1	J	401	HIS	CA-CB-CG	9.66	123.46	113.80
1	K	401	HIS	CA-CB-CG	9.65	123.45	113.80
1	N	401	HIS	CA-CB-CG	9.64	123.44	113.80
1	I	401	HIS	CA-CB-CG	9.64	123.44	113.80
1	M	401	HIS	CA-CB-CG	9.64	123.44	113.80
1	H	401	HIS	CA-CB-CG	9.63	123.43	113.80
1	K	283	ASP	CA-CB-CG	-9.63	102.97	112.60
1	H	283	ASP	CA-CB-CG	-9.61	102.99	112.60
1	L	224	ASP	N-CA-CB	9.52	124.25	110.16
1	N	224	ASP	N-CA-CB	9.51	124.23	110.16
1	M	224	ASP	N-CA-CB	9.51	124.23	110.16
1	F	316	ASP	N-CA-CB	9.32	123.95	110.16
1	A	316	ASP	N-CA-CB	9.31	123.95	110.16
1	B	316	ASP	N-CA-CB	9.31	123.94	110.16
1	C	316	ASP	N-CA-CB	9.31	123.94	110.16
1	E	316	ASP	N-CA-CB	9.31	123.93	110.16
1	M	283	ASP	CA-CB-CG	-9.30	103.30	112.60
1	N	283	ASP	CA-CB-CG	-9.30	103.30	112.60
1	G	316	ASP	N-CA-CB	9.30	123.92	110.16
1	D	316	ASP	N-CA-CB	9.29	123.91	110.16
1	L	283	ASP	CA-CB-CG	-9.29	103.31	112.60
1	J	300	VAL	CB-CA-C	-9.29	98.81	111.63
1	I	300	VAL	CB-CA-C	-9.28	98.83	111.63
1	G	221	LEU	CA-C-N	-9.26	109.98	122.85
1	G	221	LEU	C-N-CA	-9.26	109.98	122.85
1	B	221	LEU	CA-C-N	-9.25	110.00	122.85
1	B	221	LEU	C-N-CA	-9.25	110.00	122.85
1	F	221	LEU	CA-C-N	-9.24	110.00	122.85
1	F	221	LEU	C-N-CA	-9.24	110.00	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LEU	CA-C-N	-9.24	110.00	122.85
1	A	221	LEU	C-N-CA	-9.24	110.00	122.85
1	D	221	LEU	CA-C-N	-9.23	110.02	122.85
1	D	221	LEU	C-N-CA	-9.23	110.02	122.85
1	E	221	LEU	CA-C-N	-9.23	110.02	122.85
1	E	221	LEU	C-N-CA	-9.23	110.02	122.85
1	E	192	GLY	CA-C-N	-9.23	109.99	122.72
1	E	192	GLY	C-N-CA	-9.23	109.99	122.72
1	A	192	GLY	CA-C-N	-9.22	110.00	122.72
1	A	192	GLY	C-N-CA	-9.22	110.00	122.72
1	C	221	LEU	CA-C-N	-9.22	110.03	122.85
1	C	221	LEU	C-N-CA	-9.22	110.03	122.85
1	F	52	ASP	CA-C-N	-9.22	103.35	121.41
1	F	52	ASP	C-N-CA	-9.22	103.35	121.41
1	G	52	ASP	CA-C-N	-9.22	103.34	121.41
1	G	52	ASP	C-N-CA	-9.22	103.34	121.41
1	D	192	GLY	CA-C-N	-9.21	110.00	122.72
1	D	192	GLY	C-N-CA	-9.21	110.00	122.72
1	C	52	ASP	CA-C-N	-9.21	103.35	121.41
1	C	52	ASP	C-N-CA	-9.21	103.35	121.41
1	F	192	GLY	CA-C-N	-9.21	110.01	122.72
1	F	192	GLY	C-N-CA	-9.21	110.01	122.72
1	A	52	ASP	CA-C-N	-9.21	103.36	121.41
1	A	52	ASP	C-N-CA	-9.21	103.36	121.41
1	D	52	ASP	CA-C-N	-9.21	103.36	121.41
1	D	52	ASP	C-N-CA	-9.21	103.36	121.41
1	K	115	ASP	CA-CB-CG	-9.19	103.41	112.60
1	B	52	ASP	CA-C-N	-9.19	103.40	121.41
1	B	52	ASP	C-N-CA	-9.19	103.40	121.41
1	E	52	ASP	CA-C-N	-9.19	103.41	121.41
1	E	52	ASP	C-N-CA	-9.19	103.41	121.41
1	L	300	VAL	CB-CA-C	-9.18	98.97	111.63
1	J	224	ASP	N-CA-CB	9.18	123.74	110.16
1	N	300	VAL	CB-CA-C	-9.18	98.97	111.63
1	J	283	ASP	CA-CB-CG	-9.17	103.43	112.60
1	J	115	ASP	CA-CB-CG	-9.17	103.43	112.60
1	I	224	ASP	N-CA-CB	9.17	123.73	110.16
1	I	283	ASP	CA-CB-CG	-9.16	103.44	112.60
1	M	115	ASP	CA-CB-CG	-9.16	103.44	112.60
1	H	115	ASP	CA-CB-CG	-9.15	103.45	112.60
1	K	300	VAL	CB-CA-C	-9.15	99.00	111.63
1	L	115	ASP	CA-CB-CG	-9.14	103.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	115	ASP	CA-CB-CG	-9.13	103.47	112.60
1	M	300	VAL	CB-CA-C	-9.13	99.03	111.63
1	H	300	VAL	CB-CA-C	-9.12	99.05	111.63
1	I	303	GLU	CB-CA-C	-9.12	95.35	110.85
1	N	115	ASP	CA-CB-CG	-9.11	103.49	112.60
1	J	303	GLU	CB-CA-C	-9.09	95.40	110.85
1	E	49	ILE	N-CA-CB	-8.96	100.61	111.90
1	A	49	ILE	N-CA-CB	-8.95	100.62	111.90
1	C	49	ILE	N-CA-CB	-8.95	100.63	111.90
1	G	49	ILE	N-CA-CB	-8.94	100.63	111.90
1	B	49	ILE	N-CA-CB	-8.94	100.64	111.90
1	D	401	HIS	CA-CB-CG	8.94	122.74	113.80
1	F	49	ILE	N-CA-CB	-8.93	100.64	111.90
1	N	208	PRO	O-C-N	-8.92	110.60	122.64
1	D	49	ILE	N-CA-CB	-8.91	100.67	111.90
1	F	401	HIS	CA-CB-CG	8.91	122.71	113.80
1	B	401	HIS	CA-CB-CG	8.90	122.70	113.80
1	E	401	HIS	CA-CB-CG	8.90	122.70	113.80
1	A	401	HIS	CA-CB-CG	8.89	122.69	113.80
1	C	401	HIS	CA-CB-CG	8.87	122.67	113.80
1	G	401	HIS	CA-CB-CG	8.87	122.67	113.80
1	L	369	VAL	N-CA-CB	8.80	122.50	110.54
1	K	369	VAL	N-CA-CB	8.79	122.50	110.54
1	J	369	VAL	N-CA-CB	8.79	122.49	110.54
1	M	369	VAL	N-CA-CB	8.79	122.49	110.54
1	I	369	VAL	N-CA-CB	8.78	122.49	110.54
1	M	229	ASN	CA-CB-CG	8.77	121.37	112.60
1	H	369	VAL	N-CA-CB	8.76	122.46	110.54
1	N	369	VAL	N-CA-CB	8.76	122.46	110.54
1	H	224	ASP	N-CA-CB	8.74	123.10	110.16
1	K	224	ASP	N-CA-CB	8.72	123.07	110.16
1	H	303	GLU	CB-CA-C	-8.63	96.18	110.85
1	K	303	GLU	CB-CA-C	-8.63	96.18	110.85
1	H	265	ASN	CA-CB-CG	-8.55	104.05	112.60
1	D	252	GLU	N-CA-CB	8.51	122.34	110.01
1	G	252	GLU	N-CA-CB	8.51	122.34	110.01
1	B	252	GLU	N-CA-CB	8.50	122.34	110.01
1	C	252	GLU	N-CA-CB	8.50	122.34	110.01
1	A	252	GLU	N-CA-CB	8.49	122.33	110.01
1	F	252	GLU	N-CA-CB	8.49	122.32	110.01
1	E	252	GLU	N-CA-CB	8.49	122.32	110.01
1	J	265	ASN	CA-CB-CG	-8.43	104.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	207	LYS	CB-CA-C	8.40	126.73	110.17
1	K	265	ASN	CA-CB-CG	-8.38	104.22	112.60
1	C	39	VAL	N-CA-CB	8.34	126.64	111.21
1	F	39	VAL	N-CA-CB	8.33	126.63	111.21
1	A	39	VAL	N-CA-CB	8.33	126.62	111.21
1	G	39	VAL	N-CA-CB	8.33	126.62	111.21
1	E	39	VAL	N-CA-CB	8.33	126.61	111.21
1	N	185	ASP	CB-CA-C	8.32	124.36	110.79
1	H	185	ASP	CB-CA-C	8.32	124.36	110.79
1	I	185	ASP	CB-CA-C	8.32	124.35	110.79
1	D	39	VAL	N-CA-CB	8.32	126.60	111.21
1	L	185	ASP	CB-CA-C	8.32	124.35	110.79
1	B	39	VAL	N-CA-CB	8.31	126.59	111.21
1	J	185	ASP	CB-CA-C	8.31	124.34	110.79
1	M	185	ASP	CB-CA-C	8.31	124.34	110.79
1	C	196	ASP	CA-CB-CG	-8.30	104.30	112.60
1	D	273	VAL	CB-CA-C	-8.24	99.11	111.80
1	B	273	VAL	CB-CA-C	-8.23	99.13	111.80
1	C	273	VAL	CB-CA-C	-8.23	99.13	111.80
1	F	273	VAL	CB-CA-C	-8.23	99.13	111.80
1	G	273	VAL	CB-CA-C	-8.23	99.13	111.80
1	A	273	VAL	CB-CA-C	-8.22	99.13	111.80
1	E	273	VAL	CB-CA-C	-8.22	99.14	111.80
1	D	411	VAL	CB-CA-C	-8.16	100.60	111.70
1	G	411	VAL	CB-CA-C	-8.16	100.60	111.70
1	F	411	VAL	CB-CA-C	-8.16	100.61	111.70
1	A	411	VAL	CB-CA-C	-8.15	100.61	111.70
1	M	266	THR	N-CA-CB	8.15	122.11	110.12
1	E	411	VAL	CB-CA-C	-8.15	100.62	111.70
1	N	266	THR	N-CA-CB	8.15	122.09	110.12
1	H	243	ALA	N-CA-CB	8.14	122.62	110.40
1	B	411	VAL	CB-CA-C	-8.14	100.63	111.70
1	C	411	VAL	CB-CA-C	-8.14	100.63	111.70
1	H	266	THR	N-CA-CB	8.13	122.08	110.12
1	K	243	ALA	N-CA-CB	8.13	122.60	110.40
1	K	266	THR	N-CA-CB	8.12	122.06	110.12
1	C	34	LYS	N-CA-CB	8.12	121.78	110.01
1	I	266	THR	N-CA-CB	8.12	122.06	110.12
1	L	303	GLU	CB-CA-C	-8.12	97.05	110.85
1	N	303	GLU	CB-CA-C	-8.12	97.05	110.85
1	M	303	GLU	CB-CA-C	-8.12	97.05	110.85
1	A	34	LYS	N-CA-CB	8.12	121.78	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	LYS	N-CA-CB	8.11	121.77	110.01
1	L	266	THR	N-CA-CB	8.11	122.04	110.12
1	D	34	LYS	N-CA-CB	8.11	121.77	110.01
1	F	34	LYS	N-CA-CB	8.11	121.76	110.01
1	M	243	ALA	N-CA-CB	8.10	122.55	110.40
1	E	34	LYS	N-CA-CB	8.10	121.75	110.01
1	G	34	LYS	N-CA-CB	8.09	121.75	110.01
1	N	207	LYS	CD-CE-NZ	8.09	137.79	111.90
1	J	266	THR	N-CA-CB	8.09	122.01	110.12
1	N	243	ALA	N-CA-CB	8.07	122.51	110.40
1	J	243	ALA	N-CA-CB	8.07	122.51	110.40
1	I	243	ALA	N-CA-CB	8.07	122.50	110.40
1	B	367	GLU	CB-CA-C	-8.06	97.41	110.79
1	L	243	ALA	N-CA-CB	8.06	122.49	110.40
1	D	367	GLU	CB-CA-C	-8.06	97.42	110.79
1	F	367	GLU	CB-CA-C	-8.06	97.42	110.79
1	C	367	GLU	CB-CA-C	-8.05	97.42	110.79
1	H	206	ASN	CA-CB-CG	-8.05	104.55	112.60
1	A	367	GLU	CB-CA-C	-8.05	97.43	110.79
1	E	367	GLU	CB-CA-C	-8.04	97.45	110.79
1	G	367	GLU	CB-CA-C	-8.04	97.45	110.79
1	A	115	ASP	CA-CB-CG	-8.03	104.58	112.60
1	C	252	GLU	CB-CG-CD	8.01	126.21	112.60
1	C	321	LYS	N-CA-C	-8.00	102.51	111.71
1	D	321	LYS	N-CA-C	-7.99	102.52	111.71
1	G	321	LYS	N-CA-C	-7.99	102.52	111.71
1	B	321	LYS	N-CA-C	-7.99	102.52	111.71
1	E	321	LYS	N-CA-C	-7.99	102.53	111.71
1	D	252	GLU	CB-CG-CD	7.98	126.17	112.60
1	A	321	LYS	N-CA-C	-7.98	102.53	111.71
1	F	252	GLU	CB-CG-CD	7.98	126.16	112.60
1	G	252	GLU	CB-CG-CD	7.98	126.16	112.60
1	A	252	GLU	CB-CG-CD	7.97	126.15	112.60
1	E	252	GLU	CB-CG-CD	7.97	126.15	112.60
1	B	252	GLU	CB-CG-CD	7.97	126.14	112.60
1	F	321	LYS	N-CA-C	-7.96	102.56	111.71
1	N	50	THR	CB-CA-C	7.96	123.37	110.88
1	H	483	GLU	CB-CG-CD	7.95	126.12	112.60
1	J	483	GLU	CB-CG-CD	7.95	126.12	112.60
1	K	483	GLU	CB-CG-CD	7.95	126.12	112.60
1	N	483	GLU	CB-CG-CD	7.95	126.11	112.60
1	J	50	THR	CB-CA-C	7.95	123.36	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	LYS	N-CA-CB	7.95	121.80	110.12
1	L	483	GLU	CB-CG-CD	7.95	126.11	112.60
1	F	326	ASN	CA-CB-CG	7.95	120.55	112.60
1	C	311	LYS	N-CA-CB	7.94	121.79	110.12
1	K	50	THR	CB-CA-C	7.94	123.34	110.88
1	G	311	LYS	N-CA-CB	7.94	121.79	110.12
1	M	50	THR	CB-CA-C	7.94	123.34	110.88
1	M	483	GLU	CB-CG-CD	7.93	126.09	112.60
1	L	50	THR	CB-CA-C	7.93	123.33	110.88
1	G	326	ASN	CA-CB-CG	7.93	120.53	112.60
1	A	311	LYS	N-CA-CB	7.93	121.78	110.12
1	B	326	ASN	CA-CB-CG	7.93	120.53	112.60
1	A	326	ASN	CA-CB-CG	7.92	120.52	112.60
1	B	311	LYS	N-CA-CB	7.92	121.77	110.12
1	E	311	LYS	N-CA-CB	7.92	121.76	110.12
1	H	50	THR	CB-CA-C	7.92	123.32	110.88
1	F	311	LYS	N-CA-CB	7.92	121.76	110.12
1	I	483	GLU	CB-CG-CD	7.92	126.06	112.60
1	I	50	THR	CB-CA-C	7.91	123.30	110.88
1	E	326	ASN	CA-CB-CG	7.91	120.51	112.60
1	C	326	ASN	CA-CB-CG	7.90	120.50	112.60
1	D	326	ASN	CA-CB-CG	7.89	120.49	112.60
1	N	252	GLU	CB-CA-C	-7.88	98.51	110.88
1	L	252	GLU	CB-CA-C	-7.87	98.53	110.88
1	K	482	THR	N-CA-CB	7.87	121.80	110.16
1	M	482	THR	N-CA-CB	7.87	121.80	110.16
1	H	482	THR	N-CA-CB	7.87	121.80	110.16
1	M	252	GLU	CB-CA-C	-7.87	98.53	110.88
1	N	482	THR	N-CA-CB	7.86	121.80	110.16
1	J	482	THR	N-CA-CB	7.86	121.79	110.16
1	L	482	THR	N-CA-CB	7.86	121.79	110.16
1	I	482	THR	N-CA-CB	7.82	121.74	110.16
1	K	377	ALA	N-CA-CB	7.80	124.42	111.08
1	N	377	ALA	N-CA-CB	7.79	124.39	111.08
1	H	377	ALA	N-CA-CB	7.77	124.37	111.08
1	I	377	ALA	N-CA-CB	7.77	124.37	111.08
1	J	377	ALA	N-CA-CB	7.77	124.37	111.08
1	L	377	ALA	N-CA-CB	7.77	124.37	111.08
1	M	377	ALA	N-CA-CB	7.77	124.37	111.08
1	B	115	ASP	CA-CB-CG	-7.76	104.83	112.60
1	F	115	ASP	CA-CB-CG	-7.76	104.84	112.60
1	G	115	ASP	CA-CB-CG	-7.75	104.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	ASP	CA-CB-CG	-7.73	104.87	112.60
1	J	107	VAL	N-CA-CB	7.67	120.97	110.54
1	E	115	ASP	CA-CB-CG	-7.63	104.97	112.60
1	C	115	ASP	CA-CB-CG	-7.62	104.98	112.60
1	A	196	ASP	CA-CB-CG	-7.60	105.00	112.60
1	F	11	ASP	O-C-N	-7.60	113.33	122.22
1	C	11	ASP	O-C-N	-7.59	113.33	122.22
1	B	11	ASP	O-C-N	-7.59	113.34	122.22
1	A	11	ASP	O-C-N	-7.58	113.35	122.22
1	G	11	ASP	O-C-N	-7.58	113.35	122.22
1	D	11	ASP	O-C-N	-7.58	113.35	122.22
1	E	11	ASP	O-C-N	-7.58	113.35	122.22
1	K	37	ASN	CB-CA-C	7.57	123.46	109.54
1	J	37	ASN	CB-CA-C	7.55	123.43	109.54
1	L	37	ASN	CB-CA-C	7.55	123.43	109.54
1	N	208	PRO	CA-C-O	-7.54	106.87	120.60
1	N	37	ASN	CB-CA-C	7.54	123.42	109.54
1	H	37	ASN	CB-CA-C	7.54	123.41	109.54
1	M	37	ASN	CB-CA-C	7.54	123.41	109.54
1	I	37	ASN	CB-CA-C	7.53	123.40	109.54
1	B	258	ALA	N-CA-CB	7.52	120.91	110.01
1	C	258	ALA	N-CA-CB	7.52	120.91	110.01
1	D	258	ALA	N-CA-CB	7.52	120.91	110.01
1	A	258	ALA	N-CA-CB	7.51	120.91	110.01
1	J	397	GLU	CB-CA-C	7.51	123.26	110.79
1	K	397	GLU	CB-CA-C	7.51	123.25	110.79
1	H	397	GLU	CB-CA-C	7.51	123.25	110.79
1	E	258	ALA	N-CA-CB	7.50	120.89	110.01
1	M	397	GLU	CB-CA-C	7.50	123.25	110.79
1	L	397	GLU	CB-CA-C	7.50	123.24	110.79
1	F	258	ALA	N-CA-CB	7.50	120.88	110.01
1	D	193	MET	O-C-N	-7.49	114.81	123.27
1	G	258	ALA	N-CA-CB	7.49	120.87	110.01
1	I	397	GLU	CB-CA-C	7.49	123.22	110.79
1	H	368	ARG	CB-CA-C	-7.48	99.13	110.88
1	F	193	MET	O-C-N	-7.48	114.82	123.27
1	N	397	GLU	CB-CA-C	7.48	123.21	110.79
1	M	368	ARG	CB-CA-C	-7.48	99.14	110.88
1	K	368	ARG	CB-CA-C	-7.47	99.14	110.88
1	N	368	ARG	CB-CA-C	-7.47	99.15	110.88
1	L	107	VAL	N-CA-CB	7.47	120.70	110.54
1	A	193	MET	O-C-N	-7.47	114.83	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	86	GLY	N-CA-C	-7.46	106.20	115.08
1	L	368	ARG	CB-CA-C	-7.46	99.17	110.88
1	N	86	GLY	N-CA-C	-7.45	106.22	115.08
1	K	86	GLY	N-CA-C	-7.45	106.22	115.08
1	I	86	GLY	N-CA-C	-7.44	106.22	115.08
1	B	192	GLY	CA-C-N	-7.44	110.00	122.64
1	B	192	GLY	C-N-CA	-7.44	110.00	122.64
1	J	86	GLY	N-CA-C	-7.44	106.23	115.08
1	J	368	ARG	CB-CA-C	-7.44	99.20	110.88
1	C	59	GLU	N-CA-CB	-7.43	97.93	110.41
1	E	193	MET	O-C-N	-7.43	114.88	123.27
1	D	59	GLU	N-CA-CB	-7.43	97.93	110.41
1	I	368	ARG	CB-CA-C	-7.42	99.22	110.88
1	E	59	GLU	N-CA-CB	-7.42	97.94	110.41
1	L	86	GLY	N-CA-C	-7.42	106.25	115.08
1	H	86	GLY	N-CA-C	-7.42	106.25	115.08
1	A	59	GLU	N-CA-CB	-7.42	97.95	110.41
1	G	59	GLU	N-CA-CB	-7.42	97.95	110.41
1	B	59	GLU	N-CA-CB	-7.40	97.97	110.41
1	F	59	GLU	N-CA-CB	-7.40	97.98	110.41
1	C	87	ASP	N-CA-CB	7.39	122.79	111.56
1	I	107	VAL	N-CA-CB	7.39	120.59	110.54
1	G	87	ASP	N-CA-CB	7.38	122.78	111.56
1	A	87	ASP	N-CA-CB	7.38	122.78	111.56
1	E	87	ASP	N-CA-CB	7.37	122.77	111.56
1	F	195	PHE	CA-CB-CG	-7.37	106.43	113.80
1	K	107	VAL	N-CA-CB	7.37	120.56	110.54
1	F	369	VAL	N-CA-CB	7.36	120.55	110.54
1	E	369	VAL	N-CA-CB	7.35	120.54	110.54
1	C	369	VAL	N-CA-CB	7.35	120.54	110.54
1	A	369	VAL	N-CA-CB	7.33	120.51	110.54
1	B	369	VAL	N-CA-CB	7.33	120.51	110.54
1	D	369	VAL	N-CA-CB	7.33	120.51	110.54
1	M	379	ILE	CB-CA-C	-7.33	99.71	110.62
1	F	463	SER	N-CA-CB	7.32	120.89	110.12
1	G	369	VAL	N-CA-CB	7.32	120.50	110.54
1	H	379	ILE	CB-CA-C	-7.32	99.71	110.62
1	J	379	ILE	CB-CA-C	-7.32	99.72	110.62
1	I	379	ILE	CB-CA-C	-7.31	99.72	110.62
1	K	379	ILE	CB-CA-C	-7.30	99.73	110.62
1	L	379	ILE	CB-CA-C	-7.30	99.74	110.62
1	N	379	ILE	CB-CA-C	-7.30	99.75	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	463	SER	N-CA-CB	7.29	120.83	110.12
1	A	463	SER	N-CA-CB	7.29	120.83	110.12
1	G	463	SER	N-CA-CB	7.29	120.83	110.12
1	D	463	SER	N-CA-CB	7.27	120.81	110.12
1	G	192	GLY	CA-C-N	-7.27	112.69	122.72
1	G	192	GLY	C-N-CA	-7.27	112.69	122.72
1	N	240	VAL	CA-CB-CG2	-7.27	98.04	110.40
1	G	34	LYS	CB-CA-C	7.27	122.29	110.88
1	B	463	SER	N-CA-CB	7.26	120.80	110.12
1	F	34	LYS	CB-CA-C	7.26	122.27	110.88
1	A	34	LYS	CB-CA-C	7.25	122.27	110.88
1	E	34	LYS	CB-CA-C	7.25	122.27	110.88
1	K	56	VAL	CB-CA-C	-7.25	102.35	112.14
1	D	34	LYS	CB-CA-C	7.25	122.27	110.88
1	C	34	LYS	CB-CA-C	7.24	122.25	110.88
1	C	463	SER	N-CA-CB	7.24	120.76	110.12
1	H	56	VAL	CB-CA-C	-7.24	102.36	112.14
1	M	240	VAL	CA-CB-CG2	-7.24	98.09	110.40
1	J	56	VAL	CB-CA-C	-7.24	102.37	112.14
1	M	56	VAL	CB-CA-C	-7.24	102.37	112.14
1	B	34	LYS	CB-CA-C	7.23	122.23	110.88
1	I	56	VAL	CB-CA-C	-7.23	102.38	112.14
1	L	56	VAL	CB-CA-C	-7.23	102.38	112.14
1	N	59	GLU	CB-CA-C	7.22	122.78	110.79
1	N	56	VAL	CB-CA-C	-7.22	102.39	112.14
1	D	39	VAL	CA-C-N	-7.22	112.82	123.00
1	D	39	VAL	C-N-CA	-7.22	112.82	123.00
1	G	200	LEU	CD1-CG-CD2	7.22	126.68	110.80
1	J	59	GLU	CB-CA-C	7.22	122.77	110.79
1	K	59	GLU	CB-CA-C	7.22	122.77	110.79
1	A	371	LYS	CB-CA-C	7.22	122.30	110.90
1	F	371	LYS	CB-CA-C	7.22	122.30	110.90
1	I	240	VAL	CA-CB-CG2	-7.22	98.13	110.40
1	L	240	VAL	CA-CB-CG2	-7.21	98.14	110.40
1	B	371	LYS	CB-CA-C	7.21	122.29	110.90
1	H	59	GLU	CB-CA-C	7.21	122.76	110.79
1	G	371	LYS	CB-CA-C	7.21	122.29	110.90
1	M	59	GLU	CB-CA-C	7.21	122.75	110.79
1	B	149	THR	CB-CA-C	-7.21	99.56	110.88
1	C	371	LYS	CB-CA-C	7.21	122.29	110.90
1	E	371	LYS	CB-CA-C	7.21	122.28	110.90
1	F	39	VAL	CA-C-N	-7.20	112.84	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	39	VAL	C-N-CA	-7.20	112.84	123.00
1	L	59	GLU	CB-CA-C	7.20	122.75	110.79
1	B	39	VAL	CA-C-N	-7.20	112.86	123.00
1	B	39	VAL	C-N-CA	-7.20	112.86	123.00
1	I	59	GLU	CB-CA-C	7.20	122.73	110.79
1	A	39	VAL	CA-C-N	-7.19	112.86	123.00
1	A	39	VAL	C-N-CA	-7.19	112.86	123.00
1	D	371	LYS	CB-CA-C	7.19	122.27	110.90
1	J	240	VAL	CA-CB-CG2	-7.19	98.17	110.40
1	H	240	VAL	CA-CB-CG2	-7.19	98.17	110.40
1	D	457	ASN	CA-CB-CG	-7.19	105.41	112.60
1	G	39	VAL	CA-C-N	-7.19	112.86	123.00
1	G	39	VAL	C-N-CA	-7.19	112.86	123.00
1	K	240	VAL	CA-CB-CG2	-7.18	98.19	110.40
1	C	39	VAL	CA-C-N	-7.18	112.88	123.00
1	C	39	VAL	C-N-CA	-7.18	112.88	123.00
1	E	39	VAL	CA-C-N	-7.17	112.89	123.00
1	E	39	VAL	C-N-CA	-7.17	112.89	123.00
1	F	149	THR	CB-CA-C	-7.15	99.65	110.88
1	M	107	VAL	N-CA-CB	7.15	120.27	110.54
1	D	149	THR	CB-CA-C	-7.15	99.65	110.88
1	F	457	ASN	CA-CB-CG	-7.15	105.45	112.60
1	H	107	VAL	N-CA-CB	7.15	120.26	110.54
1	B	457	ASN	CA-CB-CG	-7.13	105.47	112.60
1	N	107	VAL	N-CA-CB	7.13	120.24	110.54
1	E	457	ASN	CA-CB-CG	-7.12	105.47	112.60
1	C	457	ASN	CA-CB-CG	-7.12	105.48	112.60
1	A	149	THR	CB-CA-C	-7.11	99.71	110.88
1	A	457	ASN	CA-CB-CG	-7.11	105.49	112.60
1	E	149	THR	CB-CA-C	-7.11	99.72	110.88
1	C	149	THR	CB-CA-C	-7.11	99.72	110.88
1	G	149	THR	CB-CA-C	-7.11	99.72	110.88
1	G	457	ASN	CA-CB-CG	-7.09	105.51	112.60
1	H	56	VAL	N-CA-CB	7.09	120.18	110.54
1	N	296	THR	N-CA-CB	7.09	120.54	110.12
1	K	56	VAL	N-CA-CB	7.08	120.17	110.54
1	M	56	VAL	N-CA-CB	7.08	120.16	110.54
1	L	296	THR	N-CA-CB	7.07	120.52	110.12
1	H	296	THR	N-CA-CB	7.07	120.52	110.12
1	J	296	THR	N-CA-CB	7.07	120.52	110.12
1	K	296	THR	N-CA-CB	7.07	120.51	110.12
1	I	56	VAL	N-CA-CB	7.07	120.15	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	296	THR	N-CA-CB	7.07	120.51	110.12
1	I	296	THR	N-CA-CB	7.07	120.51	110.12
1	J	56	VAL	N-CA-CB	7.07	120.15	110.54
1	L	56	VAL	N-CA-CB	7.06	120.15	110.54
1	N	56	VAL	N-CA-CB	7.06	120.14	110.54
1	N	6	VAL	CB-CA-C	-7.04	100.34	110.83
1	I	6	VAL	CB-CA-C	-7.03	100.35	110.83
1	H	6	VAL	CB-CA-C	-7.03	100.36	110.83
1	H	365	LEU	CB-CA-C	7.03	122.45	110.79
1	J	365	LEU	CB-CA-C	7.03	122.45	110.79
1	I	365	LEU	CB-CA-C	7.02	122.45	110.79
1	L	6	VAL	CB-CA-C	-7.02	100.37	110.83
1	K	365	LEU	CB-CA-C	7.02	122.44	110.79
1	M	6	VAL	CB-CA-C	-7.02	100.37	110.83
1	K	6	VAL	CB-CA-C	-7.02	100.37	110.83
1	M	365	LEU	CB-CA-C	7.02	122.44	110.79
1	J	6	VAL	CB-CA-C	-7.01	100.38	110.83
1	L	365	LEU	CB-CA-C	7.01	122.43	110.79
1	N	365	LEU	CB-CA-C	7.01	122.42	110.79
1	I	363	GLU	CB-CA-C	6.99	122.39	110.79
1	J	363	GLU	CB-CA-C	6.98	122.38	110.79
1	G	73	MET	CB-CA-C	-6.97	99.88	110.90
1	M	34	LYS	CB-CA-C	6.97	124.05	110.67
1	D	73	MET	CB-CA-C	-6.97	99.89	110.90
1	A	73	MET	CB-CA-C	-6.96	99.90	110.90
1	H	34	LYS	CB-CA-C	6.96	124.04	110.67
1	H	363	GLU	CB-CA-C	6.96	122.34	110.79
1	J	34	LYS	CB-CA-C	6.96	124.03	110.67
1	K	34	LYS	CB-CA-C	6.96	124.03	110.67
1	I	34	LYS	CB-CA-C	6.96	124.02	110.67
1	L	363	GLU	CB-CA-C	6.95	122.33	110.79
1	L	34	LYS	CB-CA-C	6.95	124.02	110.67
1	B	73	MET	CB-CA-C	-6.95	99.92	110.90
1	E	73	MET	CB-CA-C	-6.95	99.92	110.90
1	N	34	LYS	CB-CA-C	6.95	124.02	110.67
1	C	73	MET	CB-CA-C	-6.95	99.92	110.90
1	M	363	GLU	CB-CA-C	6.95	122.33	110.79
1	N	363	GLU	CB-CA-C	6.95	122.32	110.79
1	F	73	MET	CB-CA-C	-6.94	99.93	110.90
1	K	363	GLU	CB-CA-C	6.94	122.32	110.79
1	E	334	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	334	ASP	CA-CB-CG	6.92	119.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	229	ASN	CA-CB-CG	6.89	119.49	112.60
1	F	87	ASP	N-CA-CB	6.88	122.03	111.56
1	A	334	ASP	CA-CB-CG	6.87	119.47	112.60
1	I	229	ASN	CA-CB-CG	6.87	119.47	112.60
1	C	334	ASP	CA-CB-CG	6.86	119.46	112.60
1	D	87	ASP	N-CA-CB	6.86	121.98	111.56
1	D	334	ASP	CA-CB-CG	6.85	119.45	112.60
1	F	324	VAL	N-CA-CB	-6.85	100.20	111.44
1	G	324	VAL	N-CA-CB	-6.85	100.21	111.44
1	G	334	ASP	CA-CB-CG	6.85	119.45	112.60
1	D	173	GLY	CA-C-N	-6.84	110.04	122.43
1	D	173	GLY	C-N-CA	-6.84	110.04	122.43
1	F	334	ASP	CA-CB-CG	6.84	119.44	112.60
1	E	173	GLY	CA-C-N	-6.84	110.05	122.43
1	E	173	GLY	C-N-CA	-6.84	110.05	122.43
1	E	324	VAL	N-CA-CB	-6.84	100.22	111.44
1	I	242	LYS	CA-CB-CG	6.84	127.78	114.10
1	A	324	VAL	N-CA-CB	-6.84	100.23	111.44
1	C	324	VAL	N-CA-CB	-6.83	100.23	111.44
1	D	324	VAL	N-CA-CB	-6.83	100.23	111.44
1	F	401	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	J	242	LYS	CA-CB-CG	6.83	127.76	114.10
1	C	304	GLU	CB-CA-C	-6.83	100.16	110.88
1	B	324	VAL	N-CA-CB	-6.83	100.24	111.44
1	A	173	GLY	CA-C-N	-6.82	110.08	122.43
1	A	173	GLY	C-N-CA	-6.82	110.08	122.43
1	C	173	GLY	CA-C-N	-6.82	110.08	122.43
1	C	173	GLY	C-N-CA	-6.82	110.08	122.43
1	G	173	GLY	CA-C-N	-6.82	110.08	122.43
1	G	173	GLY	C-N-CA	-6.82	110.08	122.43
1	G	304	GLU	CB-CA-C	-6.82	100.17	110.88
1	D	304	GLU	CB-CA-C	-6.82	100.17	110.88
1	B	173	GLY	CA-C-N	-6.82	110.09	122.43
1	B	173	GLY	C-N-CA	-6.82	110.09	122.43
1	E	304	GLU	CB-CA-C	-6.82	100.17	110.88
1	F	173	GLY	CA-C-N	-6.82	110.09	122.43
1	F	173	GLY	C-N-CA	-6.82	110.09	122.43
1	C	401	HIS	CB-CG-CD2	-6.82	122.34	131.20
1	A	304	GLU	CB-CA-C	-6.80	100.20	110.88
1	N	242	LYS	CA-CB-CG	6.80	127.71	114.10
1	B	401	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	B	304	GLU	CB-CA-C	-6.80	100.20	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	GLU	CB-CA-C	-6.80	100.21	110.88
1	F	247	LEU	CB-CA-C	-6.79	97.28	109.71
1	A	247	LEU	CB-CA-C	-6.79	97.28	109.71
1	D	247	LEU	CB-CA-C	-6.79	97.28	109.71
1	E	247	LEU	CB-CA-C	-6.79	97.28	109.71
1	E	401	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	G	401	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	B	247	LEU	CB-CA-C	-6.79	97.29	109.71
1	G	247	LEU	CB-CA-C	-6.78	97.30	109.71
1	D	401	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	C	247	LEU	CB-CA-C	-6.78	97.31	109.71
1	F	283	ASP	CA-CB-CG	-6.76	105.84	112.60
1	A	401	HIS	CB-CG-CD2	-6.76	122.41	131.20
1	L	242	LYS	CA-CB-CG	6.76	127.63	114.10
1	D	36	ARG	CA-C-N	6.76	134.45	121.54
1	D	36	ARG	C-N-CA	6.76	134.45	121.54
1	D	251	ALA	N-CA-CB	-6.76	100.63	110.70
1	N	411	VAL	CB-CA-C	-6.76	101.17	110.90
1	F	36	ARG	CA-C-N	6.75	134.43	121.54
1	F	36	ARG	C-N-CA	6.75	134.43	121.54
1	I	411	VAL	CB-CA-C	-6.75	101.18	110.90
1	N	208	PRO	N-CA-CB	-6.75	96.16	103.25
1	B	36	ARG	CA-C-N	6.75	134.43	121.54
1	B	36	ARG	C-N-CA	6.75	134.43	121.54
1	A	251	ALA	N-CA-CB	-6.75	100.65	110.70
1	E	251	ALA	N-CA-CB	-6.75	100.65	110.70
1	C	36	ARG	CA-C-N	6.74	134.42	121.54
1	C	36	ARG	C-N-CA	6.74	134.42	121.54
1	E	36	ARG	CA-C-N	6.74	134.42	121.54
1	E	36	ARG	C-N-CA	6.74	134.42	121.54
1	G	251	ALA	N-CA-CB	-6.74	100.66	110.70
1	L	265	ASN	CA-CB-CG	-6.73	105.87	112.60
1	B	251	ALA	N-CA-CB	-6.73	100.67	110.70
1	C	251	ALA	N-CA-CB	-6.73	100.67	110.70
1	F	251	ALA	N-CA-CB	-6.73	100.67	110.70
1	I	36	ARG	N-CA-CB	6.73	120.72	110.70
1	A	36	ARG	CA-C-N	6.73	134.39	121.54
1	A	36	ARG	C-N-CA	6.73	134.39	121.54
1	C	283	ASP	CA-CB-CG	-6.73	105.87	112.60
1	G	283	ASP	CA-CB-CG	-6.71	105.89	112.60
1	G	36	ARG	CA-C-N	6.71	134.36	121.54
1	G	36	ARG	C-N-CA	6.71	134.36	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	36	ARG	N-CA-CB	6.71	120.69	110.70
1	A	283	ASP	CA-CB-CG	-6.70	105.90	112.60
1	G	201	SER	CA-C-N	6.70	128.21	119.84
1	G	201	SER	C-N-CA	6.70	128.21	119.84
1	L	255	GLU	N-CA-CB	6.70	119.94	110.36
1	D	283	ASP	CA-CB-CG	-6.70	105.91	112.60
1	J	36	ARG	N-CA-CB	6.68	120.66	110.70
1	E	40	LEU	CB-CA-C	-6.68	99.07	110.16
1	H	36	ARG	N-CA-CB	6.68	120.65	110.70
1	A	40	LEU	CB-CA-C	-6.68	99.07	110.16
1	I	265	ASN	CA-CB-CG	-6.68	105.92	112.60
1	B	40	LEU	CB-CA-C	-6.67	99.08	110.16
1	G	40	LEU	CB-CA-C	-6.67	99.08	110.16
1	E	283	ASP	CA-CB-CG	-6.67	105.93	112.60
1	C	40	LEU	CB-CA-C	-6.67	99.09	110.16
1	I	361	ASP	CA-CB-CG	-6.67	105.93	112.60
1	D	40	LEU	CB-CA-C	-6.67	99.09	110.16
1	N	36	ARG	N-CA-CB	6.67	120.63	110.70
1	B	283	ASP	CA-CB-CG	-6.66	105.94	112.60
1	D	196	ASP	CA-CB-CG	-6.66	105.94	112.60
1	J	361	ASP	CA-CB-CG	-6.66	105.94	112.60
1	M	361	ASP	CA-CB-CG	-6.66	105.94	112.60
1	F	40	LEU	CB-CA-C	-6.66	99.11	110.16
1	F	140	ASP	N-CA-CB	-6.66	100.87	110.45
1	L	36	ARG	N-CA-CB	6.66	120.62	110.70
1	A	515	ILE	N-CA-CB	6.65	118.33	110.55
1	C	140	ASP	N-CA-CB	-6.65	100.88	110.45
1	K	361	ASP	CA-CB-CG	-6.65	105.95	112.60
1	N	361	ASP	CA-CB-CG	-6.65	105.95	112.60
1	A	140	ASP	N-CA-CB	-6.64	100.88	110.45
1	B	140	ASP	N-CA-CB	-6.64	100.88	110.45
1	C	515	ILE	N-CA-CB	6.64	118.32	110.55
1	J	523	ASP	N-CA-CB	6.64	119.74	110.17
1	B	515	ILE	N-CA-CB	6.64	118.32	110.55
1	H	361	ASP	CA-CB-CG	-6.64	105.96	112.60
1	M	36	ARG	N-CA-CB	6.64	120.59	110.70
1	E	140	ASP	N-CA-CB	-6.64	100.89	110.45
1	L	361	ASP	CA-CB-CG	-6.64	105.96	112.60
1	D	140	ASP	N-CA-CB	-6.64	100.89	110.45
1	J	359	ASP	CA-CB-CG	-6.64	105.96	112.60
1	D	515	ILE	N-CA-CB	6.63	118.31	110.55
1	E	515	ILE	N-CA-CB	6.63	118.31	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	523	ASP	N-CA-CB	6.63	119.72	110.17
1	L	523	ASP	N-CA-CB	6.63	119.72	110.17
1	F	515	ILE	N-CA-CB	6.63	118.31	110.55
1	G	515	ILE	N-CA-CB	6.63	118.30	110.55
1	N	523	ASP	N-CA-CB	6.63	119.71	110.17
1	G	140	ASP	N-CA-CB	-6.62	100.91	110.45
1	K	359	ASP	CA-CB-CG	-6.62	105.98	112.60
1	D	230	ILE	CA-C-N	-6.62	111.60	120.54
1	D	230	ILE	C-N-CA	-6.62	111.60	120.54
1	F	230	ILE	CA-C-N	-6.62	111.60	120.54
1	F	230	ILE	C-N-CA	-6.62	111.60	120.54
1	M	523	ASP	N-CA-CB	6.62	119.71	110.17
1	K	523	ASP	N-CA-CB	6.62	119.70	110.17
1	B	230	ILE	CA-C-N	-6.62	111.61	120.54
1	B	230	ILE	C-N-CA	-6.62	111.61	120.54
1	A	230	ILE	CA-C-N	-6.62	111.61	120.54
1	A	230	ILE	C-N-CA	-6.62	111.61	120.54
1	G	230	ILE	CA-C-N	-6.62	111.61	120.54
1	G	230	ILE	C-N-CA	-6.62	111.61	120.54
1	N	359	ASP	CA-CB-CG	-6.62	105.98	112.60
1	M	359	ASP	CA-CB-CG	-6.61	105.99	112.60
1	L	359	ASP	CA-CB-CG	-6.61	105.99	112.60
1	E	230	ILE	CA-C-N	-6.61	111.61	120.54
1	E	230	ILE	C-N-CA	-6.61	111.61	120.54
1	H	359	ASP	CA-CB-CG	-6.61	105.99	112.60
1	C	153	ASN	N-CA-CB	6.61	121.66	110.49
1	H	523	ASP	N-CA-CB	6.61	119.68	110.17
1	C	230	ILE	CA-C-N	-6.61	111.62	120.54
1	C	230	ILE	C-N-CA	-6.61	111.62	120.54
1	A	153	ASN	N-CA-CB	6.60	121.64	110.49
1	G	153	ASN	N-CA-CB	6.60	121.64	110.49
1	H	18	ARG	CD-NE-CZ	6.60	133.63	124.40
1	E	153	ASN	N-CA-CB	6.59	121.63	110.49
1	I	359	ASP	CA-CB-CG	-6.59	106.01	112.60
1	I	18	ARG	CD-NE-CZ	6.58	133.61	124.40
1	K	311	LYS	CB-CA-C	6.56	121.68	110.79
1	N	18	ARG	CD-NE-CZ	6.54	133.56	124.40
1	H	311	LYS	CB-CA-C	6.54	121.65	110.79
1	L	18	ARG	CD-NE-CZ	6.54	133.56	124.40
1	J	18	ARG	CD-NE-CZ	6.54	133.55	124.40
1	M	18	ARG	CD-NE-CZ	6.54	133.55	124.40
1	B	273	VAL	N-CA-CB	6.53	120.01	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	273	VAL	N-CA-CB	6.53	120.01	111.19
1	A	273	VAL	N-CA-CB	6.53	120.00	111.19
1	C	273	VAL	N-CA-CB	6.53	120.00	111.19
1	D	273	VAL	N-CA-CB	6.52	120.00	111.19
1	F	273	VAL	N-CA-CB	6.52	120.00	111.19
1	E	273	VAL	N-CA-CB	6.52	120.00	111.19
1	J	140	ASP	CA-CB-CG	6.52	119.12	112.60
1	B	87	ASP	N-CA-CB	6.51	121.46	111.56
1	K	18	ARG	CD-NE-CZ	6.51	133.52	124.40
1	N	40	LEU	CB-CA-C	-6.50	99.02	109.75
1	E	172	GLU	N-CA-CB	6.50	119.44	110.01
1	K	40	LEU	CB-CA-C	-6.50	99.02	109.75
1	L	140	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	172	GLU	N-CA-CB	6.50	119.43	110.01
1	N	140	ASP	CA-CB-CG	6.50	119.09	112.60
1	A	172	GLU	N-CA-CB	6.49	119.43	110.01
1	L	40	LEU	CB-CA-C	-6.49	99.04	109.75
1	H	40	LEU	CB-CA-C	-6.49	99.04	109.75
1	F	172	GLU	N-CA-CB	6.49	119.42	110.01
1	M	140	ASP	CA-CB-CG	6.49	119.09	112.60
1	I	40	LEU	CB-CA-C	-6.49	99.05	109.75
1	M	40	LEU	CB-CA-C	-6.49	99.05	109.75
1	J	40	LEU	CB-CA-C	-6.49	99.05	109.75
1	D	172	GLU	N-CA-CB	6.48	119.41	110.01
1	G	172	GLU	N-CA-CB	6.48	119.41	110.01
1	H	140	ASP	CA-CB-CG	6.48	119.08	112.60
1	C	172	GLU	N-CA-CB	6.48	119.40	110.01
1	N	265	ASN	CA-CB-CG	-6.47	106.12	112.60
1	I	140	ASP	CA-CB-CG	6.47	119.07	112.60
1	K	140	ASP	CA-CB-CG	6.47	119.07	112.60
1	M	311	LYS	CB-CA-C	6.45	121.49	110.79
1	L	10	ASN	N-CA-C	-6.44	104.26	111.28
1	L	311	LYS	CB-CA-C	6.44	121.48	110.79
1	F	315	GLU	CA-C-N	6.43	129.43	120.29
1	F	315	GLU	C-N-CA	6.43	129.43	120.29
1	H	334	ASP	CB-CA-C	6.43	122.00	112.09
1	K	334	ASP	CB-CA-C	6.43	122.00	112.09
1	D	153	ASN	CB-CA-C	6.43	123.21	110.42
1	N	311	LYS	CB-CA-C	6.43	121.46	110.79
1	N	10	ASN	N-CA-C	-6.42	104.28	111.28
1	F	80	LYS	CB-CA-C	6.42	121.77	110.85
1	G	80	LYS	CB-CA-C	6.42	121.77	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	315	GLU	CA-C-N	6.42	129.41	120.29
1	G	315	GLU	C-N-CA	6.42	129.41	120.29
1	J	334	ASP	CB-CA-C	6.42	121.98	112.09
1	A	80	LYS	CB-CA-C	6.42	121.76	110.85
1	B	315	GLU	CA-C-N	6.42	129.40	120.29
1	B	315	GLU	C-N-CA	6.42	129.40	120.29
1	E	80	LYS	CB-CA-C	6.42	121.76	110.85
1	A	315	GLU	CA-C-N	6.41	129.40	120.29
1	A	315	GLU	C-N-CA	6.41	129.40	120.29
1	E	315	GLU	CA-C-N	6.41	129.40	120.29
1	E	315	GLU	C-N-CA	6.41	129.40	120.29
1	I	334	ASP	CB-CA-C	6.41	121.97	112.09
1	B	80	LYS	CB-CA-C	6.41	121.75	110.85
1	C	80	LYS	CB-CA-C	6.41	121.75	110.85
1	L	334	ASP	CB-CA-C	6.41	121.96	112.09
1	D	80	LYS	CB-CA-C	6.41	121.74	110.85
1	M	334	ASP	CB-CA-C	6.41	121.96	112.09
1	C	315	GLU	CA-C-N	6.40	129.38	120.29
1	C	315	GLU	C-N-CA	6.40	129.38	120.29
1	I	10	ASN	N-CA-C	-6.39	104.31	111.28
1	K	10	ASN	N-CA-C	-6.39	104.31	111.28
1	D	315	GLU	CA-C-N	6.39	129.37	120.29
1	D	315	GLU	C-N-CA	6.39	129.37	120.29
1	J	10	ASN	N-CA-C	-6.39	104.31	111.28
1	N	334	ASP	CB-CA-C	6.39	121.93	112.09
1	F	153	ASN	CB-CA-C	6.39	123.13	110.42
1	J	311	LYS	CB-CA-C	6.38	121.38	110.79
1	C	27	VAL	N-CA-C	6.37	116.52	110.53
1	D	27	VAL	N-CA-C	6.37	116.52	110.53
1	G	27	VAL	N-CA-C	6.37	116.52	110.53
1	A	27	VAL	N-CA-C	6.36	116.51	110.53
1	E	27	VAL	N-CA-C	6.36	116.51	110.53
1	F	27	VAL	N-CA-C	6.36	116.51	110.53
1	I	311	LYS	CB-CA-C	6.36	121.35	110.79
1	B	27	VAL	N-CA-C	6.36	116.50	110.53
1	H	10	ASN	N-CA-C	-6.34	104.37	111.28
1	I	252	GLU	CB-CA-C	-6.31	100.97	110.88
1	M	10	ASN	N-CA-C	-6.31	104.40	111.28
1	K	297	GLY	N-CA-C	-6.30	106.73	114.92
1	I	297	GLY	N-CA-C	-6.29	106.74	114.92
1	K	458	CYS	N-CA-CB	6.29	119.37	110.12
1	J	252	GLU	CB-CA-C	-6.29	101.01	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	297	GLY	N-CA-C	-6.29	106.74	114.92
1	I	458	CYS	N-CA-CB	6.29	119.36	110.12
1	L	261	THR	N-CA-CB	6.28	119.12	110.01
1	J	458	CYS	N-CA-CB	6.28	119.36	110.12
1	N	458	CYS	N-CA-CB	6.28	119.35	110.12
1	G	244	GLY	N-CA-C	-6.28	107.05	115.21
1	H	458	CYS	N-CA-CB	6.28	119.34	110.12
1	J	297	GLY	N-CA-C	-6.28	106.76	114.92
1	H	297	GLY	N-CA-C	-6.27	106.77	114.92
1	N	297	GLY	N-CA-C	-6.27	106.77	114.92
1	M	458	CYS	N-CA-CB	6.27	119.33	110.12
1	I	64	ASP	CB-CA-C	6.26	120.36	109.65
1	J	255	GLU	N-CA-CB	6.26	119.32	110.36
1	L	64	ASP	CB-CA-C	6.26	120.36	109.65
1	L	458	CYS	N-CA-CB	6.26	119.33	110.12
1	N	219	PHE	CA-CB-CG	6.26	120.06	113.80
1	C	244	GLY	N-CA-C	-6.26	107.08	115.21
1	L	20	VAL	N-CA-CB	6.26	119.05	110.54
1	A	244	GLY	N-CA-C	-6.25	107.08	115.21
1	D	244	GLY	N-CA-C	-6.25	107.08	115.21
1	G	199	TYR	O-C-N	-6.25	114.27	122.59
1	H	20	VAL	N-CA-CB	6.25	119.05	110.54
1	E	244	GLY	N-CA-C	-6.25	107.08	115.21
1	J	20	VAL	N-CA-CB	6.25	119.04	110.54
1	K	64	ASP	CB-CA-C	6.25	120.33	109.65
1	H	64	ASP	CB-CA-C	6.24	120.33	109.65
1	M	64	ASP	CB-CA-C	6.24	120.33	109.65
1	N	20	VAL	N-CA-CB	6.24	119.03	110.54
1	J	64	ASP	CB-CA-C	6.24	120.32	109.65
1	F	244	GLY	N-CA-C	-6.24	107.10	115.21
1	I	20	VAL	N-CA-CB	6.24	119.02	110.54
1	M	20	VAL	N-CA-CB	6.24	119.02	110.54
1	N	64	ASP	CB-CA-C	6.24	120.31	109.65
1	B	244	GLY	N-CA-C	-6.23	107.11	115.21
1	M	297	GLY	N-CA-C	-6.23	106.82	114.92
1	B	254	VAL	CB-CA-C	-6.23	101.17	111.32
1	K	20	VAL	N-CA-CB	6.22	119.00	110.54
1	G	49	ILE	CA-C-N	-6.22	112.03	122.29
1	G	49	ILE	C-N-CA	-6.22	112.03	122.29
1	A	49	ILE	CA-C-N	-6.22	112.03	122.29
1	A	49	ILE	C-N-CA	-6.22	112.03	122.29
1	B	87	ASP	CA-CB-CG	-6.22	106.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	49	ILE	CA-C-N	-6.22	112.03	122.29
1	F	49	ILE	C-N-CA	-6.22	112.03	122.29
1	J	228	SER	N-CA-CB	6.22	119.02	110.01
1	A	254	VAL	CB-CA-C	-6.21	101.19	111.32
1	C	49	ILE	CA-C-N	-6.21	112.04	122.29
1	C	49	ILE	C-N-CA	-6.21	112.04	122.29
1	E	49	ILE	CA-C-N	-6.21	112.04	122.29
1	E	49	ILE	C-N-CA	-6.21	112.04	122.29
1	C	254	VAL	CB-CA-C	-6.21	101.20	111.32
1	E	254	VAL	CB-CA-C	-6.21	101.20	111.32
1	B	49	ILE	CA-C-N	-6.21	112.05	122.29
1	B	49	ILE	C-N-CA	-6.21	112.05	122.29
1	G	254	VAL	CB-CA-C	-6.20	101.21	111.32
1	D	254	VAL	CB-CA-C	-6.20	101.21	111.32
1	D	49	ILE	CA-C-N	-6.20	112.06	122.29
1	D	49	ILE	C-N-CA	-6.20	112.06	122.29
1	F	254	VAL	CB-CA-C	-6.20	101.22	111.32
1	K	188	ASP	CA-CB-CG	6.19	118.79	112.60
1	G	185	ASP	CA-CB-CG	-6.18	106.42	112.60
1	N	188	ASP	CA-CB-CG	6.17	118.78	112.60
1	H	188	ASP	CA-CB-CG	6.17	118.77	112.60
1	M	255	GLU	N-CA-CB	6.17	119.19	110.36
1	K	459	GLY	N-CA-C	-6.17	106.90	114.92
1	J	188	ASP	CA-CB-CG	6.17	118.77	112.60
1	I	188	ASP	CA-CB-CG	6.16	118.76	112.60
1	L	188	ASP	CA-CB-CG	6.16	118.75	112.60
1	J	459	GLY	N-CA-C	-6.15	106.93	114.92
1	H	459	GLY	N-CA-C	-6.14	106.94	114.92
1	K	255	GLU	N-CA-CB	6.14	119.14	110.36
1	I	410	GLY	N-CA-C	-6.13	105.42	112.29
1	I	459	GLY	N-CA-C	-6.13	106.96	114.92
1	L	459	GLY	N-CA-C	-6.12	106.96	114.92
1	H	255	GLU	N-CA-CB	6.12	119.12	110.36
1	L	410	GLY	N-CA-C	-6.12	105.44	112.29
1	I	255	GLU	N-CA-CB	6.11	119.10	110.36
1	N	207	LYS	O-C-N	-6.11	114.29	121.32
1	N	459	GLY	N-CA-C	-6.10	106.98	114.92
1	M	390	LYS	CB-CA-C	6.10	120.92	110.79
1	H	371	LYS	N-CA-CB	-6.10	101.17	110.01
1	I	390	LYS	CB-CA-C	6.10	120.91	110.79
1	M	459	GLY	N-CA-C	-6.09	107.00	114.92
1	J	390	LYS	CB-CA-C	6.09	120.90	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	371	LYS	N-CA-CB	-6.09	101.18	110.01
1	M	371	LYS	N-CA-CB	-6.09	101.18	110.01
1	N	410	GLY	N-CA-C	-6.08	105.47	112.29
1	H	390	LYS	CB-CA-C	6.08	120.89	110.79
1	J	371	LYS	N-CA-CB	-6.08	101.19	110.01
1	H	410	GLY	N-CA-C	-6.08	105.48	112.29
1	L	390	LYS	CB-CA-C	6.08	120.88	110.79
1	M	410	GLY	N-CA-C	-6.08	105.48	112.29
1	N	390	LYS	CB-CA-C	6.08	120.88	110.79
1	K	390	LYS	CB-CA-C	6.07	120.87	110.79
1	N	255	GLU	N-CA-CB	6.07	119.05	110.36
1	N	371	LYS	N-CA-CB	-6.07	101.21	110.01
1	L	371	LYS	N-CA-CB	-6.07	101.21	110.01
1	L	257	GLU	CB-CA-C	-6.06	101.36	110.88
1	L	257	GLU	CB-CG-CD	6.06	122.91	112.60
1	L	206	ASN	CB-CA-C	-6.06	108.34	117.07
1	K	410	GLY	N-CA-C	-6.06	105.50	112.29
1	I	371	LYS	N-CA-CB	-6.06	101.23	110.01
1	J	410	GLY	N-CA-C	-6.05	105.52	112.29
1	D	168	LYS	CB-CA-C	6.04	120.31	110.95
1	I	208	PRO	CA-C-N	6.04	130.26	120.60
1	I	208	PRO	C-N-CA	6.04	130.26	120.60
1	A	168	LYS	CB-CA-C	6.04	120.31	110.95
1	G	168	LYS	CB-CA-C	6.03	120.30	110.95
1	C	168	LYS	CB-CA-C	6.03	120.30	110.95
1	F	168	LYS	CB-CA-C	6.03	120.30	110.95
1	J	518	GLU	CB-CG-CD	6.03	122.85	112.60
1	E	168	LYS	CB-CA-C	6.03	120.29	110.95
1	H	229	ASN	CA-CB-CG	6.03	118.63	112.60
1	K	314	LEU	N-CA-CB	6.03	118.98	110.12
1	D	60	ILE	N-CA-C	6.02	117.46	108.54
1	B	168	LYS	CB-CA-C	6.02	120.29	110.95
1	L	219	PHE	CA-CB-CG	6.02	119.82	113.80
1	H	401	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	G	200	LEU	CB-CA-C	-6.02	103.63	114.52
1	K	206	ASN	CB-CA-C	-6.02	108.41	117.07
1	A	60	ILE	N-CA-C	6.01	117.44	108.54
1	E	60	ILE	N-CA-C	6.01	117.44	108.54
1	F	60	ILE	N-CA-C	6.01	117.44	108.54
1	A	272	LYS	N-CA-CB	-6.01	100.99	110.06
1	C	60	ILE	N-CA-C	6.01	117.44	108.54
1	G	60	ILE	N-CA-C	6.01	117.44	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	219	PHE	CA-CB-CG	6.01	119.81	113.80
1	B	60	ILE	N-CA-C	6.01	117.43	108.54
1	I	389	MET	CB-CA-C	6.00	120.76	110.79
1	H	228	SER	N-CA-CB	6.00	118.72	110.01
1	E	272	LYS	N-CA-CB	-6.00	101.00	110.06
1	L	518	GLU	CB-CG-CD	6.00	122.80	112.60
1	F	272	LYS	N-CA-CB	-6.00	101.00	110.06
1	G	272	LYS	N-CA-CB	-6.00	101.00	110.06
1	K	401	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	N	389	MET	CB-CA-C	6.00	120.75	110.79
1	L	401	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	D	272	LYS	N-CA-CB	-6.00	101.01	110.06
1	J	389	MET	CB-CA-C	6.00	120.74	110.79
1	L	389	MET	CB-CA-C	5.99	120.74	110.79
1	M	401	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	B	272	LYS	N-CA-CB	-5.99	101.02	110.06
1	K	389	MET	CB-CA-C	5.99	120.73	110.79
1	M	389	MET	CB-CA-C	5.99	120.73	110.79
1	K	518	GLU	CB-CG-CD	5.99	122.78	112.60
1	H	389	MET	CB-CA-C	5.99	120.73	110.79
1	C	272	LYS	N-CA-CB	-5.98	101.03	110.06
1	I	219	PHE	CA-CB-CG	5.98	119.78	113.80
1	I	401	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	I	518	GLU	CB-CG-CD	5.98	122.77	112.60
1	N	401	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	H	219	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	198	GLY	CA-C-N	5.96	130.19	121.31
1	A	198	GLY	C-N-CA	5.96	130.19	121.31
1	J	401	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	M	219	PHE	CA-CB-CG	5.95	119.75	113.80
1	H	518	GLU	CB-CG-CD	5.95	122.71	112.60
1	M	518	GLU	CB-CG-CD	5.94	122.70	112.60
1	K	416	GLY	N-CA-C	-5.93	107.06	115.30
1	L	416	GLY	N-CA-C	-5.93	107.06	115.30
1	M	27	VAL	CB-CA-C	5.93	120.14	112.14
1	M	416	GLY	N-CA-C	-5.92	107.06	115.30
1	I	261	THR	N-CA-CB	5.92	118.60	110.01
1	K	228	SER	N-CA-CB	5.92	118.59	110.01
1	N	518	GLU	CB-CG-CD	5.92	122.66	112.60
1	A	5	ASP	N-CA-C	-5.92	99.55	109.07
1	D	5	ASP	N-CA-C	-5.92	99.55	109.07
1	E	5	ASP	N-CA-C	-5.92	99.54	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5	ASP	N-CA-C	-5.92	99.54	109.07
1	I	27	VAL	CB-CA-C	5.92	120.13	112.14
1	J	27	VAL	CB-CA-C	5.92	120.13	112.14
1	J	416	GLY	N-CA-C	-5.92	107.08	115.30
1	F	5	ASP	N-CA-C	-5.91	99.56	109.07
1	N	416	GLY	N-CA-C	-5.91	107.09	115.30
1	H	27	VAL	CB-CA-C	5.91	120.11	112.14
1	B	5	ASP	N-CA-C	-5.91	99.56	109.07
1	C	5	ASP	N-CA-C	-5.91	99.56	109.07
1	L	27	VAL	CB-CA-C	5.90	120.10	112.14
1	K	27	VAL	CB-CA-C	5.90	120.10	112.14
1	J	229	ASN	CA-CB-CG	5.89	118.50	112.60
1	I	416	GLY	N-CA-C	-5.89	107.11	115.30
1	N	27	VAL	CB-CA-C	5.89	120.10	112.14
1	H	416	GLY	N-CA-C	-5.89	107.11	115.30
1	N	228	SER	N-CA-CB	5.87	118.53	110.01
1	K	229	ASN	CA-CB-CG	5.87	118.47	112.60
1	G	311	LYS	N-CA-C	-5.87	104.89	111.28
1	F	461	GLU	CA-C-N	5.86	125.34	119.24
1	F	461	GLU	C-N-CA	5.86	125.34	119.24
1	D	311	LYS	N-CA-C	-5.86	104.89	111.28
1	E	311	LYS	N-CA-C	-5.86	104.89	111.28
1	E	461	GLU	CA-C-N	5.86	125.33	119.24
1	E	461	GLU	C-N-CA	5.86	125.33	119.24
1	A	311	LYS	N-CA-C	-5.86	104.89	111.28
1	C	311	LYS	N-CA-C	-5.86	104.90	111.28
1	B	311	LYS	N-CA-C	-5.85	104.90	111.28
1	F	311	LYS	N-CA-C	-5.84	104.91	111.28
1	A	461	GLU	CA-C-N	5.84	125.31	119.24
1	A	461	GLU	C-N-CA	5.84	125.31	119.24
1	C	461	GLU	CA-C-N	5.84	125.31	119.24
1	C	461	GLU	C-N-CA	5.84	125.31	119.24
1	G	461	GLU	CA-C-N	5.84	125.31	119.24
1	G	461	GLU	C-N-CA	5.84	125.31	119.24
1	B	461	GLU	CA-C-N	5.83	125.31	119.24
1	B	461	GLU	C-N-CA	5.83	125.31	119.24
1	D	461	GLU	CA-C-N	5.83	125.31	119.24
1	D	461	GLU	C-N-CA	5.83	125.31	119.24
1	B	198	GLY	CA-C-N	5.83	130.00	121.31
1	B	198	GLY	C-N-CA	5.83	130.00	121.31
1	I	228	SER	N-CA-CB	5.83	118.46	110.01
1	L	520	MET	N-CA-CB	5.82	120.96	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	520	MET	N-CA-CB	5.82	120.95	110.83
1	J	361	ASP	CB-CA-C	5.82	120.44	110.79
1	N	520	MET	N-CA-CB	5.81	120.94	110.83
1	D	380	LYS	CB-CA-C	5.81	119.60	110.19
1	I	361	ASP	CB-CA-C	5.81	120.43	110.79
1	H	520	MET	N-CA-CB	5.80	120.93	110.83
1	J	520	MET	N-CA-CB	5.80	120.92	110.83
1	J	10	ASN	CA-CB-CG	-5.80	106.80	112.60
1	H	361	ASP	CB-CA-C	5.80	120.41	110.79
1	I	520	MET	N-CA-CB	5.79	120.91	110.83
1	K	520	MET	N-CA-CB	5.79	120.91	110.83
1	N	361	ASP	CB-CA-C	5.79	120.40	110.79
1	B	206	ASN	CA-CB-CG	-5.79	106.81	112.60
1	L	361	ASP	CB-CA-C	5.79	120.40	110.79
1	M	361	ASP	CB-CA-C	5.79	120.40	110.79
1	G	185	ASP	CA-C-N	-5.79	113.36	122.73
1	G	185	ASP	C-N-CA	-5.79	113.36	122.73
1	G	380	LYS	CB-CA-C	5.79	119.56	110.19
1	K	361	ASP	CB-CA-C	5.79	120.39	110.79
1	G	473	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	380	LYS	CB-CA-C	5.78	119.56	110.19
1	M	10	ASN	CA-CB-CG	-5.78	106.82	112.60
1	D	205	ILE	CA-C-N	-5.78	110.50	121.54
1	D	205	ILE	C-N-CA	-5.78	110.50	121.54
1	E	380	LYS	CB-CA-C	5.78	119.55	110.19
1	C	380	LYS	CB-CA-C	5.78	119.55	110.19
1	B	380	LYS	CB-CA-C	5.77	119.55	110.19
1	H	10	ASN	CA-CB-CG	-5.77	106.83	112.60
1	F	380	LYS	CB-CA-C	5.77	119.54	110.19
1	L	10	ASN	CA-CB-CG	-5.77	106.83	112.60
1	A	301	ILE	CB-CA-C	5.76	119.91	111.33
1	C	301	ILE	CB-CA-C	5.76	119.91	111.33
1	C	473	ASP	CA-CB-CG	-5.75	106.85	112.60
1	D	301	ILE	CB-CA-C	5.75	119.90	111.33
1	I	10	ASN	CA-CB-CG	-5.75	106.85	112.60
1	K	10	ASN	CA-CB-CG	-5.75	106.85	112.60
1	D	473	ASP	CA-CB-CG	-5.75	106.85	112.60
1	N	10	ASN	CA-CB-CG	-5.75	106.85	112.60
1	G	301	ILE	CB-CA-C	5.75	119.90	111.33
1	B	301	ILE	CB-CA-C	5.75	119.89	111.33
1	E	473	ASP	CA-CB-CG	-5.75	106.85	112.60
1	F	301	ILE	CB-CA-C	5.74	119.89	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	473	ASP	CA-CB-CG	-5.74	106.86	112.60
1	E	301	ILE	CB-CA-C	5.74	119.88	111.33
1	B	473	ASP	CA-CB-CG	-5.74	106.86	112.60
1	E	87	ASP	CA-CB-CG	-5.74	106.86	112.60
1	C	286	LYS	N-CA-CB	-5.73	101.69	110.12
1	K	411	VAL	CB-CA-C	-5.73	102.64	110.90
1	D	286	LYS	N-CA-CB	-5.73	101.69	110.12
1	G	286	LYS	N-CA-CB	-5.73	101.70	110.12
1	G	87	ASP	CA-CB-CG	-5.72	106.88	112.60
1	B	286	LYS	N-CA-CB	-5.72	101.71	110.12
1	A	473	ASP	CA-CB-CG	-5.72	106.88	112.60
1	L	411	VAL	CB-CA-C	-5.72	102.67	110.90
1	A	286	LYS	N-CA-CB	-5.71	101.72	110.12
1	F	286	LYS	N-CA-CB	-5.71	101.72	110.12
1	E	286	LYS	N-CA-CB	-5.71	101.73	110.12
1	J	411	VAL	CB-CA-C	-5.71	102.68	110.90
1	M	206	ASN	CA-CB-CG	-5.70	106.90	112.60
1	C	87	ASP	CA-CB-CG	-5.70	106.91	112.60
1	E	402	ALA	N-CA-CB	-5.70	101.73	110.16
1	K	415	GLY	N-CA-C	-5.70	107.46	115.32
1	M	411	VAL	CB-CA-C	-5.70	102.70	110.90
1	L	415	GLY	N-CA-C	-5.69	107.46	115.32
1	H	411	VAL	CB-CA-C	-5.69	102.70	110.90
1	I	415	GLY	N-CA-C	-5.69	107.47	115.32
1	G	402	ALA	N-CA-CB	-5.68	101.75	110.16
1	B	402	ALA	N-CA-CB	-5.68	101.75	110.16
1	M	153	ASN	CB-CA-C	-5.68	103.34	112.09
1	M	197	ARG	CB-CA-C	5.68	121.73	110.42
1	A	402	ALA	N-CA-CB	-5.68	101.75	110.16
1	D	402	ALA	N-CA-CB	-5.68	101.75	110.16
1	M	415	GLY	N-CA-C	-5.68	107.48	115.32
1	J	153	ASN	CB-CA-C	-5.68	103.35	112.09
1	A	87	ASP	CA-CB-CG	-5.67	106.92	112.60
1	I	232	GLU	CB-CA-C	-5.67	101.37	110.79
1	F	402	ALA	N-CA-CB	-5.67	101.76	110.16
1	K	153	ASN	CB-CA-C	-5.67	103.36	112.09
1	C	402	ALA	N-CA-CB	-5.67	101.77	110.16
1	E	46	ALA	N-CA-CB	-5.66	102.40	110.04
1	J	415	GLY	N-CA-C	-5.66	107.51	115.32
1	H	153	ASN	CB-CA-C	-5.66	103.38	112.09
1	L	197	ARG	CB-CA-C	5.66	121.68	110.42
1	I	153	ASN	CB-CA-C	-5.66	103.38	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	153	ASN	CB-CA-C	-5.66	103.38	112.09
1	D	46	ALA	N-CA-CB	-5.65	102.41	110.04
1	F	46	ALA	N-CA-CB	-5.65	102.41	110.04
1	B	46	ALA	N-CA-CB	-5.65	102.41	110.04
1	N	153	ASN	CB-CA-C	-5.65	103.39	112.09
1	N	415	GLY	N-CA-C	-5.65	107.52	115.32
1	A	46	ALA	N-CA-CB	-5.65	102.42	110.04
1	H	415	GLY	N-CA-C	-5.64	107.53	115.32
1	B	358	SER	CA-C-N	5.64	127.84	120.28
1	B	358	SER	C-N-CA	5.64	127.84	120.28
1	C	46	ALA	N-CA-CB	-5.64	102.43	110.04
1	G	358	SER	CA-C-N	5.64	127.83	120.28
1	G	358	SER	C-N-CA	5.64	127.83	120.28
1	G	46	ALA	N-CA-CB	-5.64	102.43	110.04
1	C	358	SER	CA-C-N	5.63	127.83	120.28
1	C	358	SER	C-N-CA	5.63	127.83	120.28
1	L	228	SER	N-CA-CB	5.63	118.18	110.01
1	D	358	SER	CA-C-N	5.63	127.82	120.28
1	D	358	SER	C-N-CA	5.63	127.82	120.28
1	F	358	SER	CA-C-N	5.63	127.82	120.28
1	F	358	SER	C-N-CA	5.63	127.82	120.28
1	A	358	SER	CA-C-N	5.63	127.82	120.28
1	A	358	SER	C-N-CA	5.63	127.82	120.28
1	L	353	ILE	CB-CA-C	-5.63	104.55	112.14
1	M	353	ILE	CB-CA-C	-5.62	104.55	112.14
1	J	353	ILE	CB-CA-C	-5.62	104.55	112.14
1	E	358	SER	CA-C-N	5.62	127.81	120.28
1	E	358	SER	C-N-CA	5.62	127.81	120.28
1	A	194	GLN	N-CA-CB	-5.62	101.25	110.68
1	E	194	GLN	N-CA-CB	-5.62	101.25	110.68
1	I	181	THR	N-CA-C	-5.62	104.85	110.97
1	G	194	GLN	N-CA-CB	-5.61	101.25	110.68
1	I	353	ILE	CB-CA-C	-5.61	104.56	112.14
1	H	252	GLU	CB-CA-C	-5.61	102.07	110.88
1	D	194	GLN	N-CA-CB	-5.61	101.26	110.68
1	F	457	ASN	CB-CA-C	5.61	122.03	110.31
1	H	353	ILE	CB-CA-C	-5.61	104.57	112.14
1	K	252	GLU	CB-CA-C	-5.61	102.08	110.88
1	N	353	ILE	CB-CA-C	-5.61	104.57	112.14
1	B	147	VAL	CB-CA-C	-5.60	104.57	112.14
1	C	41	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	194	GLN	N-CA-CB	-5.60	101.27	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	359	ASP	CB-CA-C	5.60	120.09	110.79
1	E	41	ASP	CA-CB-CG	5.60	118.20	112.60
1	K	353	ILE	CB-CA-C	-5.60	104.58	112.14
1	D	457	ASN	CB-CA-C	5.60	122.02	110.31
1	A	359	ASP	CB-CA-C	5.60	120.08	110.79
1	D	41	ASP	CA-CB-CG	5.60	118.20	112.60
1	G	359	ASP	CB-CA-C	5.60	120.08	110.79
1	E	359	ASP	CB-CA-C	5.59	120.08	110.79
1	B	359	ASP	CB-CA-C	5.59	120.07	110.79
1	G	521	VAL	CB-CA-C	-5.59	102.17	110.33
1	I	75	LYS	N-CA-CB	5.59	118.34	110.12
1	A	521	VAL	CB-CA-C	-5.59	102.17	110.33
1	C	521	VAL	CB-CA-C	-5.59	102.17	110.33
1	D	521	VAL	CB-CA-C	-5.59	102.17	110.33
1	F	359	ASP	CB-CA-C	5.59	120.07	110.79
1	D	87	ASP	CA-CB-CG	-5.59	107.01	112.60
1	A	41	ASP	CA-CB-CG	5.59	118.19	112.60
1	F	147	VAL	CB-CA-C	-5.59	104.60	112.14
1	F	521	VAL	CB-CA-C	-5.59	102.17	110.33
1	B	521	VAL	CB-CA-C	-5.58	102.18	110.33
1	C	359	ASP	CB-CA-C	5.58	120.06	110.79
1	C	147	VAL	CB-CA-C	-5.58	104.61	112.14
1	D	147	VAL	CB-CA-C	-5.58	104.61	112.14
1	A	147	VAL	CB-CA-C	-5.57	104.61	112.14
1	G	147	VAL	CB-CA-C	-5.57	104.61	112.14
1	M	75	LYS	N-CA-CB	5.57	118.31	110.12
1	N	75	LYS	N-CA-CB	5.57	118.31	110.12
1	B	41	ASP	CA-CB-CG	5.57	118.17	112.60
1	E	147	VAL	CB-CA-C	-5.57	104.63	112.14
1	H	75	LYS	N-CA-CB	5.56	118.30	110.12
1	K	75	LYS	N-CA-CB	5.56	118.30	110.12
1	F	87	ASP	CA-CB-CG	-5.56	107.04	112.60
1	A	515	ILE	CA-C-N	-5.56	115.61	122.84
1	A	515	ILE	C-N-CA	-5.56	115.61	122.84
1	E	521	VAL	CB-CA-C	-5.56	102.22	110.33
1	G	41	ASP	CA-CB-CG	5.56	118.16	112.60
1	G	515	ILE	CA-C-N	-5.56	115.62	122.84
1	G	515	ILE	C-N-CA	-5.56	115.62	122.84
1	A	181	THR	N-CA-C	-5.55	105.38	111.82
1	B	153	ASN	N-CA-CB	5.55	119.88	110.49
1	J	152	ALA	CB-CA-C	5.55	120.01	110.79
1	D	515	ILE	CA-C-N	-5.55	115.62	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	515	ILE	C-N-CA	-5.55	115.62	122.84
1	J	75	LYS	N-CA-CB	5.55	118.28	110.12
1	L	75	LYS	N-CA-CB	5.55	118.28	110.12
1	C	515	ILE	CA-C-N	-5.55	115.63	122.84
1	C	515	ILE	C-N-CA	-5.55	115.63	122.84
1	D	181	THR	N-CA-C	-5.55	105.38	111.82
1	L	152	ALA	CB-CA-C	5.55	120.00	110.79
1	C	181	THR	N-CA-C	-5.55	105.39	111.82
1	F	181	THR	N-CA-C	-5.55	105.39	111.82
1	B	181	THR	N-CA-C	-5.54	105.39	111.82
1	G	181	THR	N-CA-C	-5.54	105.39	111.82
1	H	317	LEU	CB-CA-C	-5.54	100.17	109.65
1	J	317	LEU	CB-CA-C	-5.54	100.17	109.65
1	E	181	THR	N-CA-C	-5.54	105.39	111.82
1	H	152	ALA	CB-CA-C	5.54	119.99	110.79
1	I	152	ALA	CB-CA-C	5.54	119.99	110.79
1	K	152	ALA	CB-CA-C	5.54	119.98	110.79
1	B	515	ILE	CA-C-N	-5.54	115.64	122.84
1	B	515	ILE	C-N-CA	-5.54	115.64	122.84
1	C	272	LYS	CB-CG-CD	5.54	124.03	111.30
1	E	515	ILE	CA-C-N	-5.53	115.65	122.84
1	E	515	ILE	C-N-CA	-5.53	115.65	122.84
1	F	41	ASP	CA-CB-CG	5.53	118.13	112.60
1	F	173	GLY	N-CA-C	-5.53	104.05	112.51
1	F	515	ILE	CA-C-N	-5.53	115.65	122.84
1	F	515	ILE	C-N-CA	-5.53	115.65	122.84
1	B	173	GLY	N-CA-C	-5.53	104.05	112.51
1	B	272	LYS	CB-CG-CD	5.53	124.02	111.30
1	N	152	ALA	CB-CA-C	5.53	119.97	110.79
1	C	246	PRO	N-CA-CB	5.53	109.19	103.38
1	F	272	LYS	CB-CG-CD	5.53	124.01	111.30
1	E	246	PRO	N-CA-CB	5.52	109.18	103.38
1	M	152	ALA	CB-CA-C	5.52	119.96	110.79
1	A	173	GLY	N-CA-C	-5.52	104.06	112.51
1	B	246	PRO	N-CA-CB	5.52	109.18	103.38
1	C	173	GLY	N-CA-C	-5.52	104.06	112.51
1	A	393	LYS	CB-CA-C	-5.52	101.63	110.79
1	E	173	GLY	N-CA-C	-5.52	104.06	112.51
1	F	246	PRO	N-CA-CB	5.52	109.17	103.38
1	B	393	LYS	CB-CA-C	-5.52	101.63	110.79
1	D	393	LYS	CB-CA-C	-5.52	101.63	110.79
1	G	173	GLY	N-CA-C	-5.52	104.07	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	PRO	N-CA-CB	5.51	109.17	103.38
1	D	272	LYS	CB-CG-CD	5.51	123.98	111.30
1	E	197	ARG	CB-CA-C	5.51	122.01	111.48
1	E	393	LYS	CB-CA-C	-5.51	101.64	110.79
1	G	272	LYS	CB-CG-CD	5.51	123.98	111.30
1	D	173	GLY	N-CA-C	-5.51	104.08	112.51
1	F	393	LYS	CB-CA-C	-5.51	101.64	110.79
1	G	393	LYS	CB-CA-C	-5.51	101.64	110.79
1	I	317	LEU	CB-CA-C	-5.51	100.23	109.65
1	G	197	ARG	CB-CA-C	5.50	122.00	111.48
1	K	317	LEU	CB-CA-C	-5.50	100.24	109.65
1	L	110	GLY	N-CA-C	-5.50	107.67	115.43
1	C	393	LYS	CB-CA-C	-5.50	101.66	110.79
1	C	197	ARG	CB-CA-C	5.50	121.98	111.48
1	E	272	LYS	CB-CG-CD	5.50	123.95	111.30
1	I	110	GLY	N-CA-C	-5.50	107.67	115.43
1	A	272	LYS	CB-CG-CD	5.50	123.95	111.30
1	D	246	PRO	N-CA-CB	5.50	109.15	103.38
1	F	194	GLN	N-CA-CB	-5.50	101.27	110.83
1	M	110	GLY	N-CA-C	-5.50	107.68	115.43
1	M	317	LEU	CB-CA-C	-5.50	100.25	109.65
1	G	246	PRO	N-CA-CB	5.49	109.15	103.38
1	M	181	THR	N-CA-C	-5.49	105.19	111.07
1	K	310	GLU	CA-CB-CG	5.48	125.06	114.10
1	F	396	VAL	CB-CA-C	-5.48	104.74	112.14
1	H	310	GLU	CA-CB-CG	5.48	125.06	114.10
1	L	317	LEU	CB-CA-C	-5.48	100.28	109.65
1	B	396	VAL	CB-CA-C	-5.47	104.75	112.14
1	J	155	ASP	CA-CB-CG	5.47	118.07	112.60
1	N	110	GLY	N-CA-C	-5.47	107.71	115.43
1	A	396	VAL	CB-CA-C	-5.47	104.76	112.14
1	G	457	ASN	CB-CA-C	5.47	121.74	110.31
1	J	110	GLY	N-CA-C	-5.47	107.72	115.43
1	C	396	VAL	CB-CA-C	-5.47	104.76	112.14
1	E	396	VAL	CB-CA-C	-5.47	104.76	112.14
1	I	36	ARG	CB-CA-C	5.47	120.09	110.36
1	M	155	ASP	CA-CB-CG	5.46	118.06	112.60
1	G	396	VAL	CB-CA-C	-5.46	104.77	112.14
1	H	36	ARG	CB-CA-C	5.46	120.08	110.36
1	D	396	VAL	CB-CA-C	-5.46	104.77	112.14
1	L	155	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	457	ASN	CB-CA-C	5.46	121.72	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	155	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	457	ASN	CB-CA-C	5.46	121.72	110.31
1	K	155	ASP	CA-CB-CG	5.46	118.06	112.60
1	M	36	ARG	CB-CA-C	5.46	120.07	110.36
1	N	179	ASP	CA-CB-CG	-5.46	107.14	112.60
1	E	457	ASN	CB-CA-C	5.45	121.71	110.31
1	L	190	VAL	CA-C-N	-5.45	111.12	121.54
1	L	190	VAL	C-N-CA	-5.45	111.12	121.54
1	L	36	ARG	CB-CA-C	5.45	120.06	110.36
1	N	36	ARG	CB-CA-C	5.45	120.06	110.36
1	K	18	ARG	CB-CG-CD	5.45	123.83	111.30
1	K	36	ARG	CB-CA-C	5.45	120.06	110.36
1	J	36	ARG	CB-CA-C	5.45	120.06	110.36
1	I	155	ASP	CA-CB-CG	5.45	118.05	112.60
1	L	232	GLU	CB-CA-C	-5.44	101.75	110.79
1	N	310	GLU	CA-CB-CG	5.44	124.97	114.10
1	J	18	ARG	CB-CG-CD	5.44	123.80	111.30
1	H	110	GLY	N-CA-C	-5.43	107.77	115.43
1	B	457	ASN	CB-CA-C	5.43	121.66	110.31
1	H	18	ARG	CB-CG-CD	5.43	123.78	111.30
1	M	18	ARG	CB-CG-CD	5.42	123.77	111.30
1	K	110	GLY	N-CA-C	-5.42	107.79	115.43
1	G	389	MET	CB-CA-C	-5.41	101.80	110.79
1	N	18	ARG	CB-CG-CD	5.41	123.75	111.30
1	N	155	ASP	CA-CB-CG	5.41	118.01	112.60
1	E	389	MET	CB-CA-C	-5.41	101.81	110.79
1	L	18	ARG	CB-CG-CD	5.41	123.75	111.30
1	H	25	ASP	CA-CB-CG	-5.41	107.19	112.60
1	F	389	MET	CB-CA-C	-5.41	101.82	110.79
1	M	310	GLU	CA-CB-CG	5.40	124.91	114.10
1	I	18	ARG	CB-CG-CD	5.40	123.73	111.30
1	I	25	ASP	CA-CB-CG	-5.40	107.20	112.60
1	C	389	MET	CB-CA-C	-5.40	101.83	110.79
1	G	277	LYS	CA-CB-CG	5.40	124.89	114.10
1	D	389	MET	CB-CA-C	-5.39	101.84	110.79
1	A	389	MET	CB-CA-C	-5.39	101.84	110.79
1	B	389	MET	CB-CA-C	-5.39	101.85	110.79
1	K	25	ASP	CA-CB-CG	-5.39	107.21	112.60
1	B	277	LYS	CA-CB-CG	5.38	124.87	114.10
1	C	277	LYS	CA-CB-CG	5.38	124.87	114.10
1	D	277	LYS	CA-CB-CG	5.38	124.86	114.10
1	A	28	LYS	N-CA-C	5.38	118.94	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LYS	CA-CB-CG	5.38	124.85	114.10
1	D	28	LYS	N-CA-C	5.38	118.94	112.38
1	F	277	LYS	CA-CB-CG	5.38	124.86	114.10
1	L	25	ASP	CA-CB-CG	-5.38	107.22	112.60
1	C	28	LYS	N-CA-C	5.38	118.94	112.38
1	E	28	LYS	N-CA-C	5.37	118.93	112.38
1	K	196	ASP	CA-CB-CG	-5.37	107.23	112.60
1	L	51	LYS	N-CA-C	-5.37	105.59	111.82
1	N	25	ASP	CA-CB-CG	-5.37	107.23	112.60
1	B	28	LYS	N-CA-C	5.37	118.92	112.38
1	E	277	LYS	CA-CB-CG	5.37	124.83	114.10
1	B	197	ARG	CA-C-N	-5.36	116.77	122.67
1	B	197	ARG	C-N-CA	-5.36	116.77	122.67
1	J	25	ASP	CA-CB-CG	-5.36	107.24	112.60
1	G	28	LYS	N-CA-C	5.36	118.92	112.38
1	K	219	PHE	CA-CB-CG	5.36	119.16	113.80
1	J	310	GLU	CA-CB-CG	5.36	124.81	114.10
1	L	310	GLU	CA-CB-CG	5.35	124.81	114.10
1	M	51	LYS	N-CA-C	-5.35	105.61	111.82
1	F	28	LYS	N-CA-C	5.35	118.91	112.38
1	H	306	GLY	N-CA-C	-5.35	107.97	114.92
1	A	330	THR	CB-CA-C	-5.34	100.93	109.75
1	H	51	LYS	N-CA-C	-5.34	105.62	111.82
1	C	330	THR	CB-CA-C	-5.34	100.93	109.75
1	K	51	LYS	N-CA-C	-5.34	105.63	111.82
1	N	51	LYS	N-CA-C	-5.34	105.63	111.82
1	F	330	THR	CB-CA-C	-5.34	100.94	109.75
1	L	306	GLY	N-CA-C	-5.34	107.98	114.92
1	M	25	ASP	CA-CB-CG	-5.34	107.26	112.60
1	D	197	ARG	CB-CA-C	5.33	122.00	111.22
1	N	317	LEU	CB-CA-C	-5.33	100.53	109.65
1	A	197	ARG	CB-CA-C	5.33	122.00	111.22
1	G	330	THR	CB-CA-C	-5.33	100.95	109.75
1	E	18	ARG	CB-CG-CD	5.33	123.55	111.30
1	I	310	GLU	CA-CB-CG	5.33	124.76	114.10
1	B	330	THR	CB-CA-C	-5.33	100.96	109.75
1	G	516	THR	CA-C-N	5.33	130.62	122.95
1	G	516	THR	C-N-CA	5.33	130.62	122.95
1	D	330	THR	CB-CA-C	-5.33	100.96	109.75
1	J	51	LYS	N-CA-C	-5.32	105.64	111.82
1	B	197	ARG	CB-CA-C	5.32	121.97	111.22
1	E	330	THR	CB-CA-C	-5.32	100.97	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	197	ARG	CB-CA-C	5.32	121.97	111.22
1	A	516	THR	CA-C-N	5.32	130.61	122.95
1	A	516	THR	C-N-CA	5.32	130.61	122.95
1	F	516	THR	CA-C-N	5.32	130.60	122.95
1	F	516	THR	C-N-CA	5.32	130.60	122.95
1	B	281	PHE	CA-CB-CG	-5.31	108.49	113.80
1	D	516	THR	CA-C-N	5.31	130.60	122.95
1	D	516	THR	C-N-CA	5.31	130.60	122.95
1	B	516	THR	CA-C-N	5.31	130.60	122.95
1	B	516	THR	C-N-CA	5.31	130.60	122.95
1	M	434	GLU	N-CA-CB	5.31	117.93	110.12
1	A	281	PHE	CA-CB-CG	-5.31	108.49	113.80
1	B	18	ARG	CB-CG-CD	5.31	123.51	111.30
1	C	516	THR	CA-C-N	5.31	130.60	122.95
1	C	516	THR	C-N-CA	5.31	130.60	122.95
1	K	306	GLY	N-CA-C	-5.31	108.02	114.92
1	M	306	GLY	N-CA-C	-5.31	108.02	114.92
1	I	306	GLY	N-CA-C	-5.31	108.02	114.92
1	I	383	ALA	N-CA-CB	5.31	119.34	110.85
1	C	18	ARG	CB-CG-CD	5.30	123.50	111.30
1	D	18	ARG	CB-CG-CD	5.30	123.50	111.30
1	K	434	GLU	N-CA-CB	5.30	117.92	110.12
1	L	383	ALA	N-CA-CB	5.30	119.34	110.85
1	G	18	ARG	CB-CG-CD	5.30	123.50	111.30
1	H	383	ALA	N-CA-CB	5.30	119.33	110.85
1	J	383	ALA	N-CA-CB	5.30	119.33	110.85
1	M	383	ALA	N-CA-CB	5.30	119.33	110.85
1	N	314	LEU	N-CA-CB	5.30	117.91	110.12
1	N	383	ALA	N-CA-CB	5.30	119.33	110.85
1	F	18	ARG	CB-CG-CD	5.30	123.49	111.30
1	E	516	THR	CA-C-N	5.30	130.58	122.95
1	E	516	THR	C-N-CA	5.30	130.58	122.95
1	H	434	GLU	N-CA-CB	5.30	117.91	110.12
1	I	51	LYS	N-CA-C	-5.29	105.68	111.82
1	I	434	GLU	N-CA-CB	5.29	117.90	110.12
1	K	383	ALA	N-CA-CB	5.29	119.32	110.85
1	G	281	PHE	CA-CB-CG	-5.29	108.51	113.80
1	L	434	GLU	N-CA-CB	5.29	117.90	110.12
1	J	14	VAL	N-CA-CB	5.29	117.73	110.54
1	K	14	VAL	N-CA-CB	5.29	117.73	110.54
1	G	161	LEU	CB-CA-C	-5.29	102.51	110.92
1	N	14	VAL	N-CA-CB	5.29	117.73	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	434	GLU	N-CA-CB	5.29	117.89	110.12
1	A	18	ARG	CB-CG-CD	5.28	123.45	111.30
1	J	434	GLU	N-CA-CB	5.28	117.89	110.12
1	I	14	VAL	N-CA-CB	5.28	117.72	110.54
1	F	227	ILE	CA-C-N	5.28	127.62	120.44
1	F	227	ILE	C-N-CA	5.28	127.62	120.44
1	I	62	LEU	N-CA-CB	5.28	119.19	110.69
1	A	161	LEU	CB-CA-C	-5.28	102.53	110.92
1	L	14	VAL	N-CA-CB	5.28	117.72	110.54
1	C	281	PHE	CA-CB-CG	-5.28	108.52	113.80
1	F	161	LEU	CB-CA-C	-5.27	102.53	110.92
1	M	14	VAL	N-CA-CB	5.27	117.71	110.54
1	B	161	LEU	CB-CA-C	-5.27	102.54	110.92
1	C	312	ALA	CB-CA-C	5.27	119.24	109.54
1	K	62	LEU	N-CA-CB	5.27	119.18	110.69
1	D	161	LEU	CB-CA-C	-5.27	102.54	110.92
1	C	161	LEU	CB-CA-C	-5.27	102.54	110.92
1	M	62	LEU	N-CA-CB	5.27	119.17	110.69
1	F	281	PHE	CA-CB-CG	-5.27	108.53	113.80
1	H	14	VAL	N-CA-CB	5.27	117.70	110.54
1	H	62	LEU	N-CA-CB	5.27	119.17	110.69
1	B	312	ALA	CB-CA-C	5.26	119.22	109.54
1	L	62	LEU	N-CA-CB	5.26	119.16	110.69
1	B	63	GLU	CB-CG-CD	5.26	121.54	112.60
1	D	63	GLU	CB-CG-CD	5.26	121.54	112.60
1	E	312	ALA	CB-CA-C	5.26	119.22	109.54
1	J	62	LEU	N-CA-CB	5.26	119.16	110.69
1	F	312	ALA	CB-CA-C	5.26	119.21	109.54
1	J	306	GLY	N-CA-C	-5.26	108.09	114.92
1	A	227	ILE	CA-C-N	5.25	127.58	120.44
1	A	227	ILE	C-N-CA	5.25	127.58	120.44
1	A	312	ALA	CB-CA-C	5.25	119.20	109.54
1	F	63	GLU	CB-CG-CD	5.25	121.53	112.60
1	E	281	PHE	CA-CB-CG	-5.25	108.55	113.80
1	G	312	ALA	CB-CA-C	5.25	119.20	109.54
1	D	227	ILE	CA-C-N	5.25	127.58	120.44
1	D	227	ILE	C-N-CA	5.25	127.58	120.44
1	E	161	LEU	CB-CA-C	-5.25	102.58	110.92
1	B	227	ILE	CA-C-N	5.25	127.58	120.44
1	B	227	ILE	C-N-CA	5.25	127.58	120.44
1	C	227	ILE	CA-C-N	5.25	127.58	120.44
1	C	227	ILE	C-N-CA	5.25	127.58	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	312	ALA	CB-CA-C	5.25	119.19	109.54
1	H	305	ILE	N-CA-CB	5.25	117.68	110.54
1	N	62	LEU	N-CA-CB	5.25	119.14	110.69
1	N	306	GLY	N-CA-C	-5.25	108.10	114.92
1	A	63	GLU	CB-CG-CD	5.24	121.51	112.60
1	D	281	PHE	CA-CB-CG	-5.24	108.56	113.80
1	G	63	GLU	CB-CG-CD	5.24	121.51	112.60
1	C	63	GLU	CB-CG-CD	5.24	121.51	112.60
1	N	352	GLN	N-CA-CB	5.24	117.82	110.12
1	G	227	ILE	CA-C-N	5.24	127.56	120.44
1	G	227	ILE	C-N-CA	5.24	127.56	120.44
1	J	305	ILE	N-CA-CB	5.24	117.66	110.54
1	E	63	GLU	CB-CG-CD	5.23	121.50	112.60
1	E	227	ILE	CA-C-N	5.23	127.56	120.44
1	E	227	ILE	C-N-CA	5.23	127.56	120.44
1	H	239	ALA	N-CA-CB	-5.23	102.44	110.12
1	A	277	LYS	CB-CA-C	-5.22	98.97	109.68
1	I	232	GLU	N-CA-CB	5.22	117.80	110.12
1	K	305	ILE	N-CA-CB	5.22	117.64	110.54
1	E	277	LYS	CB-CA-C	-5.22	98.98	109.68
1	B	277	LYS	CB-CA-C	-5.22	98.98	109.68
1	C	153	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	D	368	ARG	CB-CA-C	-5.22	102.65	110.90
1	H	352	GLN	N-CA-CB	5.22	117.79	110.12
1	K	352	GLN	N-CA-CB	5.22	117.79	110.12
1	C	277	LYS	CB-CA-C	-5.22	98.98	109.68
1	G	277	LYS	CB-CA-C	-5.22	98.99	109.68
1	B	368	ARG	CB-CA-C	-5.21	102.66	110.90
1	F	368	ARG	CB-CA-C	-5.21	102.66	110.90
1	G	368	ARG	CB-CA-C	-5.21	102.66	110.90
1	I	352	GLN	N-CA-CB	5.21	117.78	110.12
1	D	277	LYS	CB-CA-C	-5.21	99.00	109.68
1	J	352	GLN	N-CA-CB	5.21	117.78	110.12
1	E	368	ARG	CB-CA-C	-5.21	102.67	110.90
1	I	305	ILE	N-CA-CB	5.21	117.62	110.54
1	J	510	VAL	N-CA-CB	5.21	117.62	110.54
1	C	368	ARG	CB-CA-C	-5.21	102.68	110.90
1	F	277	LYS	CB-CA-C	-5.21	99.01	109.68
1	I	510	VAL	N-CA-CB	5.20	117.62	110.54
1	L	510	VAL	N-CA-CB	5.20	117.62	110.54
1	F	303	GLU	N-CA-CB	5.20	118.34	110.28
1	K	510	VAL	N-CA-CB	5.20	117.61	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	352	GLN	N-CA-CB	5.20	117.76	110.12
1	A	368	ARG	CB-CA-C	-5.20	102.69	110.90
1	H	510	VAL	N-CA-CB	5.20	117.61	110.54
1	M	352	GLN	N-CA-CB	5.20	117.76	110.12
1	N	510	VAL	N-CA-CB	5.19	117.60	110.54
1	G	153	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	M	321	LYS	N-CA-CB	5.19	117.54	110.01
1	M	510	VAL	N-CA-CB	5.19	117.60	110.54
1	F	272	LYS	CG-CD-CE	5.19	123.23	111.30
1	B	303	GLU	N-CA-CB	5.19	118.32	110.28
1	G	303	GLU	N-CA-CB	5.19	118.32	110.28
1	I	239	ALA	N-CA-CB	-5.19	102.50	110.12
1	B	317	LEU	N-CA-CB	-5.19	102.70	110.17
1	I	314	LEU	N-CA-CB	5.19	117.74	110.12
1	L	239	ALA	N-CA-CB	-5.19	102.50	110.12
1	E	157	THR	N-CA-CB	5.18	117.48	109.91
1	F	157	THR	N-CA-CB	5.18	117.48	109.91
1	J	314	LEU	N-CA-CB	5.18	117.74	110.12
1	N	382	GLY	N-CA-C	-5.18	105.97	111.93
1	D	157	THR	N-CA-CB	5.18	117.48	109.91
1	G	303	GLU	CB-CG-CD	5.18	121.41	112.60
1	E	303	GLU	N-CA-CB	5.18	118.31	110.28
1	B	157	THR	N-CA-CB	5.18	117.47	109.91
1	C	303	GLU	N-CA-CB	5.18	118.31	110.28
1	E	156	GLU	CB-CA-C	-5.18	99.49	110.31
1	D	303	GLU	N-CA-CB	5.18	118.31	110.28
1	D	337	GLY	N-CA-C	-5.18	105.30	111.36
1	A	157	THR	N-CA-CB	5.18	117.47	109.91
1	A	272	LYS	CG-CD-CE	5.18	123.21	111.30
1	A	303	GLU	N-CA-CB	5.18	118.30	110.28
1	I	321	LYS	N-CA-CB	5.18	117.52	110.01
1	C	157	THR	N-CA-CB	5.17	117.47	109.91
1	F	317	LEU	N-CA-CB	-5.17	102.72	110.17
1	C	156	GLU	CB-CA-C	-5.17	99.50	110.31
1	C	303	GLU	CB-CG-CD	5.17	121.39	112.60
1	D	272	LYS	CG-CD-CE	5.17	123.20	111.30
1	G	272	LYS	CG-CD-CE	5.17	123.20	111.30
1	A	156	GLU	CB-CA-C	-5.17	99.50	110.31
1	D	317	LEU	N-CA-CB	-5.17	102.72	110.17
1	E	272	LYS	CG-CD-CE	5.17	123.20	111.30
1	F	337	GLY	N-CA-C	-5.17	105.31	111.36
1	H	382	GLY	N-CA-C	-5.17	105.98	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	LYS	CG-CD-CE	5.17	123.19	111.30
1	G	156	GLU	CB-CA-C	-5.17	99.50	110.31
1	D	303	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	337	GLY	N-CA-C	-5.17	105.31	111.36
1	L	314	LEU	N-CA-CB	5.17	117.72	110.12
1	L	412	VAL	CB-CA-C	-5.17	103.80	111.19
1	E	317	LEU	N-CA-CB	-5.17	102.73	110.17
1	G	200	LEU	O-C-N	5.17	126.42	120.58
1	J	239	ALA	N-CA-CB	-5.17	102.53	110.12
1	B	337	GLY	N-CA-C	-5.16	105.32	111.36
1	C	272	LYS	CG-CD-CE	5.16	123.17	111.30
1	C	337	GLY	N-CA-C	-5.16	105.32	111.36
1	G	337	GLY	N-CA-C	-5.16	105.32	111.36
1	M	239	ALA	N-CA-CB	-5.16	102.53	110.12
1	E	337	GLY	N-CA-C	-5.16	105.32	111.36
1	G	157	THR	N-CA-CB	5.16	117.45	109.91
1	H	321	LYS	N-CA-CB	5.16	117.49	110.01
1	I	308	GLU	CB-CA-C	5.16	118.96	109.46
1	C	317	LEU	N-CA-CB	-5.16	102.74	110.17
1	E	153	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	I	170	GLY	N-CA-C	-5.16	105.18	112.81
1	A	317	LEU	N-CA-CB	-5.16	102.74	110.17
1	A	153	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	303	GLU	CB-CG-CD	5.16	121.37	112.60
1	F	156	GLU	CB-CA-C	-5.16	99.53	110.31
1	G	317	LEU	N-CA-CB	-5.16	102.75	110.17
1	N	412	VAL	CB-CA-C	-5.16	103.82	111.19
1	N	239	ALA	N-CA-CB	-5.15	102.54	110.12
1	L	170	GLY	N-CA-C	-5.15	105.18	112.81
1	L	321	LYS	N-CA-CB	5.15	117.48	110.01
1	H	412	VAL	CB-CA-C	-5.15	103.82	111.19
1	J	321	LYS	N-CA-CB	5.15	117.48	110.01
1	J	412	VAL	CB-CA-C	-5.15	103.83	111.19
1	L	382	GLY	N-CA-C	-5.15	106.01	111.93
1	A	441	LYS	CB-CA-C	5.15	119.34	110.79
1	B	303	GLU	CB-CG-CD	5.15	121.35	112.60
1	C	521	VAL	N-CA-CB	-5.15	104.00	111.52
1	E	303	GLU	CB-CG-CD	5.14	121.35	112.60
1	J	218	PRO	N-CA-CB	5.14	108.78	103.38
1	J	308	GLU	CB-CA-C	5.14	118.92	109.46
1	C	441	LYS	CB-CA-C	5.14	119.32	110.79
1	E	441	LYS	CB-CA-C	5.14	119.32	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	38	VAL	CA-C-N	-5.14	116.47	123.10
1	F	38	VAL	C-N-CA	-5.14	116.47	123.10
1	F	303	GLU	CB-CG-CD	5.14	121.34	112.60
1	F	521	VAL	N-CA-CB	-5.14	104.02	111.52
1	K	382	GLY	N-CA-C	-5.14	106.02	111.93
1	D	156	GLU	CB-CA-C	-5.14	99.57	110.31
1	D	441	LYS	CB-CA-C	5.14	119.32	110.79
1	K	412	VAL	CB-CA-C	-5.14	103.85	111.19
1	M	382	GLY	N-CA-C	-5.14	106.02	111.93
1	N	321	LYS	N-CA-CB	5.14	117.46	110.01
1	D	521	VAL	N-CA-CB	-5.13	104.02	111.52
1	I	412	VAL	CB-CA-C	-5.13	103.85	111.19
1	J	382	GLY	N-CA-C	-5.13	106.03	111.93
1	M	305	ILE	N-CA-CB	5.13	117.52	110.54
1	M	412	VAL	CB-CA-C	-5.13	103.85	111.19
1	B	156	GLU	CB-CA-C	-5.13	99.59	110.31
1	B	441	LYS	CB-CA-C	5.13	119.31	110.79
1	I	382	GLY	N-CA-C	-5.13	106.03	111.93
1	J	54	VAL	CB-CA-C	-5.13	105.40	111.97
1	K	170	GLY	N-CA-C	-5.13	105.22	112.81
1	A	38	VAL	CA-C-N	-5.13	116.48	123.10
1	A	38	VAL	C-N-CA	-5.13	116.48	123.10
1	E	198	GLY	CA-C-N	5.13	131.34	121.54
1	E	198	GLY	C-N-CA	5.13	131.34	121.54
1	G	441	LYS	CB-CA-C	5.13	119.30	110.79
1	J	170	GLY	N-CA-C	-5.13	105.22	112.81
1	F	441	LYS	CB-CA-C	5.13	119.30	110.79
1	G	521	VAL	N-CA-CB	-5.13	104.04	111.52
1	K	321	LYS	N-CA-CB	5.13	117.44	110.01
1	L	305	ILE	N-CA-CB	5.13	117.51	110.54
1	B	521	VAL	N-CA-CB	-5.12	104.04	111.52
1	B	38	VAL	CA-C-N	-5.12	116.49	123.10
1	B	38	VAL	C-N-CA	-5.12	116.49	123.10
1	A	521	VAL	N-CA-CB	-5.12	104.04	111.52
1	I	54	VAL	CB-CA-C	-5.12	105.42	111.97
1	D	38	VAL	CA-C-N	-5.12	116.50	123.10
1	D	38	VAL	C-N-CA	-5.12	116.50	123.10
1	N	54	VAL	CB-CA-C	-5.12	105.42	111.97
1	L	54	VAL	CB-CA-C	-5.12	105.42	111.97
1	M	218	PRO	N-CA-CB	5.12	108.75	103.38
1	C	38	VAL	CA-C-N	-5.12	116.50	123.10
1	C	38	VAL	C-N-CA	-5.12	116.50	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	305	ILE	N-CA-CB	5.12	117.50	110.54
1	H	170	GLY	N-CA-C	-5.11	105.24	112.81
1	H	218	PRO	N-CA-CB	5.11	108.75	103.38
1	L	218	PRO	N-CA-CB	5.11	108.75	103.38
1	M	170	GLY	N-CA-C	-5.11	105.24	112.81
1	N	261	THR	CB-CA-C	5.11	118.91	110.88
1	E	38	VAL	CA-C-N	-5.11	116.51	123.10
1	E	38	VAL	C-N-CA	-5.11	116.51	123.10
1	E	521	VAL	N-CA-CB	-5.11	104.06	111.52
1	G	38	VAL	CA-C-N	-5.11	116.51	123.10
1	G	38	VAL	C-N-CA	-5.11	116.51	123.10
1	C	25	ASP	CA-CB-CG	-5.11	107.49	112.60
1	H	54	VAL	CB-CA-C	-5.11	105.43	111.97
1	K	54	VAL	CB-CA-C	-5.11	105.43	111.97
1	M	54	VAL	CB-CA-C	-5.11	105.43	111.97
1	G	25	ASP	CA-CB-CG	-5.10	107.50	112.60
1	H	21	ASN	CA-CB-CG	-5.10	107.50	112.60
1	K	218	PRO	N-CA-CB	5.10	108.74	103.38
1	A	25	ASP	CA-CB-CG	-5.10	107.50	112.60
1	L	21	ASN	CA-CB-CG	-5.10	107.50	112.60
1	K	21	ASN	CA-CB-CG	-5.10	107.50	112.60
1	F	25	ASP	CA-CB-CG	-5.09	107.51	112.60
1	E	25	ASP	CA-CB-CG	-5.09	107.51	112.60
1	I	218	PRO	N-CA-CB	5.08	108.72	103.38
1	N	218	PRO	N-CA-CB	5.08	108.72	103.38
1	C	225	LYS	CA-C-N	-5.08	113.39	122.07
1	C	225	LYS	C-N-CA	-5.08	113.39	122.07
1	D	225	LYS	CA-C-N	-5.08	113.39	122.07
1	D	225	LYS	C-N-CA	-5.08	113.39	122.07
1	D	434	GLU	N-CA-CB	5.07	117.37	110.01
1	H	518	GLU	CA-CB-CG	5.07	124.25	114.10
1	I	21	ASN	CA-CB-CG	-5.07	107.53	112.60
1	I	251	ALA	N-CA-CB	5.07	120.13	111.66
1	M	21	ASN	CA-CB-CG	-5.07	107.53	112.60
1	D	25	ASP	CA-CB-CG	-5.07	107.53	112.60
1	E	225	LYS	CA-C-N	-5.07	113.41	122.07
1	E	225	LYS	C-N-CA	-5.07	113.41	122.07
1	A	225	LYS	CA-C-N	-5.07	113.41	122.07
1	A	225	LYS	C-N-CA	-5.07	113.41	122.07
1	B	225	LYS	CA-C-N	-5.07	113.41	122.07
1	B	225	LYS	C-N-CA	-5.07	113.41	122.07
1	C	259	LEU	N-CA-CB	5.07	117.36	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	434	GLU	N-CA-CB	5.07	117.36	110.01
1	G	259	LEU	N-CA-CB	5.07	117.36	110.01
1	B	434	GLU	N-CA-CB	5.06	117.35	110.01
1	H	196	ASP	CB-CA-C	-5.06	103.06	111.41
1	I	518	GLU	CA-CB-CG	5.06	124.22	114.10
1	L	518	GLU	CA-CB-CG	5.06	124.23	114.10
1	B	25	ASP	CA-CB-CG	-5.06	107.54	112.60
1	G	434	GLU	N-CA-CB	5.06	117.35	110.01
1	J	251	ALA	N-CA-CB	5.06	120.11	111.66
1	F	225	LYS	CA-C-N	-5.06	113.42	122.07
1	F	225	LYS	C-N-CA	-5.06	113.42	122.07
1	A	434	GLU	N-CA-CB	5.06	117.34	110.01
1	E	434	GLU	N-CA-CB	5.06	117.34	110.01
1	K	239	ALA	N-CA-CB	-5.06	102.69	110.12
1	C	434	GLU	N-CA-CB	5.05	117.34	110.01
1	G	225	LYS	CA-C-N	-5.05	113.43	122.07
1	G	225	LYS	C-N-CA	-5.05	113.43	122.07
1	M	314	LEU	N-CA-CB	5.05	117.55	110.12
1	N	21	ASN	CA-CB-CG	-5.05	107.55	112.60
1	N	518	GLU	CA-CB-CG	5.05	124.21	114.10
1	M	518	GLU	CA-CB-CG	5.05	124.20	114.10
1	H	251	ALA	N-CA-CB	5.05	120.10	111.66
1	J	21	ASN	CA-CB-CG	-5.05	107.55	112.60
1	K	518	GLU	CA-CB-CG	5.05	124.20	114.10
1	L	308	GLU	CB-CA-C	5.05	118.76	109.46
1	N	171	LYS	N-CA-C	-5.05	105.86	111.36
1	A	259	LEU	N-CA-CB	5.05	117.33	110.01
1	D	259	LEU	N-CA-CB	5.05	117.33	110.01
1	N	185	ASP	CA-C-N	-5.04	115.66	122.77
1	N	185	ASP	C-N-CA	-5.04	115.66	122.77
1	D	516	THR	CA-CB-OG1	5.04	117.17	109.60
1	E	259	LEU	N-CA-CB	5.04	117.32	110.01
1	M	251	ALA	N-CA-CB	5.04	120.08	111.66
1	M	229	ASN	N-CA-CB	-5.04	103.46	111.62
1	B	516	THR	CA-CB-OG1	5.03	117.15	109.60
1	F	259	LEU	N-CA-CB	5.03	117.31	110.01
1	M	308	GLU	CB-CA-C	5.03	118.72	109.46
1	F	516	THR	CA-CB-OG1	5.03	117.15	109.60
1	M	367	GLU	CB-CA-C	-5.03	102.44	110.79
1	N	367	GLU	CB-CA-C	-5.03	102.44	110.79
1	C	516	THR	CA-CB-OG1	5.03	117.14	109.60
1	J	518	GLU	CA-CB-CG	5.03	124.16	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	516	THR	CA-CB-OG1	5.02	117.13	109.60
1	N	251	ALA	N-CA-CB	5.02	120.05	111.66
1	K	251	ALA	N-CA-CB	5.02	120.04	111.66
1	M	228	SER	N-CA-CB	5.02	117.28	110.01
1	B	259	LEU	N-CA-CB	5.02	117.28	110.01
1	E	516	THR	CA-CB-OG1	5.01	117.12	109.60
1	M	239	ALA	CB-CA-C	5.01	119.11	110.79
1	N	261	THR	N-CA-CB	5.01	117.28	110.01
1	N	308	GLU	CB-CA-C	5.01	118.67	109.46
1	A	516	THR	CA-CB-OG1	5.00	117.11	109.60
1	B	35	GLY	N-CA-C	-5.00	105.69	112.14
1	G	35	GLY	N-CA-C	-5.00	105.69	112.14
1	L	251	ALA	N-CA-CB	5.00	120.01	111.66
1	L	367	GLU	CB-CA-C	-5.00	102.49	110.79
1	N	206	ASN	N-CA-C	-5.00	100.15	110.80

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	37	ASN	CA
1	I	37	ASN	CA
1	J	37	ASN	CA
1	K	37	ASN	CA
1	L	37	ASN	CA
1	M	37	ASN	CA
1	N	37	ASN	CA

All (231) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	190	VAL	Peptide
1	A	193	MET	Mainchain
1	A	196	ASP	Peptide
1	A	197	ARG	Peptide,Mainchain
1	A	231	ARG	Sidechain
1	A	255	GLU	Peptide
1	A	281	PHE	Peptide
1	A	284	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	29	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	296	THR	Peptide
1	A	325	ILE	Peptide
1	A	329	THR	Peptide
1	A	368	ARG	Sidechain
1	A	404	ARG	Sidechain
1	A	52	ASP	Mainchain
1	B	13	ARG	Sidechain
1	B	18	ARG	Sidechain
1	B	190	VAL	Peptide
1	B	196	ASP	Peptide
1	B	197	ARG	Peptide,Mainchain
1	B	231	ARG	Sidechain
1	B	255	GLU	Peptide
1	B	281	PHE	Peptide
1	B	284	ARG	Sidechain
1	B	285	ARG	Sidechain
1	B	29	VAL	Mainchain
1	B	296	THR	Peptide
1	B	325	ILE	Peptide
1	B	329	THR	Peptide
1	B	368	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	52	ASP	Mainchain
1	C	13	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	190	VAL	Peptide
1	C	196	ASP	Peptide
1	C	197	ARG	Peptide,Mainchain
1	C	231	ARG	Sidechain
1	C	255	GLU	Peptide
1	C	281	PHE	Peptide
1	C	284	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	29	VAL	Mainchain
1	C	296	THR	Peptide
1	C	325	ILE	Peptide
1	C	329	THR	Peptide
1	C	368	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	52	ASP	Mainchain
1	D	13	ARG	Sidechain
1	D	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	193	MET	Mainchain
1	D	196	ASP	Peptide
1	D	197	ARG	Peptide,Mainchain
1	D	231	ARG	Sidechain
1	D	255	GLU	Peptide
1	D	281	PHE	Peptide
1	D	284	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	29	VAL	Mainchain
1	D	296	THR	Peptide
1	D	325	ILE	Peptide
1	D	329	THR	Peptide
1	D	368	ARG	Sidechain
1	D	404	ARG	Sidechain
1	D	52	ASP	Mainchain
1	E	13	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	190	VAL	Peptide
1	E	193	MET	Mainchain
1	E	196	ASP	Peptide
1	E	197	ARG	Peptide,Mainchain
1	E	231	ARG	Sidechain
1	E	255	GLU	Peptide
1	E	281	PHE	Peptide
1	E	284	ARG	Sidechain
1	E	285	ARG	Sidechain
1	E	29	VAL	Mainchain
1	E	296	THR	Peptide
1	E	325	ILE	Peptide
1	E	329	THR	Peptide
1	E	368	ARG	Sidechain
1	E	404	ARG	Sidechain
1	E	52	ASP	Mainchain
1	F	13	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	190	VAL	Peptide
1	F	193	MET	Mainchain
1	F	196	ASP	Peptide
1	F	197	ARG	Peptide,Mainchain
1	F	231	ARG	Sidechain
1	F	255	GLU	Peptide
1	F	281	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	F	284	ARG	Sidechain
1	F	285	ARG	Sidechain
1	F	29	VAL	Mainchain
1	F	296	THR	Peptide
1	F	325	ILE	Peptide
1	F	329	THR	Peptide
1	F	368	ARG	Sidechain
1	F	404	ARG	Sidechain
1	F	52	ASP	Mainchain
1	G	13	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	190	VAL	Peptide
1	G	197	ARG	Peptide,Mainchain
1	G	199	TYR	Mainchain
1	G	231	ARG	Sidechain
1	G	255	GLU	Peptide
1	G	281	PHE	Peptide
1	G	284	ARG	Sidechain
1	G	285	ARG	Sidechain
1	G	29	VAL	Mainchain
1	G	296	THR	Peptide
1	G	325	ILE	Peptide
1	G	329	THR	Peptide
1	G	368	ARG	Sidechain
1	G	404	ARG	Sidechain
1	G	52	ASP	Mainchain
1	H	213	VAL	Mainchain
1	H	219	PHE	Sidechain
1	H	285	ARG	Sidechain
1	H	345	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	368	ARG	Sidechain
1	H	395	ARG	Sidechain
1	H	404	ARG	Sidechain
1	H	421	ARG	Sidechain
1	H	452	ARG	Sidechain
1	H	50	THR	Peptide
1	H	506	TYR	Sidechain
1	H	58	ARG	Sidechain
1	I	197	ARG	Mainchain
1	I	213	VAL	Mainchain
1	I	219	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	I	285	ARG	Sidechain
1	I	345	ARG	Sidechain
1	I	350	ARG	Sidechain
1	I	368	ARG	Sidechain
1	I	395	ARG	Sidechain
1	I	404	ARG	Sidechain
1	I	421	ARG	Sidechain
1	I	452	ARG	Sidechain
1	I	50	THR	Peptide
1	I	506	TYR	Sidechain
1	I	58	ARG	Sidechain
1	J	197	ARG	Mainchain
1	J	213	VAL	Mainchain
1	J	219	PHE	Sidechain
1	J	285	ARG	Sidechain
1	J	345	ARG	Sidechain
1	J	350	ARG	Sidechain
1	J	368	ARG	Sidechain
1	J	395	ARG	Sidechain
1	J	404	ARG	Sidechain
1	J	421	ARG	Sidechain
1	J	452	ARG	Sidechain
1	J	50	THR	Peptide
1	J	506	TYR	Sidechain
1	J	58	ARG	Sidechain
1	K	18	ARG	Sidechain
1	K	197	ARG	Mainchain
1	K	213	VAL	Mainchain
1	K	219	PHE	Sidechain
1	K	285	ARG	Sidechain
1	K	345	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	368	ARG	Sidechain
1	K	395	ARG	Sidechain
1	K	404	ARG	Sidechain
1	K	421	ARG	Sidechain
1	K	452	ARG	Sidechain
1	K	50	THR	Peptide
1	K	506	TYR	Sidechain
1	K	58	ARG	Sidechain
1	L	197	ARG	Mainchain
1	L	213	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	L	219	PHE	Sidechain
1	L	285	ARG	Sidechain
1	L	345	ARG	Sidechain
1	L	350	ARG	Sidechain
1	L	368	ARG	Sidechain
1	L	395	ARG	Sidechain
1	L	404	ARG	Sidechain
1	L	421	ARG	Sidechain
1	L	452	ARG	Sidechain
1	L	50	THR	Peptide
1	L	506	TYR	Sidechain
1	L	58	ARG	Sidechain
1	M	197	ARG	Mainchain
1	M	213	VAL	Mainchain
1	M	219	PHE	Sidechain
1	M	285	ARG	Sidechain
1	M	345	ARG	Sidechain
1	M	350	ARG	Sidechain
1	M	368	ARG	Sidechain
1	M	395	ARG	Sidechain
1	M	404	ARG	Sidechain
1	M	421	ARG	Sidechain
1	M	452	ARG	Sidechain
1	M	50	THR	Peptide
1	M	506	TYR	Sidechain
1	M	58	ARG	Sidechain
1	N	197	ARG	Peptide,Mainchain
1	N	206	ASN	Peptide
1	N	207	LYS	Peptide
1	N	208	PRO	Peptide
1	N	213	VAL	Mainchain
1	N	219	PHE	Sidechain
1	N	285	ARG	Sidechain
1	N	345	ARG	Sidechain
1	N	350	ARG	Sidechain
1	N	368	ARG	Sidechain
1	N	395	ARG	Sidechain
1	N	404	ARG	Sidechain
1	N	421	ARG	Sidechain
1	N	452	ARG	Sidechain
1	N	50	THR	Peptide
1	N	506	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	N	58	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	3968	226	0
1	B	3845	0	3963	238	0
1	C	3845	0	3963	238	0
1	D	3845	0	3963	242	0
1	E	3845	0	3963	232	0
1	F	3845	0	3963	239	0
1	G	3845	0	3963	238	0
1	H	3845	0	3965	259	0
1	I	3845	0	3965	257	0
1	J	3845	0	3965	264	0
1	K	3845	0	3965	266	0
1	L	3845	0	3965	263	0
1	M	3845	0	3965	264	0
1	N	3845	0	3965	278	0
2	A	1	0	0	3	0
2	B	1	0	0	3	0
2	C	1	0	0	4	0
2	D	1	0	0	3	0
2	E	1	0	0	4	0
2	F	1	0	0	3	0
2	G	1	0	0	3	0
2	H	1	0	0	5	0
2	I	1	0	0	5	0
2	J	1	0	0	5	0
2	K	1	0	0	5	0
2	L	1	0	0	5	0
2	M	1	0	0	5	0
2	N	1	0	0	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	3	0
4	D	31	0	12	2	0
4	E	31	0	12	3	0
4	F	31	0	12	2	0
4	G	31	0	12	2	0
4	H	31	0	12	4	0
4	I	31	0	12	4	0
4	J	31	0	12	5	0
4	K	31	0	12	4	0
4	L	31	0	12	5	0
4	M	31	0	12	5	0
4	N	31	0	12	5	0
All	All	54293	0	55669	3287	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 30.

All (3287) 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:D:249:ILE:HD12	1:D:262:LEU:CD1	1.30	1.62
1:C:249:ILE:HD12	1:C:262:LEU:CD1	1.30	1.61
1:E:249:ILE:HD12	1:E:262:LEU:CD1	1.30	1.60
1:B:249:ILE:HD12	1:B:262:LEU:CD1	1.30	1.59
1:N:208:PRO:CA	1:N:208:PRO:C	1.76	1.58
1:A:249:ILE:HD12	1:A:262:LEU:CD1	1.29	1.57
1:M:518:GLU:CA	1:M:518:GLU:CB	1.83	1.57
1:F:249:ILE:HD12	1:F:262:LEU:CD1	1.30	1.57
1:H:518:GLU:CA	1:H:518:GLU:CB	1.83	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:518:GLU:CA	1:N:518:GLU:CB	1.83	1.56
1:G:249:ILE:HD12	1:G:262:LEU:CD1	1.30	1.55
1:I:518:GLU:CB	1:I:518:GLU:CA	1.83	1.55
1:L:518:GLU:CB	1:L:518:GLU:CA	1.83	1.54
1:N:207:LYS:NZ	1:N:207:LYS:CE	1.70	1.53
1:K:518:GLU:CA	1:K:518:GLU:CB	1.83	1.51
1:J:518:GLU:CA	1:J:518:GLU:CB	1.83	1.51
1:F:200:LEU:HD21	1:F:254:VAL:CG2	1.12	1.46
1:D:200:LEU:HD21	1:D:254:VAL:CG2	1.12	1.46
1:E:200:LEU:HD21	1:E:254:VAL:CG2	1.12	1.45
1:A:200:LEU:HD21	1:A:254:VAL:CG2	1.12	1.44
1:C:200:LEU:HD21	1:C:254:VAL:CG2	1.12	1.42
1:B:200:LEU:HD21	1:B:254:VAL:CG2	1.12	1.42
1:A:200:LEU:CD2	1:A:254:VAL:CG2	1.87	1.41
1:C:200:LEU:CD2	1:C:254:VAL:HG21	1.32	1.40
1:D:200:LEU:CD2	1:D:254:VAL:HG21	1.32	1.39
1:B:200:LEU:CD2	1:B:254:VAL:HG21	1.32	1.39
1:A:200:LEU:CD2	1:A:254:VAL:HG21	1.32	1.37
1:E:200:LEU:CD2	1:E:254:VAL:HG21	1.32	1.36
1:F:200:LEU:CD2	1:F:254:VAL:HG21	1.32	1.35
1:M:23:LEU:CD1	1:M:60:ILE:HD12	1.58	1.34
1:C:249:ILE:CD1	1:C:262:LEU:HD11	1.59	1.33
1:M:518:GLU:CB	1:M:518:GLU:C	2.01	1.33
1:L:518:GLU:CB	1:L:518:GLU:C	2.01	1.33
1:B:249:ILE:CD1	1:B:262:LEU:HD11	1.59	1.33
1:D:249:ILE:CD1	1:D:262:LEU:HD11	1.59	1.33
1:K:23:LEU:CD1	1:K:60:ILE:HD12	1.58	1.32
1:N:518:GLU:CB	1:N:518:GLU:C	2.01	1.32
1:N:23:LEU:CD1	1:N:60:ILE:HD12	1.58	1.32
1:H:23:LEU:CD1	1:H:60:ILE:HD12	1.58	1.32
1:L:23:LEU:CD1	1:L:60:ILE:HD12	1.58	1.32
1:I:233:MET:CE	1:I:249:ILE:HD13	1.60	1.32
1:I:518:GLU:CB	1:I:518:GLU:C	2.01	1.32
1:J:23:LEU:CD1	1:J:60:ILE:HD12	1.58	1.32
1:A:249:ILE:CD1	1:A:262:LEU:HD11	1.58	1.31
1:E:249:ILE:CD1	1:E:262:LEU:HD11	1.59	1.31
1:J:518:GLU:CB	1:J:518:GLU:C	2.01	1.31
1:I:23:LEU:CD1	1:I:60:ILE:HD12	1.58	1.31
1:H:518:GLU:CB	1:H:518:GLU:C	2.02	1.31
1:K:518:GLU:CB	1:K:518:GLU:C	2.01	1.31
1:J:233:MET:CE	1:J:249:ILE:HD13	1.60	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:ILE:CD1	1:F:262:LEU:HD11	1.58	1.29
1:G:249:ILE:CD1	1:G:262:LEU:HD11	1.59	1.29
1:D:200:LEU:CD2	1:D:254:VAL:CG2	1.87	1.29
1:K:233:MET:CE	1:K:249:ILE:HD13	1.62	1.28
1:N:233:MET:CE	1:N:249:ILE:HD13	1.63	1.28
1:H:233:MET:CE	1:H:249:ILE:HD13	1.63	1.27
1:L:233:MET:CE	1:L:249:ILE:HD13	1.65	1.27
1:M:233:MET:CE	1:M:249:ILE:HD13	1.66	1.25
1:C:200:LEU:CD2	1:C:254:VAL:CG2	1.87	1.24
1:K:301:ILE:CD1	1:K:312:ALA:HB2	1.69	1.23
1:L:301:ILE:CD1	1:L:312:ALA:HB2	1.69	1.23
1:J:301:ILE:CD1	1:J:312:ALA:HB2	1.69	1.23
1:M:301:ILE:CD1	1:M:312:ALA:HB2	1.69	1.23
1:I:301:ILE:CD1	1:I:312:ALA:HB2	1.69	1.22
1:N:301:ILE:CD1	1:N:312:ALA:HB2	1.68	1.21
1:B:200:LEU:CD2	1:B:254:VAL:CG2	1.87	1.21
1:H:23:LEU:HD12	1:H:60:ILE:CD1	1.71	1.21
1:I:23:LEU:HD12	1:I:60:ILE:CD1	1.71	1.21
1:J:23:LEU:HD12	1:J:60:ILE:CD1	1.71	1.20
1:H:301:ILE:CD1	1:H:312:ALA:HB2	1.69	1.20
1:N:23:LEU:HD12	1:N:60:ILE:CD1	1.71	1.20
1:K:23:LEU:HD12	1:K:60:ILE:CD1	1.71	1.20
1:L:23:LEU:HD12	1:L:60:ILE:CD1	1.71	1.19
1:M:23:LEU:HD12	1:M:60:ILE:CD1	1.71	1.19
1:G:23:LEU:HG	1:G:60:ILE:HD12	1.21	1.18
1:F:23:LEU:HG	1:F:60:ILE:HD12	1.21	1.18
1:C:193:MET:HG2	1:C:295:LEU:HG	1.23	1.18
1:C:249:ILE:HD11	1:C:262:LEU:HD21	1.22	1.17
1:G:249:ILE:HD11	1:G:262:LEU:HD21	1.23	1.17
1:L:37:ASN:N	1:M:518:GLU:HA	1.60	1.17
1:D:249:ILE:HD11	1:D:262:LEU:HD21	1.22	1.17
1:J:37:ASN:N	1:K:518:GLU:HA	1.59	1.17
1:B:249:ILE:HD11	1:B:262:LEU:HD21	1.23	1.16
1:E:249:ILE:CD1	1:E:262:LEU:CD1	2.20	1.16
1:A:249:ILE:HD11	1:A:262:LEU:HD21	1.22	1.16
1:I:37:ASN:N	1:J:518:GLU:HA	1.59	1.16
1:K:37:ASN:N	1:L:518:GLU:HA	1.59	1.15
1:M:37:ASN:N	1:N:518:GLU:HA	1.59	1.15
1:A:23:LEU:HG	1:A:60:ILE:HD12	1.21	1.15
1:E:249:ILE:HD11	1:E:262:LEU:HD21	1.23	1.15
1:A:249:ILE:CD1	1:A:262:LEU:CD1	2.20	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:CD1	1:B:262:LEU:CD1	2.21	1.14
1:C:193:MET:HE1	1:C:292:ILE:HG23	1.26	1.14
1:E:200:LEU:CD2	1:E:254:VAL:CG2	1.87	1.14
1:F:249:ILE:HD11	1:F:262:LEU:HD21	1.22	1.14
1:G:249:ILE:CD1	1:G:262:LEU:CD1	2.21	1.13
1:E:23:LEU:HG	1:E:60:ILE:HD12	1.21	1.13
1:B:23:LEU:HG	1:B:60:ILE:HD12	1.21	1.12
1:D:249:ILE:CD1	1:D:262:LEU:CD1	2.20	1.12
1:J:233:MET:HE2	1:J:249:ILE:HD13	1.14	1.11
1:N:208:PRO:C	1:N:208:PRO:HA	1.63	1.11
1:L:301:ILE:HD13	1:L:312:ALA:HB2	1.29	1.11
1:F:200:LEU:CD2	1:F:254:VAL:CG2	1.87	1.11
1:H:301:ILE:HD13	1:H:312:ALA:HB2	1.28	1.11
1:H:518:GLU:HA	1:N:37:ASN:N	1.59	1.10
1:I:301:ILE:HD13	1:I:312:ALA:HB2	1.29	1.10
1:H:37:ASN:N	1:I:518:GLU:HA	1.59	1.10
1:M:38:VAL:HA	1:N:519:CYS:H	1.11	1.10
1:N:233:MET:HE2	1:N:249:ILE:HD13	1.12	1.10
1:H:38:VAL:HA	1:I:519:CYS:H	1.11	1.10
1:B:199:TYR:HB3	1:B:325:ILE:HD11	1.33	1.10
1:C:199:TYR:HB3	1:C:325:ILE:HD11	1.33	1.10
1:E:249:ILE:HD11	1:E:262:LEU:CD2	1.82	1.10
1:I:38:VAL:HA	1:J:519:CYS:H	1.11	1.10
1:C:23:LEU:HG	1:C:60:ILE:HD12	1.21	1.09
1:F:249:ILE:HD11	1:F:262:LEU:CD2	1.82	1.09
1:K:38:VAL:HA	1:L:519:CYS:H	1.11	1.09
1:D:249:ILE:HD11	1:D:262:LEU:CD2	1.82	1.09
1:G:200:LEU:HD11	1:G:254:VAL:HG21	1.34	1.09
1:A:150:ILE:CD1	1:A:493:ILE:HA	1.83	1.09
1:H:233:MET:HE2	1:H:249:ILE:HD13	1.11	1.09
1:I:301:ILE:CD1	1:I:312:ALA:CB	2.31	1.09
1:J:301:ILE:CD1	1:J:312:ALA:CB	2.31	1.09
1:F:249:ILE:CD1	1:F:262:LEU:CD1	2.20	1.09
1:K:301:ILE:HD13	1:K:312:ALA:HB2	1.29	1.09
1:C:150:ILE:CD1	1:C:493:ILE:HA	1.83	1.08
1:D:23:LEU:HG	1:D:60:ILE:HD12	1.21	1.08
1:G:150:ILE:CD1	1:G:493:ILE:HA	1.83	1.08
1:H:301:ILE:CD1	1:H:312:ALA:CB	2.31	1.08
1:I:233:MET:HE2	1:I:249:ILE:HD13	1.14	1.08
1:M:233:MET:HE2	1:M:249:ILE:HD13	1.09	1.08
1:G:249:ILE:HD11	1:G:262:LEU:CD2	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:519:CYS:H	1:N:38:VAL:HA	1.11	1.08
1:L:38:VAL:HA	1:M:519:CYS:H	1.11	1.08
1:N:301:ILE:CD1	1:N:312:ALA:CB	2.31	1.08
1:A:249:ILE:HD11	1:A:262:LEU:CD2	1.82	1.08
1:K:301:ILE:CD1	1:K:312:ALA:CB	2.31	1.08
1:M:301:ILE:CD1	1:M:312:ALA:CB	2.31	1.08
1:A:199:TYR:HB3	1:A:325:ILE:HD11	1.33	1.07
1:J:301:ILE:HD13	1:J:312:ALA:HB2	1.28	1.07
1:N:301:ILE:HD13	1:N:312:ALA:HB2	1.29	1.07
1:B:150:ILE:CD1	1:B:493:ILE:HA	1.84	1.07
1:C:249:ILE:HD11	1:C:262:LEU:CD2	1.82	1.07
1:E:150:ILE:CD1	1:E:493:ILE:HA	1.83	1.07
1:L:233:MET:HE2	1:L:249:ILE:HD13	1.10	1.07
1:B:249:ILE:HD11	1:B:262:LEU:CD2	1.82	1.07
1:J:38:VAL:HA	1:K:519:CYS:H	1.11	1.07
1:L:301:ILE:CD1	1:L:312:ALA:CB	2.31	1.07
1:C:249:ILE:CD1	1:C:262:LEU:CD1	2.20	1.06
1:D:150:ILE:CD1	1:D:493:ILE:HA	1.84	1.06
1:F:150:ILE:CD1	1:F:493:ILE:HA	1.84	1.06
1:H:233:MET:HE2	1:H:249:ILE:CD1	1.85	1.06
1:K:233:MET:HE2	1:K:249:ILE:HD13	1.11	1.06
1:M:233:MET:HE2	1:M:249:ILE:CD1	1.84	1.06
1:D:199:TYR:HB3	1:D:325:ILE:HD11	1.30	1.05
1:L:233:MET:HE2	1:L:249:ILE:CD1	1.85	1.05
1:K:233:MET:HE2	1:K:249:ILE:CD1	1.85	1.05
1:N:233:MET:HE2	1:N:249:ILE:CD1	1.86	1.05
1:F:199:TYR:HB3	1:F:325:ILE:HD11	1.33	1.05
1:B:193:MET:HE3	1:B:332:ILE:HD12	1.37	1.05
1:E:199:TYR:HB3	1:E:325:ILE:HD11	1.33	1.05
1:A:193:MET:HE3	1:A:332:ILE:HD12	1.37	1.05
1:G:199:TYR:HB3	1:G:325:ILE:HD11	1.33	1.04
1:M:301:ILE:HD13	1:M:312:ALA:HB2	1.29	1.04
1:J:203:TYR:CG	1:J:267:MET:SD	2.52	1.03
1:C:249:ILE:HD12	1:C:262:LEU:HD13	1.38	1.03
1:I:203:TYR:CG	1:I:267:MET:SD	2.52	1.03
1:K:203:TYR:CG	1:K:267:MET:SD	2.52	1.03
1:M:203:TYR:CG	1:M:267:MET:SD	2.51	1.03
1:H:203:TYR:CG	1:H:267:MET:SD	2.52	1.02
1:I:233:MET:HE2	1:I:249:ILE:CD1	1.88	1.02
1:J:233:MET:HE2	1:J:249:ILE:CD1	1.87	1.02
1:L:203:TYR:CG	1:L:267:MET:SD	2.51	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:518:GLU:C	1:K:518:GLU:HB3	1.83	1.02
1:N:203:TYR:CG	1:N:267:MET:SD	2.51	1.02
1:N:518:GLU:C	1:N:518:GLU:HB3	1.83	1.02
1:I:518:GLU:C	1:I:518:GLU:HB3	1.83	1.02
1:A:249:ILE:HD12	1:A:262:LEU:HD13	1.38	1.02
1:N:182:GLY:HA3	1:N:383:ALA:H	1.24	1.02
1:E:193:MET:HE3	1:E:332:ILE:HD12	1.37	1.01
1:J:233:MET:CE	1:J:249:ILE:CD1	2.37	1.01
1:D:193:MET:HE3	1:D:332:ILE:HD12	1.37	1.01
1:F:193:MET:HE3	1:F:332:ILE:HD12	1.37	1.01
1:F:249:ILE:HD12	1:F:262:LEU:HD13	1.38	1.01
1:I:233:MET:CE	1:I:249:ILE:CD1	2.37	1.00
1:L:518:GLU:C	1:L:518:GLU:HB3	1.83	1.00
1:H:233:MET:CE	1:H:249:ILE:CD1	2.39	1.00
1:J:518:GLU:C	1:J:518:GLU:HB3	1.83	1.00
1:L:182:GLY:HA3	1:L:383:ALA:H	1.24	1.00
1:N:233:MET:CE	1:N:249:ILE:CD1	2.40	1.00
1:B:249:ILE:HD12	1:B:262:LEU:HD13	1.38	1.00
1:G:249:ILE:HD12	1:G:262:LEU:HD13	1.39	1.00
1:E:249:ILE:HD12	1:E:262:LEU:HD13	1.38	1.00
1:G:200:LEU:HD22	1:G:259:LEU:HD22	1.45	0.99
1:J:182:GLY:HA3	1:J:383:ALA:H	1.24	0.99
1:D:249:ILE:CD1	1:D:262:LEU:HD21	1.93	0.99
1:J:223:ALA:HB2	1:J:309:LEU:HD21	1.44	0.99
1:M:518:GLU:C	1:M:518:GLU:HB3	1.83	0.99
1:K:223:ALA:HB2	1:K:309:LEU:HD21	1.44	0.99
1:D:249:ILE:HD12	1:D:262:LEU:HD13	1.38	0.99
1:G:200:LEU:CD1	1:G:254:VAL:HG11	1.93	0.98
1:I:223:ALA:HB2	1:I:309:LEU:HD21	1.45	0.98
1:F:249:ILE:CD1	1:F:262:LEU:HD21	1.93	0.98
1:H:518:GLU:C	1:H:518:GLU:HB3	1.83	0.98
1:K:233:MET:CE	1:K:249:ILE:CD1	2.39	0.98
1:I:182:GLY:HA3	1:I:383:ALA:H	1.24	0.98
1:M:223:ALA:HB2	1:M:309:LEU:HD21	1.43	0.98
1:A:249:ILE:CD1	1:A:262:LEU:HD21	1.93	0.98
1:H:223:ALA:HB2	1:H:309:LEU:HD21	1.44	0.98
1:H:227:ILE:HD13	1:H:233:MET:SD	2.05	0.97
1:M:182:GLY:HA3	1:M:383:ALA:H	1.24	0.97
1:C:249:ILE:CD1	1:C:262:LEU:HD21	1.93	0.97
1:L:223:ALA:HB2	1:L:309:LEU:HD21	1.43	0.97
1:E:249:ILE:CD1	1:E:262:LEU:HD21	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:227:ILE:HD13	1:J:233:MET:SD	2.04	0.97
1:L:233:MET:CE	1:L:249:ILE:CD1	2.42	0.97
1:K:227:ILE:HD13	1:K:233:MET:SD	2.05	0.97
1:G:200:LEU:HD11	1:G:254:VAL:CG2	1.94	0.97
1:B:249:ILE:CD1	1:B:262:LEU:HD21	1.93	0.97
1:G:249:ILE:CD1	1:G:262:LEU:HD21	1.93	0.97
1:I:227:ILE:HD13	1:I:233:MET:SD	2.05	0.97
1:N:223:ALA:HB2	1:N:309:LEU:HD21	1.42	0.97
1:H:182:GLY:HA3	1:H:383:ALA:H	1.27	0.97
1:A:249:ILE:HD12	1:A:262:LEU:HD11	0.97	0.97
1:E:249:ILE:HD12	1:E:262:LEU:HD11	0.97	0.96
1:F:249:ILE:HD12	1:F:262:LEU:HD11	0.97	0.96
1:K:182:GLY:HA3	1:K:383:ALA:H	1.24	0.96
1:A:249:ILE:CD1	1:A:262:LEU:CD2	2.44	0.96
1:B:249:ILE:CD1	1:B:262:LEU:CD2	2.44	0.96
1:M:227:ILE:HD13	1:M:233:MET:SD	2.06	0.96
1:L:227:ILE:HD13	1:L:233:MET:SD	2.06	0.95
1:C:249:ILE:CD1	1:C:262:LEU:CD2	2.44	0.95
1:G:249:ILE:CD1	1:G:262:LEU:CD2	2.44	0.95
1:G:249:ILE:HD12	1:G:262:LEU:HD11	0.97	0.95
1:C:249:ILE:HD12	1:C:262:LEU:HD11	0.97	0.95
1:N:227:ILE:HD13	1:N:233:MET:SD	2.05	0.95
1:B:249:ILE:HD12	1:B:262:LEU:HD11	0.97	0.94
1:D:249:ILE:HD12	1:D:262:LEU:HD11	0.97	0.94
1:D:249:ILE:CD1	1:D:262:LEU:CD2	2.44	0.94
1:E:249:ILE:CD1	1:E:262:LEU:CD2	2.44	0.94
1:C:200:LEU:HD23	1:C:254:VAL:HG21	1.49	0.93
1:B:200:LEU:HD23	1:B:254:VAL:HG21	1.49	0.93
1:F:249:ILE:CD1	1:F:262:LEU:CD2	2.44	0.93
1:M:233:MET:CE	1:M:249:ILE:CD1	2.43	0.93
1:F:220:ILE:HD13	1:F:332:ILE:HD13	1.49	0.93
1:G:220:ILE:HD13	1:G:332:ILE:HD13	1.49	0.93
1:L:242:LYS:CA	1:M:257:GLU:HA	1.99	0.93
1:M:242:LYS:CA	1:N:257:GLU:HA	1.99	0.93
1:F:200:LEU:HD23	1:F:254:VAL:HG21	1.49	0.93
1:J:203:TYR:CD2	1:J:267:MET:SD	2.62	0.93
1:N:203:TYR:CD2	1:N:267:MET:SD	2.62	0.93
1:D:23:LEU:HG	1:D:60:ILE:CD1	1.99	0.93
1:K:203:TYR:CD2	1:K:267:MET:SD	2.62	0.93
1:C:23:LEU:HG	1:C:60:ILE:CD1	1.99	0.93
1:J:242:LYS:CA	1:K:257:GLU:HA	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:203:TYR:CD2	1:L:267:MET:SD	2.62	0.92
1:A:200:LEU:HD23	1:A:254:VAL:HG21	1.49	0.92
1:A:220:ILE:HD13	1:A:332:ILE:HD13	1.50	0.92
1:H:242:LYS:CA	1:I:257:GLU:HA	1.99	0.92
1:H:257:GLU:HA	1:N:242:LYS:CA	1.99	0.92
1:M:203:TYR:CD2	1:M:267:MET:SD	2.62	0.92
1:D:200:LEU:HD23	1:D:254:VAL:HG21	1.49	0.92
1:I:203:TYR:CD2	1:I:267:MET:SD	2.62	0.92
1:E:23:LEU:HG	1:E:60:ILE:CD1	1.99	0.92
1:H:203:TYR:CD2	1:H:267:MET:SD	2.62	0.92
1:G:23:LEU:HG	1:G:60:ILE:CD1	1.98	0.92
1:B:23:LEU:HG	1:B:60:ILE:CD1	1.98	0.92
1:B:220:ILE:HD13	1:B:332:ILE:HD13	1.49	0.92
1:E:220:ILE:HD13	1:E:332:ILE:HD13	1.49	0.91
1:I:242:LYS:CA	1:J:257:GLU:HA	1.99	0.91
1:A:23:LEU:HG	1:A:60:ILE:CD1	1.98	0.91
1:C:23:LEU:HA	1:C:60:ILE:HD13	1.52	0.91
1:D:23:LEU:HA	1:D:60:ILE:HD13	1.52	0.91
1:F:23:LEU:HG	1:F:60:ILE:CD1	1.99	0.91
1:C:213:VAL:CG1	1:C:325:ILE:HG12	2.01	0.91
1:H:242:LYS:C	1:I:257:GLU:HA	1.96	0.91
1:M:242:LYS:C	1:N:257:GLU:HA	1.96	0.91
1:B:23:LEU:HA	1:B:60:ILE:HD13	1.52	0.91
1:E:213:VAL:CG1	1:E:325:ILE:HG12	2.01	0.91
1:C:220:ILE:HD13	1:C:332:ILE:HD13	1.49	0.90
1:E:23:LEU:HA	1:E:60:ILE:HD13	1.52	0.90
1:F:213:VAL:CG1	1:F:325:ILE:HG12	2.01	0.90
1:D:220:ILE:HD13	1:D:332:ILE:HD13	1.49	0.90
1:D:213:VAL:CG1	1:D:325:ILE:HG12	2.01	0.90
1:G:213:VAL:CG1	1:G:325:ILE:HG12	2.01	0.90
1:L:242:LYS:C	1:M:257:GLU:HA	1.97	0.90
1:E:200:LEU:HD23	1:E:254:VAL:HG21	1.49	0.90
1:K:242:LYS:CA	1:L:257:GLU:HA	2.01	0.90
1:A:23:LEU:HA	1:A:60:ILE:HD13	1.52	0.90
1:B:213:VAL:CG1	1:B:325:ILE:HG12	2.01	0.90
1:F:23:LEU:HA	1:F:60:ILE:HD13	1.52	0.90
1:J:23:LEU:HD12	1:J:60:ILE:HD12	0.89	0.89
1:K:223:ALA:HB3	1:K:251:ALA:HB2	1.53	0.89
1:K:23:LEU:HD12	1:K:60:ILE:HD12	0.89	0.89
1:K:193:MET:SD	1:K:292:ILE:HA	2.12	0.89
1:G:23:LEU:HA	1:G:60:ILE:HD13	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.54	0.89
1:M:23:LEU:HD12	1:M:60:ILE:HD12	0.89	0.89
1:H:257:GLU:HA	1:N:242:LYS:C	1.98	0.89
1:I:23:LEU:HD12	1:I:60:ILE:HD12	0.90	0.89
1:L:23:LEU:HD12	1:L:60:ILE:HD12	0.89	0.89
1:N:223:ALA:HB3	1:N:251:ALA:HB2	1.54	0.89
1:N:206:ASN:HA	1:N:207:LYS:HG2	1.55	0.88
1:N:206:ASN:HA	1:N:207:LYS:CG	2.04	0.88
1:I:223:ALA:HB3	1:I:251:ALA:HB2	1.52	0.88
1:I:242:LYS:C	1:J:257:GLU:HA	1.98	0.88
1:H:23:LEU:HD12	1:H:60:ILE:HD12	0.89	0.88
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.52	0.88
1:J:242:LYS:C	1:K:257:GLU:HA	1.98	0.88
1:H:223:ALA:HB3	1:H:251:ALA:HB2	1.53	0.87
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.54	0.87
1:N:23:LEU:HD12	1:N:60:ILE:HD12	0.89	0.87
1:K:242:LYS:C	1:L:257:GLU:HA	1.98	0.87
1:A:249:ILE:HD12	1:A:262:LEU:CG	2.05	0.87
1:F:150:ILE:HD12	1:F:493:ILE:HA	1.57	0.86
1:G:200:LEU:N	1:G:200:LEU:HD12	1.88	0.86
1:G:249:ILE:HD12	1:G:262:LEU:CG	2.05	0.86
1:B:249:ILE:HD12	1:B:262:LEU:CG	2.05	0.86
1:M:36:ARG:C	1:N:518:GLU:HA	2.01	0.86
1:N:204:PHE:HA	1:N:207:LYS:NZ	1.89	0.86
1:H:219:PHE:HB2	1:H:240:VAL:HG13	1.57	0.85
1:K:219:PHE:HB2	1:K:240:VAL:HG13	1.57	0.85
1:B:150:ILE:HD12	1:B:493:ILE:HA	1.57	0.85
1:F:249:ILE:HD12	1:F:262:LEU:CG	2.05	0.85
1:J:219:PHE:HB2	1:J:240:VAL:HG13	1.57	0.85
1:L:36:ARG:C	1:M:518:GLU:HA	2.01	0.85
1:N:219:PHE:HB2	1:N:240:VAL:HG13	1.57	0.85
1:E:249:ILE:HD12	1:E:262:LEU:CG	2.05	0.85
1:I:219:PHE:HB2	1:I:240:VAL:HG13	1.57	0.85
1:I:233:MET:HE1	1:I:249:ILE:HD13	1.59	0.85
1:J:36:ARG:C	1:K:518:GLU:HA	2.01	0.85
1:J:233:MET:HE1	1:J:249:ILE:HD13	1.59	0.85
1:K:36:ARG:C	1:L:518:GLU:HA	2.01	0.85
1:M:301:ILE:HD12	1:M:312:ALA:CB	2.07	0.85
1:C:249:ILE:HD12	1:C:262:LEU:CG	2.05	0.85
1:L:219:PHE:HB2	1:L:240:VAL:HG13	1.57	0.85
1:D:150:ILE:HD12	1:D:493:ILE:HA	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ILE:HD12	1:D:262:LEU:CG	2.05	0.85
1:L:301:ILE:HD12	1:L:312:ALA:CB	2.07	0.84
1:N:208:PRO:HA	1:N:208:PRO:O	1.76	0.84
1:D:193:MET:HE3	1:D:332:ILE:CD1	2.07	0.84
1:E:193:MET:HE3	1:E:332:ILE:CD1	2.07	0.84
1:H:36:ARG:C	1:I:518:GLU:HA	2.01	0.84
1:K:37:ASN:N	1:L:518:GLU:CA	2.36	0.84
1:B:193:MET:HE3	1:B:332:ILE:CD1	2.07	0.84
1:K:199:TYR:HB3	1:K:325:ILE:HD11	1.58	0.84
1:J:301:ILE:HD12	1:J:312:ALA:CB	2.07	0.83
1:M:219:PHE:HB2	1:M:240:VAL:HG13	1.57	0.83
1:E:150:ILE:HD12	1:E:493:ILE:HA	1.60	0.83
1:H:518:GLU:HA	1:N:36:ARG:C	2.01	0.83
1:I:36:ARG:C	1:J:518:GLU:HA	2.01	0.83
1:I:301:ILE:HD12	1:I:312:ALA:CB	2.07	0.83
1:A:193:MET:HE3	1:A:332:ILE:CD1	2.07	0.83
1:H:301:ILE:HD12	1:H:312:ALA:CB	2.07	0.83
1:C:150:ILE:HD12	1:C:493:ILE:HA	1.60	0.83
1:F:193:MET:HE3	1:F:332:ILE:CD1	2.07	0.83
1:K:301:ILE:HD12	1:K:312:ALA:CB	2.07	0.83
1:L:207:LYS:HE2	1:L:207:LYS:HA	1.61	0.83
1:N:301:ILE:HD12	1:N:312:ALA:CB	2.07	0.82
1:M:37:ASN:N	1:N:518:GLU:CA	2.36	0.82
1:C:223:ALA:O	1:C:251:ALA:HA	1.80	0.82
1:A:223:ALA:O	1:A:251:ALA:HA	1.80	0.82
1:N:138:CYS:N	1:N:410:GLY:HA2	1.95	0.82
1:H:138:CYS:N	1:H:410:GLY:HA2	1.95	0.82
1:L:150:ILE:HD11	1:L:493:ILE:HA	1.62	0.82
1:M:138:CYS:N	1:M:410:GLY:HA2	1.95	0.82
1:C:192:GLY:HA2	1:C:332:ILE:O	1.80	0.82
1:F:249:ILE:HD13	1:F:262:LEU:HD11	1.62	0.82
1:K:150:ILE:HD11	1:K:493:ILE:HA	1.62	0.82
1:L:38:VAL:HA	1:M:519:CYS:N	1.95	0.82
1:M:38:VAL:HA	1:N:519:CYS:N	1.94	0.82
1:G:150:ILE:HD12	1:G:493:ILE:HA	1.60	0.81
1:G:200:LEU:CD2	1:G:254:VAL:HG11	2.10	0.81
1:A:150:ILE:HD12	1:A:493:ILE:HA	1.60	0.81
1:K:38:VAL:HA	1:L:519:CYS:N	1.95	0.81
1:L:162:ILE:HD13	1:L:400:LEU:HA	1.62	0.81
1:I:138:CYS:N	1:I:410:GLY:HA2	1.95	0.81
1:L:138:CYS:N	1:L:410:GLY:HA2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:LEU:HD23	1:L:183:LEU:H	1.45	0.81
1:M:150:ILE:HD11	1:M:493:ILE:HA	1.61	0.81
1:I:38:VAL:HA	1:J:519:CYS:N	1.95	0.81
1:K:162:ILE:HD13	1:K:400:LEU:HA	1.62	0.81
1:H:38:VAL:HA	1:I:519:CYS:N	1.95	0.81
1:J:150:ILE:HD11	1:J:493:ILE:HA	1.62	0.81
1:M:162:ILE:HD13	1:M:400:LEU:HA	1.62	0.81
1:C:193:MET:HE1	1:C:292:ILE:CG2	2.09	0.81
1:J:38:VAL:HA	1:K:519:CYS:N	1.95	0.81
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.63	0.81
1:F:223:ALA:O	1:F:251:ALA:HA	1.80	0.81
1:J:162:ILE:HD13	1:J:400:LEU:HA	1.62	0.81
1:N:208:PRO:HB2	1:N:209:GLU:OE2	1.80	0.81
1:E:223:ALA:O	1:E:251:ALA:HA	1.80	0.80
1:I:162:ILE:HD13	1:I:400:LEU:HA	1.62	0.80
1:H:150:ILE:HD11	1:H:493:ILE:HA	1.61	0.80
1:N:162:ILE:HD13	1:N:400:LEU:HA	1.62	0.80
1:J:138:CYS:N	1:J:410:GLY:HA2	1.95	0.80
1:K:138:CYS:N	1:K:410:GLY:HA2	1.95	0.80
1:H:162:ILE:HD13	1:H:400:LEU:HA	1.62	0.80
1:I:150:ILE:HD11	1:I:493:ILE:HA	1.62	0.80
1:L:38:VAL:CA	1:M:519:CYS:H	1.94	0.80
1:D:137:PRO:HA	1:D:410:GLY:HA2	1.63	0.80
1:G:223:ALA:O	1:G:251:ALA:HA	1.80	0.80
1:B:223:ALA:O	1:B:251:ALA:HA	1.80	0.80
1:D:223:ALA:O	1:D:251:ALA:HA	1.80	0.80
1:G:137:PRO:HA	1:G:410:GLY:CA	2.12	0.79
1:B:137:PRO:HA	1:B:410:GLY:CA	2.12	0.79
1:B:249:ILE:HD13	1:B:262:LEU:HD11	1.62	0.79
1:D:137:PRO:HA	1:D:410:GLY:CA	2.12	0.79
1:E:137:PRO:HA	1:E:410:GLY:HA2	1.63	0.79
1:E:199:TYR:HB3	1:E:325:ILE:CD1	2.12	0.79
1:H:518:GLU:CA	1:N:37:ASN:N	2.36	0.79
1:N:150:ILE:HD11	1:N:493:ILE:HA	1.62	0.79
1:N:206:ASN:HA	1:N:207:LYS:CB	2.11	0.79
1:A:137:PRO:HA	1:A:410:GLY:CA	2.12	0.79
1:H:38:VAL:CA	1:I:519:CYS:H	1.94	0.79
1:H:519:CYS:N	1:N:38:VAL:HA	1.94	0.79
1:N:204:PHE:HD1	1:N:207:LYS:HZ1	1.29	0.79
1:F:137:PRO:HA	1:F:410:GLY:CA	2.12	0.79
1:I:199:TYR:HB3	1:I:325:ILE:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:TYR:HB3	1:C:325:ILE:CD1	2.12	0.79
1:C:137:PRO:HA	1:C:410:GLY:CA	2.12	0.79
1:C:137:PRO:HA	1:C:410:GLY:HA2	1.63	0.79
1:C:249:ILE:HD13	1:C:262:LEU:HD11	1.62	0.79
1:E:137:PRO:HA	1:E:410:GLY:CA	2.12	0.79
1:M:199:TYR:HB3	1:M:325:ILE:HD11	1.65	0.79
1:N:199:TYR:HB3	1:N:325:ILE:HD11	1.65	0.79
1:C:207:LYS:HE3	1:C:207:LYS:H	1.47	0.78
1:F:137:PRO:HA	1:F:410:GLY:HA2	1.63	0.78
1:I:38:VAL:CA	1:J:519:CYS:H	1.94	0.78
1:K:233:MET:HE1	1:K:249:ILE:HD13	1.64	0.78
1:I:301:ILE:HD12	1:I:312:ALA:HB2	1.65	0.78
1:J:199:TYR:HB3	1:J:325:ILE:HD11	1.65	0.78
1:A:137:PRO:HA	1:A:410:GLY:HA2	1.63	0.78
1:G:137:PRO:HA	1:G:410:GLY:HA2	1.63	0.78
1:L:199:TYR:HB3	1:L:325:ILE:HD11	1.65	0.78
1:N:233:MET:HE1	1:N:249:ILE:HD13	1.64	0.78
1:B:199:TYR:HB3	1:B:325:ILE:CD1	2.12	0.78
1:H:519:CYS:H	1:N:38:VAL:CA	1.94	0.78
1:I:30:THR:O	1:I:35:GLY:HA3	1.84	0.78
1:K:30:THR:O	1:K:35:GLY:HA3	1.84	0.78
1:D:300:VAL:HG23	1:D:312:ALA:HB2	1.66	0.78
1:J:37:ASN:N	1:K:518:GLU:CA	2.36	0.78
1:E:200:LEU:HB2	1:E:259:LEU:HD13	1.66	0.78
1:C:300:VAL:HG23	1:C:312:ALA:HB2	1.66	0.78
1:F:200:LEU:HB2	1:F:259:LEU:HD13	1.66	0.77
1:F:300:VAL:HG23	1:F:312:ALA:HB2	1.66	0.77
1:G:300:VAL:HG23	1:G:312:ALA:HB2	1.66	0.77
1:A:249:ILE:HD13	1:A:262:LEU:HD11	1.62	0.77
1:B:137:PRO:HA	1:B:410:GLY:HA2	1.63	0.77
1:F:199:TYR:HB3	1:F:325:ILE:CD1	2.12	0.77
1:G:23:LEU:CG	1:G:60:ILE:HD12	2.11	0.77
1:M:30:THR:O	1:M:35:GLY:HA3	1.84	0.77
1:M:295:LEU:HA	1:M:342:ILE:HD11	1.66	0.77
1:E:249:ILE:HD13	1:E:262:LEU:HD11	1.62	0.77
1:E:300:VAL:HG23	1:E:312:ALA:HB2	1.66	0.77
1:A:200:LEU:HB2	1:A:259:LEU:HD13	1.66	0.77
1:C:200:LEU:HD12	1:C:275:ALA:HB3	1.66	0.77
1:D:23:LEU:CG	1:D:60:ILE:HD12	2.11	0.77
1:J:38:VAL:CA	1:K:519:CYS:H	1.94	0.77
1:N:295:LEU:HA	1:N:342:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD12	1:A:275:ALA:HB3	1.66	0.77
1:F:192:GLY:HA2	1:F:332:ILE:O	1.85	0.77
1:H:38:VAL:HA	1:I:519:CYS:O	1.85	0.77
1:H:295:LEU:HA	1:H:342:ILE:HD11	1.66	0.77
1:K:38:VAL:CA	1:L:519:CYS:H	1.94	0.77
1:L:30:THR:O	1:L:35:GLY:HA3	1.84	0.77
1:C:150:ILE:HD13	1:C:493:ILE:HG23	1.67	0.77
1:D:200:LEU:HD12	1:D:275:ALA:HB3	1.66	0.77
1:K:182:GLY:CA	1:K:383:ALA:H	1.98	0.77
1:A:300:VAL:HG23	1:A:312:ALA:HB2	1.66	0.77
1:A:199:TYR:HB3	1:A:325:ILE:CD1	2.12	0.77
1:B:300:VAL:HG23	1:B:312:ALA:HB2	1.66	0.77
1:D:200:LEU:HB2	1:D:259:LEU:HD13	1.66	0.77
1:F:150:ILE:CD1	1:F:493:ILE:HG23	2.15	0.77
1:F:200:LEU:HD12	1:F:275:ALA:HB3	1.66	0.77
1:J:30:THR:O	1:J:35:GLY:HA3	1.84	0.77
1:J:301:ILE:HD12	1:J:312:ALA:HB2	1.65	0.77
1:L:295:LEU:HA	1:L:342:ILE:HD11	1.66	0.77
1:N:187:LEU:HD12	1:N:378:VAL:O	1.85	0.77
1:D:150:ILE:CD1	1:D:493:ILE:HG23	2.15	0.77
1:G:200:LEU:CG	1:G:254:VAL:HG11	2.14	0.77
1:G:249:ILE:HD13	1:G:262:LEU:HD11	1.62	0.77
1:K:177:VAL:HG22	1:K:379:ILE:HB	1.67	0.77
1:N:30:THR:O	1:N:35:GLY:HA3	1.84	0.77
1:B:200:LEU:HB2	1:B:259:LEU:HD13	1.66	0.77
1:I:182:GLY:CA	1:I:383:ALA:H	1.98	0.77
1:B:150:ILE:CD1	1:B:493:ILE:HG23	2.15	0.76
1:E:192:GLY:HA2	1:E:332:ILE:O	1.85	0.76
1:G:150:ILE:HD13	1:G:493:ILE:HG23	1.67	0.76
1:H:519:CYS:O	1:N:38:VAL:HA	1.85	0.76
1:I:38:VAL:HA	1:J:519:CYS:O	1.85	0.76
1:B:356:ALA:HB1	1:B:361:ASP:HB2	1.68	0.76
1:C:193:MET:CE	1:C:292:ILE:HG23	2.11	0.76
1:F:23:LEU:CG	1:F:60:ILE:HD12	2.11	0.76
1:H:30:THR:O	1:H:35:GLY:HA3	1.84	0.76
1:H:233:MET:HE1	1:H:249:ILE:HD13	1.64	0.76
1:I:295:LEU:HA	1:I:342:ILE:HD11	1.66	0.76
1:J:38:VAL:HA	1:K:519:CYS:O	1.84	0.76
1:E:150:ILE:HD13	1:E:493:ILE:HG23	1.67	0.76
1:B:200:LEU:HD12	1:B:275:ALA:HB3	1.66	0.76
1:C:356:ALA:HB1	1:C:361:ASP:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLY:HA2	1:D:332:ILE:O	1.85	0.76
1:K:38:VAL:HA	1:L:519:CYS:O	1.85	0.76
1:A:192:GLY:HA2	1:A:332:ILE:O	1.85	0.76
1:D:200:LEU:HD12	1:D:275:ALA:CB	2.16	0.76
1:L:249:ILE:HB	1:L:275:ALA:HB2	1.68	0.76
1:C:200:LEU:HB2	1:C:259:LEU:HD13	1.66	0.76
1:G:192:GLY:HA2	1:G:332:ILE:O	1.85	0.76
1:G:193:MET:SD	1:G:292:ILE:HA	2.26	0.76
1:H:249:ILE:HB	1:H:275:ALA:HB2	1.68	0.76
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.68	0.76
1:C:200:LEU:HD12	1:C:275:ALA:CB	2.16	0.76
1:F:150:ILE:HD13	1:F:493:ILE:HG23	1.68	0.76
1:F:200:LEU:HD12	1:F:275:ALA:CB	2.16	0.76
1:G:199:TYR:HB3	1:G:325:ILE:CD1	2.12	0.76
1:M:249:ILE:HB	1:M:275:ALA:HB2	1.68	0.76
1:N:206:ASN:OD1	1:N:213:VAL:HG23	1.84	0.76
1:D:150:ILE:HD13	1:D:493:ILE:HG23	1.68	0.76
1:E:200:LEU:HD12	1:E:275:ALA:CB	2.16	0.76
1:H:37:ASN:N	1:I:518:GLU:CA	2.36	0.76
1:J:182:GLY:CA	1:J:383:ALA:H	1.98	0.76
1:L:38:VAL:HA	1:M:519:CYS:O	1.85	0.76
1:L:279:PRO:O	1:L:285:ARG:HA	1.85	0.76
1:M:169:VAL:CG1	1:M:377:ALA:HB3	2.16	0.76
1:N:249:ILE:HB	1:N:275:ALA:HB2	1.68	0.76
1:A:200:LEU:HD12	1:A:275:ALA:CB	2.16	0.76
1:A:356:ALA:HB1	1:A:361:ASP:HB2	1.68	0.76
1:B:192:GLY:HA2	1:B:332:ILE:O	1.85	0.76
1:E:200:LEU:HD12	1:E:275:ALA:HB3	1.66	0.76
1:K:137:PRO:HA	1:K:410:GLY:HA3	1.66	0.76
1:K:249:ILE:HB	1:K:275:ALA:HB2	1.68	0.76
1:K:279:PRO:O	1:K:285:ARG:HA	1.85	0.76
1:L:137:PRO:HA	1:L:410:GLY:HA3	1.66	0.76
1:L:182:GLY:CA	1:L:383:ALA:H	1.98	0.76
1:M:38:VAL:HA	1:N:519:CYS:O	1.85	0.76
1:M:137:PRO:HA	1:M:410:GLY:HA3	1.66	0.76
1:M:279:PRO:O	1:M:285:ARG:HA	1.85	0.76
1:B:200:LEU:HD12	1:B:275:ALA:CB	2.16	0.76
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.68	0.76
1:D:249:ILE:HD13	1:D:262:LEU:HD11	1.62	0.76
1:H:137:PRO:HA	1:H:410:GLY:HA3	1.66	0.76
1:I:137:PRO:HA	1:I:410:GLY:HA3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:279:PRO:O	1:I:285:ARG:HA	1.86	0.76
1:J:137:PRO:HA	1:J:410:GLY:HA3	1.66	0.76
1:K:295:LEU:HA	1:K:342:ILE:HD11	1.66	0.76
1:M:38:VAL:CA	1:N:519:CYS:H	1.94	0.76
1:N:137:PRO:HA	1:N:410:GLY:HA3	1.66	0.76
1:C:23:LEU:CG	1:C:60:ILE:HD12	2.11	0.75
1:J:279:PRO:O	1:J:285:ARG:HA	1.86	0.75
1:J:295:LEU:HA	1:J:342:ILE:HD11	1.66	0.75
1:M:182:GLY:CA	1:M:383:ALA:H	1.98	0.75
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.68	0.75
1:N:182:GLY:CA	1:N:383:ALA:H	1.98	0.75
1:D:356:ALA:HB1	1:D:361:ASP:HB2	1.68	0.75
1:J:169:VAL:CG1	1:J:377:ALA:HB3	2.16	0.75
1:H:182:GLY:CA	1:H:383:ALA:H	1.98	0.75
1:H:279:PRO:O	1:H:285:ARG:HA	1.85	0.75
1:I:169:VAL:CG1	1:I:377:ALA:HB3	2.16	0.75
1:K:169:VAL:CG1	1:K:377:ALA:HB3	2.16	0.75
1:C:207:LYS:HB2	1:C:208:PRO:HD3	1.68	0.75
1:L:169:VAL:CG1	1:L:377:ALA:HB3	2.16	0.75
1:H:169:VAL:CG1	1:H:377:ALA:HB3	2.16	0.75
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.68	0.75
1:G:356:ALA:HB1	1:G:361:ASP:HB2	1.68	0.75
1:I:249:ILE:HB	1:I:275:ALA:HB2	1.68	0.75
1:M:301:ILE:HD12	1:M:312:ALA:HB2	1.65	0.75
1:N:169:VAL:CG1	1:N:377:ALA:HB3	2.16	0.75
1:B:150:ILE:HD13	1:B:493:ILE:HG23	1.68	0.74
1:H:138:CYS:H	1:H:410:GLY:HA2	1.52	0.74
1:J:249:ILE:HB	1:J:275:ALA:HB2	1.68	0.74
1:N:138:CYS:H	1:N:410:GLY:HA2	1.52	0.74
1:F:240:VAL:HG11	1:F:247:LEU:HB2	1.68	0.74
1:A:150:ILE:HD13	1:A:493:ILE:HG23	1.67	0.74
1:D:150:ILE:HD11	1:D:493:ILE:HA	1.68	0.74
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.68	0.74
1:E:356:ALA:HB1	1:E:361:ASP:HB2	1.68	0.74
1:M:138:CYS:H	1:M:410:GLY:HA2	1.52	0.74
1:N:204:PHE:HA	1:N:207:LYS:HZ1	1.49	0.74
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.68	0.74
1:E:381:VAL:HG21	1:E:393:LYS:N	2.03	0.74
1:F:356:ALA:HB1	1:F:361:ASP:HB2	1.68	0.74
1:E:23:LEU:CG	1:E:60:ILE:HD12	2.11	0.74
1:N:279:PRO:O	1:N:285:ARG:HA	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:VAL:HG21	1:D:393:LYS:N	2.03	0.74
1:A:38:VAL:HG21	1:A:56:VAL:CG2	2.18	0.74
1:B:38:VAL:HG21	1:B:56:VAL:CG2	2.18	0.74
1:C:38:VAL:HG21	1:C:56:VAL:CG2	2.18	0.74
1:D:38:VAL:HG21	1:D:56:VAL:CG2	2.18	0.74
1:G:38:VAL:HG21	1:G:56:VAL:CG2	2.18	0.74
1:N:301:ILE:HD12	1:N:312:ALA:HB2	1.65	0.74
1:A:150:ILE:HD11	1:A:493:ILE:HA	1.69	0.73
1:B:222:LEU:HD21	1:B:292:ILE:HG22	1.70	0.73
1:E:38:VAL:HG21	1:E:56:VAL:CG2	2.18	0.73
1:F:222:LEU:HD21	1:F:292:ILE:HG22	1.70	0.73
1:G:150:ILE:HD11	1:G:493:ILE:HA	1.69	0.73
1:B:23:LEU:CG	1:B:60:ILE:HD12	2.11	0.73
1:B:150:ILE:HD11	1:B:493:ILE:HA	1.68	0.73
1:C:381:VAL:HG21	1:C:393:LYS:N	2.03	0.73
1:F:38:VAL:HG21	1:F:56:VAL:CG2	2.18	0.73
1:I:301:ILE:CD1	1:I:312:ALA:HB1	2.18	0.73
1:C:222:LEU:HD21	1:C:292:ILE:HG22	1.70	0.73
1:G:222:LEU:HD21	1:G:292:ILE:HG22	1.70	0.73
1:K:301:ILE:CD1	1:K:312:ALA:HB1	2.18	0.73
1:L:301:ILE:CD1	1:L:312:ALA:HB1	2.18	0.73
1:M:36:ARG:C	1:N:518:GLU:CA	2.62	0.73
1:A:222:LEU:HD21	1:A:292:ILE:HG22	1.70	0.73
1:C:262:LEU:HD22	1:C:273:VAL:HG11	1.71	0.73
1:E:222:LEU:HD21	1:E:292:ILE:HG22	1.70	0.73
1:F:381:VAL:HG21	1:F:393:LYS:N	2.03	0.73
1:H:301:ILE:CD1	1:H:312:ALA:HB1	2.18	0.73
1:I:36:ARG:C	1:J:518:GLU:CA	2.62	0.73
1:A:313:THR:H	1:A:316:ASP:HB3	1.54	0.73
1:B:313:THR:H	1:B:316:ASP:HB3	1.54	0.73
1:G:313:THR:H	1:G:316:ASP:HB3	1.54	0.73
1:I:138:CYS:H	1:I:410:GLY:HA2	1.52	0.73
1:K:36:ARG:C	1:L:518:GLU:CA	2.62	0.73
1:F:150:ILE:HD11	1:F:493:ILE:HA	1.68	0.73
1:H:518:GLU:CA	1:N:36:ARG:C	2.62	0.73
1:A:262:LEU:HD22	1:A:273:VAL:HG11	1.71	0.73
1:A:381:VAL:HG21	1:A:393:LYS:N	2.03	0.73
1:B:381:VAL:HG21	1:B:393:LYS:N	2.03	0.73
1:D:222:LEU:HD21	1:D:292:ILE:HG22	1.71	0.73
1:I:37:ASN:N	1:J:518:GLU:CA	2.36	0.73
1:G:262:LEU:HD22	1:G:273:VAL:HG11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:138:CYS:H	1:L:410:GLY:HA2	1.52	0.73
1:C:313:THR:H	1:C:316:ASP:HB3	1.54	0.72
1:F:193:MET:CE	1:F:332:ILE:HD12	2.19	0.72
1:G:381:VAL:HG21	1:G:393:LYS:N	2.03	0.72
1:F:313:THR:H	1:F:316:ASP:HB3	1.54	0.72
1:E:313:THR:H	1:E:316:ASP:HB3	1.54	0.72
1:N:301:ILE:CD1	1:N:312:ALA:HB1	2.18	0.72
1:G:150:ILE:CD1	1:G:493:ILE:HG23	2.20	0.72
1:K:207:LYS:HA	1:K:207:LYS:HE3	1.70	0.72
1:C:150:ILE:CD1	1:C:493:ILE:HG23	2.20	0.72
1:D:262:LEU:HD22	1:D:273:VAL:HG11	1.71	0.72
1:D:313:THR:H	1:D:316:ASP:HB3	1.54	0.72
1:E:150:ILE:CD1	1:E:493:ILE:HG23	2.20	0.72
1:E:193:MET:CE	1:E:332:ILE:HD12	2.19	0.72
1:G:193:MET:HG2	1:G:295:LEU:HG	1.71	0.72
1:G:312:ALA:HB1	1:G:316:ASP:CG	2.15	0.72
1:M:301:ILE:CD1	1:M:312:ALA:HB1	2.18	0.72
1:N:205:ILE:O	1:N:207:LYS:HG2	1.89	0.72
1:A:162:ILE:HD13	1:A:400:LEU:CA	2.20	0.72
1:H:36:ARG:C	1:I:518:GLU:CA	2.62	0.72
1:J:223:ALA:HB1	1:J:225:LYS:HD2	1.72	0.72
1:G:200:LEU:CD1	1:G:254:VAL:CG1	2.68	0.72
1:B:206:ASN:HB3	1:B:208:PRO:HD2	1.70	0.71
1:B:262:LEU:HD22	1:B:273:VAL:HG11	1.71	0.71
1:D:193:MET:CE	1:D:332:ILE:HD12	2.19	0.71
1:F:312:ALA:HB1	1:F:316:ASP:CG	2.15	0.71
1:A:23:LEU:CG	1:A:60:ILE:HD12	2.11	0.71
1:K:243:ALA:HB2	1:L:256:GLY:O	1.90	0.71
1:A:150:ILE:CD1	1:A:493:ILE:HG23	2.20	0.71
1:B:312:ALA:HB1	1:B:316:ASP:CG	2.15	0.71
1:E:312:ALA:HB1	1:E:316:ASP:CG	2.15	0.71
1:H:243:ALA:HB2	1:I:256:GLY:O	1.90	0.71
1:J:138:CYS:H	1:J:410:GLY:HA2	1.52	0.71
1:L:243:ALA:HB2	1:M:256:GLY:O	1.90	0.71
1:M:233:MET:HE1	1:M:249:ILE:HD13	1.71	0.71
1:M:243:ALA:HB2	1:N:256:GLY:O	1.90	0.71
1:C:162:ILE:HD13	1:C:400:LEU:CA	2.20	0.71
1:C:312:ALA:HB1	1:C:316:ASP:CG	2.15	0.71
1:E:162:ILE:HD13	1:E:400:LEU:CA	2.20	0.71
1:H:256:GLY:O	1:N:243:ALA:HB2	1.90	0.71
1:F:162:ILE:HD13	1:F:400:LEU:CA	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:LEU:HD22	1:F:273:VAL:HG11	1.71	0.71
1:I:223:ALA:HB1	1:I:225:LYS:HD2	1.72	0.71
1:J:36:ARG:C	1:K:518:GLU:CA	2.62	0.71
1:N:23:LEU:HD13	1:N:60:ILE:HD12	1.70	0.71
1:E:150:ILE:HD11	1:E:493:ILE:HA	1.70	0.71
1:F:249:ILE:CD1	1:F:262:LEU:CG	2.67	0.71
1:A:312:ALA:HB1	1:A:316:ASP:CG	2.15	0.71
1:H:199:TYR:HB3	1:H:325:ILE:HD11	1.72	0.71
1:L:36:ARG:C	1:M:518:GLU:CA	2.62	0.71
1:D:312:ALA:HB1	1:D:316:ASP:CG	2.15	0.71
1:D:162:ILE:HD13	1:D:400:LEU:CA	2.20	0.70
1:E:262:LEU:HD22	1:E:273:VAL:HG11	1.71	0.70
1:J:301:ILE:CD1	1:J:312:ALA:HB1	2.18	0.70
1:C:150:ILE:HD11	1:C:493:ILE:HA	1.70	0.70
1:H:217:SER:HA	1:H:320:ALA:O	1.91	0.70
1:K:223:ALA:HB1	1:K:225:LYS:HD2	1.73	0.70
1:G:193:MET:HE2	1:G:295:LEU:HD12	1.72	0.70
1:J:243:ALA:HB2	1:K:256:GLY:O	1.90	0.70
1:H:301:ILE:HD12	1:H:312:ALA:HB2	1.65	0.70
1:J:23:LEU:HD13	1:J:60:ILE:HD12	1.70	0.70
1:B:162:ILE:HD13	1:B:400:LEU:CA	2.20	0.70
1:B:195:PHE:CE1	1:B:330:THR:HB	2.26	0.70
2:C:1525:PO4:P	4:C:1527:ATP:O1G	2.50	0.70
1:K:138:CYS:H	1:K:410:GLY:HA2	1.52	0.70
1:B:200:LEU:CB	1:B:259:LEU:HD13	2.22	0.70
2:D:1525:PO4:P	4:D:1527:ATP:O1G	2.49	0.70
1:C:200:LEU:CB	1:C:259:LEU:HD13	2.22	0.70
1:F:207:LYS:H	1:F:207:LYS:HE2	1.55	0.70
1:H:223:ALA:HB1	1:H:225:LYS:HD2	1.73	0.70
1:K:153:ASN:N	1:K:154:SER:HA	2.06	0.70
1:L:233:MET:HE1	1:L:249:ILE:HD13	1.69	0.70
1:N:223:ALA:O	1:N:251:ALA:HA	1.92	0.70
1:A:200:LEU:CB	1:A:259:LEU:HD13	2.22	0.70
1:A:220:ILE:HD12	1:A:296:THR:HG21	1.74	0.70
2:F:1525:PO4:P	4:F:1527:ATP:O1G	2.49	0.70
1:H:153:ASN:N	1:H:154:SER:HA	2.06	0.70
1:D:199:TYR:HB3	1:D:325:ILE:CD1	2.16	0.70
1:F:200:LEU:CB	1:F:259:LEU:HD13	2.22	0.70
1:I:223:ALA:O	1:I:251:ALA:HA	1.92	0.70
1:G:162:ILE:HD13	1:G:400:LEU:CA	2.20	0.70
1:N:153:ASN:N	1:N:154:SER:HA	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:217:SER:HA	1:N:320:ALA:O	1.91	0.70
2:A:1525:PO4:P	4:A:1527:ATP:O1G	2.50	0.69
1:G:309:LEU:HD22	1:G:312:ALA:HB3	1.74	0.69
1:K:52:ASP:OD1	2:K:1525:PO4:P	2.50	0.69
1:K:192:GLY:O	1:K:375:GLY:HA2	1.92	0.69
1:L:223:ALA:O	1:L:251:ALA:HA	1.92	0.69
1:A:309:LEU:HD22	1:A:312:ALA:HB3	1.74	0.69
1:C:192:GLY:HA3	1:C:376:VAL:HG23	1.73	0.69
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.74	0.69
1:I:243:ALA:HB2	1:J:256:GLY:O	1.90	0.69
1:K:223:ALA:O	1:K:251:ALA:HA	1.92	0.69
1:L:242:LYS:HB2	1:M:257:GLU:O	1.92	0.69
1:N:52:ASP:OD1	2:N:1525:PO4:P	2.50	0.69
1:B:220:ILE:HD12	1:B:296:THR:HG21	1.74	0.69
1:C:309:LEU:HD22	1:C:312:ALA:HB3	1.74	0.69
2:E:1525:PO4:P	4:E:1527:ATP:O1G	2.50	0.69
1:L:52:ASP:OD1	2:L:1525:PO4:P	2.50	0.69
1:M:153:ASN:N	1:M:154:SER:HA	2.06	0.69
1:D:200:LEU:CB	1:D:259:LEU:HD13	2.22	0.69
1:E:200:LEU:CB	1:E:259:LEU:HD13	2.22	0.69
1:I:217:SER:HA	1:I:320:ALA:O	1.91	0.69
1:J:217:SER:HA	1:J:320:ALA:O	1.91	0.69
2:B:1525:PO4:P	4:B:1527:ATP:O1G	2.50	0.69
1:D:309:LEU:HD22	1:D:312:ALA:HB3	1.74	0.69
1:E:202:PRO:O	1:E:205:ILE:HG13	1.92	0.69
1:F:309:LEU:HD22	1:F:312:ALA:HB3	1.74	0.69
1:G:249:ILE:CD1	1:G:262:LEU:CG	2.67	0.69
1:I:52:ASP:OD1	2:I:1525:PO4:P	2.50	0.69
1:M:52:ASP:OD1	2:M:1525:PO4:P	2.50	0.69
1:B:309:LEU:HD22	1:B:312:ALA:HB3	1.75	0.69
1:D:249:ILE:CD1	1:D:262:LEU:CG	2.67	0.69
1:L:223:ALA:HB2	1:L:309:LEU:CD2	2.20	0.69
2:G:1525:PO4:P	4:G:1527:ATP:O1G	2.50	0.69
1:H:23:LEU:HD13	1:H:60:ILE:HD12	1.71	0.69
1:L:153:ASN:N	1:L:154:SER:HA	2.06	0.69
1:M:217:SER:HA	1:M:320:ALA:O	1.91	0.69
1:E:309:LEU:HD22	1:E:312:ALA:HB3	1.74	0.69
1:H:223:ALA:O	1:H:251:ALA:HA	1.92	0.69
1:H:257:GLU:O	1:N:242:LYS:HB2	1.93	0.69
1:J:153:ASN:N	1:J:154:SER:HA	2.06	0.69
1:J:223:ALA:O	1:J:251:ALA:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:PRO:HA	1:L:410:GLY:CA	2.23	0.69
1:M:223:ALA:O	1:M:251:ALA:HA	1.92	0.69
1:J:242:LYS:HB2	1:K:257:GLU:O	1.93	0.69
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.75	0.69
1:B:193:MET:CE	1:B:332:ILE:HD12	2.18	0.69
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.74	0.69
1:H:52:ASP:OD1	2:H:1525:PO4:P	2.50	0.69
1:K:217:SER:HA	1:K:320:ALA:O	1.91	0.69
1:L:217:SER:HA	1:L:320:ALA:O	1.91	0.69
1:M:223:ALA:HB2	1:M:309:LEU:CD2	2.20	0.69
1:K:177:VAL:HG22	1:K:379:ILE:CG2	2.23	0.68
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.76	0.68
1:C:193:MET:HE3	1:C:332:ILE:HD12	1.73	0.68
1:N:223:ALA:HB2	1:N:309:LEU:CD2	2.20	0.68
1:E:249:ILE:CD1	1:E:262:LEU:CG	2.67	0.68
1:G:193:MET:CG	1:G:295:LEU:HG	2.22	0.68
1:I:153:ASN:N	1:I:154:SER:HA	2.06	0.68
1:K:137:PRO:HA	1:K:410:GLY:CA	2.23	0.68
1:L:23:LEU:HD13	1:L:60:ILE:HD12	1.71	0.68
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.75	0.68
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.74	0.68
1:G:183:LEU:HA	1:G:383:ALA:H	1.59	0.68
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.76	0.68
1:J:52:ASP:OD1	2:J:1525:PO4:P	2.50	0.68
1:K:223:ALA:HB2	1:K:309:LEU:CD2	2.21	0.68
1:A:193:MET:CE	1:A:332:ILE:HD12	2.18	0.68
1:D:220:ILE:HD12	1:D:296:THR:HG21	1.74	0.68
1:E:220:ILE:HD12	1:E:296:THR:HG21	1.74	0.68
1:H:169:VAL:HG23	1:H:170:GLY:O	1.93	0.68
1:A:183:LEU:HA	1:A:383:ALA:H	1.59	0.68
1:F:183:LEU:HA	1:F:383:ALA:H	1.59	0.68
1:H:137:PRO:HA	1:H:410:GLY:CA	2.23	0.68
1:I:242:LYS:HB2	1:J:257:GLU:O	1.93	0.68
1:M:178:GLU:O	1:M:380:LYS:HA	1.94	0.68
1:N:137:PRO:HA	1:N:410:GLY:CA	2.23	0.68
1:G:193:MET:CE	1:G:296:THR:HG23	2.24	0.68
1:I:178:GLU:O	1:I:380:LYS:HA	1.94	0.68
1:K:178:GLU:O	1:K:380:LYS:HA	1.94	0.68
1:L:178:GLU:O	1:L:380:LYS:HA	1.94	0.68
1:M:223:ALA:HB1	1:M:225:LYS:HD2	1.76	0.68
1:N:223:ALA:HB1	1:N:225:LYS:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:LEU:HA	1:E:383:ALA:H	1.59	0.68
1:I:137:PRO:HA	1:I:410:GLY:CA	2.23	0.68
1:J:168:LYS:CG	1:J:187:LEU:HD21	2.24	0.68
1:H:203:TYR:CD1	1:H:267:MET:SD	2.88	0.67
1:I:169:VAL:HG23	1:I:170:GLY:O	1.93	0.67
1:J:137:PRO:HA	1:J:410:GLY:CA	2.23	0.67
1:J:169:VAL:HG23	1:J:170:GLY:O	1.93	0.67
1:I:203:TYR:CD1	1:I:267:MET:SD	2.87	0.67
1:L:223:ALA:HB1	1:L:225:LYS:HD2	1.76	0.67
1:B:183:LEU:HA	1:B:383:ALA:H	1.59	0.67
1:D:183:LEU:HA	1:D:383:ALA:H	1.59	0.67
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.75	0.67
1:J:223:ALA:HB2	1:J:309:LEU:CD2	2.22	0.67
1:K:169:VAL:HG23	1:K:170:GLY:O	1.93	0.67
1:M:137:PRO:HA	1:M:410:GLY:CA	2.23	0.67
1:N:203:TYR:CD1	1:N:267:MET:SD	2.87	0.67
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.75	0.67
1:L:169:VAL:HG23	1:L:170:GLY:O	1.93	0.67
1:G:227:ILE:HB	1:G:258:ALA:HB2	1.77	0.67
1:K:203:TYR:CD1	1:K:267:MET:SD	2.87	0.67
1:K:243:ALA:HA	1:L:260:ALA:HB2	1.77	0.67
1:M:169:VAL:HG23	1:M:170:GLY:O	1.93	0.67
1:A:162:ILE:HD13	1:A:400:LEU:HA	1.77	0.67
1:A:249:ILE:CD1	1:A:262:LEU:CG	2.67	0.67
1:C:183:LEU:HA	1:C:383:ALA:H	1.59	0.67
1:G:162:ILE:HD13	1:G:400:LEU:HA	1.77	0.67
1:A:227:ILE:HB	1:A:258:ALA:HB2	1.77	0.67
1:B:227:ILE:HB	1:B:258:ALA:HB2	1.77	0.67
1:E:162:ILE:HD13	1:E:400:LEU:HA	1.77	0.67
1:H:178:GLU:O	1:H:380:LYS:HA	1.94	0.67
1:H:243:ALA:HA	1:I:260:ALA:HB2	1.77	0.67
1:N:178:GLU:O	1:N:380:LYS:HA	1.94	0.67
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.75	0.67
1:H:223:ALA:HB2	1:H:309:LEU:CD2	2.21	0.67
1:N:204:PHE:C	1:N:207:LYS:HE2	2.20	0.67
1:C:227:ILE:HB	1:C:258:ALA:HB2	1.77	0.67
1:L:243:ALA:CA	1:M:256:GLY:O	2.43	0.67
1:B:194:GLN:CG	1:B:329:THR:HG21	2.25	0.67
1:C:249:ILE:CD1	1:C:262:LEU:CG	2.67	0.67
1:D:213:VAL:HG13	1:D:325:ILE:HG12	1.76	0.67
1:L:203:TYR:CD1	1:L:267:MET:SD	2.87	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:203:TYR:CD1	1:M:267:MET:SD	2.87	0.67
1:F:162:ILE:HD13	1:F:400:LEU:HA	1.77	0.66
1:F:213:VAL:HG13	1:F:325:ILE:HG12	1.77	0.66
1:F:227:ILE:HB	1:F:258:ALA:HB2	1.77	0.66
1:H:256:GLY:O	1:N:243:ALA:CA	2.43	0.66
1:H:295:LEU:HD23	1:H:342:ILE:HD13	1.78	0.66
1:N:295:LEU:HD23	1:N:342:ILE:HD13	1.77	0.66
1:B:162:ILE:HD13	1:B:400:LEU:HA	1.77	0.66
1:B:271:VAL:HG12	1:B:273:VAL:CG2	2.26	0.66
1:D:162:ILE:HD13	1:D:400:LEU:HA	1.77	0.66
1:E:279:PRO:O	1:E:285:ARG:HA	1.95	0.66
1:F:279:PRO:O	1:F:285:ARG:HA	1.95	0.66
1:I:223:ALA:HB2	1:I:309:LEU:CD2	2.22	0.66
1:J:203:TYR:CD1	1:J:267:MET:SD	2.87	0.66
1:K:243:ALA:CA	1:L:256:GLY:O	2.43	0.66
1:A:271:VAL:HG12	1:A:273:VAL:CG2	2.26	0.66
1:D:227:ILE:HB	1:D:258:ALA:HB2	1.77	0.66
1:M:243:ALA:CA	1:N:256:GLY:O	2.43	0.66
1:C:271:VAL:HG12	1:C:273:VAL:CG2	2.26	0.66
1:C:279:PRO:O	1:C:285:ARG:HA	1.95	0.66
1:D:271:VAL:HG12	1:D:273:VAL:CG2	2.26	0.66
1:E:271:VAL:HG12	1:E:273:VAL:CG2	2.26	0.66
1:G:213:VAL:HG13	1:G:325:ILE:HG12	1.76	0.66
1:H:243:ALA:CA	1:I:256:GLY:O	2.43	0.66
1:N:206:ASN:CA	1:N:207:LYS:HG2	2.24	0.66
1:A:200:LEU:HB2	1:A:259:LEU:CD1	2.25	0.66
1:E:227:ILE:HB	1:E:258:ALA:HB2	1.77	0.66
1:F:271:VAL:HG12	1:F:273:VAL:CG2	2.26	0.66
1:G:271:VAL:HG12	1:G:273:VAL:CG2	2.26	0.66
1:H:199:TYR:CE1	1:H:202:PRO:HA	2.31	0.66
1:K:223:ALA:CB	1:K:309:LEU:HD21	2.25	0.66
1:D:200:LEU:HB2	1:D:259:LEU:CD1	2.25	0.66
1:B:249:ILE:CD1	1:B:262:LEU:CG	2.67	0.66
1:E:200:LEU:HB2	1:E:259:LEU:CD1	2.25	0.66
1:B:213:VAL:HG13	1:B:325:ILE:HG12	1.76	0.66
1:C:162:ILE:HD13	1:C:400:LEU:HA	1.77	0.66
1:I:295:LEU:HD23	1:I:342:ILE:HD13	1.78	0.66
1:B:200:LEU:HB2	1:B:259:LEU:CD1	2.26	0.65
1:B:279:PRO:O	1:B:285:ARG:HA	1.95	0.65
1:D:279:PRO:O	1:D:285:ARG:HA	1.95	0.65
1:E:195:PHE:CE2	1:E:292:ILE:HD13	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:PRO:O	1:G:285:ARG:HA	1.95	0.65
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.78	0.65
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.78	0.65
1:I:243:ALA:CA	1:J:256:GLY:O	2.43	0.65
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.78	0.65
1:E:213:VAL:HG13	1:E:325:ILE:HG12	1.76	0.65
1:H:149:THR:O	1:H:154:SER:HA	1.97	0.65
1:I:249:ILE:O	1:I:275:ALA:HA	1.97	0.65
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.78	0.65
1:J:243:ALA:CA	1:K:256:GLY:O	2.43	0.65
1:L:149:THR:O	1:L:154:SER:HA	1.97	0.65
1:M:249:ILE:O	1:M:275:ALA:HA	1.97	0.65
1:A:162:ILE:HD13	1:A:400:LEU:N	2.12	0.65
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.78	0.65
1:J:179:ASP:OD2	1:J:389:MET:HE2	1.96	0.65
1:B:162:ILE:HD13	1:B:400:LEU:N	2.12	0.65
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.78	0.65
1:G:193:MET:SD	1:G:295:LEU:HG	2.36	0.65
1:K:149:THR:O	1:K:154:SER:HA	1.97	0.65
1:H:249:ILE:O	1:H:275:ALA:HA	1.97	0.65
1:J:249:ILE:O	1:J:275:ALA:HA	1.97	0.65
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.78	0.65
1:C:200:LEU:HB2	1:C:259:LEU:CD1	2.26	0.65
1:F:200:LEU:HB2	1:F:259:LEU:CD1	2.25	0.65
1:J:149:THR:O	1:J:154:SER:HA	1.97	0.65
1:K:249:ILE:O	1:K:275:ALA:HA	1.97	0.65
1:M:295:LEU:HD23	1:M:342:ILE:HD13	1.78	0.65
1:A:279:PRO:O	1:A:285:ARG:HA	1.95	0.65
1:J:295:LEU:HD23	1:J:342:ILE:HD13	1.78	0.65
1:M:223:ALA:CB	1:M:309:LEU:HD21	2.23	0.65
1:C:195:PHE:CE2	1:C:292:ILE:HD13	2.31	0.65
1:M:149:THR:O	1:M:154:SER:HA	1.97	0.65
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.78	0.65
1:A:195:PHE:CE2	1:A:292:ILE:HD13	2.31	0.65
1:D:195:PHE:CE2	1:D:292:ILE:HD13	2.31	0.65
1:G:161:LEU:HD11	1:G:185:ASP:HB3	1.79	0.65
1:G:195:PHE:CE2	1:G:292:ILE:HD13	2.31	0.65
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.78	0.65
1:D:223:ALA:HA	1:D:309:LEU:HD23	1.79	0.64
1:I:23:LEU:HD13	1:I:60:ILE:HD12	1.70	0.64
1:J:168:LYS:HG3	1:J:187:LEU:HD21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HD13	1:C:400:LEU:N	2.12	0.64
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.78	0.64
1:G:70:GLY:HA2	1:G:73:MET:HE3	1.78	0.64
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.78	0.64
1:N:149:THR:O	1:N:154:SER:HA	1.97	0.64
1:C:223:ALA:HA	1:C:309:LEU:HD23	1.79	0.64
1:K:223:ALA:HB3	1:K:251:ALA:CB	2.25	0.64
1:E:162:ILE:HD13	1:E:400:LEU:N	2.12	0.64
1:L:249:ILE:O	1:L:275:ALA:HA	1.97	0.64
1:M:223:ALA:HB3	1:M:251:ALA:CB	2.26	0.64
1:N:223:ALA:CB	1:N:309:LEU:HD21	2.23	0.64
1:B:197:ARG:HG3	1:B:198:GLY:O	1.97	0.64
1:E:223:ALA:HA	1:E:309:LEU:HD23	1.79	0.64
1:L:223:ALA:CB	1:L:309:LEU:HD21	2.23	0.64
1:G:162:ILE:HD13	1:G:400:LEU:N	2.12	0.64
1:M:301:ILE:HD11	1:M:316:ASP:OD2	1.98	0.64
1:N:202:PRO:O	1:N:205:ILE:HG13	1.98	0.64
1:C:213:VAL:HG13	1:C:325:ILE:HG12	1.76	0.64
1:J:202:PRO:O	1:J:205:ILE:HG13	1.98	0.64
1:L:202:PRO:O	1:L:205:ILE:HG13	1.98	0.64
1:L:223:ALA:HB3	1:L:251:ALA:CB	2.26	0.64
1:L:295:LEU:HD23	1:L:342:ILE:HD13	1.78	0.64
1:L:301:ILE:HD11	1:L:316:ASP:OD2	1.97	0.64
1:A:223:ALA:HA	1:A:309:LEU:HD23	1.79	0.64
1:D:162:ILE:HD13	1:D:400:LEU:N	2.12	0.64
1:G:202:PRO:O	1:G:205:ILE:HG13	1.98	0.64
1:J:223:ALA:CB	1:J:309:LEU:HD21	2.26	0.64
1:K:295:LEU:HD23	1:K:342:ILE:HD13	1.77	0.64
1:G:223:ALA:HA	1:G:309:LEU:HD23	1.79	0.64
1:J:223:ALA:HB3	1:J:251:ALA:CB	2.25	0.64
1:K:295:LEU:HA	1:K:342:ILE:CD1	2.27	0.64
1:K:301:ILE:HD11	1:K:316:ASP:OD2	1.98	0.64
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.78	0.64
1:N:249:ILE:O	1:N:275:ALA:HA	1.97	0.64
1:C:221:LEU:HD11	1:C:309:LEU:HD21	1.80	0.64
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.78	0.64
2:H:1525:PO4:P	4:H:1527:ATP:O3G	2.56	0.64
1:A:227:ILE:HD12	1:A:258:ALA:CB	2.29	0.63
1:B:223:ALA:HA	1:B:309:LEU:HD23	1.79	0.63
1:C:202:PRO:O	1:C:205:ILE:HG13	1.98	0.63
1:D:221:LEU:HD11	1:D:309:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:ILE:HD13	1:F:400:LEU:N	2.12	0.63
1:I:149:THR:O	1:I:154:SER:HA	1.97	0.63
1:I:202:PRO:O	1:I:205:ILE:HG13	1.98	0.63
1:K:23:LEU:HD13	1:K:60:ILE:HD12	1.71	0.63
1:N:223:ALA:HB3	1:N:251:ALA:CB	2.26	0.63
1:N:295:LEU:HA	1:N:342:ILE:CD1	2.27	0.63
1:G:200:LEU:HD13	1:G:254:VAL:HG11	1.79	0.63
1:H:295:LEU:HA	1:H:342:ILE:CD1	2.27	0.63
1:J:295:LEU:HA	1:J:342:ILE:CD1	2.27	0.63
2:L:1525:PO4:P	4:L:1527:ATP:O3G	2.56	0.63
1:M:295:LEU:HA	1:M:342:ILE:CD1	2.27	0.63
2:M:1525:PO4:P	4:M:1527:ATP:O3G	2.56	0.63
2:N:1525:PO4:P	4:N:1527:ATP:O3G	2.56	0.63
1:B:202:PRO:O	1:B:205:ILE:HG13	1.98	0.63
1:G:221:LEU:HD11	1:G:309:LEU:HD21	1.80	0.63
1:H:301:ILE:HD11	1:H:316:ASP:OD2	1.99	0.63
2:K:1525:PO4:P	4:K:1527:ATP:O3G	2.56	0.63
1:L:221:LEU:HA	1:L:317:LEU:HG	1.80	0.63
1:A:199:TYR:CB	1:A:325:ILE:HD11	2.21	0.63
1:F:221:LEU:HD11	1:F:309:LEU:HD21	1.80	0.63
1:M:202:PRO:O	1:M:205:ILE:HG13	1.98	0.63
1:M:242:LYS:CB	1:N:257:GLU:HA	2.27	0.63
1:B:221:LEU:HD11	1:B:309:LEU:HD21	1.80	0.63
1:F:223:ALA:HA	1:F:309:LEU:HD23	1.79	0.63
1:F:227:ILE:HD12	1:F:258:ALA:CB	2.29	0.63
1:N:196:ASP:OD1	1:N:329:THR:HG22	1.99	0.63
1:N:221:LEU:HA	1:N:317:LEU:HG	1.79	0.63
1:D:227:ILE:HD12	1:D:258:ALA:CB	2.29	0.63
1:H:202:PRO:O	1:H:205:ILE:HG13	1.98	0.63
1:I:223:ALA:HB3	1:I:251:ALA:CB	2.25	0.63
2:J:1525:PO4:P	4:J:1527:ATP:O3G	2.56	0.63
1:L:295:LEU:HA	1:L:342:ILE:CD1	2.27	0.63
1:M:221:LEU:HA	1:M:317:LEU:HG	1.80	0.63
1:N:301:ILE:HD11	1:N:316:ASP:OD2	1.98	0.63
1:E:227:ILE:HD12	1:E:258:ALA:CB	2.29	0.63
1:F:224:ASP:O	1:F:303:GLU:HB2	1.99	0.63
1:G:227:ILE:HD12	1:G:258:ALA:CB	2.29	0.63
1:C:145:ALA:HA	1:C:159:GLY:O	1.99	0.63
1:D:197:ARG:HG3	1:D:198:GLY:O	1.99	0.63
1:E:224:ASP:O	1:E:303:GLU:HB2	1.99	0.63
1:D:145:ALA:HA	1:D:159:GLY:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:O	1:D:303:GLU:HB2	1.99	0.63
1:G:224:ASP:O	1:G:303:GLU:HB2	1.99	0.63
1:H:223:ALA:HB3	1:H:251:ALA:CB	2.25	0.63
1:I:295:LEU:HA	1:I:342:ILE:CD1	2.27	0.63
1:I:301:ILE:HD11	1:I:316:ASP:OD2	1.98	0.63
1:J:301:ILE:HD11	1:J:316:ASP:OD2	1.99	0.63
1:K:202:PRO:O	1:K:205:ILE:HG13	1.98	0.63
1:C:224:ASP:O	1:C:303:GLU:HB2	1.99	0.62
1:E:145:ALA:HA	1:E:159:GLY:O	1.99	0.62
1:I:149:THR:HA	1:I:155:ASP:O	1.99	0.62
1:A:511:ALA:O	1:A:515:ILE:HG13	2.00	0.62
1:B:227:ILE:HD12	1:B:258:ALA:CB	2.29	0.62
1:D:202:PRO:O	1:D:205:ILE:HG13	1.98	0.62
1:E:221:LEU:HD11	1:E:309:LEU:HD21	1.80	0.62
1:N:149:THR:HA	1:N:155:ASP:O	2.00	0.62
1:B:224:ASP:O	1:B:303:GLU:HB2	1.99	0.62
1:C:227:ILE:HD12	1:C:258:ALA:CB	2.29	0.62
1:E:511:ALA:O	1:E:515:ILE:HG13	2.00	0.62
1:F:511:ALA:O	1:F:515:ILE:HG13	2.00	0.62
1:G:511:ALA:O	1:G:515:ILE:HG13	2.00	0.62
1:K:221:LEU:HA	1:K:317:LEU:HG	1.80	0.62
1:A:221:LEU:HD11	1:A:309:LEU:HD21	1.80	0.62
1:B:145:ALA:HA	1:B:159:GLY:O	1.99	0.62
1:I:223:ALA:CB	1:I:309:LEU:HD21	2.26	0.62
1:J:192:GLY:O	1:J:375:GLY:HA2	1.99	0.62
1:A:145:ALA:HA	1:A:159:GLY:O	1.99	0.62
1:H:149:THR:HA	1:H:155:ASP:O	2.00	0.62
1:N:240:VAL:CG2	1:N:317:LEU:HD22	2.30	0.62
1:F:145:ALA:HA	1:F:159:GLY:O	1.99	0.62
1:F:207:LYS:H	1:F:207:LYS:CE	2.12	0.62
2:I:1525:PO4:P	4:I:1527:ATP:O3G	2.56	0.62
1:J:149:THR:HA	1:J:155:ASP:O	2.00	0.62
1:J:151:SER:CB	1:J:399:ALA:HA	2.30	0.62
1:M:149:THR:HA	1:M:155:ASP:O	2.00	0.62
1:A:224:ASP:O	1:A:303:GLU:HB2	1.99	0.62
1:B:511:ALA:O	1:B:515:ILE:HG13	2.00	0.62
1:C:511:ALA:O	1:C:515:ILE:HG13	2.00	0.62
1:D:240:VAL:CG1	1:D:271:VAL:HG13	2.30	0.62
1:G:145:ALA:HA	1:G:159:GLY:O	1.99	0.62
1:G:240:VAL:CG1	1:G:271:VAL:HG13	2.30	0.62
1:J:240:VAL:CG2	1:J:317:LEU:HD22	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:GLN:HA	1:K:75:LYS:HD2	1.82	0.62
1:L:192:GLY:O	1:L:375:GLY:HA2	1.99	0.62
1:D:511:ALA:O	1:D:515:ILE:HG13	2.00	0.62
1:L:384:ALA:HA	1:L:385:THR:C	2.25	0.62
1:M:240:VAL:CG2	1:M:317:LEU:HD22	2.30	0.62
1:B:204:PHE:CE1	1:B:273:VAL:O	2.53	0.61
1:E:240:VAL:CG1	1:E:271:VAL:HG13	2.30	0.61
1:F:165:ALA:HB2	1:F:187:LEU:HD11	1.82	0.61
1:F:240:VAL:CG1	1:F:271:VAL:HG13	2.30	0.61
1:I:151:SER:CB	1:I:399:ALA:HA	2.30	0.61
1:J:72:GLN:HA	1:J:75:LYS:HD2	1.82	0.61
1:L:72:GLN:HA	1:L:75:LYS:HD2	1.82	0.61
1:H:223:ALA:CB	1:H:309:LEU:HD21	2.25	0.61
1:I:72:GLN:HA	1:I:75:LYS:HD2	1.82	0.61
1:K:151:SER:CB	1:K:399:ALA:HA	2.30	0.61
1:M:151:SER:CB	1:M:399:ALA:HA	2.30	0.61
1:N:151:SER:CB	1:N:399:ALA:HA	2.30	0.61
1:N:192:GLY:O	1:N:375:GLY:HA2	1.99	0.61
1:C:204:PHE:CE1	1:C:273:VAL:O	2.53	0.61
1:F:204:PHE:CE1	1:F:273:VAL:O	2.53	0.61
1:H:192:GLY:O	1:H:375:GLY:HA2	1.99	0.61
1:I:384:ALA:HA	1:I:385:THR:C	2.25	0.61
1:L:151:SER:CB	1:L:399:ALA:HA	2.30	0.61
1:H:151:SER:CB	1:H:399:ALA:HA	2.30	0.61
1:B:240:VAL:CG1	1:B:271:VAL:HG13	2.30	0.61
1:H:72:GLN:HA	1:H:75:LYS:HD2	1.82	0.61
1:H:221:LEU:HA	1:H:317:LEU:HG	1.81	0.61
1:K:177:VAL:HG22	1:K:379:ILE:CB	2.30	0.61
1:K:240:VAL:CG2	1:K:317:LEU:HD22	2.30	0.61
1:L:149:THR:HA	1:L:155:ASP:O	1.99	0.61
1:L:189:VAL:HA	1:L:377:ALA:HA	1.83	0.61
1:L:240:VAL:CG2	1:L:317:LEU:HD22	2.30	0.61
1:D:169:VAL:HB	1:D:173:GLY:HA3	1.82	0.61
1:I:192:GLY:O	1:I:375:GLY:HA2	1.99	0.61
1:A:204:PHE:CE1	1:A:273:VAL:O	2.53	0.61
1:H:189:VAL:HA	1:H:377:ALA:HA	1.83	0.61
1:J:384:ALA:HA	1:J:385:THR:C	2.25	0.61
1:K:384:ALA:HA	1:K:385:THR:C	2.25	0.61
1:M:23:LEU:HD13	1:M:60:ILE:HD12	1.70	0.61
1:M:384:ALA:HA	1:M:385:THR:C	2.25	0.61
1:E:169:VAL:HB	1:E:173:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:PHE:CE1	1:G:273:VAL:O	2.53	0.61
1:N:189:VAL:HA	1:N:377:ALA:HA	1.83	0.61
1:C:169:VAL:HB	1:C:173:GLY:HA3	1.83	0.61
1:D:204:PHE:CE1	1:D:273:VAL:O	2.53	0.61
1:I:221:LEU:HA	1:I:317:LEU:HG	1.81	0.61
1:J:221:LEU:HA	1:J:317:LEU:HG	1.80	0.61
1:B:200:LEU:CD1	1:B:259:LEU:HD13	2.31	0.61
1:E:220:ILE:HD13	1:E:332:ILE:CD1	2.27	0.61
1:F:220:ILE:HD13	1:F:332:ILE:CD1	2.27	0.61
1:K:189:VAL:HA	1:K:377:ALA:HA	1.83	0.61
1:K:480:ALA:O	1:K:483:GLU:HG2	2.01	0.61
1:M:192:GLY:O	1:M:375:GLY:HA2	1.99	0.61
1:N:72:GLN:HA	1:N:75:LYS:HD2	1.82	0.61
1:B:169:VAL:HB	1:B:173:GLY:HA3	1.82	0.60
1:I:240:VAL:CG2	1:I:317:LEU:HD22	2.30	0.60
1:K:149:THR:HA	1:K:155:ASP:O	2.00	0.60
1:A:169:VAL:HB	1:A:173:GLY:HA3	1.82	0.60
1:D:200:LEU:CD1	1:D:259:LEU:HD13	2.31	0.60
1:H:240:VAL:HG22	1:H:317:LEU:HD22	1.84	0.60
1:L:480:ALA:O	1:L:483:GLU:HG2	2.01	0.60
1:M:72:GLN:HA	1:M:75:LYS:HD2	1.82	0.60
1:N:480:ALA:O	1:N:483:GLU:HG2	2.01	0.60
1:B:199:TYR:CB	1:B:325:ILE:HD11	2.21	0.60
1:D:52:ASP:OD1	2:D:1525:PO4:P	2.60	0.60
1:F:169:VAL:HB	1:F:173:GLY:HA3	1.83	0.60
1:G:169:VAL:HB	1:G:173:GLY:HA3	1.82	0.60
1:G:217:SER:HA	1:G:320:ALA:O	2.02	0.60
1:H:240:VAL:CG2	1:H:317:LEU:HD22	2.30	0.60
1:M:480:ALA:O	1:M:483:GLU:HG2	2.01	0.60
1:H:384:ALA:HA	1:H:385:THR:C	2.25	0.60
1:I:169:VAL:HG12	1:I:377:ALA:HB3	1.83	0.60
1:I:240:VAL:HG22	1:I:317:LEU:HD22	1.84	0.60
1:J:169:VAL:HG12	1:J:377:ALA:HB3	1.83	0.60
1:J:189:VAL:HA	1:J:377:ALA:HA	1.83	0.60
1:A:217:SER:HA	1:A:320:ALA:O	2.02	0.60
1:C:200:LEU:CD1	1:C:259:LEU:HD13	2.31	0.60
1:C:240:VAL:CG1	1:C:271:VAL:HG13	2.30	0.60
1:D:199:TYR:CB	1:D:325:ILE:HD11	2.20	0.60
1:F:217:SER:HA	1:F:320:ALA:O	2.02	0.60
1:A:240:VAL:CG1	1:A:271:VAL:HG13	2.30	0.60
1:D:220:ILE:HD13	1:D:332:ILE:CD1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:CD1	1:E:259:LEU:HD13	2.31	0.60
1:F:52:ASP:OD1	2:F:1525:PO4:P	2.60	0.60
1:G:220:ILE:HD13	1:G:332:ILE:CD1	2.27	0.60
1:K:192:GLY:HA3	1:K:332:ILE:O	2.02	0.60
1:A:200:LEU:CD1	1:A:259:LEU:HD13	2.31	0.60
1:H:480:ALA:O	1:H:483:GLU:HG2	2.01	0.60
1:I:480:ALA:O	1:I:483:GLU:HG2	2.01	0.60
1:B:52:ASP:OD1	2:B:1525:PO4:P	2.60	0.60
1:F:200:LEU:CD1	1:F:259:LEU:HD13	2.31	0.60
1:K:127:ALA:HB2	1:K:426:LEU:HD11	1.84	0.60
1:A:200:LEU:HB3	1:A:259:LEU:HD22	1.84	0.60
1:F:199:TYR:CB	1:F:325:ILE:HD11	2.21	0.60
1:J:240:VAL:HG22	1:J:317:LEU:HD22	1.84	0.60
1:M:193:MET:SD	1:M:292:ILE:HA	2.42	0.60
1:N:240:VAL:HG22	1:N:317:LEU:HD22	1.83	0.60
1:A:220:ILE:HD13	1:A:332:ILE:CD1	2.27	0.59
1:B:217:SER:HA	1:B:320:ALA:O	2.02	0.59
1:B:220:ILE:HD13	1:B:332:ILE:CD1	2.27	0.59
1:J:193:MET:SD	1:J:292:ILE:HA	2.42	0.59
1:M:127:ALA:HB2	1:M:426:LEU:HD11	1.84	0.59
1:N:127:ALA:HB2	1:N:426:LEU:HD11	1.84	0.59
1:C:220:ILE:HD13	1:C:332:ILE:CD1	2.27	0.59
1:J:127:ALA:HB2	1:J:426:LEU:HD11	1.84	0.59
1:K:204:PHE:CD1	1:K:273:VAL:O	2.55	0.59
1:L:127:ALA:HB2	1:L:426:LEU:HD11	1.84	0.59
1:M:242:LYS:HB3	1:N:257:GLU:HA	1.83	0.59
1:N:204:PHE:CD1	1:N:273:VAL:O	2.55	0.59
1:N:384:ALA:HA	1:N:385:THR:C	2.25	0.59
1:D:200:LEU:HB3	1:D:259:LEU:HD22	1.84	0.59
1:J:204:PHE:CD1	1:J:273:VAL:O	2.55	0.59
1:L:193:MET:SD	1:L:292:ILE:HA	2.42	0.59
1:C:200:LEU:HB3	1:C:259:LEU:HD22	1.84	0.59
1:E:217:SER:HA	1:E:320:ALA:O	2.02	0.59
1:I:193:MET:SD	1:I:292:ILE:HA	2.42	0.59
1:I:204:PHE:CD1	1:I:273:VAL:O	2.55	0.59
1:L:174:VAL:HG12	1:L:376:VAL:HG13	1.83	0.59
1:H:193:MET:SD	1:H:292:ILE:HA	2.42	0.59
1:H:301:ILE:HD11	1:H:312:ALA:CB	2.32	0.59
1:I:127:ALA:HB2	1:I:426:LEU:HD11	1.84	0.59
1:J:192:GLY:HA3	1:J:332:ILE:O	2.03	0.59
1:K:169:VAL:HG12	1:K:377:ALA:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:240:VAL:HG22	1:K:317:LEU:HD22	1.83	0.59
1:N:193:MET:SD	1:N:292:ILE:HA	2.42	0.59
1:G:52:ASP:OD1	2:G:1525:PO4:P	2.61	0.59
1:J:480:ALA:O	1:J:483:GLU:HG2	2.01	0.59
1:L:204:PHE:CD1	1:L:273:VAL:O	2.55	0.59
1:M:23:LEU:HD23	1:M:74:VAL:HG13	1.85	0.59
1:M:204:PHE:CD1	1:M:273:VAL:O	2.55	0.59
1:A:52:ASP:OD1	2:A:1525:PO4:P	2.61	0.59
1:H:127:ALA:HB2	1:H:426:LEU:HD11	1.84	0.59
1:H:169:VAL:HG12	1:H:377:ALA:HB3	1.83	0.59
1:N:23:LEU:HD23	1:N:74:VAL:HG13	1.84	0.59
1:H:23:LEU:HD23	1:H:74:VAL:HG13	1.84	0.59
1:K:242:LYS:HG3	1:L:257:GLU:O	2.03	0.59
1:L:192:GLY:HA3	1:L:332:ILE:O	2.03	0.59
1:H:165:ALA:O	1:H:169:VAL:HG22	2.03	0.59
1:H:204:PHE:CD1	1:H:273:VAL:O	2.55	0.59
2:J:1525:PO4:P	4:J:1527:ATP:O1A	2.61	0.59
1:M:165:ALA:O	1:M:169:VAL:HG22	2.03	0.59
1:M:240:VAL:HG22	1:M:317:LEU:HD22	1.83	0.59
1:M:243:ALA:CB	1:N:256:GLY:O	2.51	0.59
2:N:1525:PO4:P	4:N:1527:ATP:O1A	2.61	0.59
1:G:199:TYR:CB	1:G:325:ILE:HD11	2.21	0.59
1:L:165:ALA:O	1:L:169:VAL:HG22	2.03	0.59
1:M:169:VAL:HG12	1:M:377:ALA:HB3	1.83	0.59
1:M:420:ILE:HD12	1:M:451:LEU:HD13	1.85	0.59
2:M:1525:PO4:P	4:M:1527:ATP:O1A	2.61	0.59
1:N:165:ALA:O	1:N:169:VAL:HG22	2.03	0.59
1:E:52:ASP:OD1	2:E:1525:PO4:P	2.61	0.58
1:H:256:GLY:O	1:N:243:ALA:CB	2.51	0.58
1:H:298:GLY:HA3	1:H:318:GLY:HA3	1.86	0.58
1:I:243:ALA:CB	1:J:256:GLY:O	2.51	0.58
1:J:243:ALA:CB	1:K:256:GLY:O	2.51	0.58
1:J:298:GLY:HA3	1:J:318:GLY:HA3	1.85	0.58
1:K:165:ALA:O	1:K:169:VAL:HG22	2.03	0.58
1:L:175:ILE:HG22	1:L:176:THR:N	2.17	0.58
1:M:242:LYS:HB3	1:N:257:GLU:CA	2.31	0.58
1:N:169:VAL:HG12	1:N:377:ALA:HB3	1.83	0.58
1:B:195:PHE:CZ	1:B:330:THR:HB	2.38	0.58
1:H:243:ALA:CB	1:I:256:GLY:O	2.51	0.58
2:I:1525:PO4:P	4:I:1527:ATP:O1A	2.61	0.58
1:K:301:ILE:HD12	1:K:312:ALA:HB2	1.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1525:PO4:P	4:K:1527:ATP:O1A	2.61	0.58
1:L:23:LEU:HD23	1:L:74:VAL:HG13	1.85	0.58
1:L:240:VAL:HG22	1:L:317:LEU:HD22	1.84	0.58
2:L:1525:PO4:P	4:L:1527:ATP:O1A	2.61	0.58
1:N:192:GLY:HA3	1:N:332:ILE:O	2.03	0.58
1:I:169:VAL:HB	1:I:173:GLY:HA3	1.85	0.58
1:N:420:ILE:HD12	1:N:451:LEU:HD13	1.86	0.58
1:C:52:ASP:OD1	2:C:1525:PO4:P	2.61	0.58
1:G:221:LEU:HD13	1:G:236:VAL:HG21	1.86	0.58
1:H:169:VAL:HB	1:H:173:GLY:HA3	1.85	0.58
2:H:1525:PO4:P	4:H:1527:ATP:O1A	2.61	0.58
1:I:298:GLY:HA3	1:I:318:GLY:HA3	1.85	0.58
1:J:169:VAL:HB	1:J:173:GLY:HA3	1.85	0.58
1:A:221:LEU:HD13	1:A:236:VAL:HG21	1.86	0.58
1:D:217:SER:HA	1:D:320:ALA:O	2.02	0.58
1:E:199:TYR:CB	1:E:325:ILE:HD11	2.21	0.58
1:G:200:LEU:CD1	1:G:200:LEU:N	2.64	0.58
1:I:165:ALA:O	1:I:169:VAL:HG22	2.03	0.58
1:K:298:GLY:HA3	1:K:318:GLY:HA3	1.86	0.58
1:B:200:LEU:HB3	1:B:259:LEU:HD22	1.84	0.58
1:C:199:TYR:CB	1:C:325:ILE:HD11	2.21	0.58
1:E:200:LEU:HB3	1:E:259:LEU:HD22	1.84	0.58
1:F:200:LEU:HB3	1:F:259:LEU:HD22	1.84	0.58
1:F:221:LEU:HD13	1:F:236:VAL:HG21	1.86	0.58
1:H:192:GLY:HA3	1:H:332:ILE:O	2.03	0.58
1:I:206:ASN:CG	1:I:207:LYS:H	2.12	0.58
1:L:152:ALA:HB3	1:L:155:ASP:H	1.69	0.58
1:L:169:VAL:HG12	1:L:377:ALA:HB3	1.83	0.58
1:L:243:ALA:CB	1:M:256:GLY:O	2.51	0.58
1:L:420:ILE:HD12	1:L:451:LEU:HD13	1.86	0.58
1:N:199:TYR:CB	1:N:325:ILE:HD11	2.34	0.58
1:N:298:GLY:HA3	1:N:318:GLY:HA3	1.85	0.58
1:I:192:GLY:HA3	1:I:332:ILE:O	2.02	0.58
1:J:162:ILE:HD13	1:J:400:LEU:CA	2.34	0.58
1:C:217:SER:HA	1:C:320:ALA:O	2.02	0.58
1:H:519:CYS:O	1:N:39:VAL:N	2.37	0.58
1:I:301:ILE:HD11	1:I:312:ALA:CB	2.32	0.58
1:K:169:VAL:HB	1:K:173:GLY:HA3	1.85	0.58
1:G:200:LEU:HD11	1:G:254:VAL:CG1	2.33	0.58
1:H:38:VAL:CA	1:I:519:CYS:O	2.52	0.58
1:I:152:ALA:HB3	1:I:155:ASP:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:LEU:HD23	1:J:74:VAL:HG13	1.84	0.58
1:J:152:ALA:HB3	1:J:155:ASP:H	1.69	0.58
1:J:165:ALA:O	1:J:169:VAL:HG22	2.03	0.58
1:K:162:ILE:HD13	1:K:400:LEU:CA	2.34	0.58
1:N:169:VAL:HB	1:N:173:GLY:HA3	1.85	0.58
1:B:293:ALA:HB1	1:B:299:THR:HA	1.85	0.58
1:F:293:ALA:HB1	1:F:299:THR:HA	1.86	0.58
1:G:293:ALA:HB1	1:G:299:THR:HA	1.85	0.58
1:H:420:ILE:HD12	1:H:451:LEU:HD13	1.85	0.58
1:I:23:LEU:HD23	1:I:74:VAL:HG13	1.84	0.58
1:K:23:LEU:HD23	1:K:74:VAL:HG13	1.84	0.58
1:K:39:VAL:N	1:L:519:CYS:O	2.37	0.58
1:K:242:LYS:CB	1:L:257:GLU:HA	2.34	0.58
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.85	0.58
1:M:192:GLY:HA3	1:M:332:ILE:O	2.03	0.58
1:C:293:ALA:HB1	1:C:299:THR:HA	1.85	0.57
1:H:39:VAL:N	1:I:519:CYS:O	2.37	0.57
1:I:38:VAL:CA	1:J:519:CYS:O	2.52	0.57
1:K:152:ALA:HB3	1:K:155:ASP:H	1.69	0.57
1:L:298:GLY:HA3	1:L:318:GLY:HA3	1.85	0.57
1:M:199:TYR:CB	1:M:325:ILE:HD11	2.34	0.57
1:I:162:ILE:HD13	1:I:400:LEU:CA	2.34	0.57
1:M:298:GLY:HA3	1:M:318:GLY:HA3	1.85	0.57
1:B:221:LEU:HD13	1:B:236:VAL:HG21	1.86	0.57
1:C:224:ASP:HA	1:C:289:LEU:HD13	1.86	0.57
1:F:381:VAL:HG22	1:F:382:GLY:N	2.20	0.57
1:G:300:VAL:CG2	1:G:312:ALA:HB2	2.33	0.57
1:H:353:ILE:HD11	1:H:369:VAL:CG2	2.35	0.57
1:I:353:ILE:HD11	1:I:369:VAL:CG2	2.35	0.57
1:I:420:ILE:HD12	1:I:451:LEU:HD13	1.85	0.57
1:J:39:VAL:N	1:K:519:CYS:O	2.37	0.57
1:D:224:ASP:HA	1:D:289:LEU:HD13	1.86	0.57
1:G:199:TYR:C	1:G:200:LEU:HD12	2.29	0.57
1:G:381:VAL:HG22	1:G:382:GLY:N	2.20	0.57
1:I:301:ILE:HD11	1:I:312:ALA:HB1	1.85	0.57
1:I:524:LEU:HG	1:I:525:PRO:N	2.20	0.57
1:K:243:ALA:CB	1:L:256:GLY:O	2.51	0.57
1:N:152:ALA:HB3	1:N:155:ASP:H	1.69	0.57
1:E:221:LEU:HD13	1:E:236:VAL:HG21	1.86	0.57
1:E:300:VAL:CG2	1:E:312:ALA:HB2	2.33	0.57
1:F:300:VAL:CG2	1:F:312:ALA:HB2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:LEU:CD1	1:G:254:VAL:HG21	2.22	0.57
1:I:39:VAL:N	1:J:519:CYS:O	2.37	0.57
1:J:207:LYS:HE2	1:J:207:LYS:CA	2.34	0.57
1:L:301:ILE:HD12	1:L:312:ALA:HB2	1.65	0.57
1:M:39:VAL:N	1:N:519:CYS:O	2.37	0.57
1:M:353:ILE:HD11	1:M:369:VAL:CG2	2.35	0.57
1:E:381:VAL:HG22	1:E:382:GLY:N	2.20	0.57
1:J:301:ILE:HD11	1:J:312:ALA:HB1	1.85	0.57
1:J:420:ILE:HD12	1:J:451:LEU:HD13	1.86	0.57
1:K:353:ILE:HD11	1:K:369:VAL:CG2	2.35	0.57
1:L:36:ARG:O	1:M:518:GLU:HB2	2.05	0.57
1:A:300:VAL:CG2	1:A:312:ALA:HB2	2.33	0.57
1:E:200:LEU:HB3	1:E:259:LEU:CD2	2.35	0.57
1:E:293:ALA:HB1	1:E:299:THR:HA	1.86	0.57
1:F:23:LEU:HA	1:F:60:ILE:CD1	2.32	0.57
1:H:301:ILE:HD11	1:H:312:ALA:HB1	1.85	0.57
1:I:240:VAL:HG11	1:I:247:LEU:HA	1.87	0.57
1:J:36:ARG:O	1:K:518:GLU:HB2	2.05	0.57
1:J:240:VAL:HG11	1:J:247:LEU:HA	1.87	0.57
1:J:524:LEU:HG	1:J:525:PRO:N	2.20	0.57
1:K:301:ILE:HD11	1:K:312:ALA:CB	2.32	0.57
1:K:524:LEU:HG	1:K:525:PRO:N	2.20	0.57
1:L:199:TYR:CB	1:L:325:ILE:HD11	2.34	0.57
1:M:524:LEU:HG	1:M:525:PRO:N	2.20	0.57
1:N:240:VAL:HG11	1:N:247:LEU:HA	1.87	0.57
1:N:353:ILE:HD11	1:N:369:VAL:CG2	2.35	0.57
1:C:221:LEU:HD13	1:C:236:VAL:HG21	1.86	0.57
1:D:293:ALA:HB1	1:D:299:THR:HA	1.86	0.57
1:E:240:VAL:HG21	1:E:247:LEU:HB2	1.87	0.57
1:F:192:GLY:HA3	1:F:376:VAL:HG23	1.86	0.57
1:F:240:VAL:HG21	1:F:247:LEU:HB2	1.87	0.57
1:G:224:ASP:HA	1:G:289:LEU:HD13	1.86	0.57
1:G:240:VAL:HG21	1:G:247:LEU:HB2	1.87	0.57
1:H:518:GLU:HB2	1:N:36:ARG:O	2.05	0.57
1:L:524:LEU:HG	1:L:525:PRO:N	2.20	0.57
1:A:240:VAL:HG21	1:A:247:LEU:HB2	1.87	0.57
1:D:221:LEU:HD13	1:D:236:VAL:HG21	1.86	0.57
1:D:240:VAL:HG21	1:D:247:LEU:HB2	1.87	0.57
1:E:192:GLY:HA3	1:E:376:VAL:HG23	1.86	0.57
1:H:240:VAL:HG11	1:H:247:LEU:HA	1.87	0.57
1:H:524:LEU:HG	1:H:525:PRO:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:HB1	1:A:299:THR:HA	1.86	0.57
1:D:381:VAL:HG22	1:D:382:GLY:N	2.20	0.57
1:E:38:VAL:HG21	1:E:56:VAL:HG22	1.87	0.57
1:G:192:GLY:HA3	1:G:376:VAL:HG23	1.86	0.57
1:H:519:CYS:O	1:N:38:VAL:CA	2.52	0.57
1:I:518:GLU:HB3	1:I:519:CYS:N	2.19	0.57
1:J:353:ILE:HD11	1:J:369:VAL:CG2	2.35	0.57
1:J:518:GLU:HB3	1:J:519:CYS:N	2.19	0.57
1:L:39:VAL:N	1:M:519:CYS:O	2.37	0.57
1:L:162:ILE:HD13	1:L:400:LEU:CA	2.34	0.57
1:L:206:ASN:OD1	1:L:207:LYS:HD2	2.05	0.57
1:B:300:VAL:CG2	1:B:312:ALA:HB2	2.33	0.56
1:D:300:VAL:CG2	1:D:312:ALA:HB2	2.33	0.56
1:F:224:ASP:HA	1:F:289:LEU:HD13	1.86	0.56
1:H:36:ARG:O	1:I:518:GLU:HB2	2.05	0.56
1:I:36:ARG:O	1:J:518:GLU:HB2	2.05	0.56
1:N:524:LEU:HG	1:N:525:LEU:N	2.20	0.56
1:B:192:GLY:HA3	1:B:376:VAL:HG23	1.86	0.56
1:B:224:ASP:HA	1:B:289:LEU:HD13	1.86	0.56
1:C:200:LEU:HB3	1:C:259:LEU:CD2	2.35	0.56
1:H:152:ALA:HB3	1:H:155:ASP:H	1.69	0.56
1:N:518:GLU:HB3	1:N:519:CYS:N	2.19	0.56
1:A:224:ASP:HA	1:A:289:LEU:HD13	1.86	0.56
1:B:38:VAL:HG21	1:B:56:VAL:HG22	1.87	0.56
1:B:200:LEU:HB3	1:B:259:LEU:CD2	2.35	0.56
1:C:38:VAL:HG21	1:C:56:VAL:HG22	1.86	0.56
1:D:200:LEU:HB3	1:D:259:LEU:CD2	2.35	0.56
1:F:38:VAL:HG21	1:F:56:VAL:HG22	1.87	0.56
1:K:518:GLU:HB3	1:K:519:CYS:N	2.19	0.56
1:L:38:VAL:CA	1:M:519:CYS:O	2.52	0.56
1:M:240:VAL:HG11	1:M:247:LEU:HA	1.87	0.56
1:A:207:LYS:HB2	1:A:208:PRO:HD3	1.87	0.56
1:A:381:VAL:HG22	1:A:382:GLY:N	2.20	0.56
1:B:240:VAL:HG21	1:B:247:LEU:HB2	1.87	0.56
1:C:23:LEU:HA	1:C:60:ILE:CD1	2.32	0.56
1:E:200:LEU:HD12	1:E:259:LEU:HD13	1.88	0.56
1:E:224:ASP:HA	1:E:289:LEU:HD13	1.86	0.56
1:F:200:LEU:HD12	1:F:259:LEU:HD13	1.88	0.56
1:K:36:ARG:O	1:L:518:GLU:HB2	2.05	0.56
1:K:38:VAL:CA	1:L:519:CYS:O	2.52	0.56
1:K:240:VAL:HG11	1:K:247:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:VAL:HB	1:L:173:GLY:HA3	1.85	0.56
1:M:152:ALA:HB3	1:M:155:ASP:H	1.69	0.56
1:A:38:VAL:HG21	1:A:56:VAL:HG22	1.87	0.56
1:C:300:VAL:CG2	1:C:312:ALA:HB2	2.33	0.56
1:H:518:GLU:HB3	1:H:519:CYS:N	2.19	0.56
1:J:100:ILE:HD13	1:J:514:MET:SD	2.46	0.56
1:L:100:ILE:HD13	1:L:514:MET:SD	2.46	0.56
1:D:150:ILE:HD11	1:D:493:ILE:HG23	1.88	0.56
1:D:192:GLY:HA3	1:D:376:VAL:HG23	1.86	0.56
1:H:240:VAL:HG21	1:H:247:LEU:HD13	1.88	0.56
1:K:301:ILE:HD11	1:K:312:ALA:HB1	1.85	0.56
1:M:36:ARG:O	1:N:518:GLU:HB2	2.05	0.56
1:A:192:GLY:HA3	1:A:376:VAL:HG23	1.86	0.56
1:D:38:VAL:HG21	1:D:56:VAL:HG22	1.87	0.56
1:D:521:VAL:CG1	1:E:59:GLU:HB3	2.36	0.56
1:E:521:VAL:CG1	1:F:59:GLU:HB3	2.36	0.56
1:F:187:LEU:CD1	1:F:379:ILE:HG12	2.35	0.56
1:F:200:LEU:HB3	1:F:259:LEU:CD2	2.35	0.56
1:H:100:ILE:HD13	1:H:514:MET:SD	2.46	0.56
1:L:240:VAL:HG11	1:L:247:LEU:HA	1.87	0.56
1:N:301:ILE:HD11	1:N:312:ALA:HB1	1.86	0.56
1:B:31:LEU:HB2	1:B:90:THR:HG21	1.88	0.56
1:C:240:VAL:HG21	1:C:247:LEU:HB2	1.87	0.56
1:C:312:ALA:HB1	1:C:316:ASP:OD2	2.06	0.56
1:D:200:LEU:HD12	1:D:259:LEU:HD13	1.88	0.56
1:F:521:VAL:CG1	1:G:59:GLU:HB3	2.36	0.56
1:J:243:ALA:HA	1:K:260:ALA:HB2	1.88	0.56
1:L:301:ILE:HD11	1:L:312:ALA:HB1	1.86	0.56
1:M:518:GLU:HB3	1:M:519:CYS:N	2.19	0.56
1:A:200:LEU:HB3	1:A:259:LEU:CD2	2.35	0.56
1:B:312:ALA:HB1	1:B:316:ASP:OD2	2.06	0.56
1:H:302:SER:HB2	1:H:305:ILE:H	1.71	0.56
1:I:240:VAL:HG21	1:I:247:LEU:HD13	1.88	0.56
1:K:206:ASN:HB2	1:K:213:VAL:HG23	1.88	0.56
1:L:353:ILE:HD11	1:L:369:VAL:CG2	2.35	0.56
1:B:381:VAL:HG22	1:B:382:GLY:N	2.19	0.56
1:F:150:ILE:HD11	1:F:493:ILE:HG23	1.87	0.56
1:F:312:ALA:HB1	1:F:316:ASP:OD2	2.06	0.56
1:H:239:ALA:HB1	1:H:314:LEU:HB3	1.88	0.56
1:M:38:VAL:CA	1:N:519:CYS:O	2.52	0.56
1:M:100:ILE:HD13	1:M:514:MET:SD	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:301:ILE:HD11	1:M:312:ALA:HB1	1.86	0.56
1:N:240:VAL:HG21	1:N:247:LEU:HD13	1.87	0.56
1:C:193:MET:CE	1:C:332:ILE:HD12	2.36	0.55
1:C:200:LEU:HD12	1:C:259:LEU:HD13	1.88	0.55
1:C:521:VAL:CG1	1:D:59:GLU:HB3	2.36	0.55
1:I:239:ALA:HB1	1:I:314:LEU:HB3	1.88	0.55
1:J:240:VAL:HG21	1:J:247:LEU:HD13	1.88	0.55
1:A:59:GLU:HB3	1:G:521:VAL:CG1	2.36	0.55
1:A:200:LEU:HD21	1:A:254:VAL:HG21	1.04	0.55
1:D:191:GLU:HG3	1:D:342:ILE:CD1	2.37	0.55
1:F:202:PRO:O	1:F:205:ILE:HG13	2.05	0.55
1:G:38:VAL:HG21	1:G:56:VAL:HG22	1.87	0.55
1:G:312:ALA:HB1	1:G:316:ASP:OD2	2.06	0.55
1:L:183:LEU:HG	1:L:183:LEU:O	2.06	0.55
1:N:239:ALA:HB1	1:N:314:LEU:HB3	1.88	0.55
1:J:290:GLN:HA	1:J:300:VAL:CG2	2.37	0.55
1:K:100:ILE:HD13	1:K:514:MET:SD	2.46	0.55
1:K:302:SER:HB2	1:K:305:ILE:H	1.71	0.55
1:M:162:ILE:HD13	1:M:400:LEU:CA	2.34	0.55
1:B:150:ILE:HD11	1:B:493:ILE:HG23	1.88	0.55
1:I:100:ILE:HD13	1:I:514:MET:SD	2.46	0.55
1:J:206:ASN:CG	1:J:207:LYS:H	2.15	0.55
1:C:381:VAL:HG22	1:C:382:GLY:N	2.20	0.55
1:D:312:ALA:HB1	1:D:316:ASP:OD2	2.06	0.55
1:K:240:VAL:HG11	1:K:247:LEU:CB	2.37	0.55
1:K:240:VAL:HG21	1:K:247:LEU:HD13	1.88	0.55
1:L:518:GLU:HB3	1:L:519:CYS:N	2.19	0.55
1:N:100:ILE:HD13	1:N:514:MET:SD	2.46	0.55
1:N:221:LEU:HD13	1:N:317:LEU:HD11	1.89	0.55
1:B:200:LEU:HD12	1:B:259:LEU:HD13	1.88	0.55
1:I:243:ALA:HA	1:J:260:ALA:HB2	1.88	0.55
1:J:38:VAL:CA	1:K:519:CYS:O	2.52	0.55
1:J:203:TYR:CD1	1:J:267:MET:HE1	2.42	0.55
1:J:240:VAL:HG11	1:J:247:LEU:CB	2.37	0.55
1:K:193:MET:CE	1:K:295:LEU:HD12	2.36	0.55
1:A:521:VAL:CG1	1:B:59:GLU:HB3	2.36	0.55
1:B:521:VAL:CG1	1:C:59:GLU:HB3	2.36	0.55
1:D:23:LEU:HA	1:D:60:ILE:CD1	2.32	0.55
1:D:190:VAL:HB	1:D:334:ASP:HB2	1.89	0.55
1:D:406:ALA:HB1	1:D:411:VAL:HG13	1.89	0.55
1:H:203:TYR:CD1	1:H:267:MET:HE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:240:VAL:HG11	1:M:247:LEU:CB	2.37	0.55
1:E:312:ALA:HB1	1:E:316:ASP:OD2	2.06	0.55
1:F:31:LEU:HB2	1:F:90:THR:HG21	1.89	0.55
1:N:240:VAL:HG11	1:N:247:LEU:CB	2.35	0.55
1:A:200:LEU:HD12	1:A:259:LEU:HD13	1.88	0.55
1:A:312:ALA:HB1	1:A:316:ASP:OD2	2.06	0.55
1:D:31:LEU:HB2	1:D:90:THR:HG21	1.89	0.55
1:F:207:LYS:HE2	1:F:207:LYS:N	2.21	0.55
1:G:193:MET:CE	1:G:295:LEU:HB3	2.37	0.55
1:H:240:VAL:HG11	1:H:247:LEU:CB	2.37	0.55
1:H:243:ALA:CA	1:I:260:ALA:HB2	2.37	0.55
1:J:199:TYR:CB	1:J:325:ILE:HD11	2.34	0.55
1:K:203:TYR:CD1	1:K:267:MET:HE1	2.42	0.55
1:A:197:ARG:HG3	1:A:198:GLY:O	2.07	0.54
1:I:181:THR:O	1:I:383:ALA:HB3	2.08	0.54
1:I:240:VAL:HG11	1:I:247:LEU:CB	2.37	0.54
1:J:239:ALA:HB1	1:J:314:LEU:HB3	1.88	0.54
1:L:240:VAL:HG21	1:L:247:LEU:HD13	1.87	0.54
1:A:213:VAL:HG13	1:A:325:ILE:HG12	1.89	0.54
1:E:406:ALA:HB1	1:E:411:VAL:HG13	1.89	0.54
1:F:150:ILE:CD1	1:F:493:ILE:CA	2.74	0.54
1:F:150:ILE:HD13	1:F:493:ILE:CG2	2.36	0.54
1:L:301:ILE:HD11	1:L:312:ALA:CB	2.32	0.54
1:M:239:ALA:HB1	1:M:314:LEU:HB3	1.88	0.54
1:H:207:LYS:HE2	1:H:207:LYS:CA	2.38	0.54
1:I:221:LEU:HD13	1:I:317:LEU:HD11	1.89	0.54
1:L:242:LYS:C	1:M:257:GLU:CA	2.78	0.54
1:M:240:VAL:HG21	1:M:247:LEU:HD13	1.87	0.54
1:M:290:GLN:HA	1:M:300:VAL:CG2	2.38	0.54
1:A:224:ASP:CG	1:A:302:SER:HA	2.33	0.54
1:B:224:ASP:CG	1:B:302:SER:HA	2.33	0.54
1:I:242:LYS:C	1:J:257:GLU:CA	2.78	0.54
1:K:221:LEU:HD13	1:K:317:LEU:HD11	1.90	0.54
1:M:243:ALA:N	1:N:256:GLY:C	2.66	0.54
1:N:221:LEU:HD21	1:N:309:LEU:HD22	1.88	0.54
1:B:137:PRO:HA	1:B:410:GLY:HA3	1.90	0.54
1:C:406:ALA:HB1	1:C:411:VAL:HG13	1.89	0.54
1:F:206:ASN:HB3	1:F:208:PRO:HD2	1.90	0.54
1:G:241:ALA:HA	1:G:271:VAL:HG22	1.90	0.54
1:I:243:ALA:N	1:J:256:GLY:C	2.66	0.54
1:L:240:VAL:HG11	1:L:247:LEU:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:ALA:N	1:M:256:GLY:C	2.66	0.54
1:C:224:ASP:CG	1:C:302:SER:HA	2.33	0.54
1:D:224:ASP:CG	1:D:302:SER:HA	2.33	0.54
1:H:256:GLY:C	1:N:243:ALA:N	2.66	0.54
1:I:290:GLN:HA	1:I:300:VAL:CG2	2.37	0.54
1:J:302:SER:HB2	1:J:305:ILE:H	1.72	0.54
1:K:137:PRO:CA	1:K:410:GLY:HA3	2.36	0.54
1:A:241:ALA:HA	1:A:271:VAL:HG22	1.90	0.54
1:B:150:ILE:HD13	1:B:493:ILE:CG2	2.37	0.54
1:E:200:LEU:CB	1:E:259:LEU:CD1	2.86	0.54
1:H:260:ALA:HB2	1:N:243:ALA:CA	2.38	0.54
1:H:260:ALA:HB2	1:N:243:ALA:HA	1.88	0.54
1:J:221:LEU:HD13	1:J:317:LEU:HD11	1.90	0.54
1:N:221:LEU:HD22	1:N:236:VAL:HG11	1.90	0.54
1:C:464:VAL:HG22	1:J:464:VAL:HG22	1.90	0.54
1:D:150:ILE:CD1	1:D:493:ILE:CA	2.74	0.54
1:G:224:ASP:CG	1:G:302:SER:HA	2.33	0.54
1:I:189:VAL:HA	1:I:377:ALA:HA	1.89	0.54
1:K:243:ALA:N	1:L:256:GLY:C	2.66	0.54
1:L:239:ALA:HB1	1:L:314:LEU:HB3	1.88	0.54
1:M:60:ILE:HA	1:N:6:VAL:HG21	1.90	0.54
1:M:203:TYR:CD1	1:M:267:MET:HE1	2.43	0.54
1:A:150:ILE:HD13	1:A:493:ILE:CG2	2.37	0.54
1:C:31:LEU:HB2	1:C:90:THR:HG21	1.90	0.54
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.38	0.54
1:D:464:VAL:HG22	1:K:464:VAL:HG22	1.90	0.54
1:E:23:LEU:HA	1:E:60:ILE:CD1	2.32	0.54
1:E:224:ASP:CG	1:E:302:SER:HA	2.33	0.54
1:H:6:VAL:HG21	1:N:60:ILE:HA	1.90	0.54
1:H:242:LYS:HG3	1:I:257:GLU:O	2.07	0.54
1:L:221:LEU:HD13	1:L:317:LEU:HD11	1.90	0.54
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.90	0.54
1:E:31:LEU:HB2	1:E:90:THR:HG21	1.90	0.54
1:E:213:VAL:HG11	1:E:325:ILE:HG12	1.87	0.54
1:F:193:MET:SD	1:F:292:ILE:HG23	2.48	0.54
1:H:221:LEU:HD13	1:H:317:LEU:HD11	1.90	0.54
1:I:243:ALA:CA	1:J:260:ALA:HB2	2.38	0.54
1:J:243:ALA:CA	1:K:260:ALA:HB2	2.38	0.54
1:J:243:ALA:N	1:K:256:GLY:C	2.66	0.54
1:D:137:PRO:HA	1:D:410:GLY:HA3	1.90	0.53
1:F:406:ALA:HB1	1:F:411:VAL:HG13	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:LEU:HB2	1:G:90:THR:HG21	1.90	0.53
1:G:193:MET:SD	1:G:295:LEU:HB3	2.48	0.53
1:I:23:LEU:HA	1:I:60:ILE:HD13	1.90	0.53
1:K:150:ILE:CD1	1:K:494:LEU:H	2.22	0.53
1:K:242:LYS:C	1:L:257:GLU:CA	2.78	0.53
1:N:290:GLN:HA	1:N:300:VAL:CG2	2.38	0.53
1:A:23:LEU:HA	1:A:60:ILE:CD1	2.32	0.53
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.39	0.53
1:B:464:VAL:HG22	1:I:464:VAL:HG22	1.90	0.53
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.39	0.53
1:F:241:ALA:HA	1:F:271:VAL:HG22	1.90	0.53
1:I:199:TYR:CB	1:I:325:ILE:HD11	2.34	0.53
1:J:23:LEU:HA	1:J:60:ILE:HD13	1.90	0.53
1:J:221:LEU:HD21	1:J:309:LEU:HD22	1.90	0.53
1:K:243:ALA:CA	1:L:260:ALA:HB2	2.37	0.53
1:K:290:GLN:HA	1:K:300:VAL:CG2	2.38	0.53
1:N:162:ILE:HD13	1:N:400:LEU:CA	2.34	0.53
1:N:206:ASN:C	1:N:208:PRO:N	2.66	0.53
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.38	0.53
1:D:193:MET:SD	1:D:292:ILE:HG23	2.48	0.53
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.38	0.53
1:E:193:MET:SD	1:E:292:ILE:HA	2.49	0.53
1:G:150:ILE:HD13	1:G:493:ILE:CG2	2.37	0.53
1:H:290:GLN:HA	1:H:300:VAL:CG2	2.38	0.53
1:J:242:LYS:C	1:K:257:GLU:CA	2.78	0.53
1:L:221:LEU:HD22	1:L:236:VAL:HG11	1.90	0.53
1:L:290:GLN:HA	1:L:300:VAL:CG2	2.38	0.53
1:M:221:LEU:HD13	1:M:317:LEU:HD11	1.90	0.53
1:A:200:LEU:HD11	1:A:254:VAL:CA	2.12	0.53
1:A:406:ALA:HB1	1:A:411:VAL:HG13	1.89	0.53
1:B:193:MET:SD	1:B:292:ILE:HG23	2.48	0.53
1:C:38:VAL:HG11	1:C:56:VAL:HG22	1.91	0.53
1:F:137:PRO:HA	1:F:410:GLY:HA3	1.90	0.53
1:F:200:LEU:CB	1:F:259:LEU:CD1	2.86	0.53
1:H:137:PRO:CA	1:H:410:GLY:HA3	2.36	0.53
1:H:221:LEU:HD21	1:H:309:LEU:HD22	1.90	0.53
1:I:221:LEU:HD21	1:I:309:LEU:HD22	1.90	0.53
1:K:221:LEU:HD21	1:K:309:LEU:HD22	1.89	0.53
1:L:150:ILE:CD1	1:L:494:LEU:H	2.22	0.53
1:L:243:ALA:CA	1:M:260:ALA:HB2	2.39	0.53
1:L:255:GLU:CD	1:L:256:GLY:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:MET:SD	1:A:292:ILE:HG23	2.48	0.53
1:B:406:ALA:HB1	1:B:411:VAL:HG13	1.88	0.53
1:H:60:ILE:HA	1:I:6:VAL:HG21	1.90	0.53
1:H:243:ALA:N	1:I:256:GLY:C	2.66	0.53
1:L:60:ILE:HA	1:M:6:VAL:HG21	1.90	0.53
1:M:229:ASN:HD22	1:M:230:ILE:H	1.56	0.53
1:M:518:GLU:CB	1:M:518:GLU:O	2.54	0.53
1:N:137:PRO:CA	1:N:410:GLY:HA3	2.36	0.53
1:D:200:LEU:CB	1:D:259:LEU:CD1	2.86	0.53
1:D:213:VAL:HG11	1:D:325:ILE:HG12	1.88	0.53
1:D:241:ALA:HA	1:D:271:VAL:HG22	1.90	0.53
1:H:31:LEU:CB	1:H:90:THR:HG21	2.39	0.53
1:H:242:LYS:CB	1:I:257:GLU:HA	2.38	0.53
1:J:221:LEU:CG	1:J:309:LEU:HD22	2.39	0.53
1:K:221:LEU:HD22	1:K:236:VAL:HG11	1.91	0.53
1:K:239:ALA:HB1	1:K:314:LEU:HB3	1.89	0.53
1:L:221:LEU:HD21	1:L:309:LEU:HD22	1.89	0.53
1:M:221:LEU:HD21	1:M:309:LEU:HD22	1.89	0.53
1:B:193:MET:SD	1:B:292:ILE:HA	2.49	0.53
1:G:406:ALA:HB1	1:G:411:VAL:HG13	1.89	0.53
1:I:31:LEU:CB	1:I:90:THR:HG21	2.39	0.53
1:I:302:SER:HB2	1:I:305:ILE:H	1.72	0.53
1:N:203:TYR:CD1	1:N:267:MET:HE1	2.44	0.53
1:A:137:PRO:HA	1:A:410:GLY:HA3	1.90	0.53
1:C:241:ALA:HA	1:C:271:VAL:HG22	1.90	0.53
1:E:241:ALA:HA	1:E:271:VAL:HG22	1.90	0.53
1:E:464:VAL:HG22	1:L:464:VAL:HG22	1.91	0.53
1:F:193:MET:SD	1:F:292:ILE:HA	2.49	0.53
1:F:224:ASP:CG	1:F:302:SER:HA	2.33	0.53
1:K:31:LEU:CB	1:K:90:THR:HG21	2.39	0.53
1:M:150:ILE:CD1	1:M:494:LEU:H	2.22	0.53
1:M:221:LEU:HD22	1:M:236:VAL:HG11	1.91	0.53
1:M:243:ALA:CA	1:N:260:ALA:HB2	2.39	0.53
1:N:31:LEU:CB	1:N:90:THR:HG21	2.39	0.53
1:N:518:GLU:CB	1:N:518:GLU:O	2.54	0.53
1:A:193:MET:SD	1:A:292:ILE:HA	2.49	0.53
1:B:200:LEU:CB	1:B:259:LEU:CD1	2.86	0.53
1:B:241:ALA:HA	1:B:271:VAL:HG22	1.90	0.53
1:D:38:VAL:HG11	1:D:56:VAL:HG22	1.91	0.53
1:D:196:ASP:OD1	1:D:329:THR:HG22	2.08	0.53
1:E:193:MET:SD	1:E:292:ILE:HG23	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.39	0.53
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.38	0.53
1:I:60:ILE:HA	1:J:6:VAL:HG21	1.90	0.53
1:J:60:ILE:HA	1:K:6:VAL:HG21	1.90	0.53
1:M:302:SER:HB2	1:M:305:ILE:H	1.74	0.53
1:G:240:VAL:HG12	1:G:271:VAL:HG13	1.91	0.53
1:I:203:TYR:CD1	1:I:267:MET:HE1	2.44	0.53
1:L:23:LEU:HA	1:L:60:ILE:HD13	1.90	0.53
1:M:23:LEU:HA	1:M:60:ILE:HD13	1.90	0.53
1:A:174:VAL:H	1:A:376:VAL:HG22	1.74	0.52
1:A:464:VAL:HG22	1:H:464:VAL:HG22	1.91	0.52
1:E:240:VAL:HG12	1:E:271:VAL:HG13	1.91	0.52
1:H:23:LEU:HA	1:H:60:ILE:HD13	1.90	0.52
1:H:162:ILE:HD13	1:H:400:LEU:CA	2.34	0.52
1:J:31:LEU:CB	1:J:90:THR:HG21	2.39	0.52
1:J:150:ILE:CD1	1:J:494:LEU:H	2.22	0.52
1:D:193:MET:SD	1:D:292:ILE:HA	2.49	0.52
1:F:174:VAL:H	1:F:376:VAL:HG22	1.74	0.52
1:I:221:LEU:CG	1:I:309:LEU:HD22	2.39	0.52
1:N:150:ILE:CD1	1:N:494:LEU:H	2.22	0.52
1:D:150:ILE:HD13	1:D:493:ILE:CG2	2.37	0.52
1:I:137:PRO:CA	1:I:410:GLY:HA3	2.36	0.52
1:K:60:ILE:HA	1:L:6:VAL:HG21	1.90	0.52
1:L:31:LEU:CB	1:L:90:THR:HG21	2.39	0.52
1:L:243:ALA:HA	1:M:260:ALA:HB2	1.90	0.52
1:E:220:ILE:CD1	1:E:332:ILE:HD13	2.33	0.52
1:F:213:VAL:HG11	1:F:325:ILE:HG12	1.88	0.52
1:G:197:ARG:HG3	1:G:198:GLY:O	2.10	0.52
1:H:150:ILE:CD1	1:H:494:LEU:H	2.22	0.52
1:K:23:LEU:HA	1:K:60:ILE:HD13	1.90	0.52
1:L:203:TYR:CD1	1:L:267:MET:HE1	2.44	0.52
1:M:31:LEU:CB	1:M:90:THR:HG21	2.39	0.52
1:N:221:LEU:HB2	1:N:317:LEU:HD21	1.91	0.52
1:A:328:ASP:O	1:A:329:THR:HG23	2.10	0.52
1:B:328:ASP:O	1:B:329:THR:HG23	2.10	0.52
1:B:381:VAL:HB	1:B:393:LYS:HA	1.92	0.52
1:C:381:VAL:HB	1:C:393:LYS:HA	1.92	0.52
1:E:150:ILE:HD13	1:E:493:ILE:CG2	2.37	0.52
1:F:183:LEU:HA	1:F:383:ALA:N	2.25	0.52
1:H:220:ILE:HD12	1:H:296:THR:CG2	2.40	0.52
1:B:38:VAL:HG11	1:B:56:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:VAL:O	1:E:41:ASP:CB	2.58	0.52
1:E:174:VAL:H	1:E:376:VAL:HG22	1.74	0.52
1:F:464:VAL:HG22	1:M:464:VAL:HG22	1.91	0.52
1:J:221:LEU:HD22	1:J:236:VAL:HG11	1.92	0.52
1:L:191:GLU:CG	1:L:192:GLY:H	2.21	0.52
1:L:220:ILE:HD12	1:L:296:THR:CG2	2.40	0.52
1:M:137:PRO:CA	1:M:410:GLY:HA3	2.36	0.52
1:N:23:LEU:HA	1:N:60:ILE:HD13	1.89	0.52
1:N:221:LEU:CG	1:N:309:LEU:HD22	2.40	0.52
1:A:521:VAL:O	1:B:41:ASP:CB	2.58	0.52
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.92	0.52
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.92	0.52
1:G:183:LEU:HA	1:G:383:ALA:N	2.25	0.52
1:I:247:LEU:O	1:I:273:VAL:HA	2.10	0.52
1:E:38:VAL:HG11	1:E:56:VAL:HG22	1.91	0.52
1:G:328:ASP:O	1:G:329:THR:HG23	2.10	0.52
1:J:194:GLN:OE1	1:J:329:THR:HG21	2.09	0.52
1:K:207:LYS:HA	1:K:207:LYS:CE	2.35	0.52
1:K:221:LEU:HB2	1:K:317:LEU:HD21	1.92	0.52
1:K:247:LEU:O	1:K:273:VAL:HA	2.10	0.52
1:L:247:LEU:O	1:L:273:VAL:HA	2.10	0.52
1:M:247:LEU:O	1:M:273:VAL:HA	2.10	0.52
1:A:200:LEU:CB	1:A:259:LEU:CD1	2.86	0.52
1:B:37:ASN:ND2	1:B:49:ILE:HG23	2.25	0.52
1:B:521:VAL:O	1:C:41:ASP:CB	2.58	0.52
1:C:328:ASP:O	1:C:329:THR:HG23	2.10	0.52
1:E:183:LEU:HA	1:E:383:ALA:N	2.25	0.52
1:F:521:VAL:O	1:G:41:ASP:CB	2.58	0.52
1:G:464:VAL:HG22	1:N:464:VAL:HG22	1.91	0.52
1:H:221:LEU:CG	1:H:309:LEU:HD22	2.39	0.52
1:K:221:LEU:CG	1:K:309:LEU:HD22	2.39	0.52
1:L:221:LEU:HB2	1:L:317:LEU:HD21	1.92	0.52
1:N:302:SER:HB2	1:N:305:ILE:H	1.74	0.52
1:A:37:ASN:ND2	1:A:49:ILE:HG23	2.25	0.52
1:A:41:ASP:CB	1:G:521:VAL:O	2.58	0.52
1:C:37:ASN:ND2	1:C:49:ILE:HG23	2.25	0.52
1:K:220:ILE:HD12	1:K:296:THR:CG2	2.40	0.52
1:L:518:GLU:CB	1:L:518:GLU:O	2.54	0.52
1:M:221:LEU:CG	1:M:309:LEU:HD22	2.40	0.52
1:C:521:VAL:O	1:D:41:ASP:CB	2.58	0.51
1:D:381:VAL:HB	1:D:393:LYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:221:LEU:HB2	1:J:317:LEU:HD21	1.92	0.51
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.92	0.51
1:D:37:ASN:ND2	1:D:49:ILE:HG23	2.25	0.51
1:D:521:VAL:HG11	1:E:59:GLU:HB3	1.93	0.51
1:E:150:ILE:CD1	1:E:493:ILE:CA	2.74	0.51
1:E:521:VAL:HG11	1:F:59:GLU:HB3	1.92	0.51
1:E:521:VAL:O	1:F:41:ASP:CB	2.58	0.51
1:N:204:PHE:HA	1:N:207:LYS:CE	2.40	0.51
1:A:34:LYS:HB2	1:A:458:CYS:HA	1.92	0.51
1:A:521:VAL:HG11	1:B:59:GLU:HB3	1.93	0.51
1:C:174:VAL:H	1:C:376:VAL:HG22	1.74	0.51
1:C:521:VAL:HG11	1:D:59:GLU:HB3	1.93	0.51
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.92	0.51
1:D:174:VAL:H	1:D:376:VAL:HG22	1.74	0.51
1:G:174:VAL:H	1:G:376:VAL:HG22	1.74	0.51
1:H:247:LEU:O	1:H:273:VAL:HA	2.10	0.51
1:I:221:LEU:HD22	1:I:236:VAL:HG11	1.91	0.51
1:J:511:ALA:O	1:J:515:ILE:HG13	2.11	0.51
1:B:207:LYS:HB2	1:B:208:PRO:HD3	1.92	0.51
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.93	0.51
1:C:150:ILE:HD13	1:C:493:ILE:CG2	2.37	0.51
1:C:207:LYS:CB	1:C:208:PRO:HD3	2.40	0.51
1:G:34:LYS:HB2	1:G:458:CYS:HA	1.92	0.51
1:H:221:LEU:HD22	1:H:236:VAL:HG11	1.91	0.51
1:I:221:LEU:HB2	1:I:317:LEU:HD21	1.92	0.51
1:N:247:LEU:O	1:N:273:VAL:HA	2.10	0.51
1:B:174:VAL:H	1:B:376:VAL:HG22	1.74	0.51
1:B:195:PHE:CZ	1:B:330:THR:CB	2.94	0.51
1:B:521:VAL:HG11	1:C:59:GLU:HB3	1.93	0.51
1:E:37:ASN:ND2	1:E:49:ILE:HG23	2.25	0.51
1:E:475:ASN:ND2	1:E:489:ILE:HD11	2.26	0.51
1:F:161:LEU:HD11	1:F:185:ASP:HB3	1.93	0.51
1:G:23:LEU:HA	1:G:60:ILE:CD1	2.32	0.51
1:G:38:VAL:HG11	1:G:56:VAL:HG22	1.91	0.51
1:G:52:ASP:CB	1:G:55:SER:H	2.24	0.51
1:H:221:LEU:HB2	1:H:317:LEU:HD21	1.92	0.51
1:H:511:ALA:O	1:H:515:ILE:HG13	2.11	0.51
1:J:30:THR:C	1:J:35:GLY:HA3	2.36	0.51
1:J:220:ILE:HD12	1:J:296:THR:CG2	2.40	0.51
2:K:1525:PO4:P	4:K:1527:ATP:PG	3.09	0.51
1:L:137:PRO:CA	1:L:410:GLY:HA3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:220:ILE:HD12	1:M:296:THR:CG2	2.40	0.51
1:M:221:LEU:HB2	1:M:317:LEU:HD21	1.92	0.51
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.93	0.51
1:A:59:GLU:HB3	1:G:521:VAL:HG11	1.93	0.51
1:A:183:LEU:HA	1:A:383:ALA:N	2.25	0.51
1:B:240:VAL:HG12	1:B:271:VAL:HG13	1.91	0.51
1:C:141:SER:O	1:C:163:ALA:HB1	2.11	0.51
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.93	0.51
1:C:213:VAL:HG11	1:C:325:ILE:HG12	1.87	0.51
1:D:34:LYS:HB2	1:D:458:CYS:HA	1.92	0.51
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.93	0.51
1:D:183:LEU:HA	1:D:383:ALA:N	2.25	0.51
1:F:52:ASP:HB3	1:F:55:SER:H	1.75	0.51
1:F:328:ASP:O	1:F:329:THR:HG23	2.10	0.51
1:F:521:VAL:HG11	1:G:59:GLU:HB3	1.92	0.51
1:G:37:ASN:ND2	1:G:49:ILE:HG23	2.25	0.51
2:I:1525:PO4:P	4:I:1527:ATP:PG	3.09	0.51
2:J:1525:PO4:P	4:J:1527:ATP:PG	3.09	0.51
1:K:183:LEU:H	1:K:183:LEU:HD23	1.76	0.51
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.93	0.51
1:A:475:ASN:ND2	1:A:489:ILE:HD11	2.26	0.51
1:C:34:LYS:HB2	1:C:458:CYS:HA	1.92	0.51
1:D:225:LYS:CB	1:D:308:GLU:HA	2.41	0.51
1:D:328:ASP:O	1:D:329:THR:HG23	2.10	0.51
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.93	0.51
1:G:193:MET:HE3	1:G:332:ILE:HD12	1.93	0.51
1:H:77:VAL:HG22	1:H:510:VAL:HB	1.92	0.51
1:I:150:ILE:CD1	1:I:494:LEU:H	2.22	0.51
1:J:137:PRO:CA	1:J:410:GLY:HA3	2.37	0.51
1:K:511:ALA:O	1:K:515:ILE:HG13	2.11	0.51
2:L:1525:PO4:P	4:L:1527:ATP:PG	3.09	0.51
1:M:189:VAL:HA	1:M:377:ALA:HA	1.93	0.51
1:N:77:VAL:HG22	1:N:510:VAL:HB	1.92	0.51
1:N:169:VAL:HG23	1:N:170:GLY:O	2.10	0.51
1:N:240:VAL:HG11	1:N:247:LEU:CA	2.40	0.51
1:A:141:SER:O	1:A:163:ALA:HB1	2.11	0.51
1:C:183:LEU:HA	1:C:383:ALA:N	2.25	0.51
1:C:225:LYS:CB	1:C:308:GLU:HA	2.41	0.51
1:C:475:ASN:ND2	1:C:489:ILE:HD11	2.26	0.51
1:D:52:ASP:HB3	1:D:55:SER:H	1.75	0.51
1:E:52:ASP:CB	1:E:55:SER:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:SER:O	1:E:163:ALA:HB1	2.11	0.51
1:E:328:ASP:O	1:E:329:THR:HG23	2.10	0.51
1:F:34:LYS:HB2	1:F:458:CYS:HA	1.92	0.51
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.93	0.51
2:H:1525:PO4:P	4:H:1527:ATP:PG	3.09	0.51
1:I:220:ILE:HD12	1:I:296:THR:CG2	2.40	0.51
1:L:240:VAL:HG11	1:L:247:LEU:CA	2.41	0.51
1:N:240:VAL:HG11	1:N:247:LEU:HB2	1.93	0.51
1:B:141:SER:O	1:B:163:ALA:HB1	2.11	0.51
1:B:225:LYS:CB	1:B:308:GLU:HA	2.41	0.51
1:C:240:VAL:HG12	1:C:271:VAL:HG13	1.91	0.51
1:E:225:LYS:CB	1:E:308:GLU:HA	2.41	0.51
1:F:37:ASN:ND2	1:F:49:ILE:HG23	2.25	0.51
1:F:240:VAL:HG12	1:F:271:VAL:HG13	1.91	0.51
1:G:475:ASN:ND2	1:G:489:ILE:HD11	2.26	0.51
1:H:207:LYS:HE2	1:H:207:LYS:N	2.24	0.51
1:H:518:GLU:CB	1:H:518:GLU:O	2.54	0.51
1:J:183:LEU:HD23	1:J:183:LEU:H	1.76	0.51
1:L:302:SER:HB2	1:L:305:ILE:H	1.74	0.51
1:M:77:VAL:HG22	1:M:510:VAL:HB	1.92	0.51
1:N:511:ALA:O	1:N:515:ILE:HG13	2.11	0.51
1:A:381:VAL:HB	1:A:393:LYS:HA	1.92	0.51
1:B:52:ASP:CB	1:B:55:SER:H	2.24	0.51
1:C:52:ASP:CB	1:C:55:SER:H	2.24	0.51
1:C:194:GLN:CG	1:C:329:THR:HG21	2.41	0.51
1:C:200:LEU:CB	1:C:259:LEU:CD1	2.86	0.51
1:F:381:VAL:HB	1:F:393:LYS:HA	1.92	0.51
1:G:141:SER:O	1:G:163:ALA:HB1	2.11	0.51
1:L:30:THR:C	1:L:35:GLY:HA3	2.36	0.51
1:L:221:LEU:CG	1:L:309:LEU:HD22	2.40	0.51
1:N:220:ILE:HD12	1:N:296:THR:CG2	2.40	0.51
1:N:221:LEU:CD2	1:N:309:LEU:HD22	2.41	0.51
1:A:38:VAL:HG11	1:A:56:VAL:HG22	1.91	0.50
1:D:475:ASN:ND2	1:D:489:ILE:HD11	2.26	0.50
1:E:161:LEU:HD11	1:E:185:ASP:HB3	1.93	0.50
1:F:38:VAL:HG11	1:F:56:VAL:HG22	1.91	0.50
1:F:141:SER:O	1:F:163:ALA:HB1	2.11	0.50
1:H:30:THR:C	1:H:35:GLY:HA3	2.36	0.50
1:H:240:VAL:HG11	1:H:247:LEU:CA	2.42	0.50
1:J:247:LEU:O	1:J:273:VAL:HA	2.10	0.50
1:M:249:ILE:HB	1:M:275:ALA:CB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HD11	1:A:185:ASP:HB3	1.93	0.50
1:B:34:LYS:HB2	1:B:458:CYS:HA	1.92	0.50
1:B:100:ILE:HD13	1:B:514:MET:SD	2.52	0.50
1:D:194:GLN:CG	1:D:329:THR:HG21	2.41	0.50
1:G:100:ILE:HD13	1:G:514:MET:SD	2.52	0.50
1:G:193:MET:HE2	1:G:296:THR:HG23	1.93	0.50
1:H:257:GLU:CA	1:N:242:LYS:C	2.78	0.50
1:I:206:ASN:HB3	1:I:208:PRO:HD2	1.93	0.50
1:J:240:VAL:HG11	1:J:247:LEU:CA	2.41	0.50
1:K:177:VAL:HG12	1:K:393:LYS:HE2	1.93	0.50
1:M:183:LEU:HD23	1:M:183:LEU:H	1.76	0.50
1:M:196:ASP:CG	1:M:329:THR:HG22	2.35	0.50
1:M:240:VAL:HG11	1:M:247:LEU:CA	2.41	0.50
1:A:100:ILE:HD13	1:A:514:MET:SD	2.52	0.50
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.93	0.50
1:L:77:VAL:HG22	1:L:510:VAL:HB	1.92	0.50
1:L:511:ALA:O	1:L:515:ILE:HG13	2.11	0.50
1:A:240:VAL:HG12	1:A:271:VAL:HG13	1.91	0.50
1:C:100:ILE:HD13	1:C:514:MET:SD	2.52	0.50
1:C:137:PRO:HA	1:C:410:GLY:HA3	1.90	0.50
1:D:166:MET:O	1:D:170:GLY:HA2	2.12	0.50
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.93	0.50
1:G:166:MET:O	1:G:170:GLY:HA2	2.12	0.50
1:G:213:VAL:HG11	1:G:325:ILE:HG12	1.88	0.50
1:I:30:THR:C	1:I:35:GLY:HA3	2.36	0.50
2:M:1525:PO4:P	4:M:1527:ATP:PG	3.09	0.50
1:N:205:ILE:C	1:N:207:LYS:HG2	2.36	0.50
2:N:1525:PO4:P	4:N:1527:ATP:PG	3.09	0.50
1:A:166:MET:O	1:A:170:GLY:HA2	2.12	0.50
1:A:200:LEU:HD11	1:A:254:VAL:HA	1.94	0.50
1:B:183:LEU:HA	1:B:383:ALA:N	2.25	0.50
1:B:194:GLN:O	1:B:371:LYS:HB3	2.12	0.50
1:D:161:LEU:HD11	1:D:185:ASP:HB3	1.93	0.50
1:D:240:VAL:HG12	1:D:271:VAL:HG13	1.91	0.50
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.93	0.50
1:F:100:ILE:HD13	1:F:514:MET:SD	2.52	0.50
1:F:475:ASN:ND2	1:F:489:ILE:HD11	2.26	0.50
1:G:194:GLN:CG	1:G:329:THR:HG21	2.41	0.50
1:G:381:VAL:HB	1:G:393:LYS:HA	1.92	0.50
1:K:190:VAL:HG21	1:K:333:ILE:HD13	1.94	0.50
1:K:193:MET:HE2	1:K:295:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASP:HB3	1:B:55:SER:H	1.76	0.50
1:G:225:LYS:CB	1:G:308:GLU:HA	2.41	0.50
1:G:255:GLU:HB2	1:G:259:LEU:H	1.77	0.50
1:I:77:VAL:HG22	1:I:510:VAL:HB	1.92	0.50
1:J:77:VAL:HG22	1:J:510:VAL:HB	1.92	0.50
1:K:30:THR:C	1:K:35:GLY:HA3	2.36	0.50
1:K:221:LEU:CD2	1:K:309:LEU:HD22	2.42	0.50
1:L:191:GLU:HG2	1:L:192:GLY:H	1.75	0.50
1:L:221:LEU:CD2	1:L:309:LEU:HD22	2.42	0.50
1:N:204:PHE:HD1	1:N:207:LYS:NZ	2.06	0.50
1:N:249:ILE:HB	1:N:275:ALA:CB	2.40	0.50
1:A:194:GLN:CG	1:A:329:THR:HG21	2.41	0.50
1:B:255:GLU:HB2	1:B:259:LEU:H	1.77	0.50
1:C:166:MET:O	1:C:170:GLY:HA2	2.12	0.50
1:E:34:LYS:HB2	1:E:458:CYS:HA	1.92	0.50
1:E:194:GLN:CG	1:E:329:THR:HG21	2.41	0.50
1:E:381:VAL:HB	1:E:393:LYS:HA	1.92	0.50
1:F:200:LEU:HD12	1:F:275:ALA:HB1	1.93	0.50
1:G:150:ILE:CD1	1:G:493:ILE:CA	2.74	0.50
1:G:406:ALA:HB1	1:G:411:VAL:CG1	2.42	0.50
1:J:168:LYS:HG2	1:J:187:LEU:HD21	1.93	0.50
1:M:511:ALA:O	1:M:515:ILE:HG13	2.11	0.50
1:N:183:LEU:HD23	1:N:183:LEU:H	1.76	0.50
1:C:224:ASP:HA	1:C:289:LEU:CD1	2.42	0.50
1:C:249:ILE:HD11	1:C:262:LEU:HD22	1.87	0.50
1:D:255:GLU:HB2	1:D:259:LEU:H	1.77	0.50
1:E:147:VAL:HG22	1:E:494:LEU:HB2	1.94	0.50
1:E:166:MET:O	1:E:170:GLY:HA2	2.12	0.50
1:F:147:VAL:HG22	1:F:494:LEU:HB2	1.94	0.50
1:G:382:GLY:O	1:G:389:MET:HA	2.12	0.50
1:I:511:ALA:O	1:I:515:ILE:HG13	2.11	0.50
1:J:190:VAL:HG21	1:J:333:ILE:HD13	1.94	0.50
1:J:242:LYS:CB	1:K:257:GLU:HA	2.41	0.50
1:J:255:GLU:CD	1:J:256:GLY:H	2.20	0.50
1:K:182:GLY:HA3	1:K:383:ALA:N	2.09	0.50
1:A:52:ASP:CB	1:A:55:SER:H	2.24	0.50
1:A:224:ASP:HA	1:A:289:LEU:CD1	2.42	0.50
1:A:225:LYS:CB	1:A:308:GLU:HA	2.41	0.50
1:B:147:VAL:HG22	1:B:494:LEU:HB2	1.94	0.50
1:B:213:VAL:HG11	1:B:325:ILE:HG12	1.88	0.50
1:B:406:ALA:HB1	1:B:411:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:GLY:O	1:C:389:MET:HA	2.12	0.50
1:D:141:SER:O	1:D:163:ALA:HB1	2.11	0.50
1:E:240:VAL:HG21	1:E:247:LEU:HD13	1.94	0.50
1:E:382:GLY:O	1:E:389:MET:HA	2.12	0.50
1:F:224:ASP:HA	1:F:289:LEU:CD1	2.42	0.50
1:K:240:VAL:HG11	1:K:247:LEU:CA	2.41	0.50
1:M:30:THR:C	1:M:35:GLY:HA3	2.36	0.50
1:M:221:LEU:CD2	1:M:309:LEU:HD22	2.42	0.50
1:A:225:LYS:HB2	1:A:308:GLU:HA	1.94	0.49
1:B:475:ASN:ND2	1:B:489:ILE:HD11	2.26	0.49
1:D:100:ILE:HD13	1:D:514:MET:SD	2.52	0.49
1:D:191:GLU:HG3	1:D:342:ILE:HD12	1.93	0.49
1:G:200:LEU:CD2	1:G:254:VAL:CG1	2.86	0.49
1:I:190:VAL:HG21	1:I:333:ILE:HD13	1.94	0.49
1:I:221:LEU:HG	1:I:309:LEU:HD22	1.94	0.49
1:K:152:ALA:HB3	1:K:155:ASP:N	2.27	0.49
1:M:152:ALA:HB3	1:M:155:ASP:N	2.27	0.49
1:M:190:VAL:HG21	1:M:333:ILE:HD13	1.94	0.49
1:M:301:ILE:HD11	1:M:312:ALA:CB	2.32	0.49
1:A:147:VAL:HG22	1:A:494:LEU:HB2	1.94	0.49
1:B:161:LEU:HD11	1:B:185:ASP:HB3	1.93	0.49
1:B:224:ASP:HA	1:B:289:LEU:CD1	2.42	0.49
1:B:225:LYS:HB2	1:B:308:GLU:HA	1.94	0.49
1:C:161:LEU:HD11	1:C:185:ASP:HB3	1.93	0.49
1:C:192:GLY:HA3	1:C:376:VAL:CG2	2.40	0.49
1:D:220:ILE:CD1	1:D:332:ILE:HD13	2.33	0.49
1:F:225:LYS:CB	1:F:308:GLU:HA	2.41	0.49
1:F:240:VAL:HG21	1:F:247:LEU:HD13	1.94	0.49
1:G:225:LYS:HB2	1:G:308:GLU:HA	1.94	0.49
1:J:224:ASP:HB2	1:J:303:GLU:H	1.77	0.49
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.94	0.49
1:L:31:LEU:HB2	1:L:90:THR:HG21	1.95	0.49
1:L:249:ILE:HB	1:L:275:ALA:CB	2.40	0.49
1:M:243:ALA:HA	1:N:260:ALA:HB2	1.93	0.49
1:N:182:GLY:HA3	1:N:383:ALA:N	2.09	0.49
1:B:166:MET:O	1:B:170:GLY:HA2	2.12	0.49
1:B:240:VAL:HG21	1:B:247:LEU:HD13	1.94	0.49
1:C:147:VAL:HG22	1:C:494:LEU:HB2	1.94	0.49
1:D:190:VAL:HG23	1:D:333:ILE:CG2	2.42	0.49
1:D:224:ASP:HA	1:D:289:LEU:CD1	2.42	0.49
1:D:240:VAL:HG21	1:D:247:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:GLY:O	1:D:389:MET:HA	2.12	0.49
1:F:225:LYS:HB2	1:F:308:GLU:HA	1.94	0.49
1:H:152:ALA:HB3	1:H:155:ASP:N	2.27	0.49
1:H:242:LYS:HG3	1:I:257:GLU:C	2.38	0.49
1:H:257:GLU:HA	1:N:242:LYS:CB	2.41	0.49
1:J:178:GLU:O	1:J:380:LYS:HA	2.12	0.49
1:K:77:VAL:HG22	1:K:510:VAL:HB	1.92	0.49
1:K:518:GLU:CB	1:K:518:GLU:O	2.54	0.49
1:C:240:VAL:HG21	1:C:247:LEU:HD13	1.94	0.49
1:D:52:ASP:CB	1:D:55:SER:H	2.25	0.49
1:E:221:LEU:HD21	1:E:309:LEU:HD11	1.95	0.49
1:F:166:MET:O	1:F:170:GLY:HA2	2.12	0.49
1:F:255:GLU:HB2	1:F:259:LEU:H	1.77	0.49
1:F:406:ALA:HB1	1:F:411:VAL:CG1	2.42	0.49
1:H:236:VAL:O	1:H:240:VAL:HG23	2.13	0.49
1:H:255:GLU:CD	1:H:256:GLY:H	2.20	0.49
1:I:31:LEU:HB2	1:I:90:THR:HG21	1.95	0.49
1:K:31:LEU:HB2	1:K:90:THR:HG21	1.95	0.49
1:K:249:ILE:HB	1:K:275:ALA:CB	2.40	0.49
1:N:224:ASP:HB2	1:N:303:GLU:H	1.78	0.49
1:A:240:VAL:HG21	1:A:247:LEU:HD13	1.94	0.49
1:A:382:GLY:O	1:A:389:MET:HA	2.12	0.49
1:A:406:ALA:HB1	1:A:411:VAL:CG1	2.42	0.49
1:B:200:LEU:HD11	1:B:254:VAL:HA	1.94	0.49
1:C:221:LEU:HD21	1:C:309:LEU:HD11	1.95	0.49
1:D:147:VAL:HG22	1:D:494:LEU:HB2	1.94	0.49
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.95	0.49
1:I:183:LEU:HD23	1:I:183:LEU:H	1.76	0.49
1:I:255:GLU:CD	1:I:256:GLY:H	2.21	0.49
1:J:227:ILE:CD1	1:J:233:MET:SD	2.92	0.49
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.94	0.49
1:J:242:LYS:HG3	1:K:257:GLU:HB2	1.94	0.49
1:K:255:GLU:CD	1:K:256:GLY:H	2.20	0.49
1:K:406:ALA:HB1	1:K:411:VAL:CG1	2.43	0.49
1:L:406:ALA:HB1	1:L:411:VAL:CG1	2.43	0.49
1:C:200:LEU:HD12	1:C:275:ALA:HB1	1.93	0.49
1:C:406:ALA:HB1	1:C:411:VAL:CG1	2.42	0.49
1:D:521:VAL:HG21	1:E:59:GLU:CB	2.43	0.49
1:E:100:ILE:HD13	1:E:514:MET:SD	2.52	0.49
1:E:137:PRO:HA	1:E:410:GLY:HA3	1.90	0.49
1:F:194:GLN:CG	1:F:329:THR:HG21	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:LEU:HG	1:H:309:LEU:HD22	1.95	0.49
1:H:406:ALA:HB1	1:H:411:VAL:CG1	2.43	0.49
1:I:240:VAL:HG11	1:I:247:LEU:CA	2.41	0.49
1:I:242:LYS:CB	1:J:257:GLU:HA	2.41	0.49
1:I:242:LYS:HG3	1:J:257:GLU:HB2	1.93	0.49
1:J:31:LEU:HB2	1:J:90:THR:HG21	1.95	0.49
1:J:221:LEU:HG	1:J:309:LEU:HD22	1.95	0.49
1:A:255:GLU:HB2	1:A:259:LEU:H	1.77	0.49
1:D:383:ALA:HA	1:D:389:MET:HB2	1.95	0.49
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.95	0.49
1:F:383:ALA:HA	1:F:389:MET:HB2	1.95	0.49
1:G:240:VAL:HG21	1:G:247:LEU:HD13	1.94	0.49
1:H:190:VAL:HG21	1:H:333:ILE:HD13	1.94	0.49
1:H:249:ILE:HB	1:H:275:ALA:CB	2.40	0.49
1:J:290:GLN:HA	1:J:300:VAL:HG21	1.95	0.49
1:L:182:GLY:HA3	1:L:383:ALA:N	2.09	0.49
1:L:224:ASP:HB2	1:L:303:GLU:H	1.78	0.49
1:M:255:GLU:CD	1:M:256:GLY:H	2.20	0.49
1:N:30:THR:C	1:N:35:GLY:HA3	2.36	0.49
1:N:255:GLU:CD	1:N:256:GLY:H	2.21	0.49
1:B:200:LEU:HD12	1:B:275:ALA:HB1	1.93	0.49
1:B:382:GLY:O	1:B:389:MET:HA	2.12	0.49
1:C:225:LYS:HB2	1:C:308:GLU:HA	1.94	0.49
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.95	0.49
1:E:383:ALA:HA	1:E:389:MET:HB2	1.95	0.49
1:F:52:ASP:CB	1:F:55:SER:H	2.25	0.49
1:F:227:ILE:HG12	1:F:309:LEU:HG	1.95	0.49
1:I:236:VAL:O	1:I:240:VAL:HG23	2.13	0.49
1:J:406:ALA:HB1	1:J:411:VAL:CG1	2.43	0.49
1:M:31:LEU:HB2	1:M:90:THR:HG21	1.95	0.49
1:N:206:ASN:HB2	1:N:213:VAL:HA	1.94	0.49
1:A:220:ILE:CD1	1:A:332:ILE:HD13	2.33	0.49
1:B:221:LEU:HD21	1:B:309:LEU:HD11	1.95	0.49
1:C:255:GLU:HB2	1:C:259:LEU:H	1.77	0.49
1:D:406:ALA:HB1	1:D:411:VAL:CG1	2.42	0.49
1:E:225:LYS:HB2	1:E:308:GLU:HA	1.94	0.49
1:E:249:ILE:HD11	1:E:262:LEU:HD22	1.87	0.49
1:E:521:VAL:HG21	1:F:59:GLU:CB	2.43	0.49
1:G:137:PRO:HA	1:G:410:GLY:HA3	1.90	0.49
1:H:31:LEU:HB2	1:H:90:THR:HG21	1.95	0.49
1:H:136:VAL:O	1:H:410:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:221:LEU:HD13	1:I:317:LEU:CD1	2.43	0.49
1:I:290:GLN:HA	1:I:300:VAL:HG21	1.95	0.49
1:M:182:GLY:HA3	1:M:383:ALA:N	2.09	0.49
1:A:383:ALA:HA	1:A:389:MET:HB2	1.95	0.49
1:B:383:ALA:HA	1:B:389:MET:HB2	1.95	0.49
1:C:383:ALA:HA	1:C:389:MET:HB2	1.95	0.49
1:D:221:LEU:HD21	1:D:309:LEU:HD11	1.95	0.49
1:E:240:VAL:CG1	1:E:247:LEU:HB2	2.42	0.49
1:G:227:ILE:HG12	1:G:309:LEU:HG	1.94	0.49
1:H:221:LEU:CD2	1:H:309:LEU:HD22	2.42	0.49
1:H:257:GLU:HB2	1:N:242:LYS:HG3	1.94	0.49
1:H:427:ALA:HA	1:H:444:LEU:HD11	1.95	0.49
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.94	0.49
1:M:136:VAL:O	1:M:410:GLY:HA3	2.13	0.49
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.96	0.48
1:E:227:ILE:HG12	1:E:309:LEU:HG	1.94	0.48
1:G:383:ALA:HA	1:G:389:MET:HB2	1.95	0.48
1:I:224:ASP:HB2	1:I:303:GLU:H	1.78	0.48
1:K:221:LEU:HG	1:K:309:LEU:HD22	1.95	0.48
1:L:290:GLN:HA	1:L:300:VAL:HG21	1.95	0.48
1:M:240:VAL:HG11	1:M:247:LEU:HB2	1.94	0.48
1:M:290:GLN:HA	1:M:300:VAL:HG21	1.95	0.48
1:M:406:ALA:HB1	1:M:411:VAL:CG1	2.43	0.48
1:N:31:LEU:HB2	1:N:90:THR:HG21	1.95	0.48
1:N:152:ALA:HB3	1:N:155:ASP:N	2.27	0.48
1:N:190:VAL:HG21	1:N:333:ILE:HD13	1.94	0.48
1:A:59:GLU:CB	1:G:521:VAL:HG21	2.43	0.48
1:D:225:LYS:HB2	1:D:308:GLU:HA	1.94	0.48
1:E:200:LEU:HD12	1:E:275:ALA:HB1	1.93	0.48
1:E:224:ASP:HA	1:E:289:LEU:CD1	2.42	0.48
1:G:206:ASN:HB3	1:G:208:PRO:HD2	1.94	0.48
1:I:152:ALA:HB3	1:I:155:ASP:N	2.27	0.48
1:I:427:ALA:HA	1:I:444:LEU:HD11	1.95	0.48
1:J:221:LEU:HD13	1:J:317:LEU:CD1	2.44	0.48
1:N:350:ARG:HD2	1:N:353:ILE:HD12	1.96	0.48
1:N:427:ALA:HA	1:N:444:LEU:HD11	1.95	0.48
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.96	0.48
1:E:255:GLU:HB2	1:E:259:LEU:H	1.77	0.48
1:F:382:GLY:O	1:F:389:MET:HA	2.12	0.48
1:G:220:ILE:CD1	1:G:332:ILE:HD13	2.33	0.48
1:H:350:ARG:HD2	1:H:353:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:221:LEU:CD2	1:I:309:LEU:HD22	2.42	0.48
1:I:518:GLU:CB	1:I:518:GLU:O	2.54	0.48
1:J:152:ALA:HB3	1:J:155:ASP:N	2.27	0.48
1:N:290:GLN:HA	1:N:300:VAL:HG21	1.95	0.48
1:B:521:VAL:HG21	1:C:59:GLU:CB	2.43	0.48
1:E:200:LEU:HD11	1:E:254:VAL:CA	2.12	0.48
1:E:406:ALA:HB1	1:E:411:VAL:CG1	2.42	0.48
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.95	0.48
1:I:240:VAL:HG11	1:I:247:LEU:HB2	1.94	0.48
1:K:221:LEU:HD13	1:K:317:LEU:CD1	2.44	0.48
1:L:152:ALA:HB3	1:L:155:ASP:N	2.27	0.48
1:M:350:ARG:HD2	1:M:353:ILE:HD12	1.96	0.48
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.96	0.48
1:D:190:VAL:HG23	1:D:333:ILE:HG23	1.96	0.48
1:G:147:VAL:HG22	1:G:494:LEU:HB2	1.94	0.48
1:K:290:GLN:HA	1:K:300:VAL:HG21	1.95	0.48
1:A:227:ILE:HG12	1:A:309:LEU:HG	1.95	0.48
1:A:311:LYS:HD3	1:A:311:LYS:HA	1.93	0.48
1:B:23:LEU:HA	1:B:60:ILE:CD1	2.32	0.48
1:B:150:ILE:CD1	1:B:493:ILE:CA	2.74	0.48
1:D:200:LEU:HD11	1:D:254:VAL:CA	2.12	0.48
1:D:240:VAL:CG1	1:D:247:LEU:HB2	2.42	0.48
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.95	0.48
1:F:521:VAL:HG21	1:G:59:GLU:CB	2.43	0.48
1:G:162:ILE:CD1	1:G:400:LEU:N	2.77	0.48
1:G:224:ASP:HA	1:G:289:LEU:CD1	2.42	0.48
1:H:221:LEU:HD13	1:H:317:LEU:CD1	2.44	0.48
1:H:240:VAL:HG11	1:H:247:LEU:HB2	1.95	0.48
1:H:290:GLN:HA	1:H:300:VAL:HG21	1.95	0.48
1:J:221:LEU:CD2	1:J:309:LEU:HD22	2.42	0.48
1:J:249:ILE:HB	1:J:275:ALA:CB	2.40	0.48
1:J:427:ALA:HA	1:J:444:LEU:HD11	1.95	0.48
1:K:274:ALA:HB1	1:K:325:ILE:HD13	1.95	0.48
1:M:224:ASP:HB2	1:M:303:GLU:H	1.78	0.48
1:A:227:ILE:HD12	1:A:258:ALA:HB1	1.96	0.48
1:B:222:LEU:CD2	1:B:292:ILE:HG22	2.42	0.48
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.95	0.48
1:C:162:ILE:CD1	1:C:400:LEU:N	2.77	0.48
1:D:309:LEU:O	1:D:312:ALA:HB3	2.14	0.48
1:E:158:VAL:HG13	1:E:396:VAL:HA	1.96	0.48
1:F:309:LEU:O	1:F:312:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:ALA:CA	1:G:271:VAL:HG22	2.44	0.48
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.96	0.48
1:H:242:LYS:C	1:I:257:GLU:CA	2.78	0.48
1:I:136:VAL:O	1:I:410:GLY:HA3	2.13	0.48
1:I:182:GLY:HA3	1:I:383:ALA:N	2.09	0.48
1:L:236:VAL:O	1:L:240:VAL:HG23	2.13	0.48
1:M:236:VAL:O	1:M:240:VAL:HG23	2.13	0.48
1:A:200:LEU:HD12	1:A:275:ALA:HB1	1.93	0.48
1:D:158:VAL:HG13	1:D:396:VAL:HA	1.96	0.48
1:D:190:VAL:CG2	1:D:333:ILE:HG22	2.43	0.48
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.96	0.48
1:F:158:VAL:HG13	1:F:396:VAL:HA	1.96	0.48
1:G:184:GLN:HG2	1:G:185:ASP:O	2.14	0.48
1:H:203:TYR:CD1	1:H:267:MET:CE	2.97	0.48
1:L:136:VAL:O	1:L:410:GLY:HA3	2.13	0.48
1:L:196:ASP:OD1	1:L:329:THR:HG22	2.14	0.48
1:A:222:LEU:CD2	1:A:292:ILE:HG22	2.42	0.48
1:D:162:ILE:CD1	1:D:400:LEU:N	2.77	0.48
1:E:222:LEU:CD2	1:E:292:ILE:HG22	2.42	0.48
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.96	0.48
1:J:207:LYS:HE2	1:J:207:LYS:N	2.28	0.48
1:J:518:GLU:CB	1:J:518:GLU:O	2.54	0.48
1:L:298:GLY:HA3	1:L:318:GLY:CA	2.44	0.48
1:M:183:LEU:HA	1:M:382:GLY:CA	2.44	0.48
1:N:236:VAL:O	1:N:240:VAL:HG23	2.14	0.48
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.95	0.48
1:A:99:ILE:CG2	1:A:120:ILE:HD13	2.44	0.48
1:A:249:ILE:HD11	1:A:262:LEU:HD22	1.87	0.48
1:A:309:LEU:O	1:A:312:ALA:HB3	2.14	0.48
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.95	0.48
1:C:213:VAL:CG2	1:C:214:GLU:N	2.77	0.48
1:E:309:LEU:O	1:E:312:ALA:HB3	2.14	0.48
1:F:221:LEU:HD21	1:F:309:LEU:HD11	1.95	0.48
1:G:207:LYS:HE2	1:G:207:LYS:HB2	1.49	0.48
1:G:311:LYS:HD3	1:G:311:LYS:HA	1.93	0.48
1:I:350:ARG:HD2	1:I:353:ILE:HD12	1.95	0.48
1:K:236:VAL:O	1:K:240:VAL:HG23	2.13	0.48
1:L:183:LEU:HD23	1:L:183:LEU:N	2.22	0.48
1:L:350:ARG:HD2	1:L:353:ILE:HD12	1.96	0.48
1:B:99:ILE:CG2	1:B:120:ILE:HD13	2.44	0.47
1:B:220:ILE:CD1	1:B:332:ILE:HD13	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LEU:HD11	1:C:254:VAL:HA	1.94	0.47
1:C:521:VAL:HG21	1:D:59:GLU:CB	2.43	0.47
1:D:190:VAL:HB	1:D:334:ASP:CB	2.44	0.47
1:D:241:ALA:CA	1:D:271:VAL:HG22	2.44	0.47
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.96	0.47
1:E:240:VAL:HG11	1:E:247:LEU:CB	2.43	0.47
1:G:200:LEU:HD22	1:G:259:LEU:CD2	2.30	0.47
1:J:183:LEU:HA	1:J:382:GLY:CA	2.44	0.47
1:K:427:ALA:HA	1:K:444:LEU:HD11	1.95	0.47
1:L:427:ALA:HA	1:L:444:LEU:HD11	1.95	0.47
1:M:242:LYS:C	1:N:257:GLU:CA	2.78	0.47
1:N:221:LEU:HD13	1:N:317:LEU:CD1	2.44	0.47
1:A:162:ILE:CD1	1:A:400:LEU:N	2.77	0.47
1:A:384:ALA:HA	1:A:385:THR:HA	1.68	0.47
1:B:162:ILE:CD1	1:B:400:LEU:N	2.77	0.47
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.96	0.47
1:B:203:TYR:N	1:B:203:TYR:HD1	2.12	0.47
1:B:227:ILE:HD12	1:B:258:ALA:HB1	1.96	0.47
1:C:220:ILE:CD1	1:C:332:ILE:HD13	2.33	0.47
1:D:200:LEU:HD12	1:D:275:ALA:HB1	1.93	0.47
1:D:222:LEU:CD2	1:D:292:ILE:HG22	2.42	0.47
1:E:99:ILE:CG2	1:E:120:ILE:HD13	2.44	0.47
1:F:311:LYS:HD3	1:F:311:LYS:HA	1.93	0.47
1:J:301:ILE:HD11	1:J:312:ALA:CB	2.32	0.47
1:B:309:LEU:O	1:B:312:ALA:HB3	2.14	0.47
1:D:99:ILE:CG2	1:D:120:ILE:HD13	2.44	0.47
1:D:213:VAL:O	1:D:324:VAL:HA	2.15	0.47
1:D:240:VAL:HG11	1:D:247:LEU:CB	2.43	0.47
1:D:278:ALA:HB2	1:D:289:LEU:CD1	2.45	0.47
1:E:213:VAL:CG2	1:E:214:GLU:N	2.77	0.47
1:E:278:ALA:HB2	1:E:289:LEU:CD1	2.45	0.47
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.97	0.47
1:F:241:ALA:CA	1:F:271:VAL:HG22	2.44	0.47
1:G:158:VAL:HG13	1:G:396:VAL:HA	1.96	0.47
1:G:222:LEU:CD2	1:G:292:ILE:HG22	2.42	0.47
1:I:189:VAL:HG22	1:I:377:ALA:HB2	1.95	0.47
1:J:214:GLU:CD	1:J:322:ARG:HE	2.22	0.47
1:K:136:VAL:O	1:K:410:GLY:HA3	2.13	0.47
1:K:183:LEU:HA	1:K:382:GLY:CA	2.44	0.47
1:K:350:ARG:HD2	1:K:353:ILE:HD12	1.96	0.47
1:M:298:GLY:HA3	1:M:318:GLY:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:VAL:O	1:N:410:GLY:HA3	2.13	0.47
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.96	0.47
1:A:221:LEU:HD21	1:A:309:LEU:HD11	1.95	0.47
1:A:241:ALA:CA	1:A:271:VAL:HG22	2.44	0.47
1:A:278:ALA:HB2	1:A:289:LEU:CD1	2.45	0.47
1:A:521:VAL:HG21	1:B:59:GLU:CB	2.43	0.47
1:B:227:ILE:HG12	1:B:309:LEU:HG	1.95	0.47
1:B:353:ILE:HD13	1:B:366:GLN:HG2	1.97	0.47
1:C:99:ILE:CG2	1:C:120:ILE:HD13	2.44	0.47
1:C:158:VAL:HG13	1:C:396:VAL:HA	1.96	0.47
1:C:227:ILE:HG12	1:C:309:LEU:HG	1.95	0.47
1:C:353:ILE:HD13	1:C:366:GLN:HG2	1.97	0.47
1:D:150:ILE:CD1	1:D:493:ILE:CG2	2.91	0.47
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.97	0.47
1:E:241:ALA:CA	1:E:271:VAL:HG22	2.44	0.47
1:E:311:LYS:HD3	1:E:311:LYS:HA	1.93	0.47
1:F:222:LEU:CD2	1:F:292:ILE:HG22	2.42	0.47
1:H:298:GLY:HA3	1:H:318:GLY:CA	2.44	0.47
1:J:136:VAL:O	1:J:410:GLY:HA3	2.13	0.47
1:L:207:LYS:HA	1:L:207:LYS:CE	2.36	0.47
1:L:221:LEU:HG	1:L:309:LEU:HD22	1.96	0.47
1:M:196:ASP:OD2	1:M:329:THR:HG22	2.14	0.47
1:M:237:LEU:CD2	1:M:247:LEU:HD23	2.44	0.47
1:M:314:LEU:O	1:M:317:LEU:HB2	2.14	0.47
1:M:427:ALA:HA	1:M:444:LEU:HD11	1.95	0.47
1:N:183:LEU:HA	1:N:382:GLY:CA	2.44	0.47
1:N:237:LEU:CD2	1:N:247:LEU:HD23	2.44	0.47
1:B:384:ALA:HA	1:B:385:THR:HA	1.68	0.47
1:C:150:ILE:CD1	1:C:493:ILE:CA	2.74	0.47
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.96	0.47
1:C:240:VAL:CG1	1:C:247:LEU:HB2	2.42	0.47
1:C:241:ALA:CA	1:C:271:VAL:HG22	2.44	0.47
1:D:353:ILE:HD13	1:D:366:GLN:HG2	1.97	0.47
1:E:213:VAL:O	1:E:324:VAL:HA	2.14	0.47
1:E:381:VAL:CG2	1:E:393:LYS:N	2.77	0.47
1:F:223:ALA:CA	1:F:309:LEU:HD23	2.45	0.47
1:G:99:ILE:CG2	1:G:120:ILE:HD13	2.44	0.47
1:H:237:LEU:CD2	1:H:247:LEU:HD23	2.45	0.47
2:H:1525:PO4:P	4:H:1527:ATP:O1G	2.73	0.47
1:I:214:GLU:CD	1:I:322:ARG:HE	2.22	0.47
1:J:237:LEU:CD2	1:J:247:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:298:GLY:HA3	1:K:318:GLY:CA	2.44	0.47
1:A:223:ALA:CA	1:A:309:LEU:HD23	2.45	0.47
1:A:353:ILE:HD13	1:A:366:GLN:HG2	1.97	0.47
1:C:213:VAL:O	1:C:324:VAL:HA	2.15	0.47
1:C:222:LEU:CD2	1:C:292:ILE:HG22	2.42	0.47
1:D:213:VAL:CG2	1:D:214:GLU:N	2.77	0.47
1:D:221:LEU:CD1	1:D:309:LEU:HD21	2.45	0.47
1:F:99:ILE:CG2	1:F:120:ILE:HD13	2.44	0.47
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.96	0.47
1:G:221:LEU:HD21	1:G:309:LEU:HD11	1.95	0.47
1:G:278:ALA:HB2	1:G:289:LEU:CD1	2.45	0.47
1:H:220:ILE:HD12	1:H:296:THR:HG21	1.96	0.47
1:I:209:GLU:H	1:I:209:GLU:CD	2.23	0.47
1:I:237:LEU:CD2	1:I:247:LEU:HD23	2.44	0.47
1:J:350:ARG:HD2	1:J:353:ILE:HD12	1.96	0.47
1:L:221:LEU:HD13	1:L:317:LEU:CD1	2.45	0.47
2:L:1525:PO4:P	4:L:1527:ATP:O1G	2.73	0.47
1:N:221:LEU:HG	1:N:309:LEU:HD22	1.96	0.47
1:B:203:TYR:N	1:B:203:TYR:CD1	2.83	0.47
1:B:221:LEU:CD1	1:B:309:LEU:HD21	2.45	0.47
1:B:278:ALA:HB2	1:B:289:LEU:CD1	2.45	0.47
1:C:309:LEU:O	1:C:312:ALA:HB3	2.14	0.47
1:D:227:ILE:HG12	1:D:309:LEU:HG	1.95	0.47
1:F:213:VAL:CG2	1:F:214:GLU:N	2.77	0.47
1:F:262:LEU:O	1:F:266:THR:HG23	2.15	0.47
1:G:213:VAL:O	1:G:324:VAL:HA	2.14	0.47
1:G:309:LEU:O	1:G:312:ALA:HB3	2.14	0.47
1:H:237:LEU:HA	1:H:247:LEU:HD22	1.97	0.47
1:I:183:LEU:HA	1:I:382:GLY:CA	2.44	0.47
1:I:220:ILE:HD12	1:I:296:THR:HG21	1.96	0.47
2:I:1525:PO4:P	4:I:1527:ATP:O1G	2.73	0.47
1:J:203:TYR:CD1	1:J:267:MET:CE	2.97	0.47
1:K:214:GLU:CD	1:K:322:ARG:HE	2.22	0.47
1:K:227:ILE:CD1	1:K:233:MET:SD	2.92	0.47
2:K:1525:PO4:P	4:K:1527:ATP:O1G	2.73	0.47
1:L:237:LEU:CD2	1:L:247:LEU:HD23	2.45	0.47
1:M:203:TYR:CD1	1:M:267:MET:CE	2.97	0.47
1:M:221:LEU:HD13	1:M:317:LEU:CD1	2.45	0.47
1:N:34:LYS:HB2	1:N:457:ASN:HB3	1.97	0.47
1:N:205:ILE:O	1:N:207:LYS:CG	2.62	0.47
2:N:1525:PO4:P	4:N:1527:ATP:O1G	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HG13	1:A:396:VAL:HA	1.96	0.47
1:C:192:GLY:H	1:C:375:GLY:HA2	1.80	0.47
1:C:221:LEU:CD1	1:C:309:LEU:HD21	2.45	0.47
1:D:223:ALA:CA	1:D:309:LEU:HD23	2.45	0.47
1:E:353:ILE:HD13	1:E:366:GLN:HG2	1.97	0.47
1:F:240:VAL:HG11	1:F:247:LEU:CB	2.43	0.47
1:G:227:ILE:HD12	1:G:258:ALA:HB1	1.96	0.47
1:H:214:GLU:CD	1:H:322:ARG:HE	2.22	0.47
1:H:314:LEU:O	1:H:317:LEU:HB2	2.14	0.47
1:J:194:GLN:HG3	1:J:329:THR:HB	1.97	0.47
1:L:206:ASN:HB2	1:L:213:VAL:HG23	1.96	0.47
1:L:209:GLU:H	1:L:209:GLU:CD	2.23	0.47
1:L:242:LYS:CB	1:M:257:GLU:HA	2.43	0.47
1:N:50:THR:HB	1:N:51:LYS:HA	1.97	0.47
1:N:237:LEU:HA	1:N:247:LEU:HD22	1.97	0.47
1:B:213:VAL:CG2	1:B:214:GLU:N	2.77	0.47
1:B:262:LEU:O	1:B:266:THR:HG23	2.15	0.47
1:C:227:ILE:HD12	1:C:258:ALA:HB1	1.96	0.47
1:C:278:ALA:HB2	1:C:289:LEU:CD1	2.45	0.47
1:F:226:LYS:HB2	1:F:252:GLU:HG3	1.96	0.47
1:G:200:LEU:HD22	1:G:254:VAL:HG11	1.96	0.47
1:G:262:LEU:O	1:G:266:THR:HG23	2.15	0.47
1:H:203:TYR:CE2	1:H:267:MET:SD	3.08	0.47
1:I:237:LEU:HA	1:I:247:LEU:HD22	1.97	0.47
1:J:236:VAL:O	1:J:240:VAL:HG23	2.13	0.47
1:K:144:ILE:HG23	1:K:403:THR:HG21	1.97	0.47
1:K:314:LEU:O	1:K:317:LEU:HB2	2.14	0.47
1:L:144:ILE:HG23	1:L:403:THR:HG21	1.97	0.47
1:N:214:GLU:CD	1:N:322:ARG:HE	2.22	0.47
1:A:204:PHE:CD1	1:A:273:VAL:O	2.68	0.47
1:B:213:VAL:O	1:B:324:VAL:HA	2.15	0.47
1:C:150:ILE:HD11	1:C:493:ILE:HG23	1.97	0.47
1:D:262:LEU:O	1:D:266:THR:HG23	2.15	0.47
1:F:162:ILE:CD1	1:F:400:LEU:N	2.77	0.47
1:F:213:VAL:O	1:F:324:VAL:HA	2.14	0.47
1:G:353:ILE:HD13	1:G:366:GLN:HG2	1.97	0.47
1:I:298:GLY:HA3	1:I:318:GLY:CA	2.44	0.47
1:J:203:TYR:CE2	1:J:267:MET:SD	3.08	0.47
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.97	0.47
1:K:34:LYS:HB2	1:K:457:ASN:HB3	1.97	0.47
1:K:237:LEU:HD13	1:K:271:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:214:GLU:CD	1:L:322:ARG:HE	2.22	0.47
1:M:237:LEU:HA	1:M:247:LEU:HD22	1.97	0.47
1:B:241:ALA:CA	1:B:271:VAL:HG22	2.44	0.46
1:E:226:LYS:HB2	1:E:252:GLU:HG3	1.96	0.46
1:G:213:VAL:CG2	1:G:214:GLU:N	2.77	0.46
1:H:34:LYS:HB2	1:H:457:ASN:HB3	1.97	0.46
1:H:182:GLY:HA3	1:H:383:ALA:N	2.11	0.46
1:J:144:ILE:HG23	1:J:403:THR:HG21	1.97	0.46
1:K:203:TYR:CD1	1:K:267:MET:CE	2.97	0.46
1:K:237:LEU:CD2	1:K:247:LEU:HD23	2.44	0.46
1:L:237:LEU:HD13	1:L:271:VAL:HG21	1.97	0.46
1:M:34:LYS:HB2	1:M:457:ASN:HB3	1.97	0.46
1:M:50:THR:HB	1:M:51:LYS:HA	1.97	0.46
1:M:411:VAL:HG21	1:M:494:LEU:HD13	1.97	0.46
1:B:158:VAL:HG13	1:B:396:VAL:HA	1.96	0.46
1:B:195:PHE:N	1:B:195:PHE:CD1	2.82	0.46
1:C:226:LYS:HB2	1:C:252:GLU:HG3	1.96	0.46
1:E:162:ILE:CD1	1:E:400:LEU:N	2.77	0.46
1:E:206:ASN:HB3	1:E:208:PRO:HD2	1.96	0.46
1:E:262:LEU:O	1:E:266:THR:HG23	2.15	0.46
1:F:204:PHE:CD1	1:F:273:VAL:O	2.68	0.46
1:F:227:ILE:HD12	1:F:258:ALA:HB1	1.96	0.46
1:F:278:ALA:HB2	1:F:289:LEU:CD1	2.45	0.46
1:I:314:LEU:O	1:I:317:LEU:HB2	2.14	0.46
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.96	0.46
1:K:242:LYS:HG3	1:L:257:GLU:C	2.40	0.46
1:L:203:TYR:CD1	1:L:267:MET:CE	2.99	0.46
2:M:1525:PO4:P	4:M:1527:ATP:O1G	2.73	0.46
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.96	0.46
1:N:233:MET:CE	1:N:249:ILE:HD11	2.42	0.46
1:N:314:LEU:O	1:N:317:LEU:HB2	2.15	0.46
1:A:353:ILE:HD13	1:A:366:GLN:CG	2.46	0.46
1:C:262:LEU:O	1:C:266:THR:HG23	2.15	0.46
1:D:204:PHE:CD1	1:D:273:VAL:O	2.68	0.46
1:D:207:LYS:N	1:D:208:PRO:HD2	2.29	0.46
1:G:207:LYS:CB	1:G:208:PRO:HD3	2.46	0.46
1:H:50:THR:HB	1:H:51:LYS:HA	1.97	0.46
1:I:144:ILE:HG23	1:I:403:THR:HG21	1.97	0.46
1:J:34:LYS:HB2	1:J:457:ASN:HB3	1.97	0.46
1:J:77:VAL:HG22	1:J:510:VAL:CG2	2.46	0.46
1:J:298:GLY:HA3	1:J:318:GLY:CA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:314:LEU:O	1:J:317:LEU:HB2	2.14	0.46
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.96	0.46
1:M:183:LEU:HA	1:M:382:GLY:HA3	1.97	0.46
1:M:214:GLU:CD	1:M:322:ARG:HE	2.22	0.46
1:N:183:LEU:HA	1:N:382:GLY:HA3	1.98	0.46
1:B:226:LYS:HB2	1:B:252:GLU:HG3	1.96	0.46
1:B:250:ILE:HD11	1:B:332:ILE:HD11	1.98	0.46
1:C:240:VAL:HG11	1:C:247:LEU:CB	2.43	0.46
1:C:250:ILE:HD11	1:C:332:ILE:HD11	1.98	0.46
1:C:308:GLU:CD	1:C:311:LYS:HZ3	2.23	0.46
1:D:250:ILE:HD11	1:D:332:ILE:HD11	1.98	0.46
1:D:311:LYS:HD3	1:D:311:LYS:HA	1.93	0.46
1:E:353:ILE:HD13	1:E:366:GLN:CG	2.46	0.46
1:G:226:LYS:HB2	1:G:252:GLU:HG3	1.96	0.46
1:H:411:VAL:HG21	1:H:494:LEU:HD13	1.97	0.46
1:I:50:THR:HB	1:I:51:LYS:HA	1.97	0.46
1:I:249:ILE:HB	1:I:275:ALA:CB	2.40	0.46
1:J:237:LEU:HD13	1:J:271:VAL:HG21	1.97	0.46
2:J:1525:PO4:P	4:J:1527:ATP:O1G	2.73	0.46
1:M:144:ILE:HG23	1:M:403:THR:HG21	1.97	0.46
1:M:221:LEU:HG	1:M:309:LEU:HD22	1.96	0.46
1:N:203:TYR:CD1	1:N:267:MET:CE	2.98	0.46
1:D:200:LEU:HD11	1:D:254:VAL:HA	1.94	0.46
1:D:226:LYS:HB2	1:D:252:GLU:HG3	1.96	0.46
1:F:209:GLU:H	1:F:209:GLU:CD	2.24	0.46
1:G:353:ILE:HD13	1:G:366:GLN:CG	2.46	0.46
1:H:237:LEU:HD13	1:H:271:VAL:HG21	1.97	0.46
1:L:314:LEU:O	1:L:317:LEU:HB2	2.14	0.46
1:B:111:MET:O	1:B:113:PRO:HD3	2.16	0.46
1:B:353:ILE:HD13	1:B:366:GLN:CG	2.46	0.46
1:E:111:MET:O	1:E:113:PRO:HD3	2.16	0.46
1:F:165:ALA:CA	1:F:187:LEU:HD21	2.46	0.46
1:F:353:ILE:HD13	1:F:366:GLN:HG2	1.97	0.46
1:H:144:ILE:HG23	1:H:403:THR:HG21	1.97	0.46
1:I:237:LEU:HD13	1:I:271:VAL:HG21	1.97	0.46
1:J:237:LEU:HA	1:J:247:LEU:HD22	1.97	0.46
1:J:411:VAL:HG21	1:J:494:LEU:HD13	1.97	0.46
1:M:220:ILE:HD12	1:M:296:THR:HG21	1.96	0.46
1:A:262:LEU:O	1:A:266:THR:HG23	2.15	0.46
1:B:204:PHE:CD1	1:B:273:VAL:O	2.68	0.46
1:B:223:ALA:CA	1:B:309:LEU:HD23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASP:OD1	1:C:329:THR:HG22	2.16	0.46
1:C:204:PHE:CD1	1:C:273:VAL:O	2.69	0.46
1:H:199:TYR:CB	1:H:325:ILE:HD11	2.41	0.46
1:K:203:TYR:CE2	1:K:267:MET:SD	3.08	0.46
1:L:40:LEU:HD21	1:L:55:SER:HB3	1.98	0.46
1:M:353:ILE:HD11	1:M:369:VAL:HG21	1.98	0.46
1:N:144:ILE:HG23	1:N:403:THR:HG21	1.97	0.46
1:A:250:ILE:HD11	1:A:332:ILE:HD11	1.98	0.46
1:B:240:VAL:CG1	1:B:247:LEU:HB2	2.42	0.46
1:C:353:ILE:HD13	1:C:366:GLN:CG	2.46	0.46
1:F:381:VAL:CG2	1:F:393:LYS:N	2.77	0.46
1:G:240:VAL:HG11	1:G:247:LEU:CB	2.43	0.46
1:K:233:MET:CE	1:K:249:ILE:HD11	2.42	0.46
1:L:50:THR:HB	1:L:51:LYS:HA	1.97	0.46
1:L:77:VAL:HG22	1:L:510:VAL:CG2	2.46	0.46
1:L:237:LEU:HA	1:L:247:LEU:HD22	1.97	0.46
1:M:40:LEU:HD21	1:M:55:SER:HB3	1.98	0.46
1:M:182:GLY:HA2	1:M:382:GLY:HA2	1.98	0.46
1:M:237:LEU:HD13	1:M:271:VAL:HG21	1.97	0.46
1:N:353:ILE:HD11	1:N:369:VAL:HG21	1.98	0.46
1:A:111:MET:O	1:A:113:PRO:HD3	2.16	0.46
1:A:209:GLU:H	1:A:209:GLU:CD	2.24	0.46
1:A:226:LYS:HB2	1:A:252:GLU:HG3	1.96	0.46
1:C:278:ALA:CB	1:C:289:LEU:HD12	2.46	0.46
1:D:278:ALA:HB2	1:D:289:LEU:HD12	1.98	0.46
1:F:220:ILE:CD1	1:F:332:ILE:HD13	2.33	0.46
1:F:353:ILE:HD13	1:F:366:GLN:CG	2.46	0.46
1:K:237:LEU:HA	1:K:247:LEU:HD22	1.97	0.46
1:N:169:VAL:HG21	1:N:175:ILE:HG13	1.98	0.46
1:N:298:GLY:HA3	1:N:318:GLY:CA	2.44	0.46
1:C:111:MET:O	1:C:113:PRO:HD3	2.16	0.46
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.16	0.46
1:H:77:VAL:HG22	1:H:510:VAL:CG2	2.46	0.46
1:H:169:VAL:HG21	1:H:175:ILE:HG13	1.98	0.46
1:I:203:TYR:CD1	1:I:267:MET:CE	2.98	0.46
1:J:29:VAL:O	1:J:35:GLY:HA2	2.16	0.46
1:J:50:THR:HB	1:J:51:LYS:HA	1.97	0.46
1:K:282:GLY:O	1:K:285:ARG:HB3	2.16	0.46
1:L:182:GLY:HA2	1:L:382:GLY:HA2	1.98	0.46
1:L:411:VAL:HG21	1:L:494:LEU:HD13	1.97	0.46
1:M:29:VAL:O	1:M:35:GLY:HA2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:77:VAL:HG22	1:N:510:VAL:CG2	2.46	0.46
1:A:150:ILE:HD11	1:A:493:ILE:HG23	1.97	0.45
1:B:521:VAL:O	1:C:41:ASP:HB3	2.16	0.45
1:C:289:LEU:HD23	1:C:289:LEU:O	2.17	0.45
1:D:353:ILE:HD13	1:D:366:GLN:CG	2.46	0.45
1:E:227:ILE:HD12	1:E:258:ALA:HB1	1.96	0.45
1:G:111:MET:O	1:G:113:PRO:HD3	2.16	0.45
1:I:169:VAL:HG21	1:I:175:ILE:HG13	1.98	0.45
1:I:227:ILE:CD1	1:I:233:MET:SD	2.92	0.45
1:K:40:LEU:HD21	1:K:55:SER:HB3	1.98	0.45
1:K:199:TYR:CB	1:K:325:ILE:HD11	2.39	0.45
1:L:34:LYS:HB2	1:L:457:ASN:HB3	1.97	0.45
1:L:183:LEU:HA	1:L:382:GLY:CA	2.45	0.45
1:B:207:LYS:HB2	1:B:207:LYS:HE2	1.62	0.45
1:C:278:ALA:HB2	1:C:289:LEU:HD12	1.98	0.45
1:D:521:VAL:O	1:E:41:ASP:HB3	2.16	0.45
1:E:250:ILE:HD11	1:E:332:ILE:HD11	1.98	0.45
1:F:278:ALA:HB2	1:F:289:LEU:HD12	1.99	0.45
1:G:223:ALA:CA	1:G:309:LEU:HD23	2.45	0.45
1:I:40:LEU:HD21	1:I:55:SER:HB3	1.98	0.45
1:I:227:ILE:HB	1:I:262:LEU:HD11	1.98	0.45
1:J:227:ILE:HB	1:J:262:LEU:HD11	1.98	0.45
1:L:227:ILE:HB	1:L:262:LEU:HD11	1.98	0.45
1:M:209:GLU:CD	1:M:209:GLU:H	2.24	0.45
1:N:40:LEU:HD21	1:N:55:SER:HB3	1.97	0.45
1:B:278:ALA:CB	1:B:289:LEU:HD12	2.46	0.45
1:D:111:MET:O	1:D:113:PRO:HD3	2.16	0.45
1:D:190:VAL:HG21	1:D:333:ILE:HG22	1.99	0.45
1:D:278:ALA:CB	1:D:289:LEU:HD12	2.46	0.45
2:D:1525:PO4:P	4:D:1527:ATP:PG	3.15	0.45
1:G:204:PHE:CD1	1:G:273:VAL:O	2.69	0.45
1:G:278:ALA:HB2	1:G:289:LEU:HD12	1.98	0.45
1:G:289:LEU:O	1:G:289:LEU:HD23	2.17	0.45
1:H:406:ALA:HB1	1:H:411:VAL:HG12	1.99	0.45
1:K:29:VAL:O	1:K:35:GLY:HA2	2.16	0.45
1:K:50:THR:HB	1:K:51:LYS:HA	1.97	0.45
1:K:77:VAL:HG22	1:K:510:VAL:CG2	2.46	0.45
1:K:183:LEU:HA	1:K:382:GLY:HA3	1.97	0.45
1:L:182:GLY:HA2	1:L:183:LEU:HA	1.57	0.45
1:M:77:VAL:HG22	1:M:510:VAL:CG2	2.46	0.45
1:N:182:GLY:HA2	1:N:382:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:VAL:O	1:D:41:ASP:HB3	2.16	0.45
1:D:402:ALA:HB1	1:D:496:PRO:HG2	1.99	0.45
1:E:200:LEU:HD11	1:E:254:VAL:HA	1.94	0.45
1:E:223:ALA:CA	1:E:309:LEU:HD23	2.45	0.45
1:F:200:LEU:HD11	1:F:254:VAL:CA	2.12	0.45
1:F:200:LEU:HD11	1:F:254:VAL:HA	1.94	0.45
1:F:272:LYS:CD	1:F:272:LYS:H	2.30	0.45
1:F:384:ALA:HA	1:F:385:THR:HA	1.68	0.45
1:G:219:PHE:HB3	1:G:317:LEU:HD11	1.98	0.45
1:H:353:ILE:HD11	1:H:369:VAL:HG21	1.98	0.45
1:I:29:VAL:O	1:I:35:GLY:HA2	2.16	0.45
1:K:227:ILE:HB	1:K:262:LEU:HD11	1.98	0.45
1:K:353:ILE:HD11	1:K:369:VAL:HG21	1.98	0.45
1:L:151:SER:HB3	1:L:399:ALA:HA	1.99	0.45
1:L:190:VAL:HG21	1:L:333:ILE:HG12	1.98	0.45
1:M:169:VAL:HG21	1:M:175:ILE:HG13	1.98	0.45
1:N:29:VAL:O	1:N:35:GLY:HA2	2.16	0.45
1:N:184:GLN:HG2	1:N:186:GLU:HG2	1.97	0.45
1:N:227:ILE:HB	1:N:262:LEU:HD11	1.97	0.45
1:N:237:LEU:HD13	1:N:271:VAL:HG21	1.97	0.45
1:A:289:LEU:HD23	1:A:289:LEU:O	2.17	0.45
1:A:521:VAL:O	1:B:41:ASP:HB3	2.16	0.45
1:B:249:ILE:HD11	1:B:262:LEU:HD22	1.87	0.45
1:E:272:LYS:H	1:E:272:LYS:CD	2.30	0.45
1:E:308:GLU:CD	1:E:311:LYS:HZ3	2.24	0.45
1:F:195:PHE:CD1	1:F:195:PHE:N	2.82	0.45
1:F:207:LYS:HB2	1:F:207:LYS:HE3	1.73	0.45
1:F:219:PHE:HB3	1:F:317:LEU:HD11	1.98	0.45
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.99	0.45
1:I:34:LYS:HB2	1:I:457:ASN:HB3	1.97	0.45
1:I:182:GLY:HA2	1:I:382:GLY:HA2	1.98	0.45
1:J:182:GLY:HA2	1:J:382:GLY:HA2	1.98	0.45
1:J:183:LEU:HA	1:J:382:GLY:HA3	1.97	0.45
1:K:151:SER:HB3	1:K:399:ALA:HA	1.99	0.45
1:K:406:ALA:HB1	1:K:411:VAL:HG12	1.98	0.45
1:K:411:VAL:HG21	1:K:494:LEU:HD13	1.97	0.45
1:L:233:MET:CE	1:L:249:ILE:HD11	2.44	0.45
1:C:402:ALA:HB1	1:C:496:PRO:HG2	1.99	0.45
1:D:289:LEU:HD23	1:D:289:LEU:O	2.17	0.45
1:E:402:ALA:HB1	1:E:496:PRO:HG2	1.99	0.45
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:LYS:HE2	1:H:207:LYS:HA	1.99	0.45
1:I:77:VAL:HG22	1:I:510:VAL:CG2	2.46	0.45
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.99	0.45
1:J:40:LEU:HD21	1:J:55:SER:HB3	1.98	0.45
1:J:209:GLU:H	1:J:209:GLU:CD	2.25	0.45
1:K:182:GLY:HA2	1:K:183:LEU:HA	1.63	0.45
1:L:29:VAL:O	1:L:35:GLY:HA2	2.16	0.45
1:L:353:ILE:HD11	1:L:369:VAL:HG21	1.98	0.45
1:A:240:VAL:HG11	1:A:247:LEU:CB	2.43	0.45
1:C:207:LYS:HE3	1:C:207:LYS:N	2.23	0.45
1:D:227:ILE:HD12	1:D:258:ALA:HB1	1.96	0.45
1:F:521:VAL:O	1:G:41:ASP:HB3	2.16	0.45
1:H:227:ILE:HB	1:H:262:LEU:HD11	1.98	0.45
1:J:151:SER:HB3	1:J:399:ALA:HA	1.99	0.45
1:J:169:VAL:HG21	1:J:175:ILE:HG13	1.99	0.45
1:M:151:SER:HB3	1:M:399:ALA:HA	1.99	0.45
1:M:203:TYR:CE2	1:M:267:MET:SD	3.09	0.45
1:A:278:ALA:CB	1:A:289:LEU:HD12	2.46	0.45
1:B:402:ALA:HB1	1:B:496:PRO:HG2	1.99	0.45
1:C:177:VAL:HG21	1:C:397:GLU:HG2	1.99	0.45
1:D:272:LYS:CD	1:D:272:LYS:H	2.30	0.45
1:E:278:ALA:CB	1:E:289:LEU:HD12	2.46	0.45
1:E:521:VAL:O	1:F:41:ASP:HB3	2.16	0.45
1:F:111:MET:O	1:F:113:PRO:HD3	2.16	0.45
1:G:272:LYS:H	1:G:272:LYS:CD	2.30	0.45
1:H:196:ASP:OD1	1:H:329:THR:HG22	2.17	0.45
1:J:196:ASP:HA	1:J:329:THR:HG22	1.98	0.45
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.99	0.45
1:L:406:ALA:HB1	1:L:411:VAL:HG12	1.98	0.45
1:A:240:VAL:CG1	1:A:247:LEU:HB2	2.42	0.45
1:B:278:ALA:HB2	1:B:289:LEU:HD12	1.98	0.45
2:F:1525:PO4:P	4:F:1527:ATP:PG	3.15	0.45
1:H:282:GLY:O	1:H:285:ARG:HB3	2.16	0.45
1:K:19:GLY:HA2	1:K:62:LEU:CD1	2.47	0.45
1:K:177:VAL:CG2	1:K:379:ILE:HB	2.42	0.45
1:K:182:GLY:HA2	1:K:382:GLY:HA2	1.98	0.45
1:L:183:LEU:H	1:L:183:LEU:CD2	2.22	0.45
1:M:227:ILE:HB	1:M:262:LEU:HD11	1.98	0.45
1:A:16:MET:SD	1:A:73:MET:HE1	2.57	0.45
1:D:308:GLU:CD	1:D:311:LYS:HZ3	2.24	0.45
1:E:16:MET:SD	1:E:73:MET:HE1	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ILE:HD11	1:F:332:ILE:HD11	1.98	0.45
1:G:384:ALA:HA	1:G:385:THR:HA	1.68	0.45
1:H:40:LEU:HD21	1:H:55:SER:HB3	1.98	0.45
1:H:517:THR:HG21	1:H:520:MET:HG3	1.99	0.45
1:I:183:LEU:HA	1:I:382:GLY:HA3	1.98	0.45
1:I:517:THR:HG21	1:I:520:MET:HG3	1.99	0.45
1:L:19:GLY:HA2	1:L:62:LEU:CD1	2.47	0.45
1:L:301:ILE:HD11	1:L:316:ASP:CG	2.42	0.45
1:M:223:ALA:HB2	1:M:309:LEU:CG	2.47	0.45
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.99	0.45
1:A:41:ASP:HB3	1:G:521:VAL:O	2.16	0.44
1:A:52:ASP:HB3	1:A:55:SER:H	1.82	0.44
1:C:219:PHE:HB3	1:C:317:LEU:HD11	1.98	0.44
1:C:461:GLU:HA	1:C:462:PRO:HD3	1.87	0.44
1:E:384:ALA:HA	1:E:385:THR:HA	1.68	0.44
1:G:278:ALA:CB	1:G:289:LEU:HD12	2.46	0.44
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.47	0.44
1:I:203:TYR:CE2	1:I:267:MET:SD	3.09	0.44
1:I:295:LEU:HD23	1:I:342:ILE:CD1	2.46	0.44
1:I:353:ILE:HD11	1:I:369:VAL:HG21	1.98	0.44
1:J:353:ILE:HD11	1:J:369:VAL:HG21	1.98	0.44
1:L:295:LEU:HD23	1:L:342:ILE:CD1	2.46	0.44
1:M:19:GLY:HA2	1:M:62:LEU:CD1	2.47	0.44
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.99	0.44
1:B:308:GLU:CD	1:B:311:LYS:HZ3	2.25	0.44
1:C:152:ALA:HB2	1:C:399:ALA:HB2	2.00	0.44
1:D:177:VAL:HG21	1:D:397:GLU:HG2	1.99	0.44
1:D:219:PHE:HB3	1:D:317:LEU:HD11	1.99	0.44
1:E:513:LEU:HB3	1:F:49:ILE:HD12	2.00	0.44
1:F:193:MET:HE2	1:F:296:THR:HG23	1.99	0.44
1:F:221:LEU:CD1	1:F:309:LEU:HD21	2.45	0.44
1:F:291:ASP:OD1	1:F:349:ILE:HD11	2.18	0.44
1:F:513:LEU:HB3	1:G:49:ILE:HD12	1.99	0.44
1:G:240:VAL:CG1	1:G:247:LEU:HB2	2.42	0.44
1:G:250:ILE:HD11	1:G:332:ILE:HD11	1.98	0.44
1:H:19:GLY:HA2	1:H:62:LEU:CD1	2.47	0.44
1:I:272:LYS:HD3	1:I:272:LYS:H	1.82	0.44
1:J:517:THR:HG21	1:J:520:MET:HG3	1.99	0.44
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.99	0.44
1:L:223:ALA:HB2	1:L:309:LEU:CG	2.47	0.44
1:A:278:ALA:HB2	1:A:289:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ALA:HB1	1:A:496:PRO:HG2	1.99	0.44
1:B:16:MET:SD	1:B:73:MET:HE1	2.58	0.44
1:B:152:ALA:HB2	1:B:399:ALA:HB2	2.00	0.44
1:B:291:ASP:OD1	1:B:349:ILE:HD11	2.18	0.44
1:B:311:LYS:HD3	1:B:311:LYS:HA	1.93	0.44
1:E:291:ASP:OD1	1:E:349:ILE:HD11	2.17	0.44
1:F:289:LEU:HD23	1:F:289:LEU:O	2.17	0.44
1:F:402:ALA:HB1	1:F:496:PRO:HG2	1.99	0.44
1:G:381:VAL:CG2	1:G:393:LYS:N	2.77	0.44
1:I:222:LEU:CD2	1:I:250:ILE:HD12	2.48	0.44
1:J:222:LEU:CD2	1:J:250:ILE:HD12	2.47	0.44
1:K:169:VAL:HG21	1:K:175:ILE:HG13	1.98	0.44
1:L:203:TYR:CE2	1:L:267:MET:SD	3.09	0.44
1:L:272:LYS:HD3	1:L:272:LYS:H	1.82	0.44
1:N:203:TYR:CE2	1:N:267:MET:SD	3.09	0.44
1:A:219:PHE:HB3	1:A:317:LEU:HD11	1.98	0.44
1:B:272:LYS:H	1:B:272:LYS:CD	2.30	0.44
1:D:513:LEU:HB3	1:E:49:ILE:HD12	2.00	0.44
1:F:16:MET:SD	1:F:73:MET:HE1	2.57	0.44
1:G:291:ASP:OD1	1:G:349:ILE:HD11	2.18	0.44
1:H:295:LEU:HD23	1:H:342:ILE:CD1	2.46	0.44
1:J:272:LYS:H	1:J:272:LYS:HD3	1.82	0.44
1:M:301:ILE:HD11	1:M:316:ASP:CG	2.43	0.44
1:N:19:GLY:HA2	1:N:62:LEU:CD1	2.47	0.44
1:N:223:ALA:HB2	1:N:309:LEU:CG	2.47	0.44
1:A:272:LYS:CD	1:A:272:LYS:H	2.30	0.44
1:B:194:GLN:HG2	1:B:329:THR:HG21	1.99	0.44
1:B:240:VAL:HG11	1:B:247:LEU:CB	2.43	0.44
1:B:289:LEU:O	1:B:289:LEU:HD23	2.17	0.44
1:C:16:MET:SD	1:C:73:MET:HE1	2.57	0.44
1:E:289:LEU:O	1:E:289:LEU:HD23	2.17	0.44
1:J:206:ASN:HB3	1:J:208:PRO:HD2	1.98	0.44
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.47	0.44
1:M:406:ALA:HB1	1:M:411:VAL:HG12	1.98	0.44
1:A:49:ILE:HD12	1:G:513:LEU:HB3	2.00	0.44
1:A:291:ASP:OD1	1:A:349:ILE:HD11	2.17	0.44
1:C:193:MET:SD	1:C:292:ILE:HG12	2.57	0.44
1:D:16:MET:SD	1:D:73:MET:HE1	2.58	0.44
1:E:193:MET:HE2	1:E:296:THR:HG23	1.99	0.44
1:H:29:VAL:O	1:H:35:GLY:HA2	2.16	0.44
1:H:218:PRO:HG3	1:H:323:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:ILE:HA	1:J:6:VAL:CG2	2.48	0.44
1:I:242:LYS:HZ1	1:J:257:GLU:CD	2.26	0.44
1:M:413:ALA:HB1	1:M:488:MET:HB2	2.00	0.44
1:N:215:LEU:HB3	1:N:246:PRO:HG2	2.00	0.44
1:N:517:THR:HG21	1:N:520:MET:HG3	1.99	0.44
1:A:193:MET:HE2	1:A:296:THR:HG23	1.99	0.44
1:C:200:LEU:HD11	1:C:254:VAL:CA	2.12	0.44
1:G:402:ALA:HB1	1:G:496:PRO:HG2	1.99	0.44
1:H:60:ILE:HA	1:I:6:VAL:CG2	2.48	0.44
1:H:215:LEU:HB3	1:H:246:PRO:HG2	2.00	0.44
1:H:224:ASP:HB2	1:H:303:GLU:H	1.82	0.44
1:J:60:ILE:HA	1:K:6:VAL:CG2	2.48	0.44
1:K:272:LYS:HD3	1:K:272:LYS:H	1.82	0.44
1:L:356:ALA:HB1	1:L:361:ASP:HB2	2.00	0.44
1:M:215:LEU:HB2	1:M:323:VAL:HG22	1.99	0.44
1:N:413:ALA:HB1	1:N:488:MET:HB2	2.00	0.44
1:A:221:LEU:CD1	1:A:309:LEU:HD21	2.45	0.44
1:C:272:LYS:CD	1:C:272:LYS:H	2.30	0.44
1:D:152:ALA:HB2	1:D:399:ALA:HB2	2.00	0.44
1:E:202:PRO:C	1:E:204:PHE:H	2.26	0.44
1:G:278:ALA:HA	1:G:279:PRO:HD3	1.72	0.44
1:I:182:GLY:HA2	1:I:183:LEU:HA	1.63	0.44
1:I:356:ALA:HB1	1:I:361:ASP:HB2	2.00	0.44
1:J:215:LEU:HB3	1:J:246:PRO:HG2	2.00	0.44
1:J:406:ALA:HB1	1:J:411:VAL:HG12	1.99	0.44
1:K:60:ILE:HA	1:L:6:VAL:CG2	2.48	0.44
1:K:215:LEU:HB3	1:K:246:PRO:HG2	2.00	0.44
1:K:356:ALA:HB1	1:K:361:ASP:HB2	2.00	0.44
1:L:215:LEU:HB3	1:L:246:PRO:HG2	2.00	0.44
1:L:240:VAL:HG21	1:L:317:LEU:HD22	2.00	0.44
1:N:272:LYS:HD3	1:N:272:LYS:H	1.82	0.44
1:A:152:ALA:HB2	1:A:399:ALA:HB2	2.00	0.44
1:A:513:LEU:HB3	1:B:49:ILE:HD12	2.00	0.44
1:B:52:ASP:HB2	1:B:55:SER:HB2	2.00	0.44
1:B:381:VAL:CG2	1:B:393:LYS:N	2.77	0.44
1:C:52:ASP:HB3	1:C:55:SER:H	1.82	0.44
1:E:219:PHE:HB3	1:E:317:LEU:HD11	1.98	0.44
1:E:278:ALA:HB2	1:E:289:LEU:HD12	1.98	0.44
1:F:52:ASP:HB2	1:F:55:SER:HB2	2.00	0.44
1:G:177:VAL:HG21	1:G:397:GLU:HG2	1.99	0.44
1:H:209:GLU:CD	1:H:209:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:237:LEU:HA	1:H:247:LEU:CD2	2.48	0.44
1:I:413:ALA:HB1	1:I:488:MET:HB2	2.00	0.44
1:J:62:LEU:HB2	1:J:68:ASN:HA	2.00	0.44
1:L:215:LEU:HB2	1:L:323:VAL:HG22	1.99	0.44
1:M:156:GLU:CD	1:M:160:LYS:HZ2	2.25	0.44
1:M:215:LEU:HB3	1:M:246:PRO:HG2	2.00	0.44
1:M:227:ILE:CD1	1:M:233:MET:SD	2.93	0.44
1:B:193:MET:HE2	1:B:296:THR:HG23	1.99	0.43
1:B:219:PHE:HB3	1:B:317:LEU:HD11	1.98	0.43
1:C:513:LEU:HB3	1:D:49:ILE:HD12	2.00	0.43
2:C:1525:PO4:P	4:C:1527:ATP:PG	3.16	0.43
1:F:278:ALA:CB	1:F:289:LEU:HD12	2.47	0.43
1:F:524:LEU:HG	1:F:525:PRO:N	2.33	0.43
1:G:201:SER:C	1:G:203:TYR:N	2.76	0.43
1:H:272:LYS:H	1:H:272:LYS:HD3	1.82	0.43
1:H:413:ALA:HB1	1:H:488:MET:HB2	2.00	0.43
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.47	0.43
1:J:242:LYS:HA	1:J:243:ALA:HA	1.12	0.43
1:J:356:ALA:HB1	1:J:361:ASP:HB2	2.00	0.43
1:K:218:PRO:HG3	1:K:323:VAL:HG13	1.99	0.43
1:L:242:LYS:HZ1	1:M:257:GLU:CD	2.26	0.43
1:N:218:PRO:HG3	1:N:323:VAL:HG13	2.00	0.43
1:B:513:LEU:HB3	1:C:49:ILE:HD12	2.00	0.43
1:C:291:ASP:OD1	1:C:349:ILE:HD11	2.18	0.43
1:D:52:ASP:HB2	1:D:55:SER:HB2	2.00	0.43
1:E:152:ALA:HB2	1:E:399:ALA:HB2	2.00	0.43
1:E:524:LEU:HG	1:E:525:PRO:N	2.33	0.43
1:G:16:MET:SD	1:G:73:MET:HE1	2.57	0.43
1:K:240:VAL:HG21	1:K:317:LEU:HD22	2.00	0.43
1:K:517:THR:HG21	1:K:520:MET:HG3	1.99	0.43
1:L:190:VAL:HG21	1:L:333:ILE:HG23	1.98	0.43
1:M:240:VAL:HG21	1:M:317:LEU:HD22	2.00	0.43
1:D:278:ALA:HB2	1:D:289:LEU:CG	2.49	0.43
1:D:291:ASP:OD1	1:D:349:ILE:HD11	2.17	0.43
1:F:177:VAL:HG21	1:F:397:GLU:HG2	1.99	0.43
1:F:240:VAL:CG1	1:F:247:LEU:HB2	2.42	0.43
1:G:220:ILE:CD1	1:G:296:THR:HG21	2.47	0.43
1:H:62:LEU:HB2	1:H:68:ASN:HA	2.00	0.43
1:H:240:VAL:HG21	1:H:317:LEU:CD2	2.49	0.43
1:H:356:ALA:HB1	1:H:361:ASP:HB2	2.00	0.43
1:I:215:LEU:HB3	1:I:246:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:PRO:HG3	1:I:323:VAL:HG13	2.00	0.43
1:I:237:LEU:HA	1:I:247:LEU:CD2	2.49	0.43
1:K:36:ARG:C	1:L:518:GLU:CB	2.92	0.43
1:L:218:PRO:HG3	1:L:323:VAL:HG13	2.00	0.43
1:L:413:ALA:HB1	1:L:488:MET:HB2	2.00	0.43
1:M:356:ALA:HB1	1:M:361:ASP:HB2	2.00	0.43
1:A:177:VAL:HA	1:A:379:ILE:O	2.19	0.43
1:A:240:VAL:HG13	1:A:245:LYS:O	2.19	0.43
1:A:278:ALA:HB2	1:A:289:LEU:CG	2.49	0.43
1:D:193:MET:HE2	1:D:296:THR:HG23	1.99	0.43
1:D:524:LEU:HG	1:D:525:PRO:N	2.33	0.43
1:I:19:GLY:HA2	1:I:62:LEU:CD1	2.47	0.43
1:I:62:LEU:HB2	1:I:68:ASN:HA	2.00	0.43
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.47	0.43
1:K:62:LEU:HB2	1:K:68:ASN:HA	2.00	0.43
1:K:77:VAL:HG22	1:K:510:VAL:CB	2.49	0.43
1:K:240:VAL:HG21	1:K:317:LEU:CD2	2.49	0.43
1:L:240:VAL:HG21	1:L:317:LEU:CD2	2.49	0.43
1:M:36:ARG:C	1:N:518:GLU:CB	2.92	0.43
1:M:60:ILE:HA	1:N:6:VAL:CG2	2.48	0.43
1:M:240:VAL:HG21	1:M:317:LEU:CD2	2.49	0.43
1:N:227:ILE:CD1	1:N:233:MET:SD	2.93	0.43
1:N:301:ILE:HD11	1:N:312:ALA:CB	2.32	0.43
1:A:150:ILE:CD1	1:A:493:ILE:CA	2.74	0.43
1:C:311:LYS:HD3	1:C:311:LYS:HA	1.93	0.43
1:D:177:VAL:HA	1:D:379:ILE:O	2.18	0.43
1:E:214:GLU:CD	1:E:322:ARG:HE	2.26	0.43
1:E:240:VAL:HG13	1:E:245:LYS:O	2.18	0.43
1:F:150:ILE:CD1	1:F:493:ILE:CG2	2.91	0.43
1:G:152:ALA:HB2	1:G:399:ALA:HB2	2.00	0.43
1:G:177:VAL:HA	1:G:379:ILE:O	2.19	0.43
1:G:240:VAL:HG13	1:G:245:LYS:O	2.18	0.43
1:H:36:ARG:C	1:I:518:GLU:CB	2.92	0.43
1:I:233:MET:CE	1:I:249:ILE:HD11	2.40	0.43
1:J:77:VAL:HG22	1:J:510:VAL:CB	2.49	0.43
1:J:240:VAL:HG21	1:J:317:LEU:CD2	2.49	0.43
1:K:169:VAL:HG21	1:K:175:ILE:CG1	2.49	0.43
1:K:223:ALA:HB2	1:K:309:LEU:CG	2.48	0.43
1:L:60:ILE:HA	1:M:6:VAL:CG2	2.48	0.43
1:N:99:ILE:CG2	1:N:120:ILE:HD13	2.49	0.43
1:N:356:ALA:HB1	1:N:361:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG13	1:B:245:LYS:O	2.18	0.43
1:B:381:VAL:HG11	1:B:393:LYS:HB2	2.00	0.43
1:C:197:ARG:HG3	1:C:198:GLY:O	2.18	0.43
1:C:223:ALA:CA	1:C:309:LEU:HD23	2.45	0.43
1:C:524:LEU:HG	1:C:525:PRO:N	2.33	0.43
1:F:240:VAL:HG13	1:F:245:LYS:O	2.18	0.43
1:F:381:VAL:HG11	1:F:393:LYS:HB2	2.00	0.43
1:G:221:LEU:CD1	1:G:309:LEU:HD21	2.45	0.43
2:G:1525:PO4:P	4:G:1527:ATP:PG	3.16	0.43
1:H:151:SER:HB3	1:H:399:ALA:HA	1.99	0.43
1:H:223:ALA:HB2	1:H:309:LEU:CG	2.48	0.43
1:I:36:ARG:C	1:J:518:GLU:CB	2.92	0.43
1:I:181:THR:HG22	1:I:182:GLY:O	2.19	0.43
1:J:36:ARG:C	1:K:518:GLU:CB	2.92	0.43
1:J:240:VAL:HG21	1:J:317:LEU:HD22	2.00	0.43
1:L:77:VAL:HG22	1:L:510:VAL:CB	2.49	0.43
1:M:99:ILE:CG2	1:M:120:ILE:HD13	2.49	0.43
1:M:229:ASN:HB3	1:M:231:ARG:HG3	2.01	0.43
1:M:272:LYS:H	1:M:272:LYS:HD3	1.82	0.43
1:M:517:THR:HG21	1:M:520:MET:HG3	2.00	0.43
1:N:240:VAL:HG21	1:N:317:LEU:HD22	2.00	0.43
2:A:1525:PO4:P	4:A:1527:ATP:PG	3.16	0.43
1:B:236:VAL:HG13	1:B:317:LEU:HD13	2.01	0.43
1:B:524:LEU:HG	1:B:525:PRO:N	2.33	0.43
1:E:177:VAL:HA	1:E:379:ILE:O	2.19	0.43
1:E:191:GLU:H	1:E:334:ASP:HA	1.84	0.43
1:G:308:GLU:CD	1:G:311:LYS:HZ3	2.27	0.43
1:I:169:VAL:HG21	1:I:175:ILE:CG1	2.49	0.43
1:J:218:PRO:HG3	1:J:323:VAL:HG13	2.00	0.43
1:J:413:ALA:HB1	1:J:488:MET:HB2	2.00	0.43
1:K:237:LEU:HA	1:K:247:LEU:CD2	2.48	0.43
1:K:301:ILE:HD11	1:K:316:ASP:CG	2.43	0.43
1:K:413:ALA:HB1	1:K:488:MET:HB2	2.00	0.43
1:L:242:LYS:HG3	1:M:257:GLU:HB2	2.00	0.43
1:M:321:LYS:HZ3	1:M:334:ASP:CG	2.27	0.43
1:N:169:VAL:HG21	1:N:175:ILE:CG1	2.49	0.43
1:A:177:VAL:HG21	1:A:397:GLU:HG2	1.99	0.43
1:A:200:LEU:HD13	1:A:259:LEU:HB2	2.00	0.43
1:A:236:VAL:HG13	1:A:317:LEU:HD13	2.01	0.43
1:C:144:ILE:CG2	1:C:163:ALA:HA	2.49	0.43
1:D:240:VAL:HG13	1:D:245:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:VAL:CG2	1:N:60:ILE:HA	2.48	0.43
1:J:179:ASP:HB3	1:J:383:ALA:HB2	2.01	0.43
1:L:517:THR:HG21	1:L:520:MET:HG3	1.99	0.43
1:M:222:LEU:CD2	1:M:250:ILE:HD12	2.48	0.43
1:N:62:LEU:HB2	1:N:68:ASN:HA	2.00	0.43
1:N:295:LEU:HD23	1:N:342:ILE:CD1	2.46	0.43
1:A:381:VAL:CG2	1:A:393:LYS:N	2.77	0.43
1:A:521:VAL:HG11	1:B:59:GLU:CG	2.49	0.43
1:B:34:LYS:NZ	1:B:483:GLU:OE2	2.52	0.43
1:B:144:ILE:CG2	1:B:163:ALA:HA	2.49	0.43
1:C:236:VAL:HG13	1:C:317:LEU:HD13	2.01	0.43
1:C:240:VAL:HG13	1:C:245:LYS:O	2.18	0.43
1:C:278:ALA:HB2	1:C:289:LEU:CG	2.49	0.43
1:E:144:ILE:CG2	1:E:163:ALA:HA	2.49	0.43
1:E:513:LEU:O	1:F:49:ILE:HD13	2.19	0.43
1:F:152:ALA:HB2	1:F:399:ALA:HB2	2.00	0.43
1:G:52:ASP:HB3	1:G:55:SER:H	1.82	0.43
1:G:381:VAL:HG11	1:G:393:LYS:HB2	2.00	0.43
1:H:227:ILE:CD1	1:H:233:MET:SD	2.92	0.43
1:I:77:VAL:HG22	1:I:510:VAL:CB	2.49	0.43
1:I:240:VAL:HG21	1:I:317:LEU:CD2	2.49	0.43
1:I:240:VAL:HG21	1:I:317:LEU:HD22	2.00	0.43
1:J:196:ASP:CG	1:J:329:THR:HG22	2.44	0.43
1:L:99:ILE:CG2	1:L:120:ILE:HD13	2.49	0.43
1:M:237:LEU:HA	1:M:247:LEU:CD2	2.48	0.43
1:N:282:GLY:O	1:N:285:ARG:HB3	2.19	0.43
1:N:301:ILE:HD11	1:N:316:ASP:CG	2.44	0.43
1:A:34:LYS:NZ	1:A:483:GLU:OE2	2.52	0.43
1:A:513:LEU:O	1:B:49:ILE:HD13	2.19	0.43
1:A:524:LEU:HG	1:A:525:PRO:N	2.33	0.43
1:B:200:LEU:HD13	1:B:259:LEU:HB2	2.00	0.43
1:C:191:GLU:H	1:C:334:ASP:HA	1.84	0.43
1:C:381:VAL:HG11	1:C:393:LYS:HB2	2.00	0.43
1:D:236:VAL:HG13	1:D:317:LEU:HD13	2.01	0.43
1:E:177:VAL:HG21	1:E:397:GLU:HG2	1.99	0.43
1:F:165:ALA:HA	1:F:187:LEU:HD21	2.01	0.43
1:F:177:VAL:HA	1:F:379:ILE:O	2.19	0.43
1:F:236:VAL:HG13	1:F:317:LEU:HD13	2.01	0.43
1:F:513:LEU:O	1:G:49:ILE:HD13	2.19	0.43
1:F:521:VAL:HG11	1:G:59:GLU:CG	2.49	0.43
1:G:236:VAL:HG13	1:G:317:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:524:LEU:HG	1:G:525:LEU:N	2.34	0.43
1:H:518:GLU:CB	1:H:519:CYS:N	2.74	0.43
1:J:237:LEU:HA	1:J:247:LEU:CD2	2.49	0.43
1:K:224:ASP:HB2	1:K:303:GLU:H	1.82	0.43
1:K:301:ILE:HG23	1:K:307:MET:HB2	2.01	0.43
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.47	0.43
1:L:237:LEU:HA	1:L:247:LEU:CD2	2.48	0.43
1:B:150:ILE:CD1	1:B:493:ILE:CG2	2.91	0.42
1:B:191:GLU:H	1:B:334:ASP:HA	1.84	0.42
1:B:206:ASN:CB	1:B:208:PRO:HD2	2.42	0.42
1:B:278:ALA:HB2	1:B:289:LEU:CG	2.49	0.42
2:B:1525:PO4:P	4:B:1527:ATP:PG	3.17	0.42
1:E:200:LEU:HD13	1:E:259:LEU:HB2	2.00	0.42
1:E:236:VAL:HG13	1:E:317:LEU:HD13	2.01	0.42
1:E:521:VAL:HG11	1:F:59:GLU:CG	2.49	0.42
2:E:1525:PO4:P	4:E:1527:ATP:PG	3.16	0.42
1:F:34:LYS:NZ	1:F:483:GLU:OE2	2.52	0.42
1:H:222:LEU:CD2	1:H:250:ILE:HD12	2.48	0.42
1:H:240:VAL:HG21	1:H:317:LEU:HD22	2.00	0.42
1:H:518:GLU:CB	1:N:36:ARG:C	2.92	0.42
1:I:298:GLY:CA	1:I:318:GLY:HA3	2.49	0.42
1:J:99:ILE:CG2	1:J:120:ILE:HD13	2.49	0.42
1:L:62:LEU:HB2	1:L:68:ASN:HA	2.00	0.42
1:M:218:PRO:HG3	1:M:323:VAL:HG13	2.00	0.42
1:M:282:GLY:O	1:M:285:ARG:HB3	2.19	0.42
1:A:220:ILE:CD1	1:A:296:THR:HG21	2.47	0.42
1:B:223:ALA:HB3	1:B:251:ALA:HA	2.02	0.42
1:C:223:ALA:HB3	1:C:251:ALA:HA	2.02	0.42
1:E:207:LYS:HB2	1:E:208:PRO:HD3	2.01	0.42
1:E:381:VAL:HG11	1:E:393:LYS:HB2	2.00	0.42
1:F:200:LEU:HD13	1:F:259:LEU:HB2	2.00	0.42
1:F:249:ILE:HD11	1:F:262:LEU:HD22	1.87	0.42
1:G:34:LYS:NZ	1:G:483:GLU:OE2	2.52	0.42
1:G:190:VAL:HB	1:G:334:ASP:HB2	2.01	0.42
1:H:182:GLY:HA2	1:H:183:LEU:HA	1.66	0.42
1:H:321:LYS:HZ3	1:H:334:ASP:CG	2.27	0.42
1:I:278:ALA:HA	1:I:279:PRO:HD3	1.87	0.42
1:J:169:VAL:HG21	1:J:175:ILE:CG1	2.49	0.42
1:J:242:LYS:HZ1	1:K:257:GLU:CD	2.26	0.42
1:L:190:VAL:HG21	1:L:333:ILE:CG1	2.49	0.42
1:L:227:ILE:HG22	1:L:262:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:LEU:HB2	1:M:68:ASN:HA	2.00	0.42
1:M:206:ASN:CG	1:M:207:LYS:H	2.25	0.42
1:N:182:GLY:HA2	1:N:183:LEU:HA	1.63	0.42
1:N:240:VAL:HG21	1:N:317:LEU:CD2	2.49	0.42
1:A:115:ASP:CG	1:A:118:ARG:HH21	2.27	0.42
1:B:214:GLU:CD	1:B:322:ARG:HE	2.26	0.42
1:C:214:GLU:CD	1:C:322:ARG:HE	2.26	0.42
1:C:278:ALA:HB2	1:C:289:LEU:HG	2.01	0.42
1:C:521:VAL:HG11	1:D:59:GLU:CG	2.49	0.42
1:D:200:LEU:HD13	1:D:259:LEU:HB2	2.00	0.42
1:E:209:GLU:CD	1:E:209:GLU:H	2.26	0.42
1:E:221:LEU:CD1	1:E:309:LEU:HD21	2.45	0.42
1:F:223:ALA:HB3	1:F:251:ALA:HA	2.02	0.42
1:G:52:ASP:HB2	1:G:55:SER:HB2	2.01	0.42
1:G:278:ALA:HB2	1:G:289:LEU:CG	2.49	0.42
1:H:169:VAL:HG21	1:H:175:ILE:CG1	2.49	0.42
1:I:223:ALA:HB2	1:I:309:LEU:CG	2.48	0.42
1:J:37:ASN:HB2	1:K:516:THR:O	2.20	0.42
1:J:223:ALA:HB2	1:J:309:LEU:CG	2.49	0.42
1:L:222:LEU:CD2	1:L:250:ILE:HD12	2.48	0.42
1:M:225:LYS:CA	1:M:303:GLU:HB2	2.50	0.42
1:A:52:ASP:HB2	1:A:55:SER:HB2	2.01	0.42
1:A:190:VAL:HB	1:A:334:ASP:HB2	2.01	0.42
1:A:214:GLU:CD	1:A:322:ARG:HE	2.26	0.42
1:A:381:VAL:HG11	1:A:393:LYS:HB2	2.00	0.42
1:B:521:VAL:HG11	1:C:59:GLU:CG	2.49	0.42
1:D:521:VAL:HG11	1:E:59:GLU:CG	2.49	0.42
1:E:52:ASP:HB2	1:E:55:SER:HB2	2.01	0.42
1:E:223:ALA:HB3	1:E:251:ALA:HA	2.02	0.42
1:E:278:ALA:HB2	1:E:289:LEU:CG	2.49	0.42
1:F:190:VAL:HB	1:F:334:ASP:HB2	2.01	0.42
1:F:278:ALA:HB2	1:F:289:LEU:CG	2.49	0.42
1:G:144:ILE:CG2	1:G:163:ALA:HA	2.49	0.42
1:G:161:LEU:HD21	1:G:185:ASP:HB3	2.00	0.42
1:G:214:GLU:CD	1:G:322:ARG:HE	2.26	0.42
1:I:99:ILE:CG2	1:I:120:ILE:HD13	2.49	0.42
1:I:301:ILE:HG23	1:I:307:MET:HB2	2.01	0.42
1:K:37:ASN:HB2	1:L:516:THR:O	2.20	0.42
1:L:36:ARG:C	1:M:518:GLU:CB	2.92	0.42
1:M:295:LEU:HD13	1:M:335:GLY:HA3	2.02	0.42
1:N:222:LEU:CD2	1:N:250:ILE:HD12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HB3	1:A:246:PRO:HG2	2.02	0.42
1:C:286:LYS:HD3	1:C:304:GLU:HA	2.01	0.42
1:D:278:ALA:HB2	1:D:289:LEU:HG	2.01	0.42
1:D:513:LEU:O	1:E:49:ILE:HD13	2.19	0.42
1:F:214:GLU:CD	1:F:322:ARG:HE	2.26	0.42
1:G:249:ILE:HD11	1:G:262:LEU:HD22	1.87	0.42
1:H:193:MET:HG2	1:H:372:LEU:HA	2.02	0.42
1:I:151:SER:HB3	1:I:399:ALA:HA	1.99	0.42
1:J:239:ALA:CB	1:J:314:LEU:HB3	2.49	0.42
1:K:99:ILE:CG2	1:K:120:ILE:HD13	2.49	0.42
1:L:227:ILE:CD1	1:L:233:MET:SD	2.93	0.42
1:M:169:VAL:HG21	1:M:175:ILE:CG1	2.49	0.42
1:M:298:GLY:CA	1:M:318:GLY:HA3	2.49	0.42
1:N:237:LEU:HA	1:N:247:LEU:CD2	2.49	0.42
1:N:295:LEU:HD13	1:N:335:GLY:HA3	2.02	0.42
1:A:49:ILE:HD13	1:G:513:LEU:O	2.19	0.42
1:A:59:GLU:CG	1:G:521:VAL:HG11	2.49	0.42
1:A:144:ILE:CG2	1:A:163:ALA:HA	2.49	0.42
1:A:191:GLU:H	1:A:334:ASP:HA	1.84	0.42
1:A:223:ALA:HB3	1:A:251:ALA:HA	2.02	0.42
1:B:513:LEU:O	1:C:49:ILE:HD13	2.19	0.42
1:C:52:ASP:HB2	1:C:55:SER:HB2	2.01	0.42
1:D:34:LYS:NZ	1:D:483:GLU:OE2	2.52	0.42
1:D:117:LYS:HZ2	1:D:121:ASP:CG	2.28	0.42
1:D:271:VAL:O	1:D:273:VAL:HG23	2.20	0.42
1:D:381:VAL:CG2	1:D:393:LYS:N	2.77	0.42
1:E:207:LYS:N	1:E:208:PRO:HD2	2.34	0.42
1:E:271:VAL:O	1:E:273:VAL:HG23	2.20	0.42
1:G:223:ALA:HB3	1:G:251:ALA:HA	2.02	0.42
1:H:295:LEU:HD13	1:H:335:GLY:HA3	2.02	0.42
1:I:37:ASN:HB2	1:J:516:THR:O	2.20	0.42
1:I:227:ILE:H	1:I:254:VAL:HG22	1.85	0.42
1:J:295:LEU:HD23	1:J:342:ILE:CD1	2.46	0.42
1:K:295:LEU:HD13	1:K:335:GLY:HA3	2.02	0.42
1:L:225:LYS:CA	1:L:303:GLU:HB2	2.50	0.42
1:L:295:LEU:HD13	1:L:335:GLY:HA3	2.02	0.42
1:M:227:ILE:HG22	1:M:262:LEU:HD21	2.01	0.42
1:M:446:ALA:O	1:M:450:PRO:HD2	2.20	0.42
1:N:193:MET:HG2	1:N:372:LEU:HA	2.02	0.42
1:B:278:ALA:HB2	1:B:289:LEU:HG	2.01	0.42
1:B:286:LYS:HD3	1:B:304:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLU:CD	1:B:501:ARG:HH22	2.28	0.42
1:C:34:LYS:NZ	1:C:483:GLU:OE2	2.52	0.42
1:D:144:ILE:CG2	1:D:163:ALA:HA	2.49	0.42
1:D:190:VAL:HB	1:D:334:ASP:CA	2.50	0.42
1:D:223:ALA:HB3	1:D:251:ALA:HA	2.02	0.42
1:D:381:VAL:HG11	1:D:393:LYS:HB2	2.00	0.42
1:D:384:ALA:HA	1:D:385:THR:HA	1.68	0.42
1:F:191:GLU:H	1:F:334:ASP:HA	1.84	0.42
1:G:150:ILE:HD11	1:G:493:ILE:HG23	1.97	0.42
1:G:191:GLU:H	1:G:334:ASP:HA	1.84	0.42
1:G:215:LEU:HB3	1:G:246:PRO:HG2	2.02	0.42
1:H:82:ASN:HA	1:H:89:THR:HG22	2.02	0.42
1:H:227:ILE:H	1:H:254:VAL:HG22	1.85	0.42
1:I:295:LEU:HD13	1:I:335:GLY:HA3	2.02	0.42
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.47	0.42
1:L:82:ASN:HA	1:L:89:THR:HG22	2.02	0.42
1:L:183:LEU:HA	1:L:382:GLY:HA3	2.01	0.42
1:M:82:ASN:HA	1:M:89:THR:HG22	2.02	0.42
1:N:239:ALA:CB	1:N:314:LEU:HB3	2.49	0.42
1:N:301:ILE:HG23	1:N:307:MET:HB2	2.01	0.42
1:N:406:ALA:HB1	1:N:411:VAL:CG1	2.49	0.42
1:N:446:ALA:O	1:N:450:PRO:HD2	2.20	0.42
1:B:166:MET:HE3	1:B:175:ILE:HD12	2.02	0.42
1:C:177:VAL:HA	1:C:379:ILE:O	2.19	0.42
1:C:271:VAL:O	1:C:273:VAL:HG23	2.20	0.42
1:E:34:LYS:NZ	1:E:483:GLU:OE2	2.52	0.42
1:F:215:LEU:HB3	1:F:246:PRO:HG2	2.02	0.42
1:F:286:LYS:HD3	1:F:304:GLU:HA	2.01	0.42
1:G:165:ALA:HB2	1:G:187:LEU:HD13	2.02	0.42
1:H:225:LYS:CA	1:H:303:GLU:HB2	2.50	0.42
1:H:239:ALA:CB	1:H:314:LEU:HB3	2.49	0.42
1:H:446:ALA:O	1:H:450:PRO:HD2	2.20	0.42
1:I:82:ASN:HA	1:I:89:THR:HG22	2.02	0.42
1:I:301:ILE:HD11	1:I:316:ASP:CG	2.44	0.42
1:I:406:ALA:HB1	1:I:411:VAL:CG1	2.50	0.42
1:I:406:ALA:HB1	1:I:411:VAL:HG12	2.02	0.42
1:J:82:ASN:HA	1:J:89:THR:HG22	2.02	0.42
1:J:295:LEU:HD13	1:J:335:GLY:HA3	2.02	0.42
1:K:222:LEU:CD2	1:K:250:ILE:HD12	2.49	0.42
1:L:282:GLY:O	1:L:285:ARG:HB3	2.19	0.42
1:M:8:PHE:HA	1:M:9:GLY:HA3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:77:VAL:HG22	1:M:510:VAL:CB	2.49	0.42
1:N:151:SER:HB3	1:N:399:ALA:HA	1.99	0.42
1:N:206:ASN:O	1:N:208:PRO:N	2.52	0.42
1:B:177:VAL:HA	1:B:379:ILE:O	2.19	0.42
1:C:270:ILE:O	1:C:271:VAL:HB	2.20	0.42
1:E:52:ASP:HB3	1:E:55:SER:H	1.83	0.42
1:F:117:LYS:HZ2	1:F:121:ASP:CG	2.28	0.42
1:F:166:MET:HE3	1:F:175:ILE:HD12	2.02	0.42
1:F:271:VAL:O	1:F:273:VAL:HG23	2.20	0.42
1:H:227:ILE:HG22	1:H:262:LEU:HD21	2.02	0.42
1:H:298:GLY:CA	1:H:318:GLY:HA3	2.49	0.42
1:I:149:THR:HG22	1:I:154:SER:HB3	2.02	0.42
1:J:227:ILE:HG22	1:J:262:LEU:HD21	2.02	0.42
1:K:82:ASN:HA	1:K:89:THR:HG22	2.02	0.42
1:K:150:ILE:HD12	1:K:494:LEU:H	1.85	0.42
1:L:239:ALA:CB	1:L:314:LEU:HB3	2.49	0.42
1:M:240:VAL:HB	1:M:247:LEU:HD22	2.02	0.42
1:N:82:ASN:HA	1:N:89:THR:HG22	2.02	0.42
1:N:406:ALA:HB1	1:N:411:VAL:HG12	2.02	0.42
1:A:165:ALA:HB2	1:A:187:LEU:HD13	2.02	0.42
1:B:215:LEU:HB3	1:B:246:PRO:HG2	2.02	0.42
1:D:166:MET:HE3	1:D:175:ILE:HD12	2.02	0.42
1:D:209:GLU:H	1:D:209:GLU:CD	2.27	0.42
1:D:270:ILE:O	1:D:271:VAL:HB	2.20	0.42
1:D:286:LYS:HD3	1:D:304:GLU:HA	2.01	0.42
1:E:190:VAL:HB	1:E:334:ASP:HB2	2.01	0.42
1:H:77:VAL:HG22	1:H:510:VAL:CB	2.49	0.42
1:H:99:ILE:CG2	1:H:120:ILE:HD13	2.49	0.42
1:H:149:THR:HG22	1:H:154:SER:HB3	2.02	0.42
1:H:301:ILE:HD11	1:H:316:ASP:CG	2.45	0.42
1:I:227:ILE:HG22	1:I:262:LEU:HD21	2.02	0.42
1:J:240:VAL:HB	1:J:247:LEU:HD22	2.02	0.42
1:K:227:ILE:H	1:K:254:VAL:HG22	1.85	0.42
1:K:227:ILE:HG22	1:K:262:LEU:HD21	2.02	0.42
1:K:309:LEU:HD23	1:K:309:LEU:HA	1.81	0.42
1:L:37:ASN:HB2	1:M:516:THR:O	2.20	0.42
1:L:190:VAL:HG23	1:L:191:GLU:O	2.20	0.42
1:M:153:ASN:N	1:M:154:SER:CA	2.82	0.42
1:M:301:ILE:HG23	1:M:307:MET:HB2	2.01	0.42
1:M:417:VAL:HG11	1:M:477:GLY:HA3	2.02	0.42
1:N:204:PHE:CA	1:N:207:LYS:HE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:227:ILE:HG22	1:N:262:LEU:HD21	2.02	0.42
1:B:200:LEU:HD11	1:B:254:VAL:CA	2.12	0.41
1:C:513:LEU:O	1:D:49:ILE:HD13	2.19	0.41
1:E:150:ILE:HD11	1:E:493:ILE:HG23	1.97	0.41
1:E:215:LEU:HB3	1:E:246:PRO:HG2	2.02	0.41
1:F:165:ALA:HB2	1:F:187:LEU:CD1	2.50	0.41
1:F:200:LEU:HD11	1:F:254:VAL:CG2	2.20	0.41
1:H:37:ASN:HB2	1:I:516:THR:O	2.20	0.41
1:I:161:LEU:HD22	1:I:379:ILE:HG23	2.02	0.41
1:J:182:GLY:HA2	1:J:183:LEU:HA	1.63	0.41
1:K:298:GLY:CA	1:K:318:GLY:HA3	2.50	0.41
1:L:161:LEU:HD22	1:L:379:ILE:HG23	2.02	0.41
1:M:31:LEU:HB3	1:M:90:THR:HG21	2.03	0.41
1:A:117:LYS:HZ2	1:A:121:ASP:CG	2.28	0.41
1:A:193:MET:CE	1:A:292:ILE:HG23	2.51	0.41
1:C:200:LEU:HD13	1:C:259:LEU:HB2	2.00	0.41
1:F:144:ILE:CG2	1:F:163:ALA:HA	2.49	0.41
1:G:286:LYS:HD3	1:G:304:GLU:HA	2.01	0.41
1:I:240:VAL:HB	1:I:247:LEU:HD22	2.02	0.41
1:L:417:VAL:HG11	1:L:477:GLY:HA3	2.02	0.41
1:A:166:MET:HE3	1:A:175:ILE:HD12	2.02	0.41
1:A:270:ILE:O	1:A:271:VAL:HB	2.20	0.41
1:A:278:ALA:HB2	1:A:289:LEU:HG	2.02	0.41
1:A:286:LYS:HD3	1:A:304:GLU:HA	2.01	0.41
1:B:190:VAL:HB	1:B:334:ASP:HB2	2.01	0.41
1:B:270:ILE:O	1:B:271:VAL:HB	2.20	0.41
1:C:117:LYS:HZ2	1:C:121:ASP:CG	2.28	0.41
1:C:254:VAL:HG12	1:C:259:LEU:HB2	2.03	0.41
1:C:381:VAL:CG2	1:C:393:LYS:N	2.77	0.41
1:D:193:MET:CE	1:D:292:ILE:HG23	2.51	0.41
1:D:214:GLU:CD	1:D:322:ARG:HE	2.26	0.41
1:E:193:MET:CE	1:E:292:ILE:HG23	2.50	0.41
1:E:270:ILE:O	1:E:271:VAL:HB	2.20	0.41
1:E:286:LYS:HD3	1:E:304:GLU:HA	2.01	0.41
1:G:409:GLU:CD	1:G:501:ARG:HH22	2.28	0.41
1:H:182:GLY:HA2	1:H:382:GLY:HA2	2.02	0.41
1:H:242:LYS:HA	1:H:243:ALA:HA	1.16	0.41
1:I:239:ALA:CB	1:I:314:LEU:HB3	2.49	0.41
1:I:417:VAL:HG11	1:I:477:GLY:HA3	2.02	0.41
1:J:233:MET:CE	1:J:249:ILE:HD11	2.40	0.41
1:J:301:ILE:HG23	1:J:307:MET:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:161:LEU:HD22	1:K:379:ILE:HG23	2.02	0.41
1:K:225:LYS:CA	1:K:303:GLU:HB2	2.50	0.41
1:L:31:LEU:HB3	1:L:90:THR:HG21	2.03	0.41
1:L:227:ILE:H	1:L:254:VAL:HG22	1.85	0.41
1:M:150:ILE:HD12	1:M:494:LEU:H	1.85	0.41
1:M:295:LEU:HD23	1:M:342:ILE:CD1	2.46	0.41
1:N:417:VAL:HG11	1:N:477:GLY:HA3	2.02	0.41
1:A:213:VAL:HG23	1:A:214:GLU:N	2.33	0.41
1:B:193:MET:CE	1:B:292:ILE:HG23	2.51	0.41
1:B:220:ILE:CD1	1:B:296:THR:HG21	2.47	0.41
1:E:165:ALA:HB2	1:E:187:LEU:HD13	2.02	0.41
1:E:278:ALA:HB2	1:E:289:LEU:HG	2.01	0.41
1:F:254:VAL:HG12	1:F:259:LEU:HB2	2.03	0.41
1:G:166:MET:HE3	1:G:175:ILE:HD12	2.02	0.41
1:G:278:ALA:HB2	1:G:289:LEU:HG	2.01	0.41
1:H:161:LEU:HD22	1:H:379:ILE:HG23	2.02	0.41
1:H:417:VAL:HG11	1:H:477:GLY:HA3	2.03	0.41
1:J:161:LEU:HD22	1:J:379:ILE:HG23	2.02	0.41
1:J:225:LYS:CA	1:J:303:GLU:HB2	2.50	0.41
1:L:446:ALA:O	1:L:450:PRO:HD2	2.20	0.41
1:M:161:LEU:HD22	1:M:379:ILE:HG23	2.03	0.41
1:M:278:ALA:HA	1:M:279:PRO:HD3	1.87	0.41
1:N:150:ILE:HD12	1:N:494:LEU:H	1.85	0.41
1:C:166:MET:HE3	1:C:175:ILE:HD12	2.02	0.41
1:C:250:ILE:HD13	1:C:292:ILE:HG21	2.02	0.41
1:D:215:LEU:HB3	1:D:246:PRO:HG2	2.02	0.41
1:D:254:VAL:HG12	1:D:259:LEU:HB2	2.03	0.41
1:D:409:GLU:CD	1:D:501:ARG:HH22	2.28	0.41
1:E:197:ARG:HG3	1:E:198:GLY:O	2.20	0.41
1:E:254:VAL:HG12	1:E:259:LEU:HB2	2.03	0.41
1:F:278:ALA:HA	1:F:279:PRO:HD3	1.72	0.41
1:I:31:LEU:HB3	1:I:90:THR:HG21	2.02	0.41
1:I:193:MET:HG2	1:I:372:LEU:HA	2.02	0.41
1:K:518:GLU:CB	1:K:519:CYS:N	2.74	0.41
1:N:77:VAL:HG22	1:N:510:VAL:CB	2.49	0.41
1:N:171:LYS:HE3	1:N:408:GLU:OE1	2.21	0.41
1:N:240:VAL:HB	1:N:247:LEU:HD22	2.02	0.41
1:B:271:VAL:O	1:B:273:VAL:HG23	2.20	0.41
1:C:223:ALA:HB3	1:C:251:ALA:CA	2.51	0.41
1:D:223:ALA:HB3	1:D:251:ALA:CA	2.51	0.41
1:D:249:ILE:HD11	1:D:262:LEU:HD22	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:MET:HE3	1:E:175:ILE:HD12	2.02	0.41
1:F:278:ALA:HB2	1:F:289:LEU:HG	2.01	0.41
1:G:271:VAL:O	1:G:273:VAL:HG23	2.20	0.41
1:H:301:ILE:HG23	1:H:307:MET:HB2	2.01	0.41
1:H:309:LEU:HA	1:H:309:LEU:HD23	1.81	0.41
1:I:150:ILE:HD12	1:I:494:LEU:H	1.85	0.41
1:I:321:LYS:HZ3	1:I:334:ASP:CG	2.28	0.41
1:I:446:ALA:O	1:I:450:PRO:HD2	2.20	0.41
1:J:149:THR:HG22	1:J:154:SER:HB3	2.02	0.41
1:K:240:VAL:HB	1:K:247:LEU:HD22	2.02	0.41
1:L:240:VAL:HB	1:L:247:LEU:HD22	2.02	0.41
1:L:301:ILE:HG23	1:L:307:MET:HB2	2.01	0.41
1:M:193:MET:HG2	1:M:372:LEU:HA	2.02	0.41
1:A:73:MET:HG2	1:B:46:ALA:CB	2.51	0.41
1:B:165:ALA:HB2	1:B:187:LEU:HD13	2.02	0.41
1:B:254:VAL:HG12	1:B:259:LEU:HB2	2.03	0.41
1:C:165:ALA:HB2	1:C:187:LEU:HD13	2.02	0.41
1:C:215:LEU:HB3	1:C:246:PRO:HG2	2.02	0.41
1:D:250:ILE:HD13	1:D:292:ILE:HG21	2.02	0.41
1:E:197:ARG:HD3	1:E:197:ARG:HA	2.02	0.41
1:H:233:MET:CE	1:H:249:ILE:HD11	2.42	0.41
1:H:516:THR:O	1:N:37:ASN:HB2	2.20	0.41
1:I:8:PHE:HA	1:I:9:GLY:HA3	1.81	0.41
1:J:31:LEU:HB3	1:J:90:THR:HG21	2.03	0.41
1:J:227:ILE:H	1:J:254:VAL:HG22	1.85	0.41
1:J:301:ILE:HD11	1:J:316:ASP:CG	2.45	0.41
1:J:446:ALA:O	1:J:450:PRO:HD2	2.20	0.41
1:K:31:LEU:HB3	1:K:90:THR:HG21	2.03	0.41
1:M:37:ASN:HB2	1:N:516:THR:O	2.20	0.41
1:N:149:THR:HG22	1:N:154:SER:HB3	2.02	0.41
1:N:227:ILE:H	1:N:254:VAL:HG22	1.85	0.41
1:A:46:ALA:CB	1:G:73:MET:HG2	2.51	0.41
1:B:236:VAL:CG1	1:B:317:LEU:HD13	2.51	0.41
1:C:409:GLU:CD	1:C:501:ARG:HH22	2.28	0.41
1:D:165:ALA:HB2	1:D:187:LEU:HD13	2.02	0.41
1:F:236:VAL:CG1	1:F:317:LEU:HD13	2.51	0.41
1:F:270:ILE:O	1:F:271:VAL:HB	2.20	0.41
1:G:193:MET:SD	1:G:295:LEU:CB	3.09	0.41
1:G:236:VAL:CG1	1:G:317:LEU:HD13	2.51	0.41
1:G:270:ILE:O	1:G:271:VAL:HB	2.20	0.41
1:H:225:LYS:HA	1:H:303:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:417:VAL:HG11	1:J:477:GLY:HA3	2.02	0.41
1:M:309:LEU:HD23	1:M:309:LEU:HA	1.81	0.41
1:N:225:LYS:CA	1:N:303:GLU:HB2	2.50	0.41
1:A:250:ILE:HD13	1:A:292:ILE:HG21	2.02	0.41
1:A:409:GLU:CD	1:A:501:ARG:HH22	2.28	0.41
1:B:144:ILE:HG23	1:B:403:THR:HG23	2.03	0.41
1:B:250:ILE:HD13	1:B:292:ILE:HG21	2.02	0.41
1:C:190:VAL:HB	1:C:334:ASP:HB2	2.01	0.41
1:C:271:VAL:HG12	1:C:273:VAL:HG22	2.02	0.41
1:D:73:MET:HG2	1:E:46:ALA:CB	2.51	0.41
1:D:190:VAL:CG2	1:D:333:ILE:CG2	2.98	0.41
1:D:236:VAL:CG1	1:D:317:LEU:HD13	2.51	0.41
1:E:236:VAL:CG1	1:E:317:LEU:HD13	2.51	0.41
1:E:250:ILE:HD13	1:E:292:ILE:HG21	2.02	0.41
2:E:1525:PO4:P	4:E:1527:ATP:O3G	2.79	0.41
1:G:254:VAL:HG12	1:G:259:LEU:HB2	2.03	0.41
1:H:150:ILE:HD12	1:H:494:LEU:H	1.85	0.41
1:H:240:VAL:HB	1:H:247:LEU:HD22	2.02	0.41
1:H:257:GLU:CD	1:N:242:LYS:HZ1	2.29	0.41
1:I:225:LYS:HA	1:I:303:GLU:HB2	2.03	0.41
1:J:150:ILE:HD12	1:J:494:LEU:H	1.85	0.41
1:K:207:LYS:HB3	1:K:208:PRO:HD3	2.03	0.41
1:K:225:LYS:HA	1:K:303:GLU:HB2	2.02	0.41
1:K:239:ALA:CB	1:K:314:LEU:HB3	2.51	0.41
1:K:278:ALA:HB3	1:K:285:ARG:HG2	2.02	0.41
1:K:417:VAL:HG11	1:K:477:GLY:HA3	2.03	0.41
1:L:149:THR:HG22	1:L:154:SER:HB3	2.02	0.41
1:L:193:MET:HG2	1:L:372:LEU:HA	2.02	0.41
1:L:201:SER:OG	1:L:267:MET:HE1	2.21	0.41
1:L:223:ALA:HB2	1:L:309:LEU:HD11	2.03	0.41
1:M:149:THR:HG22	1:M:154:SER:HB3	2.02	0.41
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.47	0.41
1:N:31:LEU:HB3	1:N:90:THR:HG21	2.03	0.41
1:N:38:VAL:HG21	1:N:56:VAL:HG22	2.03	0.41
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.29	0.41
1:N:161:LEU:HD22	1:N:379:ILE:HG23	2.03	0.41
1:N:201:SER:OG	1:N:267:MET:HE1	2.21	0.41
1:N:242:LYS:HA	1:N:243:ALA:HA	1.12	0.41
1:A:236:VAL:CG1	1:A:317:LEU:HD13	2.51	0.41
1:A:311:LYS:O	1:A:313:THR:HG23	2.21	0.41
1:E:73:MET:HG2	1:F:46:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LYS:HZ2	1:E:121:ASP:CG	2.28	0.41
1:F:193:MET:CE	1:F:292:ILE:HG23	2.50	0.41
1:F:250:ILE:HD13	1:F:292:ILE:HG21	2.02	0.41
1:F:409:GLU:CD	1:F:501:ARG:HH22	2.28	0.41
1:G:117:LYS:HZ2	1:G:121:ASP:CG	2.28	0.41
1:G:250:ILE:HD13	1:G:292:ILE:HG21	2.02	0.41
1:K:356:ALA:HB2	1:K:365:LEU:HD12	2.03	0.41
1:L:405:ALA:HB1	1:L:498:LYS:CD	2.51	0.41
1:M:182:GLY:HA2	1:M:183:LEU:HA	1.63	0.41
1:M:239:ALA:CB	1:M:314:LEU:HB3	2.50	0.41
1:A:254:VAL:HG12	1:A:259:LEU:HB2	2.03	0.40
1:C:236:VAL:CG1	1:C:317:LEU:HD13	2.51	0.40
1:E:409:GLU:CD	1:E:501:ARG:HH22	2.28	0.40
1:F:73:MET:HG2	1:G:46:ALA:CB	2.51	0.40
1:F:311:LYS:O	1:F:313:THR:HG23	2.21	0.40
1:G:200:LEU:HD13	1:G:254:VAL:CG1	2.44	0.40
1:G:209:GLU:H	1:G:209:GLU:CD	2.28	0.40
1:G:311:LYS:O	1:G:313:THR:HG23	2.21	0.40
1:H:38:VAL:HG21	1:H:56:VAL:HG22	2.04	0.40
1:H:50:THR:HG22	1:H:52:ASP:O	2.21	0.40
1:I:50:THR:HG22	1:I:52:ASP:O	2.21	0.40
1:I:225:LYS:CA	1:I:303:GLU:HB2	2.50	0.40
1:M:38:VAL:HG21	1:M:56:VAL:HG22	2.03	0.40
1:M:201:SER:OG	1:M:267:MET:HE1	2.21	0.40
1:N:338:GLU:O	1:N:342:ILE:HG13	2.22	0.40
1:N:356:ALA:HB2	1:N:365:LEU:HD12	2.04	0.40
1:B:73:MET:HG2	1:C:46:ALA:CB	2.51	0.40
1:D:201:SER:HA	1:D:202:PRO:HD3	1.98	0.40
1:D:203:TYR:N	1:D:203:TYR:CD1	2.90	0.40
1:D:311:LYS:O	1:D:313:THR:HG23	2.21	0.40
1:E:225:LYS:HB2	1:E:307:MET:O	2.22	0.40
1:G:225:LYS:HB2	1:G:307:MET:O	2.22	0.40
1:J:493:ILE:HD13	4:J:1527:ATP:C6	2.57	0.40
1:M:206:ASN:HB3	1:M:208:PRO:HD2	2.03	0.40
1:M:223:ALA:HB2	1:M:309:LEU:HD11	2.03	0.40
1:M:356:ALA:HB2	1:M:365:LEU:HD12	2.04	0.40
1:A:271:VAL:O	1:A:273:VAL:HG23	2.20	0.40
1:B:223:ALA:HB3	1:B:251:ALA:CA	2.51	0.40
1:C:193:MET:HE2	1:C:295:LEU:HB3	2.03	0.40
1:C:194:GLN:HG3	1:C:329:THR:HG21	2.03	0.40
2:C:1525:PO4:P	4:C:1527:ATP:O3G	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ALA:HB3	1:F:251:ALA:CA	2.51	0.40
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.30	0.40
1:J:193:MET:HG2	1:J:372:LEU:HA	2.02	0.40
1:J:207:LYS:HE2	1:J:207:LYS:HA	2.04	0.40
1:K:149:THR:HG22	1:K:154:SER:HB3	2.02	0.40
1:K:338:GLU:O	1:K:342:ILE:HG13	2.22	0.40
1:K:446:ALA:O	1:K:450:PRO:HD2	2.20	0.40
1:M:80:LYS:HD3	1:M:80:LYS:HA	1.98	0.40
1:A:223:ALA:HB3	1:A:251:ALA:CA	2.51	0.40
1:C:203:TYR:N	1:C:203:TYR:CD1	2.90	0.40
1:C:311:LYS:O	1:C:313:THR:HG23	2.21	0.40
1:D:223:ALA:HB1	1:D:227:ILE:HG12	2.03	0.40
1:E:311:LYS:O	1:E:313:THR:HG23	2.21	0.40
1:H:356:ALA:HB2	1:H:365:LEU:HD12	2.04	0.40
1:I:201:SER:OG	1:I:267:MET:HE1	2.21	0.40
1:J:356:ALA:HB2	1:J:365:LEU:HD12	2.04	0.40
1:K:62:LEU:HD23	1:K:62:LEU:HA	2.02	0.40
1:L:150:ILE:HD12	1:L:494:LEU:H	1.85	0.40
1:L:338:GLU:O	1:L:342:ILE:HG13	2.22	0.40
1:C:201:SER:HA	1:C:202:PRO:HD3	1.84	0.40
1:C:252:GLU:HA	1:C:289:LEU:CD1	2.52	0.40
1:D:225:LYS:HB2	1:D:307:MET:O	2.22	0.40
1:E:203:TYR:N	1:E:203:TYR:CD1	2.90	0.40
1:E:223:ALA:HB1	1:E:227:ILE:HG12	2.03	0.40
1:F:225:LYS:HB2	1:F:307:MET:O	2.22	0.40
1:H:169:VAL:HB	1:H:173:GLY:CA	2.51	0.40
1:H:338:GLU:O	1:H:342:ILE:HG13	2.22	0.40
1:H:405:ALA:HB1	1:H:498:LYS:CD	2.51	0.40
1:J:38:VAL:HG21	1:J:56:VAL:HG22	2.04	0.40
1:J:278:ALA:HA	1:J:279:PRO:HD3	1.86	0.40
1:K:161:LEU:HD21	1:K:185:ASP:HB3	2.03	0.40
1:K:213:VAL:CG1	1:K:325:ILE:HG12	2.51	0.40
1:K:405:ALA:HB1	1:K:498:LYS:CD	2.52	0.40
1:L:493:ILE:HD13	4:L:1527:ATP:C6	2.57	0.40
1:M:206:ASN:HB2	1:M:213:VAL:HG23	2.02	0.40
1:M:227:ILE:H	1:M:254:VAL:HG22	1.85	0.40
1:M:242:LYS:HA	1:M:243:ALA:HA	1.13	0.40
1:M:493:ILE:HD13	4:M:1527:ATP:C6	2.57	0.40
1:N:493:ILE:HD13	4:N:1527:ATP:C6	2.57	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%)	498 (95%)	21 (4%)	3 (1%)	21	59
1	B	522/548 (95%)	497 (95%)	23 (4%)	2 (0%)	30	67
1	C	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	21	59
1	D	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	21	59
1	E	522/548 (95%)	497 (95%)	21 (4%)	4 (1%)	16	54
1	F	522/548 (95%)	497 (95%)	21 (4%)	4 (1%)	16	54
1	G	522/548 (95%)	495 (95%)	24 (5%)	3 (1%)	21	59
1	H	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	I	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	J	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	K	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	L	522/548 (95%)	513 (98%)	9 (2%)	0	100	100
1	M	522/548 (95%)	515 (99%)	7 (1%)	0	100	100
1	N	522/548 (95%)	515 (99%)	5 (1%)	2 (0%)	30	67
All	All	7308/7672 (95%)	7087 (97%)	197 (3%)	24 (0%)	37	72

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	199	TYR
1	N	207	LYS
1	N	208	PRO
1	A	384	ALA
1	B	384	ALA
1	C	199	TYR
1	C	384	ALA
1	D	384	ALA
1	E	199	TYR

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Mol	Chain	Res	Type
1	E	384	ALA
1	F	199	TYR
1	F	384	ALA
1	G	384	ALA
1	A	271	VAL
1	B	271	VAL
1	C	271	VAL
1	D	208	PRO
1	D	271	VAL
1	E	271	VAL
1	F	271	VAL
1	G	271	VAL
1	A	199	TYR
1	E	208	PRO
1	F	208	PRO

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%)	361 (90%)	41 (10%)	7	23
1	B	402/414 (97%)	359 (89%)	43 (11%)	6	21
1	C	402/414 (97%)	361 (90%)	41 (10%)	7	23
1	D	402/414 (97%)	362 (90%)	40 (10%)	7	24
1	E	402/414 (97%)	362 (90%)	40 (10%)	7	24
1	F	402/414 (97%)	362 (90%)	40 (10%)	7	24
1	G	402/414 (97%)	361 (90%)	41 (10%)	7	23
1	H	402/414 (97%)	358 (89%)	44 (11%)	6	21
1	I	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	J	402/414 (97%)	361 (90%)	41 (10%)	7	23
1	K	402/414 (97%)	358 (89%)	44 (11%)	6	21
1	L	402/414 (97%)	362 (90%)	40 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	402/414 (97%)	355 (88%)	47 (12%)	5	18
1	N	402/414 (97%)	357 (89%)	45 (11%)	6	19
All	All	5628/5796 (97%)	5039 (90%)	589 (10%)	9	21

All (589) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	34	LYS
1	A	36	ARG
1	A	37	ASN
1	A	38	VAL
1	A	65	LYS
1	A	169	VAL
1	A	171	LYS
1	A	172	GLU
1	A	177	VAL
1	A	183	LEU
1	A	186	GLU
1	A	190	VAL
1	A	196	ASP
1	A	207	LYS
1	A	213	VAL
1	A	225	LYS
1	A	226	LYS
1	A	238	GLU
1	A	242	LYS
1	A	252	GLU
1	A	272	LYS
1	A	295	LEU
1	A	300	VAL
1	A	309	LEU
1	A	311	LYS
1	A	316	ASP
1	A	319	GLN
1	A	323	VAL
1	A	325	ILE
1	A	326	ASN
1	A	327	LYS
1	A	334	ASP
1	A	336	VAL

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Mol	Chain	Res	Type
1	A	363	GLU
1	A	404	ARG
1	A	428	ASP
1	A	453	GLN
1	A	460	GLU
1	A	484	GLU
1	A	522	THR
1	B	18	ARG
1	B	34	LYS
1	B	36	ARG
1	B	37	ASN
1	B	38	VAL
1	B	65	LYS
1	B	169	VAL
1	B	171	LYS
1	B	172	GLU
1	B	177	VAL
1	B	183	LEU
1	B	186	GLU
1	B	190	VAL
1	B	195	PHE
1	B	203	TYR
1	B	207	LYS
1	B	210	THR
1	B	213	VAL
1	B	225	LYS
1	B	226	LYS
1	B	238	GLU
1	B	242	LYS
1	B	252	GLU
1	B	272	LYS
1	B	295	LEU
1	B	300	VAL
1	B	309	LEU
1	B	311	LYS
1	B	316	ASP
1	B	319	GLN
1	B	323	VAL
1	B	325	ILE
1	B	326	ASN
1	B	327	LYS
1	B	334	ASP

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Mol	Chain	Res	Type
1	B	336	VAL
1	B	363	GLU
1	B	404	ARG
1	B	428	ASP
1	B	453	GLN
1	B	460	GLU
1	B	484	GLU
1	B	522	THR
1	C	18	ARG
1	C	34	LYS
1	C	36	ARG
1	C	37	ASN
1	C	38	VAL
1	C	65	LYS
1	C	169	VAL
1	C	171	LYS
1	C	172	GLU
1	C	177	VAL
1	C	183	LEU
1	C	186	GLU
1	C	190	VAL
1	C	193	MET
1	C	207	LYS
1	C	213	VAL
1	C	225	LYS
1	C	226	LYS
1	C	238	GLU
1	C	242	LYS
1	C	252	GLU
1	C	272	LYS
1	C	295	LEU
1	C	300	VAL
1	C	309	LEU
1	C	311	LYS
1	C	316	ASP
1	C	319	GLN
1	C	323	VAL
1	C	325	ILE
1	C	326	ASN
1	C	327	LYS
1	C	334	ASP
1	C	336	VAL

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Mol	Chain	Res	Type
1	C	363	GLU
1	C	404	ARG
1	C	428	ASP
1	C	453	GLN
1	C	460	GLU
1	C	484	GLU
1	C	522	THR
1	D	18	ARG
1	D	34	LYS
1	D	36	ARG
1	D	37	ASN
1	D	38	VAL
1	D	65	LYS
1	D	153	ASN
1	D	169	VAL
1	D	171	LYS
1	D	172	GLU
1	D	177	VAL
1	D	183	LEU
1	D	186	GLU
1	D	190	VAL
1	D	213	VAL
1	D	225	LYS
1	D	226	LYS
1	D	238	GLU
1	D	242	LYS
1	D	252	GLU
1	D	272	LYS
1	D	295	LEU
1	D	300	VAL
1	D	309	LEU
1	D	311	LYS
1	D	316	ASP
1	D	319	GLN
1	D	323	VAL
1	D	325	ILE
1	D	326	ASN
1	D	327	LYS
1	D	334	ASP
1	D	336	VAL
1	D	363	GLU
1	D	404	ARG

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Mol	Chain	Res	Type
1	D	428	ASP
1	D	453	GLN
1	D	460	GLU
1	D	484	GLU
1	D	522	THR
1	E	18	ARG
1	E	34	LYS
1	E	36	ARG
1	E	37	ASN
1	E	38	VAL
1	E	65	LYS
1	E	169	VAL
1	E	171	LYS
1	E	172	GLU
1	E	177	VAL
1	E	183	LEU
1	E	186	GLU
1	E	190	VAL
1	E	207	LYS
1	E	213	VAL
1	E	225	LYS
1	E	226	LYS
1	E	238	GLU
1	E	242	LYS
1	E	252	GLU
1	E	272	LYS
1	E	295	LEU
1	E	300	VAL
1	E	309	LEU
1	E	311	LYS
1	E	316	ASP
1	E	319	GLN
1	E	323	VAL
1	E	325	ILE
1	E	326	ASN
1	E	327	LYS
1	E	334	ASP
1	E	336	VAL
1	E	363	GLU
1	E	404	ARG
1	E	428	ASP
1	E	453	GLN

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Mol	Chain	Res	Type
1	E	460	GLU
1	E	484	GLU
1	E	522	THR
1	F	18	ARG
1	F	34	LYS
1	F	36	ARG
1	F	37	ASN
1	F	38	VAL
1	F	65	LYS
1	F	153	ASN
1	F	169	VAL
1	F	171	LYS
1	F	172	GLU
1	F	177	VAL
1	F	183	LEU
1	F	190	VAL
1	F	207	LYS
1	F	213	VAL
1	F	225	LYS
1	F	226	LYS
1	F	238	GLU
1	F	242	LYS
1	F	252	GLU
1	F	272	LYS
1	F	295	LEU
1	F	300	VAL
1	F	309	LEU
1	F	311	LYS
1	F	316	ASP
1	F	319	GLN
1	F	323	VAL
1	F	325	ILE
1	F	326	ASN
1	F	327	LYS
1	F	334	ASP
1	F	336	VAL
1	F	363	GLU
1	F	404	ARG
1	F	428	ASP
1	F	453	GLN
1	F	460	GLU
1	F	484	GLU

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Mol	Chain	Res	Type
1	F	522	THR
1	G	18	ARG
1	G	34	LYS
1	G	36	ARG
1	G	37	ASN
1	G	38	VAL
1	G	65	LYS
1	G	169	VAL
1	G	171	LYS
1	G	172	GLU
1	G	177	VAL
1	G	183	LEU
1	G	186	GLU
1	G	190	VAL
1	G	201	SER
1	G	207	LYS
1	G	213	VAL
1	G	225	LYS
1	G	226	LYS
1	G	238	GLU
1	G	242	LYS
1	G	252	GLU
1	G	272	LYS
1	G	295	LEU
1	G	300	VAL
1	G	309	LEU
1	G	311	LYS
1	G	316	ASP
1	G	319	GLN
1	G	323	VAL
1	G	325	ILE
1	G	326	ASN
1	G	327	LYS
1	G	334	ASP
1	G	336	VAL
1	G	363	GLU
1	G	404	ARG
1	G	428	ASP
1	G	453	GLN
1	G	460	GLU
1	G	484	GLU
1	G	522	THR

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Mol	Chain	Res	Type
1	H	31	LEU
1	H	37	ASN
1	H	39	VAL
1	H	48	THR
1	H	51	LYS
1	H	54	VAL
1	H	63	GLU
1	H	74	VAL
1	H	89	THR
1	H	160	LYS
1	H	166	MET
1	H	174	VAL
1	H	178	GLU
1	H	183	LEU
1	H	188	ASP
1	H	191	GLU
1	H	193	MET
1	H	195	PHE
1	H	197	ARG
1	H	207	LYS
1	H	213	VAL
1	H	225	LYS
1	H	226	LYS
1	H	231	ARG
1	H	236	VAL
1	H	238	GLU
1	H	253	ASP
1	H	257	GLU
1	H	272	LYS
1	H	289	LEU
1	H	295	LEU
1	H	321	LYS
1	H	325	ILE
1	H	358	SER
1	H	364	LYS
1	H	389	MET
1	H	391	GLU
1	H	404	ARG
1	H	408	GLU
1	H	430	ARG
1	H	460	GLU
1	H	484	GLU

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Mol	Chain	Res	Type
1	H	518	GLU
1	H	523	ASP
1	I	31	LEU
1	I	37	ASN
1	I	39	VAL
1	I	48	THR
1	I	51	LYS
1	I	54	VAL
1	I	63	GLU
1	I	74	VAL
1	I	89	THR
1	I	160	LYS
1	I	166	MET
1	I	174	VAL
1	I	178	GLU
1	I	188	ASP
1	I	191	GLU
1	I	193	MET
1	I	195	PHE
1	I	197	ARG
1	I	207	LYS
1	I	213	VAL
1	I	225	LYS
1	I	226	LYS
1	I	236	VAL
1	I	238	GLU
1	I	253	ASP
1	I	257	GLU
1	I	272	LYS
1	I	289	LEU
1	I	295	LEU
1	I	321	LYS
1	I	325	ILE
1	I	358	SER
1	I	364	LYS
1	I	389	MET
1	I	391	GLU
1	I	404	ARG
1	I	408	GLU
1	I	430	ARG
1	I	460	GLU
1	I	484	GLU

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Mol	Chain	Res	Type
1	I	518	GLU
1	I	523	ASP
1	J	31	LEU
1	J	37	ASN
1	J	39	VAL
1	J	48	THR
1	J	51	LYS
1	J	54	VAL
1	J	63	GLU
1	J	74	VAL
1	J	89	THR
1	J	160	LYS
1	J	166	MET
1	J	174	VAL
1	J	188	ASP
1	J	191	GLU
1	J	193	MET
1	J	195	PHE
1	J	197	ARG
1	J	207	LYS
1	J	213	VAL
1	J	225	LYS
1	J	226	LYS
1	J	236	VAL
1	J	238	GLU
1	J	253	ASP
1	J	257	GLU
1	J	272	LYS
1	J	289	LEU
1	J	295	LEU
1	J	321	LYS
1	J	325	ILE
1	J	358	SER
1	J	364	LYS
1	J	389	MET
1	J	391	GLU
1	J	404	ARG
1	J	408	GLU
1	J	430	ARG
1	J	460	GLU
1	J	484	GLU
1	J	518	GLU

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Mol	Chain	Res	Type
1	J	523	ASP
1	K	31	LEU
1	K	37	ASN
1	K	39	VAL
1	K	48	THR
1	K	51	LYS
1	K	54	VAL
1	K	63	GLU
1	K	74	VAL
1	K	89	THR
1	K	160	LYS
1	K	166	MET
1	K	174	VAL
1	K	178	GLU
1	K	185	ASP
1	K	188	ASP
1	K	191	GLU
1	K	193	MET
1	K	195	PHE
1	K	197	ARG
1	K	207	LYS
1	K	213	VAL
1	K	225	LYS
1	K	226	LYS
1	K	231	ARG
1	K	236	VAL
1	K	238	GLU
1	K	253	ASP
1	K	257	GLU
1	K	272	LYS
1	K	289	LEU
1	K	295	LEU
1	K	321	LYS
1	K	325	ILE
1	K	358	SER
1	K	364	LYS
1	K	389	MET
1	K	391	GLU
1	K	404	ARG
1	K	408	GLU
1	K	430	ARG
1	K	460	GLU

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Mol	Chain	Res	Type
1	K	484	GLU
1	K	518	GLU
1	K	523	ASP
1	L	31	LEU
1	L	37	ASN
1	L	39	VAL
1	L	48	THR
1	L	51	LYS
1	L	54	VAL
1	L	63	GLU
1	L	74	VAL
1	L	89	THR
1	L	160	LYS
1	L	166	MET
1	L	174	VAL
1	L	178	GLU
1	L	188	ASP
1	L	193	MET
1	L	195	PHE
1	L	197	ARG
1	L	207	LYS
1	L	213	VAL
1	L	225	LYS
1	L	226	LYS
1	L	236	VAL
1	L	238	GLU
1	L	253	ASP
1	L	272	LYS
1	L	289	LEU
1	L	295	LEU
1	L	321	LYS
1	L	325	ILE
1	L	358	SER
1	L	364	LYS
1	L	389	MET
1	L	391	GLU
1	L	404	ARG
1	L	408	GLU
1	L	430	ARG
1	L	460	GLU
1	L	484	GLU
1	L	518	GLU

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Mol	Chain	Res	Type
1	L	523	ASP
1	M	31	LEU
1	M	37	ASN
1	M	39	VAL
1	M	48	THR
1	M	51	LYS
1	M	54	VAL
1	M	63	GLU
1	M	74	VAL
1	M	89	THR
1	M	160	LYS
1	M	166	MET
1	M	172	GLU
1	M	174	VAL
1	M	178	GLU
1	M	188	ASP
1	M	191	GLU
1	M	193	MET
1	M	195	PHE
1	M	197	ARG
1	M	207	LYS
1	M	213	VAL
1	M	225	LYS
1	M	226	LYS
1	M	228	SER
1	M	229	ASN
1	M	231	ARG
1	M	232	GLU
1	M	236	VAL
1	M	242	LYS
1	M	253	ASP
1	M	257	GLU
1	M	272	LYS
1	M	289	LEU
1	M	295	LEU
1	M	321	LYS
1	M	325	ILE
1	M	358	SER
1	M	364	LYS
1	M	389	MET
1	M	391	GLU
1	M	404	ARG

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Mol	Chain	Res	Type
1	M	408	GLU
1	M	430	ARG
1	M	460	GLU
1	M	484	GLU
1	M	518	GLU
1	M	523	ASP
1	N	31	LEU
1	N	37	ASN
1	N	39	VAL
1	N	48	THR
1	N	51	LYS
1	N	54	VAL
1	N	63	GLU
1	N	74	VAL
1	N	89	THR
1	N	160	LYS
1	N	166	MET
1	N	171	LYS
1	N	174	VAL
1	N	178	GLU
1	N	186	GLU
1	N	188	ASP
1	N	191	GLU
1	N	193	MET
1	N	195	PHE
1	N	197	ARG
1	N	207	LYS
1	N	213	VAL
1	N	225	LYS
1	N	226	LYS
1	N	231	ARG
1	N	236	VAL
1	N	238	GLU
1	N	253	ASP
1	N	257	GLU
1	N	272	LYS
1	N	289	LEU
1	N	295	LEU
1	N	321	LYS
1	N	325	ILE
1	N	358	SER
1	N	364	LYS

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Mol	Chain	Res	Type
1	N	389	MET
1	N	391	GLU
1	N	404	ARG
1	N	408	GLU
1	N	430	ARG
1	N	460	GLU
1	N	484	GLU
1	N	518	GLU
1	N	523	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	401	HIS
1	B	112	ASN
1	B	290	GLN
1	B	401	HIS
1	C	112	ASN
1	C	401	HIS
1	D	112	ASN
1	D	401	HIS
1	E	112	ASN
1	E	401	HIS
1	F	112	ASN
1	G	112	ASN
1	G	401	HIS
1	H	326	ASN
1	H	366	GLN
1	H	401	HIS
1	I	326	ASN
1	I	366	GLN
1	I	401	HIS
1	I	433	ASN
1	J	326	ASN
1	J	366	GLN
1	J	401	HIS
1	J	433	ASN
1	K	326	ASN
1	K	366	GLN
1	K	401	HIS
1	K	433	ASN

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Mol	Chain	Res	Type
1	L	326	ASN
1	L	366	GLN
1	L	401	HIS
1	L	433	ASN
1	M	326	ASN
1	M	366	GLN
1	M	401	HIS
1	M	433	ASN
1	N	326	ASN
1	N	366	GLN
1	N	401	HIS
1	N	433	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 14 are modelled with single atom and 14 are monoatomic - 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	$\# Z > 2$
4	ATP	B	1527	3	32,33,33	1.63	1 (3%)	48,52,52	0.76	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	1527	3	32,33,33	1.80	3 (9%)	48,52,52	0.91	1 (2%)
4	ATP	F	1527	3	32,33,33	1.59	1 (3%)	48,52,52	0.75	1 (2%)
4	ATP	G	1527	3	32,33,33	1.80	3 (9%)	48,52,52	0.91	1 (2%)
4	ATP	J	1527	3	32,33,33	1.50	1 (3%)	48,52,52	0.86	2 (4%)
4	ATP	L	1527	3	32,33,33	1.50	1 (3%)	48,52,52	0.86	2 (4%)
4	ATP	E	1527	3	32,33,33	1.80	3 (9%)	48,52,52	0.91	1 (2%)
4	ATP	H	1527	3	32,33,33	1.51	1 (3%)	48,52,52	0.87	2 (4%)
4	ATP	K	1527	3	32,33,33	1.50	1 (3%)	48,52,52	0.87	2 (4%)
4	ATP	I	1527	3	32,33,33	1.50	1 (3%)	48,52,52	0.87	2 (4%)
4	ATP	C	1527	3	32,33,33	1.81	3 (9%)	48,52,52	0.91	1 (2%)
4	ATP	M	1527	3	32,33,33	1.50	1 (3%)	48,52,52	0.87	2 (4%)
4	ATP	N	1527	3	32,33,33	1.50	1 (3%)	48,52,52	0.86	2 (4%)
4	ATP	D	1527	3	32,33,33	1.60	1 (3%)	48,52,52	0.76	1 (2%)

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
4	ATP	B	1527	3	-	5/22/38/38	0/3/3/3
4	ATP	A	1527	3	-	4/22/38/38	0/3/3/3
4	ATP	F	1527	3	-	7/22/38/38	0/3/3/3
4	ATP	G	1527	3	-	4/22/38/38	0/3/3/3
4	ATP	J	1527	3	-	2/22/38/38	0/3/3/3
4	ATP	L	1527	3	-	2/22/38/38	0/3/3/3
4	ATP	E	1527	3	-	4/22/38/38	0/3/3/3
4	ATP	H	1527	3	-	2/22/38/38	0/3/3/3
4	ATP	K	1527	3	-	2/22/38/38	0/3/3/3
4	ATP	I	1527	3	-	2/22/38/38	0/3/3/3
4	ATP	C	1527	3	-	4/22/38/38	0/3/3/3
4	ATP	M	1527	3	-	2/22/38/38	0/3/3/3
4	ATP	N	1527	3	-	2/22/38/38	0/3/3/3
4	ATP	D	1527	3	-	7/22/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1527	ATP	PA-O3A	-8.72	1.50	1.59
4	G	1527	ATP	PA-O3A	-8.67	1.50	1.59
4	E	1527	ATP	PA-O3A	-8.67	1.50	1.59
4	A	1527	ATP	PA-O3A	-8.60	1.50	1.59
4	B	1527	ATP	PA-O3A	-8.37	1.50	1.59
4	D	1527	ATP	PA-O3A	-8.16	1.50	1.59
4	F	1527	ATP	PA-O3A	-8.12	1.50	1.59
4	H	1527	ATP	PA-O3A	-7.75	1.51	1.59
4	N	1527	ATP	PA-O3A	-7.72	1.51	1.59
4	J	1527	ATP	PA-O3A	-7.71	1.51	1.59
4	I	1527	ATP	PA-O3A	-7.71	1.51	1.59
4	L	1527	ATP	PA-O3A	-7.70	1.51	1.59
4	K	1527	ATP	PA-O3A	-7.68	1.51	1.59
4	M	1527	ATP	PA-O3A	-7.68	1.51	1.59
4	A	1527	ATP	PB-O3A	-3.45	1.55	1.59
4	G	1527	ATP	PB-O3A	-3.44	1.55	1.59
4	C	1527	ATP	PB-O3A	-3.42	1.55	1.59
4	E	1527	ATP	PB-O3A	-3.41	1.55	1.59
4	A	1527	ATP	PB-O3B	2.39	1.62	1.59
4	E	1527	ATP	PB-O3B	2.39	1.62	1.59
4	G	1527	ATP	PB-O3B	2.34	1.62	1.59
4	C	1527	ATP	PB-O3B	2.33	1.62	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1527	ATP	O2A-PA-O3A	3.36	116.34	107.27
4	E	1527	ATP	O2A-PA-O3A	3.35	116.34	107.27
4	C	1527	ATP	O2A-PA-O3A	3.35	116.33	107.27
4	A	1527	ATP	O2A-PA-O3A	3.34	116.30	107.27
4	M	1527	ATP	O2A-PA-O3A	2.50	114.04	107.27
4	K	1527	ATP	O2A-PA-O3A	2.49	114.01	107.27
4	H	1527	ATP	O2A-PA-O3A	2.49	114.01	107.27
4	I	1527	ATP	O2A-PA-O3A	2.49	114.00	107.27
4	J	1527	ATP	O2A-PA-O3A	2.49	113.99	107.27
4	L	1527	ATP	O2A-PA-O3A	2.48	113.99	107.27
4	N	1527	ATP	O2A-PA-O3A	2.47	113.94	107.27
4	F	1527	ATP	O5'-C5'-C4'	2.20	116.48	108.99
4	D	1527	ATP	O5'-C5'-C4'	2.19	116.45	108.99
4	B	1527	ATP	O5'-C5'-C4'	2.17	116.39	108.99
4	H	1527	ATP	O3G-PG-O2G	2.17	115.93	107.80
4	L	1527	ATP	O3G-PG-O2G	2.17	115.93	107.80
4	I	1527	ATP	O3G-PG-O2G	2.16	115.92	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	1527	ATP	O3G-PG-O2G	2.16	115.91	107.80
4	M	1527	ATP	O3G-PG-O2G	2.16	115.91	107.80
4	K	1527	ATP	O3G-PG-O2G	2.16	115.90	107.80
4	J	1527	ATP	O3G-PG-O2G	2.16	115.89	107.80

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1527	ATP	O4'-C4'-C5'-O5'
4	A	1527	ATP	C3'-C4'-C5'-O5'
4	C	1527	ATP	O4'-C4'-C5'-O5'
4	C	1527	ATP	C3'-C4'-C5'-O5'
4	E	1527	ATP	O4'-C4'-C5'-O5'
4	E	1527	ATP	C3'-C4'-C5'-O5'
4	G	1527	ATP	C3'-C4'-C5'-O5'
4	G	1527	ATP	O4'-C4'-C5'-O5'
4	H	1527	ATP	C4'-C5'-O5'-PA
4	I	1527	ATP	C4'-C5'-O5'-PA
4	J	1527	ATP	C4'-C5'-O5'-PA
4	K	1527	ATP	C4'-C5'-O5'-PA
4	L	1527	ATP	C4'-C5'-O5'-PA
4	M	1527	ATP	C4'-C5'-O5'-PA
4	N	1527	ATP	C4'-C5'-O5'-PA
4	B	1527	ATP	C5'-O5'-PA-O1A
4	B	1527	ATP	C5'-O5'-PA-O2A
4	B	1527	ATP	C5'-O5'-PA-O3A
4	D	1527	ATP	C5'-O5'-PA-O1A
4	D	1527	ATP	C5'-O5'-PA-O2A
4	D	1527	ATP	C5'-O5'-PA-O3A
4	F	1527	ATP	C5'-O5'-PA-O1A
4	F	1527	ATP	C5'-O5'-PA-O2A
4	F	1527	ATP	C5'-O5'-PA-O3A
4	B	1527	ATP	PG-O3B-PB-O1B
4	A	1527	ATP	PB-O3A-PA-O1A
4	B	1527	ATP	PG-O3B-PB-O2B
4	C	1527	ATP	PB-O3A-PA-O1A
4	D	1527	ATP	PG-O3B-PB-O1B
4	D	1527	ATP	PG-O3B-PB-O2B
4	E	1527	ATP	PB-O3A-PA-O1A
4	F	1527	ATP	PG-O3B-PB-O1B
4	F	1527	ATP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	G	1527	ATP	PB-O3A-PA-O1A
4	A	1527	ATP	PG-O3B-PB-O2B
4	C	1527	ATP	PG-O3B-PB-O2B
4	D	1527	ATP	PA-O3A-PB-O1B
4	D	1527	ATP	PA-O3A-PB-O2B
4	E	1527	ATP	PG-O3B-PB-O2B
4	F	1527	ATP	PA-O3A-PB-O1B
4	F	1527	ATP	PA-O3A-PB-O2B
4	G	1527	ATP	PG-O3B-PB-O2B
4	H	1527	ATP	PG-O3B-PB-O2B
4	I	1527	ATP	PG-O3B-PB-O2B
4	J	1527	ATP	PG-O3B-PB-O2B
4	K	1527	ATP	PG-O3B-PB-O2B
4	L	1527	ATP	PG-O3B-PB-O2B
4	M	1527	ATP	PG-O3B-PB-O2B
4	N	1527	ATP	PG-O3B-PB-O2B

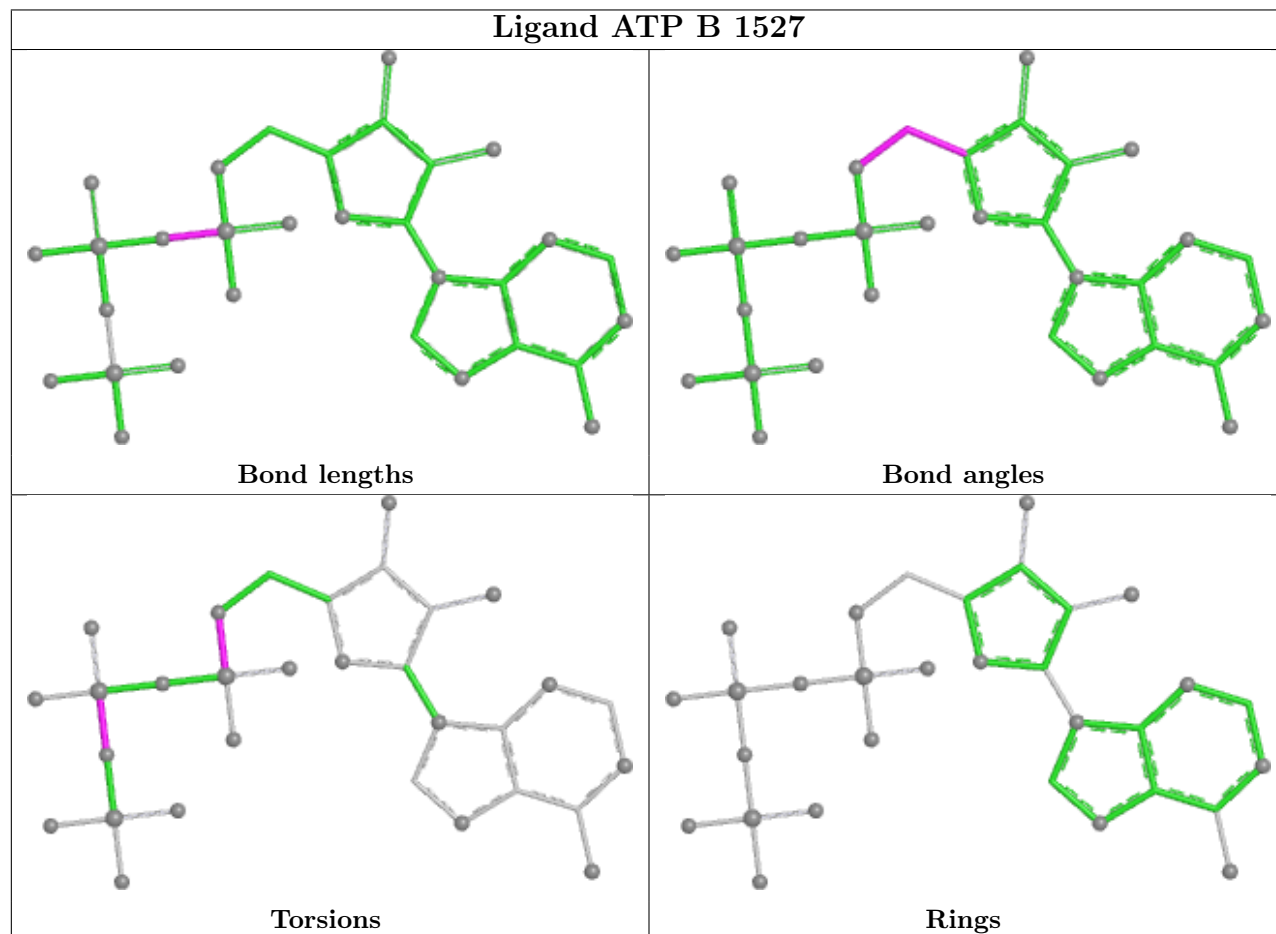
There are no ring outliers.

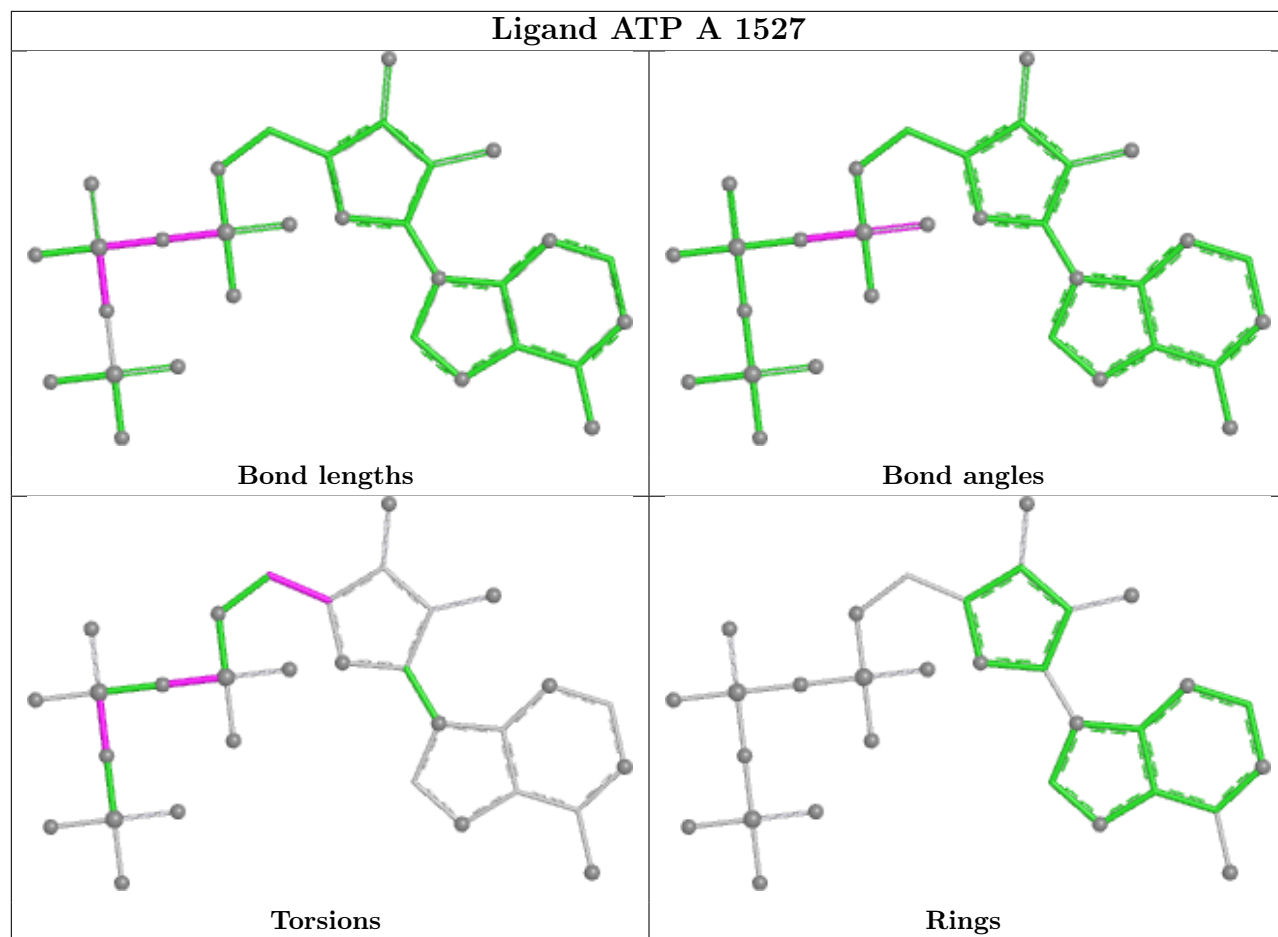
14 monomers are involved in 48 short contacts:

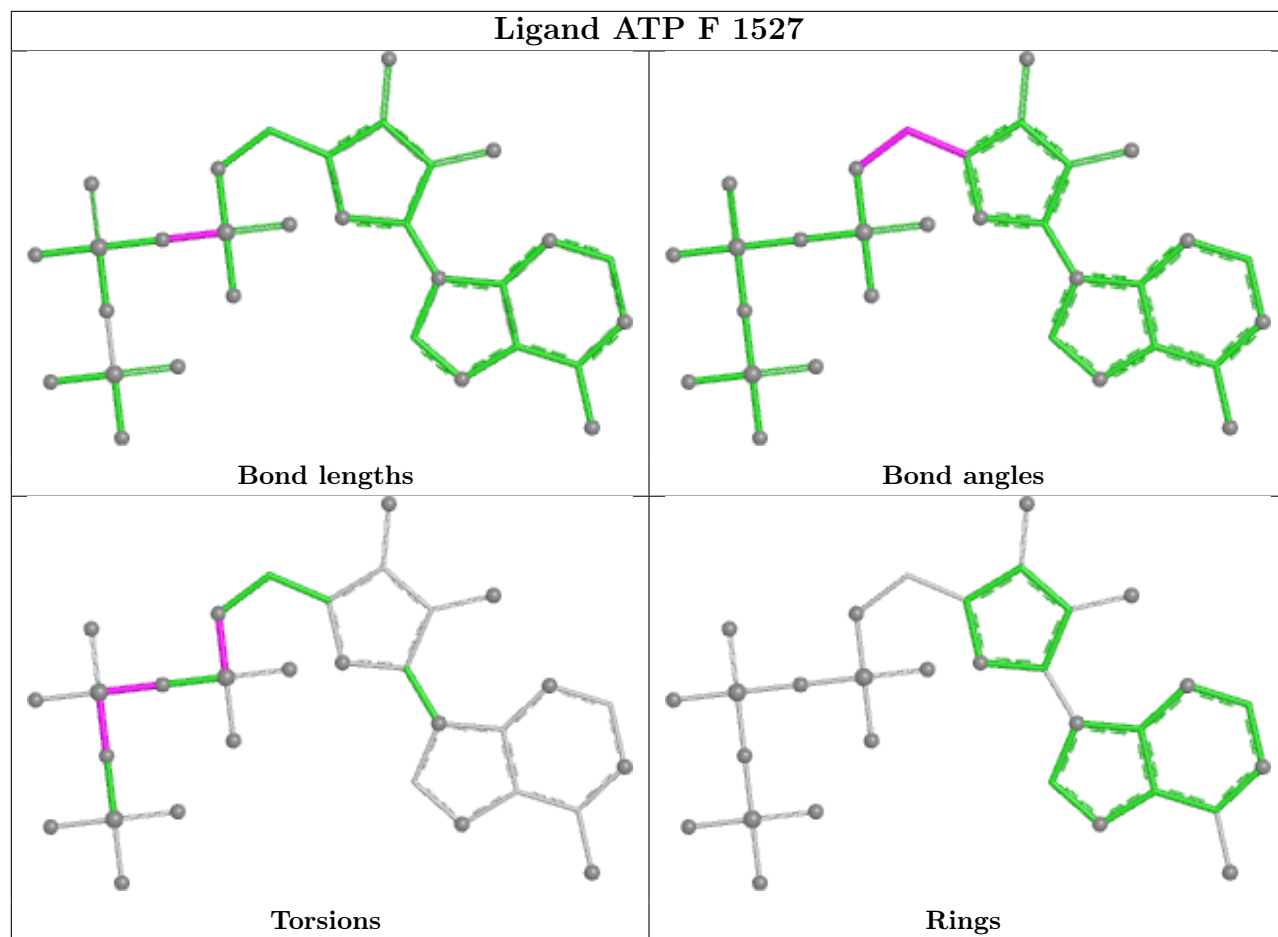
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1527	ATP	2	0
4	A	1527	ATP	2	0
4	F	1527	ATP	2	0
4	G	1527	ATP	2	0
4	J	1527	ATP	5	0
4	L	1527	ATP	5	0
4	E	1527	ATP	3	0
4	H	1527	ATP	4	0
4	K	1527	ATP	4	0
4	I	1527	ATP	4	0
4	C	1527	ATP	3	0
4	M	1527	ATP	5	0
4	N	1527	ATP	5	0
4	D	1527	ATP	2	0

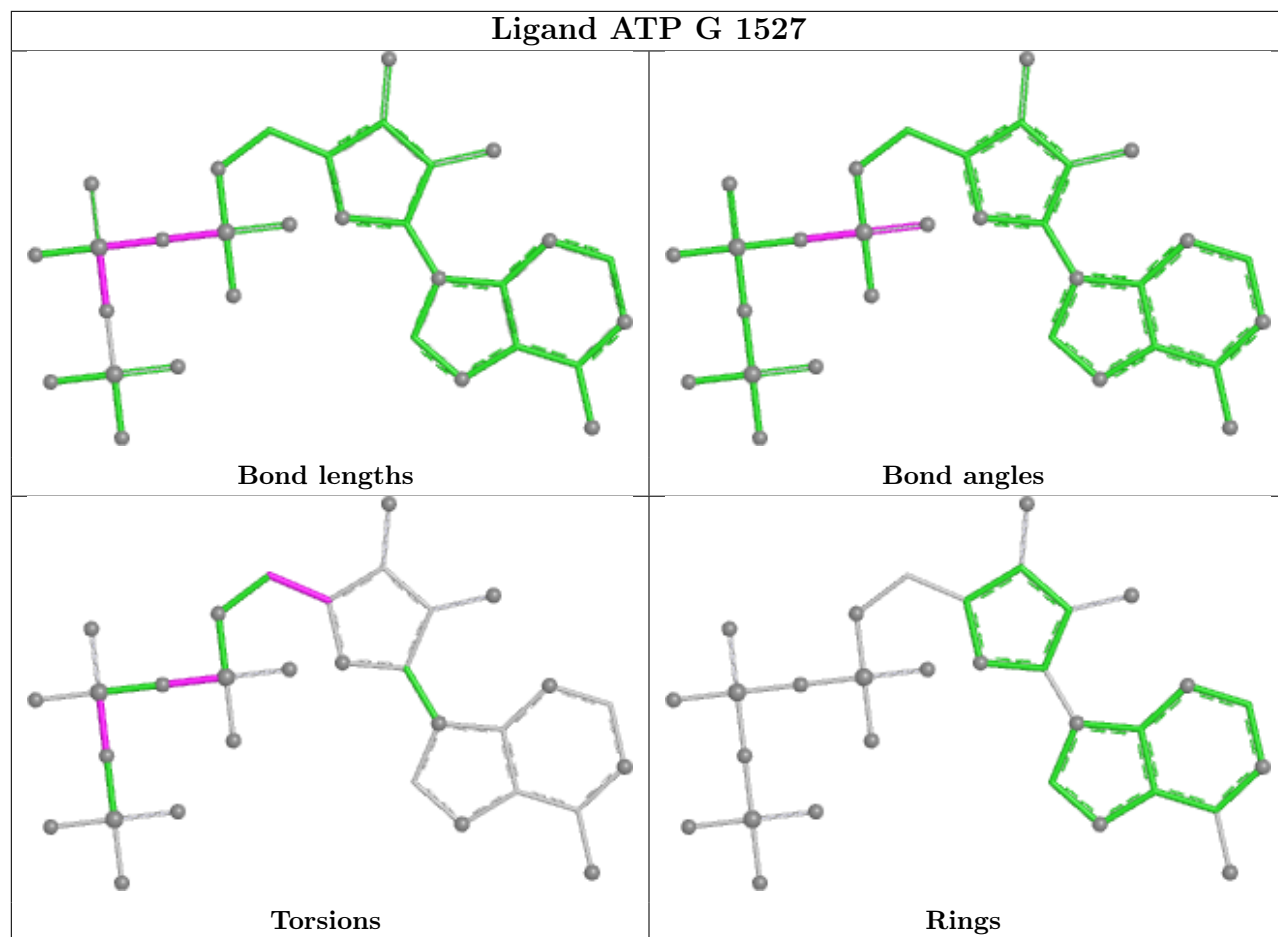
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

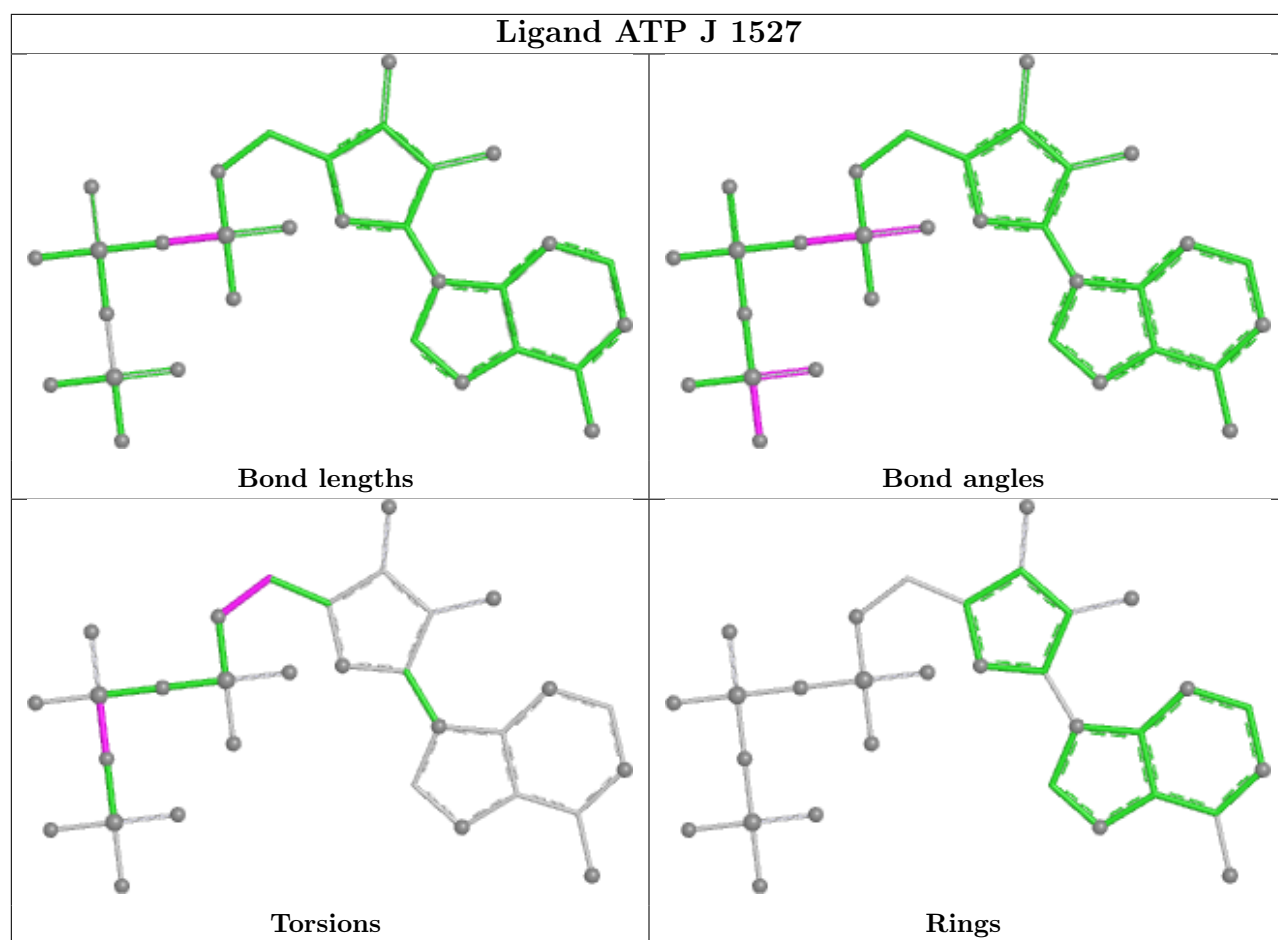
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

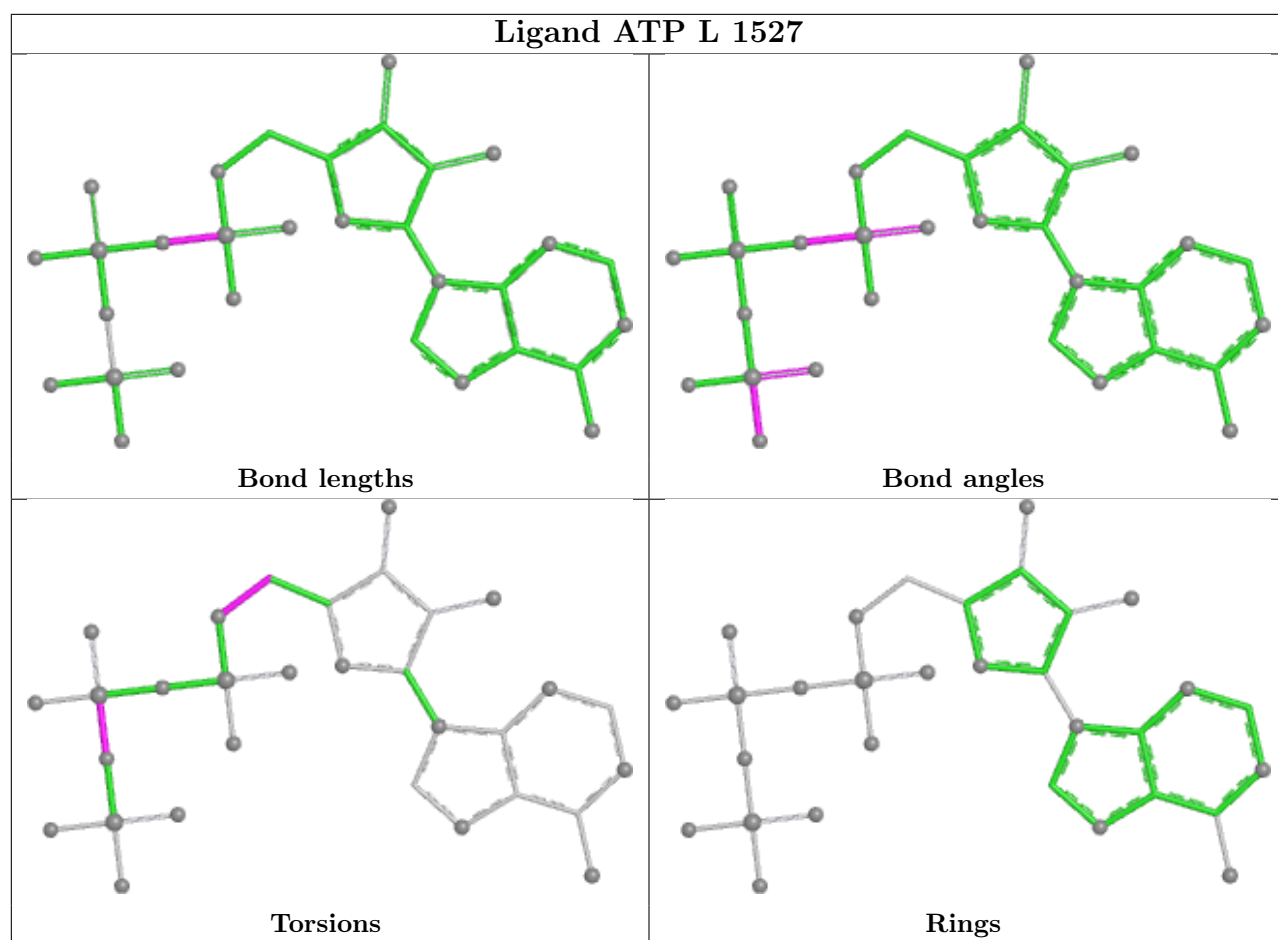


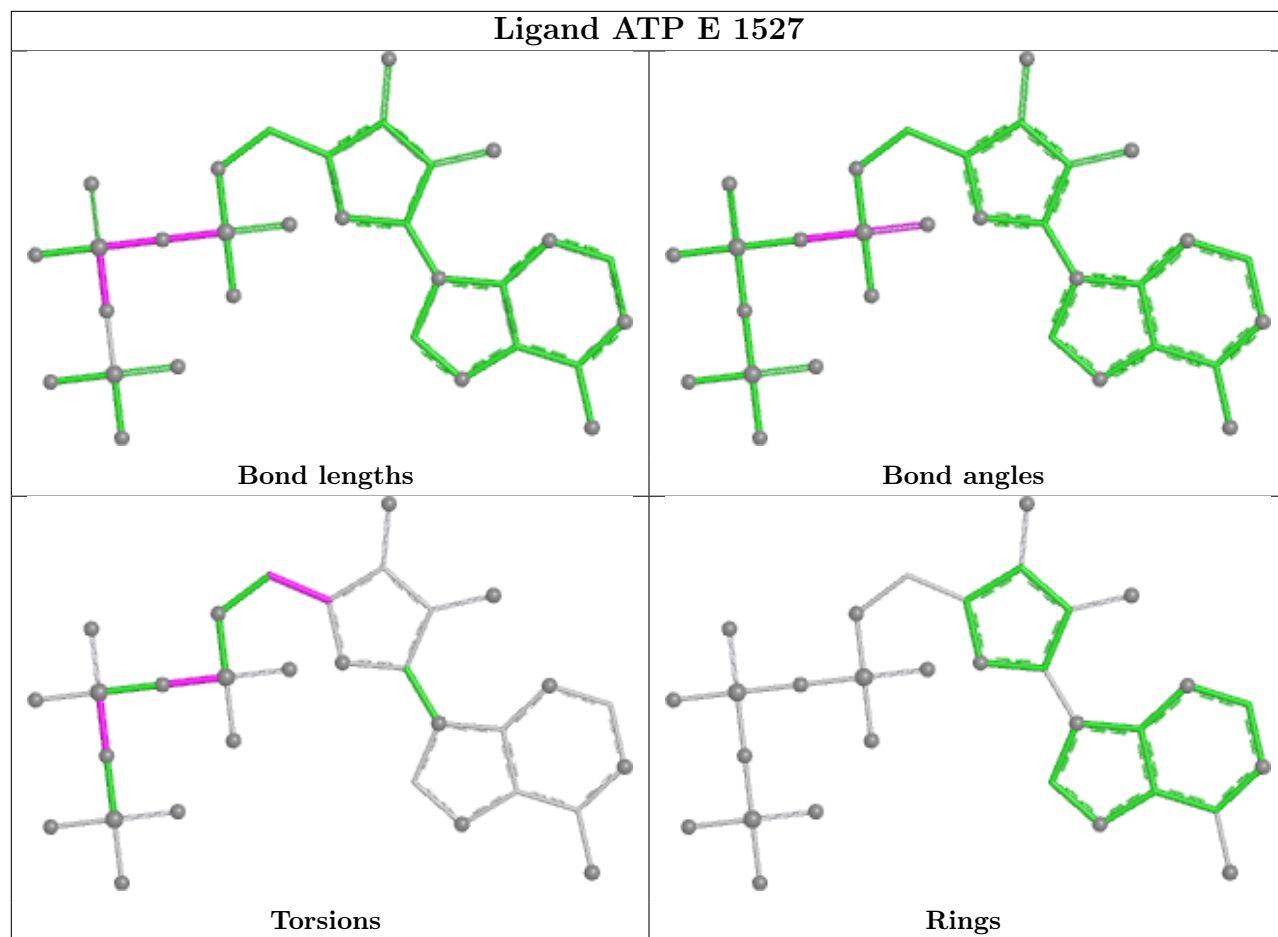


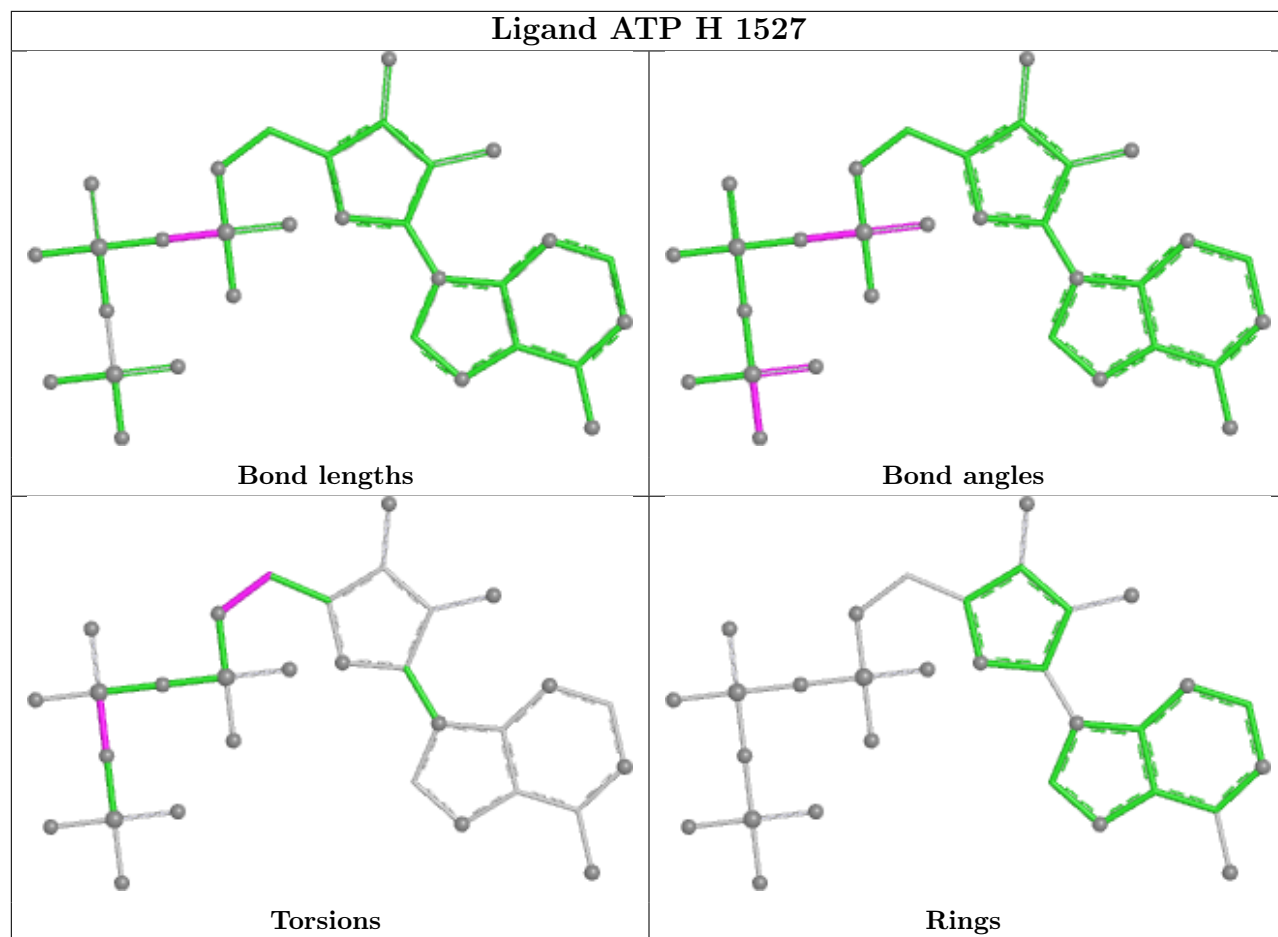


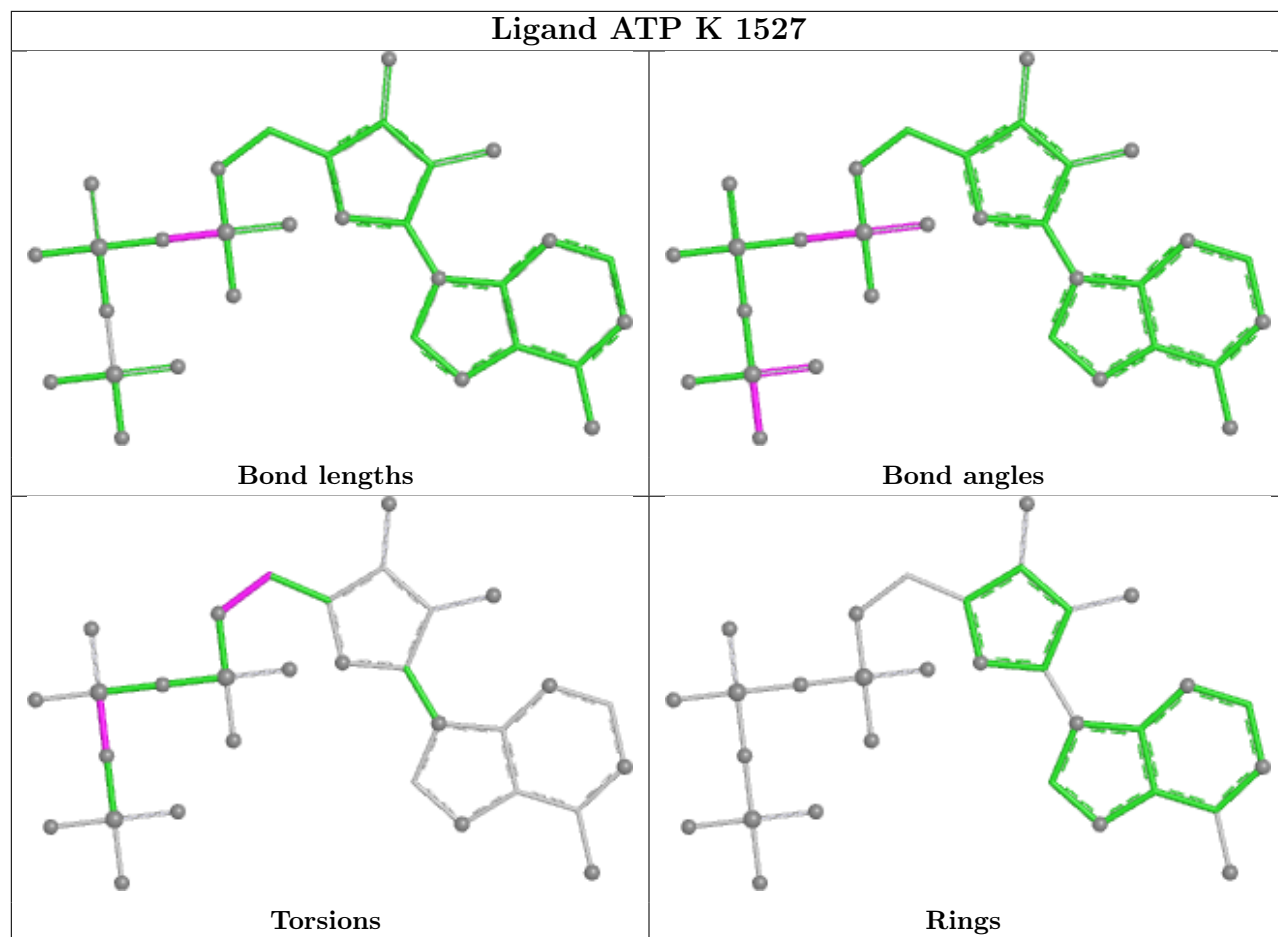


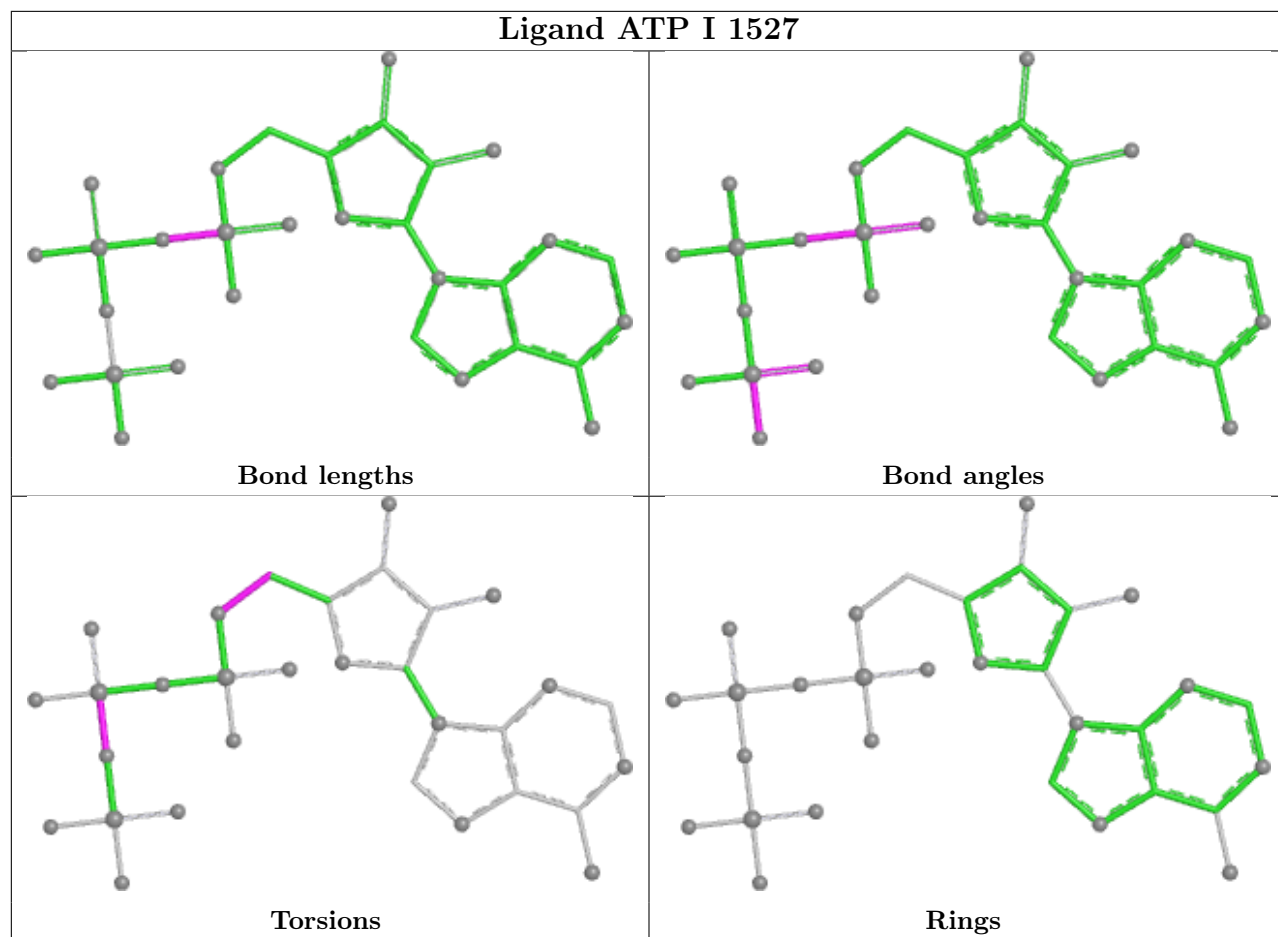


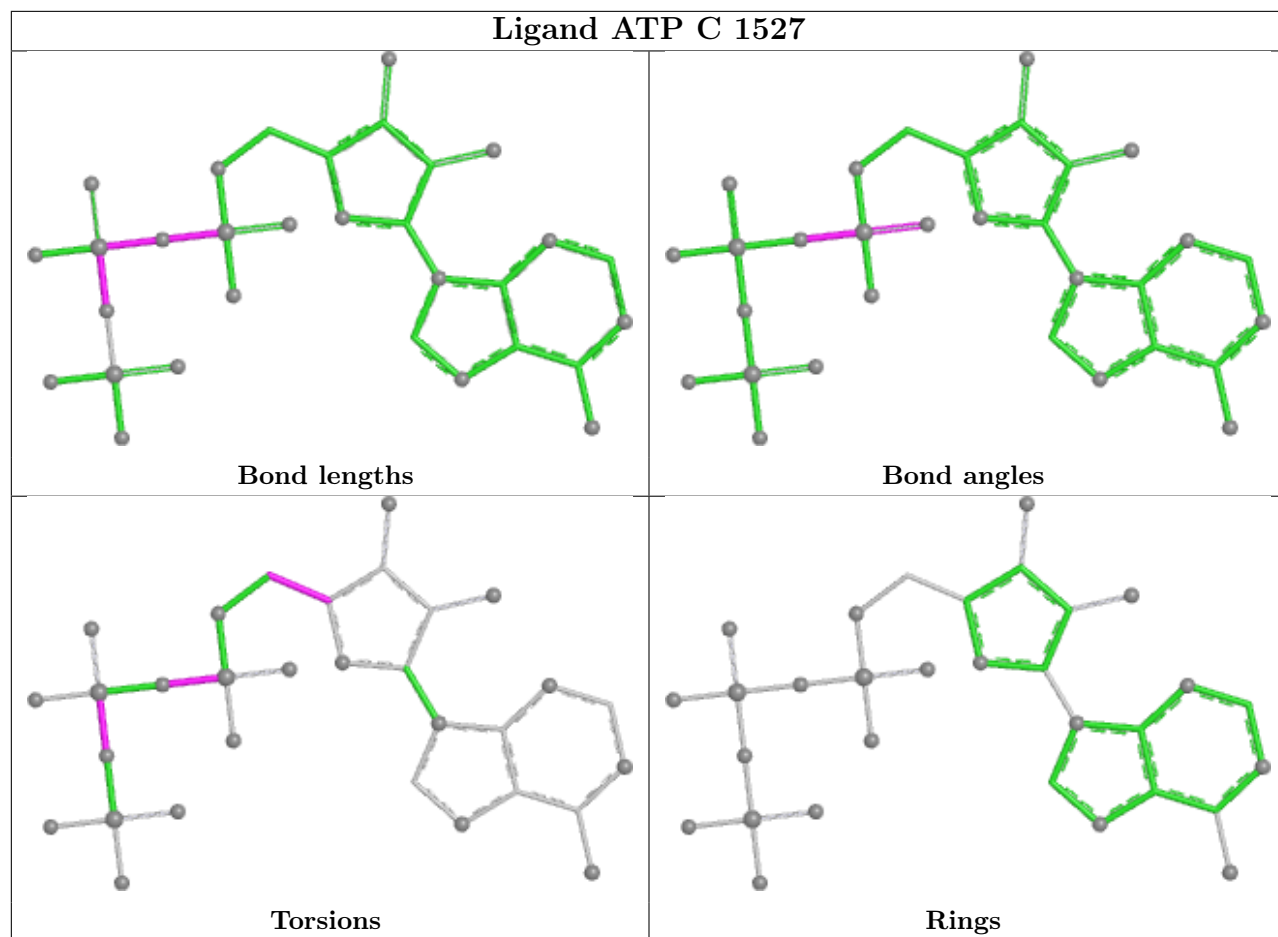


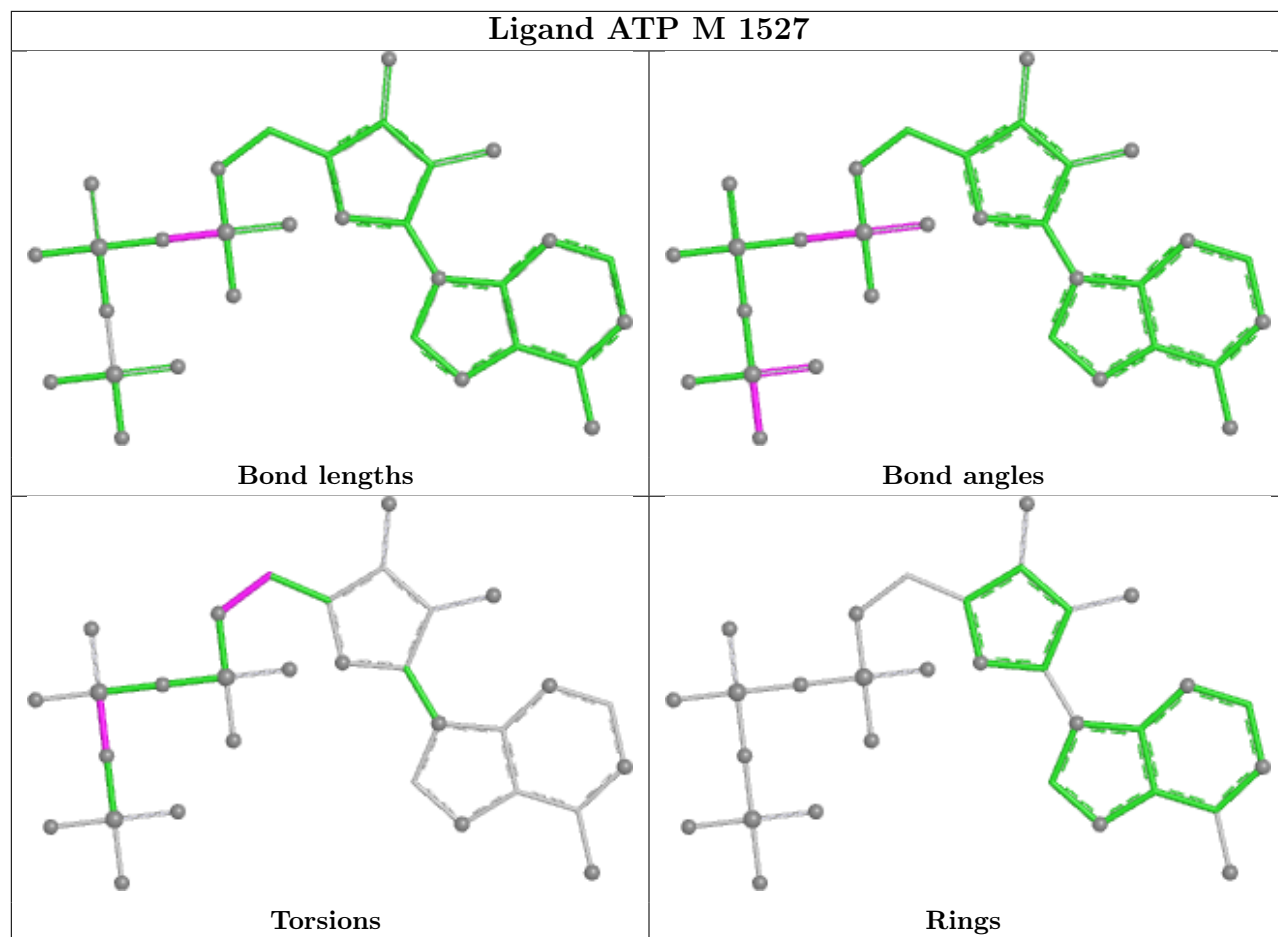


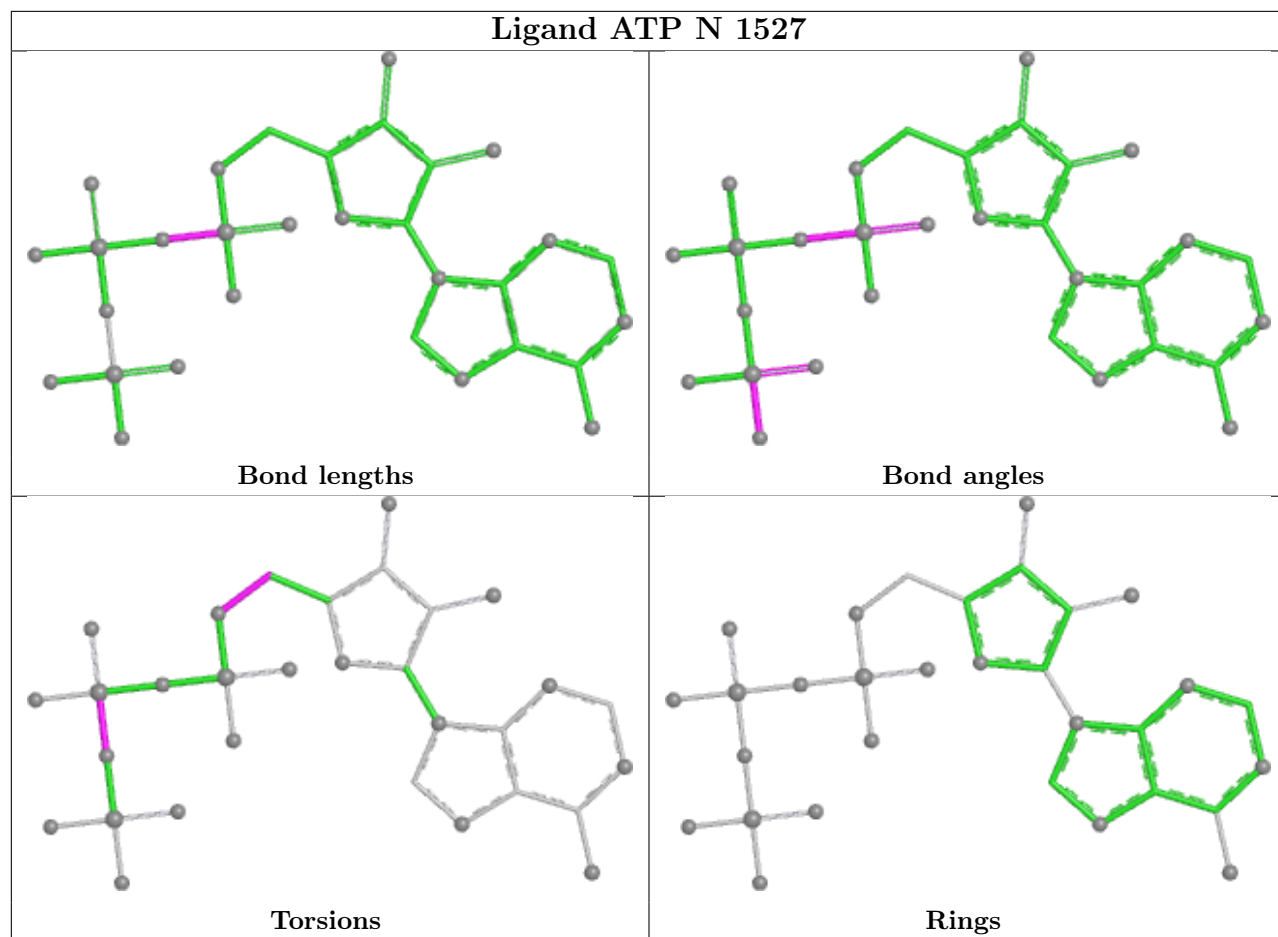


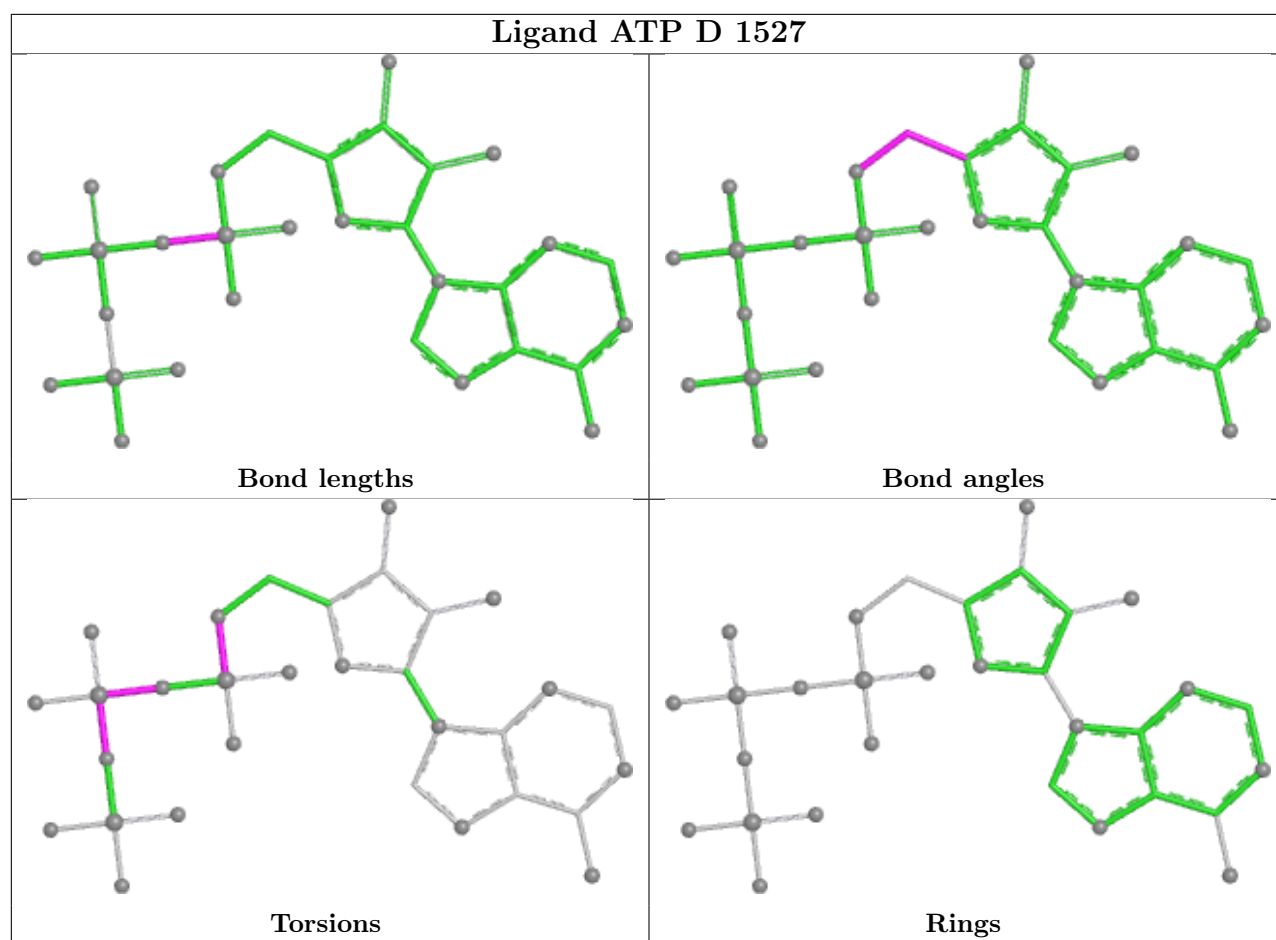












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	5
1	C	5
1	D	5
1	E	5
1	F	5
1	G	5
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:ASP	C	53:GLY	N	1.20
1	B	52:ASP	C	53:GLY	N	1.20
1	C	52:ASP	C	53:GLY	N	1.20
1	D	52:ASP	C	53:GLY	N	1.20
1	E	52:ASP	C	53:GLY	N	1.20
1	F	52:ASP	C	53:GLY	N	1.20
1	G	52:ASP	C	53:GLY	N	1.20
1	A	518:GLU	C	519:CYS	N	1.19
1	B	518:GLU	C	519:CYS	N	1.19
1	C	518:GLU	C	519:CYS	N	1.19
1	D	513:LEU	C	514:MET	N	1.19
1	D	518:GLU	C	519:CYS	N	1.19
1	E	518:GLU	C	519:CYS	N	1.19
1	F	518:GLU	C	519:CYS	N	1.19
1	G	518:GLU	C	519:CYS	N	1.19
1	A	513:LEU	C	514:MET	N	1.18
1	B	513:LEU	C	514:MET	N	1.18
1	C	513:LEU	C	514:MET	N	1.18
1	E	513:LEU	C	514:MET	N	1.18
1	F	513:LEU	C	514:MET	N	1.18
1	G	513:LEU	C	514:MET	N	1.18
1	B	213:VAL	C	214:GLU	N	1.08
1	C	213:VAL	C	214:GLU	N	1.08
1	D	213:VAL	C	214:GLU	N	1.08
1	E	213:VAL	C	214:GLU	N	1.08
1	F	213:VAL	C	214:GLU	N	1.08
1	G	213:VAL	C	214:GLU	N	1.08
1	A	7:LYS	C	8:PHE	N	1.07
1	B	7:LYS	C	8:PHE	N	1.07
1	C	7:LYS	C	8:PHE	N	1.07
1	D	7:LYS	C	8:PHE	N	1.07
1	E	7:LYS	C	8:PHE	N	1.07
1	F	7:LYS	C	8:PHE	N	1.07
1	G	7:LYS	C	8:PHE	N	1.07

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2003. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 96



Y Index: 96



Z Index: 96

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

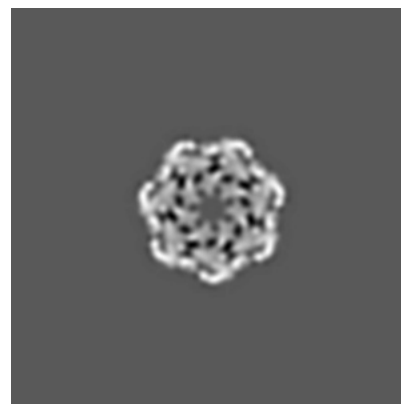
6.3.1 Primary map



X Index: 119



Y Index: 76

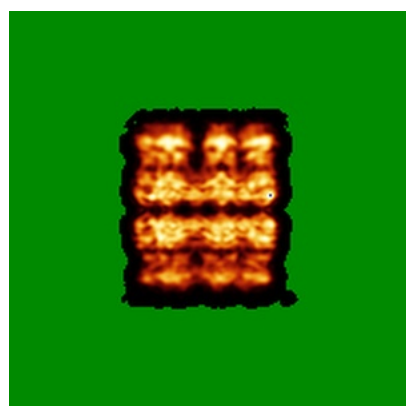


Z Index: 89

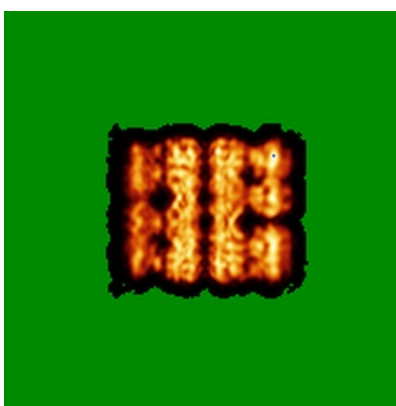
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

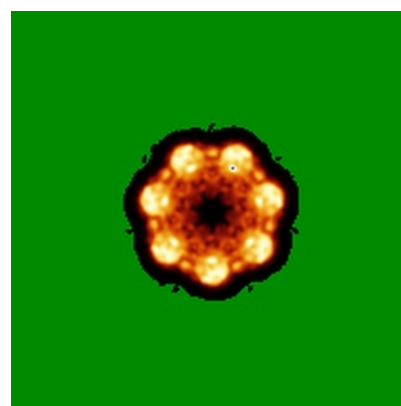
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

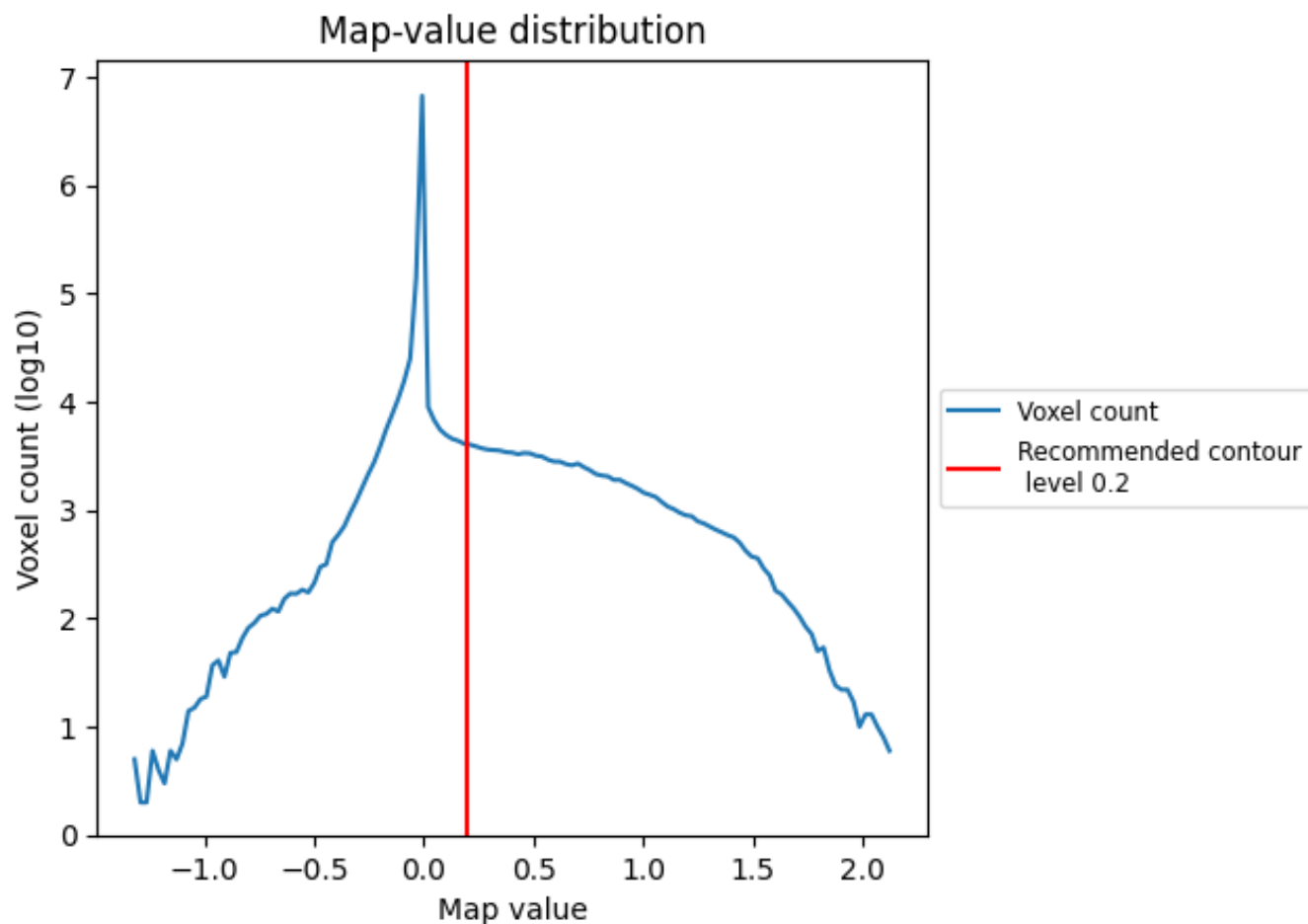
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

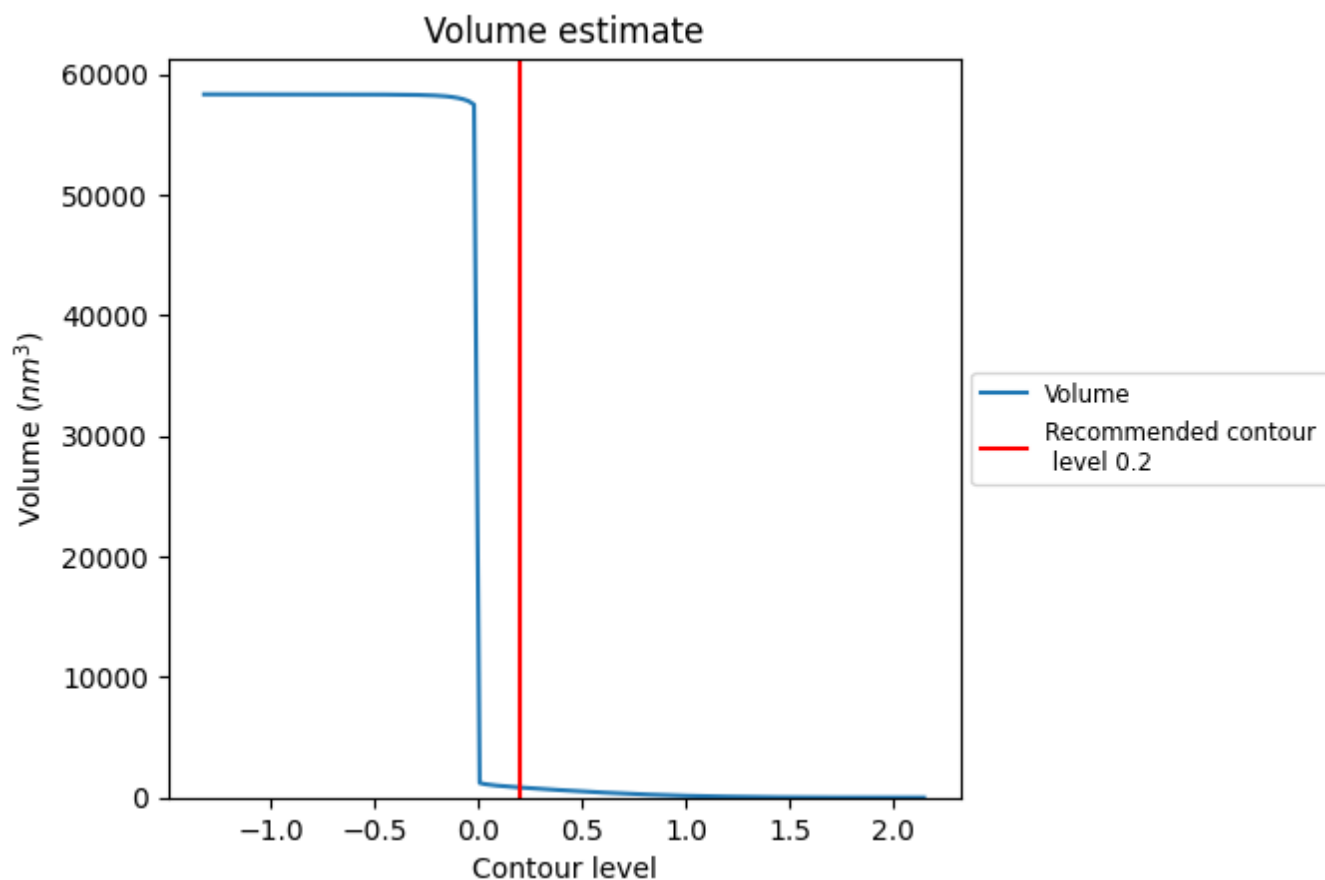
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

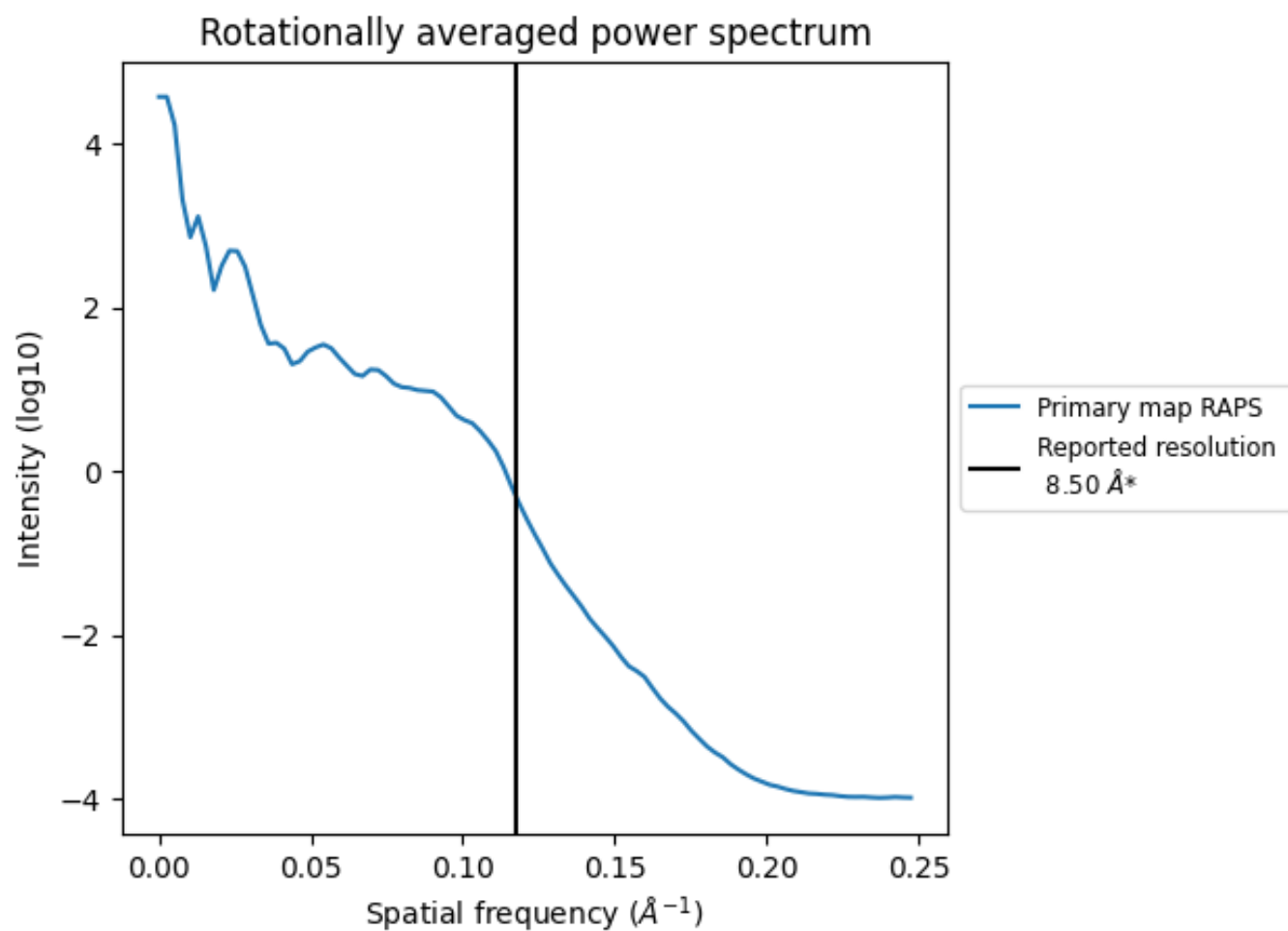
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 840 nm³; this corresponds to an approximate mass of 759 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.118 Å⁻¹

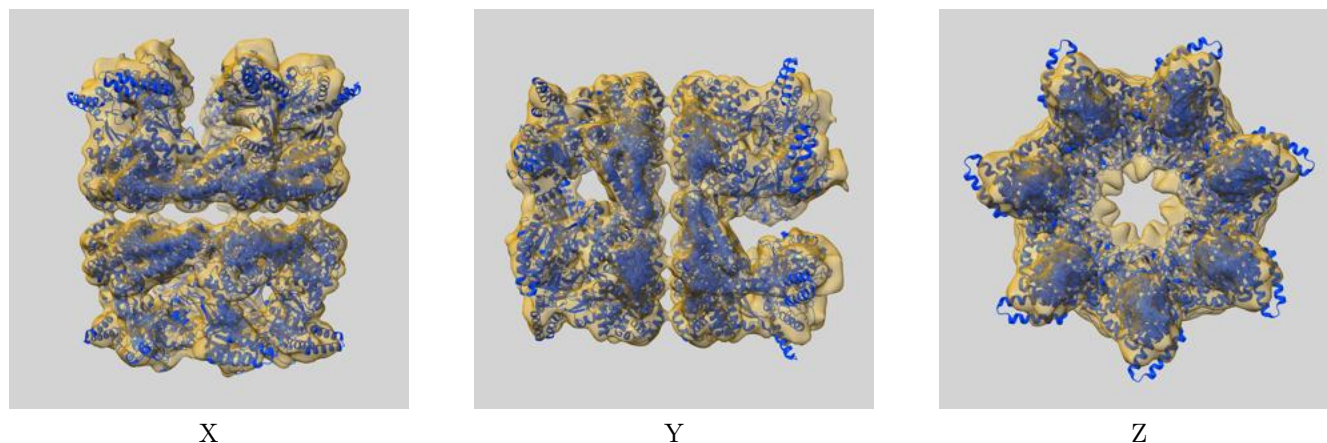
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

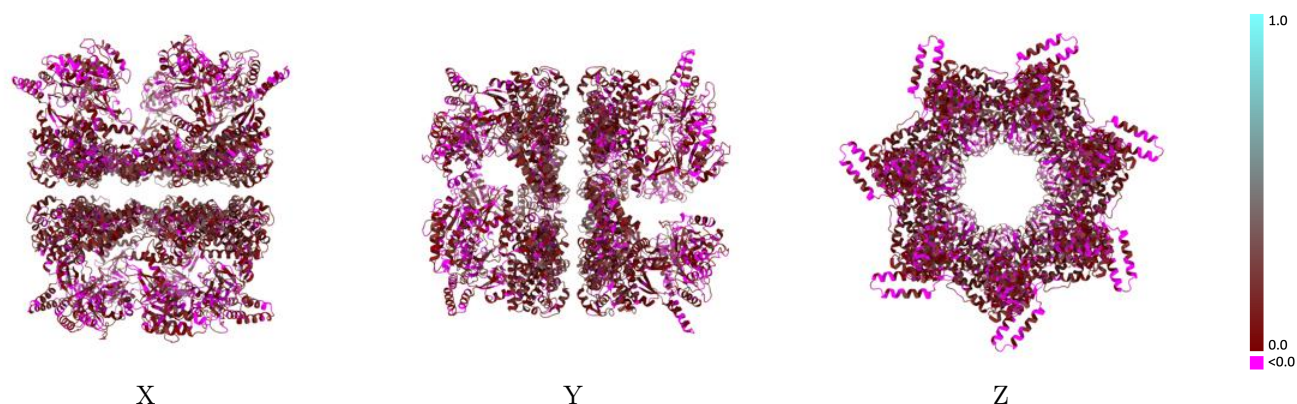
This section contains information regarding the fit between EMDB map EMD-2003 and PDB model 4AB3. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



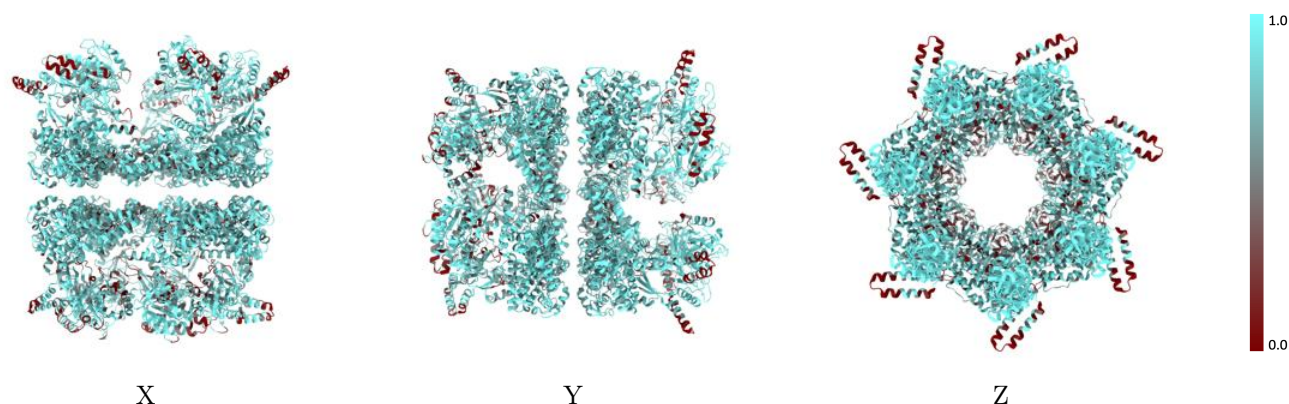
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



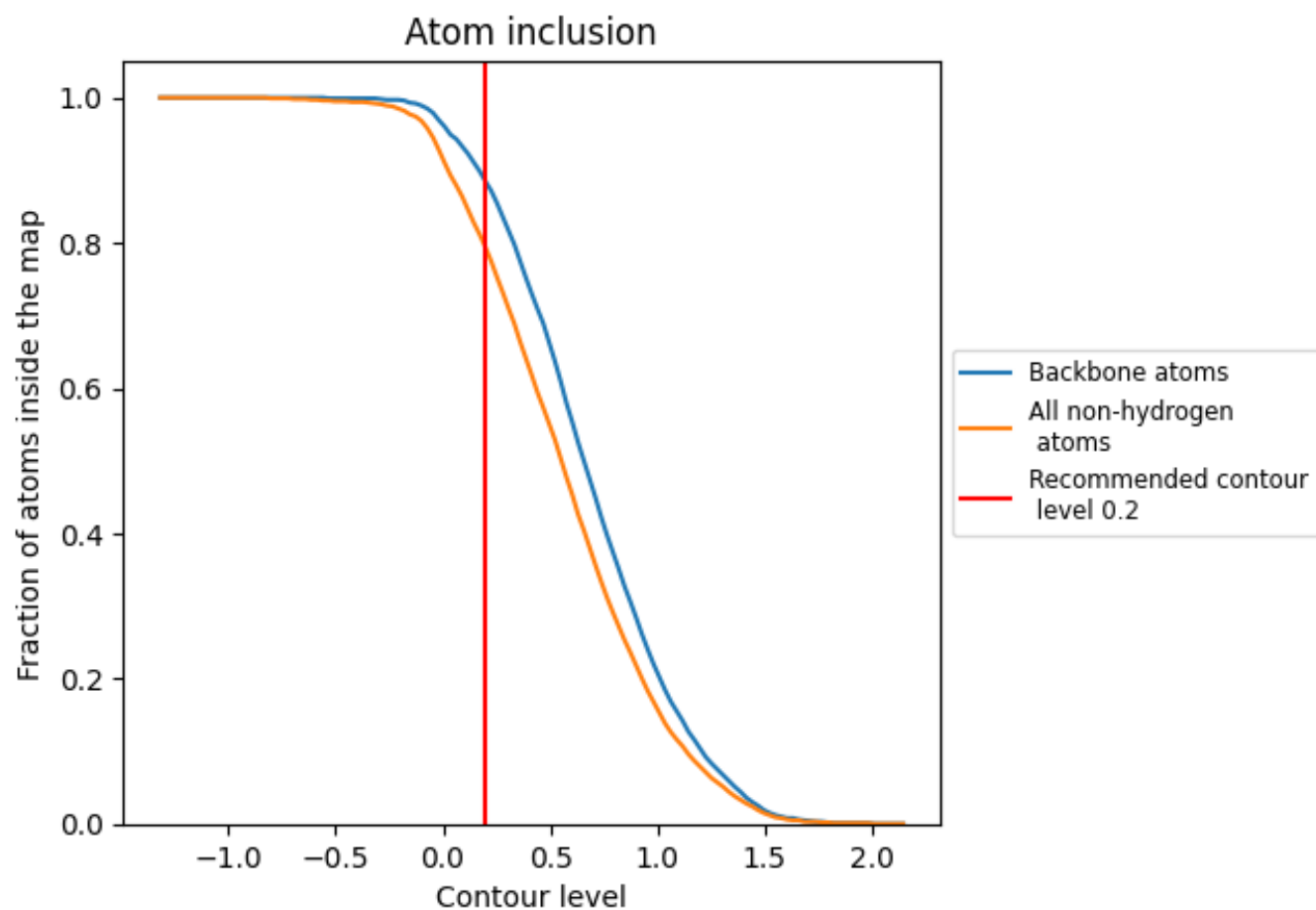
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.0910
A	 0.8040	 0.0820
B	 0.8030	 0.0830
C	 0.8030	 0.0840
D	 0.8030	 0.0850
E	 0.8040	 0.0860
F	 0.8030	 0.0840
G	 0.8030	 0.0840
H	 0.7810	 0.0970
I	 0.7830	 0.0980
J	 0.7830	 0.0980
K	 0.7820	 0.0980
L	 0.7840	 0.0980
M	 0.7830	 0.0990
N	 0.7820	 0.0980

